

9TH EUROPEAN COMBUSTION MEETING 2019

14 - 17 April, 2019 | Lisboa | Portugal

BOOK OF ABSTRACTS

EDITED BY:

Sandrina Pereira and Mário Costa



**TÉCNICO
LISBOA**

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Contents



Contents

Plenary Lectures	25
PL - 01 MILD Combustion: from ignidiffusion to temperature tailored reactors	27
PL - 02 The challenge of modelling aeronautical combustion chambers	28
PL - 03 Recent advances in soot nucleation understanding	29
PL - 04 Laser-based flame structure visualization for quantitative interpretation of combustion in small scale turbulent flows	30
PL - 05 Oxidation chemistry of oxygenated molecules	31
Poster Session 1	33
Reaction kinetics I	
S1_All_01 Exploring biofuel low-temperature chemistry with a hybrid reactive molecular-dynamics / quantum-chemistry scheme	35
S1_All_02 Detailed chemical modeling of biomass combustion in domestic heating appliances in order to reduce their polluting emissions	36
S1_All_03 Design and validation of single pulse shock tube for combustion chemistry investigations	37
S1_All_04 The thermal degradation of nitro and nitrate compounds: a study of nitromethane and isopropyl nitrate pyrolysis	38
S1_All_05 Temperature and pressure dependence of the C-O bond fission reactions of dimethoxymethane	39
S1_All_06 Byproduct formation in the thermolysis and hydrolysis of urea	40
S1_All_07 Low-temperature combustion of methylbutene isomers under engine-relevant conditions	41
S1_All_08 Pyrolysis kinetics of n-propylcyclohexane and isopropylcyclohexane at various pressures	42
S1_All_09 Study of the oxidation of the butanol isomers in a plug flow reactor	43
S1_All_10 Thermochemical study for species and reactions occurring in the S-N-O system	44
S1_All_11 Pyrene + O₂: primary reactions, reaction pathways, and influence of functional groups	45
S1_All_12 The impacts of iso-butanol blending on the low temperature autoignition behaviour gasoline and its surrogate	46
S1_All_13 Direct measurement of high-temperature rate constants and branching ratios on the pyrolysis of diethyl ether behind reflected shock waves	47

S1_All_14	Considerations in mechanism reduction applied to alcohol fuels	48
S1_All_15	An experimental and modelling study of the oxidation of cyclopentanol at high pressures	49
S1_All_16	Study of the oxidation of ammonia as an alternative to carbon-based fuels	50
S1_All_17	Experimental and modeling study of the oxidation of benzaldehyde	51
S1_All_18	Experimental analysis and 1D modelling of counterflow ammonia-methane flames	53
S1_All_19	Towards a better understanding of the combustion of oxygenated aromatic hydrocarbons. Comparing benzene, toluene, phenol and anisole with ignition delay times in a rapid compression machine	54
S1_All_20	Global quasi-linearization (GQL) for methane-air MILD combustion	55
Laminar flames I		
S1_All_21	Effects of radiation on premixed spherical flame propagation	56
S1_All_22	Stability of buoyant laminar diffusion syngas flame: impacts of H ₂ : CO	57
S1_All_23	Low dimensional chemistry manifolds applied to premixed methane/air flames under atmospheric conditions	58
S1_All_24	Effect of progress variable definition on the mass burning rate of premixed laminar flames in flamelet generated manifold methods	59
S1_All_25	The effect of droplets on laminar propagation speed of an acetone-methane flame	60
S1_All_26	Experimental study of premixed ozone-seeded DME/O ₂ cool flames on a stagnation plate burner	61
S1_All_27	1064 nm laser-induced grating spectroscopy (LIGS) measurements in flames at pressure	62
S1_All_28	An image processing routine to estimate the laminar flame speed of H ₂ -enriched biogas/air flames	63
S1_All_29	Influence of DC electric fields on laminar pre-mixed propane/air flames	64
S1_All_30	Data consistency of the burning velocity measurements using the heat flux method: syngas flames	65
S1_All_31	Propane/air flame impingement on a cylindrical surface: experimental investigation of heat transfer	66
S1_All_32	Study of laminar burning velocities and NO formation for methanol-air flames	67
S1_All_33	The H ₂ , H preferential diffusion effect on extinction behavior in SNG/air premixed symmetric flames	68
S1_All_34	Laminar burning velocities of hydrocarbons with ethanol addition	69

Solid fuels I

S1_AIII_35	Nature and origin of O-PAH compounds in biomass combustion emissions and their destruction	70
S1_AIII_36	Experimental investigation and comparison of particle-laden flows in a gas-assisted oxy-coal combustion chamber for reacting and non-reacting conditions	71
S1_AIII_37	Char emissivity measurements for coal chars	72
S1_AIII_38	Demonstration of laser-induced incandescence in single coal particle enveloping flames	73
S1_AIII_39	Heat transfer modeling using waste rubber as starting material in fluidized bed chamber	74
S1_AIII_40	Applicability investigation of a validated simulation method developed for a large scale grate incinerator for the case of a small scale pellet boiler	75
S1_AIII_41	Experimental two stage gasification of Hungarian brown coal for increased H ₂ and CO ratio in the produced synthesis gas	76
S1_AIII_42	Gasification of miscanthus x giganteus grown on heavy metal contaminated land	77
S1_AIII_43	Pyrolysis of plastic wastes for the purpose of liquid fuel production	78
S1_AIII_44	Laboratory scale pyrolysis of organic fraction and RDF from municipal solid waste	79
S1_AIII_45	Development of a vision-based monitoring system for optimizing industrial scale moving step grate biomass combustion	80
S1_AIII_46	Sewage sludge combustion in the rotary kiln	81
S1_AIII_47	Detailed analysis of single biomass particle combustion by shadowgraphy	82
S1_AIII_48	The energy aspects of biogas production from sheep manure	84
S1_AIII_49	Investigation of agriculture biomass for pyrolysis and gasification	85
S1_AIII_50	Physical and chemical characteristics of ash deposits in a utility boiler firing an Indonesian lignite	86
S1_AIII_51	Biomass for energy: excess air ratio effects on combustion characteristics of pulverized olive cake	87
S1_AIII_52	Potassium release from single burning pulverized biomass char particle	88

IC engines I

S1_AIII_53	Study on the high load potential under natural gas/diesel dual-fuel combustion in a heavy-duty engine	89
S1_AIII_54	An analysis on the combustion and performance characteristics of a hydrogen spark ignition engine with boosting condition	90

S1_AIII_55	1-methylnaphthalene LIF for the investigation of the mixture formation at diesel engine conditions and kHz repetition rates	91
S1_AIII_56	Highly resolved near-wall flame and flow measurements in an optically accessible SI engine using SO₂-PLIF and PTV	92
S1_AIII_57	Coupled experimental and numerical investigation of reactive spray processes in internal combustion engine	93
S1_AIII_58	Experimental and modeling study of 2-ethylhexyl nitrate promoting effect on a low octane gasoline surrogate	94
S1_AIII_59	A modeling study of a partial oxidation polygeneration process of fuel-rich ethanol/ozone mixtures in an HCCI engine	95
S1_AIII_60	CFD model of a spark-ignition engine fueled with several oxygenated compounds	96
S1_AIII_61	Experimental study on the knock phenomena in the individual cycles of direct-injected spark ignition engine with various stroke-to-bore ratios	97
S1_AIII_62	Numerical simulation of the prechamber processes in a lean-burn gas engine	98
S1_AIII_63	Time-resolved chemiluminescence spectroscopy of diesel and alternative fuel flames at engine relevant ambient conditions	99
S1_AIII_64	A power-to-gas process in a piston engine: exergy storage through pyrolysis of methane and ethane	100
S1_AIII_65	Investigation of the chemical stability of the laser-induced fluorescence tracer 1-methylnaphthalene at IC engine relevant conditions by supercontinuum absorption spectroscopy	101
S1_AIII_66	Comparison of fuel additives for syngas production from fuel-rich methane HCCI combustion	102
S1_AIII_67	Exploration of the high load limits in dual-fuel combustion operation	103
S1_AIII_68	Operating parameters of the biogas-diesel dual-fuel engine	104
S1_AIII_69	Active pre-chamber ignition systems: an enabler for new ICE combustion concepts	105
S1_AIII_70	Ignition characteristics of plasma reformed n-heptane in a homogeneous combustion compression ignition engine: a modeling study	106
S1_AIII_71	Ignition delay times of diluted mixtures of ammonia/methane at elevated pressures	107
 Soot and nanomaterials I		
S1_R1_72	Study of a gasoline surrogate blended with pentanol isomers: sooting tendency and flame structure analysis	108
S1_R1_73	Spray and particle characterization of a spray flame synthesis process using wide-angle light scattering (WALS)	109

S1_R1_74	Measurement of the sooting propensity of aviation fuel mixtures	110
S1_R1_75	Raman spectroscopy of soot sampled from high-pressure diffusion flames	111
S1_R1_76	Production and characterization of superhydrophilic TiO ₂ nanoparticle coatings via flame aerosol synthesis and thermophoretic deposition	112
S1_R1_77	Numerical modelling of detailed soot radiative properties of a laminar coflow sooting flame	113
S1_R1_78	Modelling soot particle inception and soot particle probe sampling	114
S1_R1_79	Formation of soot precursors in benzene-laden producer gas combustion: experimental and computational study	115
S1_R1_80	Pathways of soot precursors formation in combustion of producer gas in presence of benzene	116
S1_R1_81	Characterization of soot volume fraction and particle size inside premixed kerosene flames	117
S1_R1_82	Experimental investigation of hydrogen impact on atmospheric sooting premixed methane flames	118
S1_R1_83	Particle size distribution measurements in ethylene/toluene premixed flames	119
S1_R1_84	Soot measurements over a series of laminar pool flames of biofuels, methyl esters and blends with diesel	120
S1_R1_85	Quantification of the evolution of mean gaseous species concentrations across the sooting limit in turbulent premixed opposed jet flames	121
S1_R1_86	Numerical prediction of soot particle size distribution in a turbulent flame using the LES-PBE-PDF method	122
S1_R1_87	A reduced virtual chemistry model for soot precursors prediction in hydrocarbon-air flames	123
S1_R1_88	Influence of surrogate biofuels admixture on soot characteristics in isooctane counterflow non-premixed flames	124
S1_R1_89	Impact of spray nozzle k-factor on spray characteristics, flame propagation, and soot formation under engine-relevant conditions	125
S1_R1_90	Soot particle nanostructure from HRTEM images and reactivity towards oxidation	126
Poster Session 2		127
Turbulent combustion I		
S2_All_01	Simulation of flameless combustion in Delft lab-scale furnace using EDC model	129
S2_All_02	Reaction-diffusion manifolds (REDIMs) simplified chemistry for the simulation of laminar and turbulent CH ₄ diffusion flame	131

S2_AII_03	Application of the shadow-position mixing model to large eddy simulation with the Eulerian subgrid probability density function approach	132
S2_AII_04	The behavior of flame with the increase of turbulence intensity on low swirl combustor	133
S2_AII_05	LES modelling of nanoparticle synthesis in the SpraySyn burner	134
S2_AII_06	Comparison of LES combustion models for turbulent premixed flames at atmospheric pressures	135
S2_AII_07	Eulerian stochastic fields method and model free finite rate chemistry applied to Sydney partially premixed flame	136
S2_AII_08	Machine learning for sub-grid scale turbulent combustion modeling	137
S2_AII_09	Turbulent premixed flames in a hele-shaw cell	138
S2_AII_10	Effects of fuel composition on the minimum ignition energy and its transition for homogeneous biogas-air mixtures	139
S2_AII_11	Visualization of turbulent inverse diffusion flames at elevated pressure using OH-PLIF and OH* chemiluminescence imaging	140
S2_AII_12	Turbulent burning characteristics of hydrogen/air premixed flames in different combustion regimes	141
S2_AII_13	Flame front detection in combustion imagery based on ridges in two and three dimensions	142
S2_AII_14	Study of an opposed jet turbulent flame using the sub-grid PDF method	143
S2_AII_15	Near-wall behaviour of turbulence in flame-wall interaction of premixed turbulent combustion in boundary layers	144
S2_AII_16	Studies on the lean flammability limits of hydrogen/methane/air turbulent flames in a combustion bomb	145
S2_AII_17	Effect of equivalence ratio on turbulent premixed stratified methane-air flames	146
S2_AII_18	Combined PIV/SO₂-PLIF experiments for multi-mode combustion	147
S2_AII_19	Statistical dependence of mixture fraction and progress variable in partially-premixed combustion	148
S2_AII_20	Assessing heat release and chemical mode manifold in multi-regime combustion under experimental conditions	149
 Reaction kinetics II		
S2_AII_21	Artificial neural network prediction of emissions from primary reference fuel combustion in jet stirred reactor	150
S2_AII_22	CO-concentration and temperature measurements of fuel-rich CH₄/O₂ mixtures doped with diethyl ether behind reflected shock waves	151

S2_AII_23	Experimental study of the autoignition of isooctane/anisole mixtures at low to intermediate temperatures	152
S2_AII_24	Experimental speciation study during oxidation of n-butane in a rapid compression machine	153
S2_AII_25	High pressure ignition delay time measurements and consistent kinetic modeling of C4 - C7 ethyl esters	154
S2_AII_26	A chemical functionality approach towards the formulation of a high-fidelity surrogate fuel for FACE gasoline F	155
S2_AII_27	Experimental and modeling study of the pyrolysis and combustion of di-tert-butyl peroxide	156
S2_AII_28	Influence of CO ₂ dilution on shock tube ignition delay times of dimethyl ether/air mixtures at high pressures	157
S2_AII_29	Multi-dimensional transport phenomena of flame-wall-interactions and the REDIM method	158
S2_AII_30	The role of chemical structure in the thermal decomposition of xylan	159
S2_AII_31	Isomerisation and decomposition of alkylperoxy and hydroperoxy alkylperoxy radicals of three heptane isomers	160
S2_AII_32	Autoignition properties of liquefied natural gas (LNG): an experimental and modeling study	161
S2_AII_33	An experimental and theoretical comparison of the novel e-fuel class oxymethylene ethers	162
S2_AII_34	Reaction kinetics studies of unsaturated methyl ester: methyl crotonate	163
Diagnostics		
S2_AIII_35	A new camera-based flame stability measure for non-oscillating and oscillating combustion	164
S2_AIII_36	Image-based analysis of flames in industrial afterburner chambers using geometric constraints	165
S2_AIII_37	Application of image-based process parameters for analyzing multi-fuel burners	166
S2_AIII_38	In situ LIF and ex situ CRDS applied to NO measurement in flames: probe perturbation and absolute quantification	167
S2_AIII_39	MZI measurements on an oxidant-diluted N ₂ O/CH ₄ inverse diffusion flame	168
S2_AIII_40	Absolute SiO concentration imaging in low-pressure nanoparticle-synthesis flames via laser-induced fluorescence	169
S2_AIII_41	Investigation of the time-resolved luminescence spectra of thermographic phosphors for combustion applications	170
S2_AIII_42	High-speed OH* imaging in a twin piston rapid compression machine	171

S2_AIII_43	The application of Raman crystals as narrowband light sources for shifted vibrational CARS thermometry in sooting flames	172
S2_AIII_44	Automatic defect detection in a model combustion chamber using support vector machine	173
S2_AIII_45	Femtosecond two-photon laser-induced fluorescence imaging of atomic hydrogen in a laminar methane/air flame stimulated by nanosecond repetitively pulsed discharges	174
S2_AIII_46	Towards non-intrusive diagnostics of ethanol and hydrocarbons formed as intermediates in its flames by Raman scattering	175
S2_AIII_47	Investigation of flame propagation enhancement by a ultrashort nanosecond discharge pulse using the advanced laser-based diagnostics	177
S2_AIII_48	Phantom studies on a new evolutionary reconstruction technique applied to 3D scalar fields in the gas-phase	178
S2_AIII_49	Alternative soot detection strategies for application in aero-engine test-beds: assessment of the performance and uncertainties of time-integrated LII	179
S2_AIII_50	A novel approach to high-speed 1D Raman-scattering for combustion dynamics	180
S2_AIII_51	Characterization of UV endoscopic imaging systems for combustion applications	181
S2_AIII_52	Rayleigh temperature measurements in a non-premixed, swirl stabilized burner with iCCD and sCMOS camera systems	182
Droplets and sprays		
S2_AIII_53	Lagrangian approach to GCH₄/LOX axisymmetric spray combustion of movable pintle injector	183
S2_AIII_54	Analysis of LIF and Mie signals from single micrometric droplets for instantaneous droplet sizing in gasoline sprays	184
S2_AIII_55	VOF method: numerical analysis of single droplets impinging upon liquid films	185
S2_AIII_56	Experimental study of a droplet impact on oblique dry surface	186
S2_AIII_57	Numerical simulation of sulfur combustors with high-power-density	187
S2_AIII_58	SpraySyn – standard burner for the collaborative investigation of spray-flame synthesis of nanoparticles: droplet velocity and size of the non-reactive ethanol spray	188
S2_AIII_59	Liquid fuel MILD combustion with two stage combustion structure in a closed combustion chamber	189
S2_AIII_60	Numerical modeling of the secondary droplet break-up in spray flows	190
S2_AIII_61	Analysis of multiphase MMC coupling using DNS of a reacting double shear layer	191
S2_AIII_62	Quantifying the effect of the turbulence and break up modelling for spray simulations through a dimensionless number analysis	192

S2_AIII_63	Investigation of the sulfur dioxide absorption in water droplets	193
S2_AIII_64	A direct numerical simulation analysis of turbulent V-flames propagating into droplet-laden mixtures with an overall equivalence ratio of unity	194
S2_AIII_65	The effect of atomizing media on the flame characteristics	195
S2_AIII_66	Droplets autoignition simulations of ethanol mixtures with a reduced kinetic mechanism	196
S2_AIII_67	Uncertainty of droplet evaporation measurements and its effect on model validation	197
S2_AIII_68	Temporal and spectral correlation of acoustic and chemiluminescent signal of a liquid-fueled turbulent swirl burner	198
S2_AIII_69	Determination of the minimal acoustic signal length for fast-acting control of a liquid-fueled turbulent swirl burner by Wavelet and Fourier transform	199
S2_AIII_70	High-fidelity simulations and experiments of oxymethylene ether spray ignition	200
 Gas turbines		
S2_R1_71	The influence of film cooling flow over turbine blades from different shaped holes	201
S2_R1_72	How far can we go? Stability limit assessment of micro gas turbine combustion in diluted condition using LES.	202
S2_R1_73	Detection of high-frequency thermoacoustic combustion oscillations in a model rocket combustor	203
S2_R1_74	Early detection and prevention of blowout in a laboratory-scale gas-turbine model combustor using complex networks	204
S2_R1_75	Quantifying acoustic damping in a multi-injector annular combustor	205
S2_R1_76	Emission estimation for lean premixed methane - air flame at high pressure	206
S2_R1_77	LES-pdf of combustion dynamics in a partially premixed swirl combustor	207
S2_R1_78	A tabulated chemistry method for the LES of diluted, non-adiabatic, premixed flames including auto ignition	208
S2_R1_79	Suppression of instabilities of swirled premixed flames with minimal secondary hydrogen injection	209
S2_R1_80	Large-eddy simulation of flame dynamics during the ignition of a swirling injector unit and comparison with experiments	210
S2_R1_81	Effects of mixture stratification on thermo-acoustic instabilities in a dual-swirl gas turbine model combustor	211
S2_R1_82	Systematic CFD-CRN study of exit NO_x emission in a methane/air diffusion flame	212

S2_R1_84	Analysis of ignition processes at combustors for aero engines at high altitude conditions	213
S2_R1_84	The effects of compressibility on the response of a flame to acoustic forcing	214
S2_R1_85	Prediction of combustion instability by using a feedback transfer function approach in a model chamber	215
S2_R1_86	Simultaneous measurement of 2D mixture fraction and flame structure in a non-premixed, swirl stabilized burner	216
S2_R1_87	Assessing emission characteristics of multiphase fuel combustion under gas turbine conditions	217

Fires

S2_R1_88	Assessment of subgrid-scale turbulence-radiation interaction on the filtered mean radiative emission in large-scale pool fire simulations	218
S2_R1_89	Experimental and numerical study on the interaction between sprinkler water spray, fire plume and smoke layer	219
S2_R1_90	Laboratory investigation of the ignition of wood structural materials under the influence of spot fires	220

Poster Session 3 223

Reaction kinetics III

S3_All_01	Activation effect of diethyl ether on the partial oxidation of methane	225
S3_All_02	Estimation of sticking coefficients using mobile and immobile transition states for catalytic platinum systems	226
S3_All_03	Evaluation of polycyclic aromatic hydrocarbon formation in counterflow diffusion flames	227
S3_All_04	Combustion study of a 3-components surrogate fuel	228
S3_All_05	Mechanism and kinetic study on the pyridine low-temperature oxidation under fuel-rich condition	229
S3_All_06	Reduction of methane-air combustion kinetic model through flux analysis and optimized with adaptive Monte Carlo optimization for chemical kinetics	230
S3_All_07	An experimental and theoretical kinetic study of the reaction of hydroxyl radicals with 1,4-Pentadiene	231
S3_All_08	Combustion behaviour of ammonia blended with dimethyl ether	232
S3_All_09	Exploring the combustion chemistry of a novel lignocellulose-derived biofuel: cyclopentanol	233
S3_All_10	Comparison of methane combustion mechanisms based on shock tube and RCM ignition delay time measurements	234

S3_All_11	Comparison of detailed reaction mechanisms for nitrogen chemistry in syngas combustion systems	235
S3_All_12	Modelling study of ignition delay time characteristics of ultra-rich C1/C2 mixtures in a constant volume reactor at low-pressure	236
S3_All_13	An updated chemical kinetic model for the simulation of laminar burning velocities of premixed hydrogen-, methane-, and n-heptane/air flames	237
S3_All_14	A jet-stirred reactor study of the oxidation and pyrolysis of di-n-propyl-ether	238
S3_All_15	Determination of the rate parameters of N/H/O elementary reactions based on H ₂ /O ₂ /NO _x combustion experiments	239
S3_All_16	Experimental and modelling study of the oxidation of methane doped with ammonia	240
S3_All_17	An experimental and kinetic modeling study on the reactivity of 1,3-dioxolane under engine relevant conditions	242
S3_All_18	An experimental and modelling study of diisobutylene oxidation	243
S3_All_19	Response-surface and group-additivity methodology for estimation of thermodynamics properties of oxygen-containing organosilanes	244
S3_All_20	Global quasi-linearization (GQL) method for high dimensional detailed reaction mechanisms	245
IC Engines II		
S3_All_21	Prediction of non-premixed combustion regimes in a DI diesel engine in various operation points	246
S3_All_22	Methodology for knock investigation in spark ignition engines	247
S3_All_23	Toward direct numerical simulations of a gas engine pre-chamber	248
S3_All_24	Development of a phenomenological blending rule for the assessment of the antiknock quality of hydrocarbon fuel mixtures	249
S3_All_25	Combustion characteristics of diesel blended with sludge-derived hydrothermal liquefaction oil and its applications	250
S3_All_26	A computationally efficient combustion progress variable (CPV) approach for engine applications	251
S3_All_27	Cycle variation analysis of the partially premixed combustion (PPC) using natural flame luminosity and planar laser-induced fluorescence imaging	252
S3_All_28	Modelling of auto-ignition to premixed flame transition in a context of Dual-Fuel engine combustion	253
S3_All_29	Reactivity controlled compression ignition combustion using renewable fuels	254
S3_All_30	Experimental investigation of the impact of advanced injection strategies on a LTC concept for a single cylinder CI engine	255

Laminar flames II

S3_AIII_31	Comparison of two velocity-pressure coupling algorithms for laminar non-premixed combustion	256
S3_AIII_32	Effect of burner diameter and diluents on structure and stability of co-flow laminar diffusion flames of diluted methane fuel	257
S3_AIII_33	Analysis of $\text{CH}_2\text{O}_x\text{OH}$ as marker for fuel-rich air to pure oxy-fuel flames under higher preheat temperature and elevated pressure	258
S3_AIII_34	Numerical simulation of flames in narrow combustion chambers	259
S3_AIII_35	Features of cellular flames propagating between closely spaced parallel plates	260
S3_AIII_36	Investigation of NO_x emission for different laminar premixed CH_4-fuel blends stabilized on a flat-flame burner	261
S3_AIII_37	Laminar burning velocity and extinction strain rates of $\text{H}_2/\text{CH}_4/\text{O}_2/\text{N}_2$ in flat flames	262
S3_AIII_38	Numerical generation of multidimensional flamelet databases using an adaptive wavelet method	263
S3_AIII_39	Influence of natural gas composition and hydrogen addition on fundamental flame characteristics	264
S3_AIII_40	A DNS study of the impact of gravity on spherically expanding premixed flames	265
S3_AIII_41	Laminar premixed flames of ethanol-water-air mixtures	266
S3_AIII_42	Laminar flame speed simulations of methane-air and n-heptane-air mixtures by using an adapted mechanism	267
S3_AIII_43	Propagating edge flames in nonpremixed coflow jets under electric fields	268
S3_AIII_44	Effect of diluent addition on methane/nitrous oxide inverse diffusion flame	269
S3_AIII_45	Determination of temperature and water-concentration in fuel-rich oxy-fuel methane flames applying TDLAS	270
S3_AIII_46	Experimental investigation of synthesis gas production in fuel-rich oxy-fuel methane flames	271
S3_AIII_47	2D and 3D numerical simulation of chemiluminescent radical concentrations during side-wall quenching of premixed methane and propane flames	272
S3_AIII_48	Experimental analysis of lean hydrogen premixed flames propagating in a confined vertical channel	273
S3_AIII_49	Laminar burning velocity measurements of ethanol-air and methanol-air mixtures at atmospheric and elevated pressures on a novel heat flux method setup	274
S3_AIII_50	Flames interaction under velocity and equivalence ratio gradients	275

Porous media		
S3_AIII_51	Modeling the smoldering of a static bed of biomass with inert solids	276
S3_AIII_52	A detailed investigation on a novel combustion heat exchanger design for heating applications	277
S3_AIII_53	Development of a porous burner for low calorific gaseous fuels offering a wide operating range	278
S3_AIII_54	Experimental study on the application of the water tube in porous media burners	279
Poster Session 4		281
Propellants		
S4_AII_01	The study of combustion in gas generator with a charge of solid propellant enriched by metal	283
S4_AII_02	Development of a variable thrust water breathing engine	284
S4_AII_03	Development of cost effective high aluminum based fuel rich propellant	285
S4_AII_04	Development of controllable lab-scale hybrid motor thruster	286
S4_AII_05	Experimental determination of ignition and combustion characteristics of two insensitive propellants	287
Solid fuels II		
S4_AII_06	Thermal analysis and kinetics of biomass combustion	288
S4_AII_07	Thermal treatment of lignin rich residue from bioethanol production: preliminary study on char properties	289
S4_AII_08	Hydrogen rich syngas from updraft gasification of lignocellulosic feedstock	290
S4_AII_09	The co-oxidation study of coal and corn residue as a representative of biomass with photoionization mass spectrometry	291
S4_AII_10	PAH distribution in pig manure pyrolysis products	292
S4_AII_11	Innovative 3D CFD sewage sludge combustion modeling for furnace design optimization	294
S4_AII_12	Multi-phase reactive systems – analysis of involved time scales	296
S4_AII_13	Dust explosion characteristics of corn starch at elevated temperature and pressure and reduced oxygen concentrations	297
S4_AII_14	Combustion behavior of torrefied biochar with different constitutions of cellulose, hemicellulose, and lignin	298
S4_AII_15	Effect of CH₄ injection method on combustion and gasification efficiency of pulverized coal in the tuyere part of blast furnace	299

S4_All_16	Experimental study on reaction front propagation during biomass packed bed smouldering combustion	300
S4_All_17	Numerical simulation of raceway zone in small-scale combustion equipment for blast furnace	301
S4_All_18	Direct numerical simulations of spontaneous ignition of biomass in turbulent, high temperature particle-laden mixtures	302
S4_All_19	Kinetic modeling of the effects of Na⁺ and K⁺ on the slow pyrolysis of hemicellulose	303
S4_All_20	Modelling of particulate matter emissions from non-woody biomass combustion	304
 New concepts in combustion technology		
S4_AIII_21	Influence of the cobalt oxide coated flame holder in stabilization of inverted-methane lean flames	305
S4_AIII_22	Feasibility of natural gas pyrolysis for production of unsaturated hydrocarbons: an RCM study	306
S4_AIII_23	Plasma-assisted super-equilibrium radical generation and its effect on ignition	307
S4_AIII_24	Designing a cooking burner using biogas as fuel	308
S4_AIII_25	Partial methane oxidation via MILD combustion	309
S4_AIII_26	Experimental and numerical studies on CO₂ reforming in piston engines	310
S4_AIII_27	Autothermal and steam reforming of liquid synthetic fuels	311
S4_AIII_28	Key modeling aspects in the simulation of a cyclonic burner operated in MILD combustion conditions through flamelet generated manifold model	312
S4_AIII_29	Investigation of heterogeneous kinetic combustion of propene using novel CJSR	313
S4_AIII_30	Abatement of toluene by non-thermal plasma coupled with Cu-Co-O thin film coated on stainless steel mesh	314
S4_AIII_31	Investigation of support effect of Fe-Cu-Co thin film catalyst on the catalytic activity and stability for CO oxidation	315
S4_AIII_32	Experimental investigation of stabilization and emission characteristics of ammonia combustion in a cyclonic burner	316
S4_AIII_33	Experimental study of MILD combustion in a cyclonic burner using prevaporized liquid fuels	317
S4_AIII_34	New method of refinery gas processing into valuable petrochemicals	318
S4_AIII_35	A preliminary assessment of alternative fuels for marine engines using combustion chemistry tools	320
S4_AIII_36	Evaluation of gas turbine concepts for ammonia combustion	321

Laminar flames III

S4_AIII_37	Unsteady pure straining effects on lean premixed flames of different Lewis numbers	322
S4_AIII_38	Laminar burning velocities and laser-induced fluorescence measurements of nitric oxide formation in propyl alcohols+air flames	323
S4_AIII_39	Flame structures and local heat release rates during side-wall quenching of atmospheric methane and DME flames	324
S4_AIII_40	Influence of iron and phosphor containing additives on the laminar flame speed	325
S4_AIII_41	Measurement of laminar burning velocity of SNG fuel with various hydrogen content	326
S4_AIII_42	Experimental study of the maximum upstream location of premixed CH ₄ /air and CH ₄ /O ₂ -He flames with repetitive extinction and ignition in a quartz micro flow reactor	327
S4_AIII_43	Thermoacoustic instabilities: flame-flame interaction and boundary conditions	329
S4_AIII_44	Numerical analysis of characteristics of biogas and syngas combustion	330
S4_AIII_45	Laminar burning velocity of CH ₄ /O ₂ /N ₂ /CO ₂ flames measured by heat flux method under elevated pressure	331
S4_AIII_46	High-temperature laminar flame speed experiments in a shock tube: laminar flame speed, temperature, and species measurements	332

Poster Session 5 333

Reaction kinetics IV

S5_AII_01	Non-ideal effects in shock tubes: experiments, modeling, and simulations	335
S5_AII_02	An ignition delay time and kinetic modeling study of 1- and 2-pentene	336
S5_AII_03	Plasma assisted combustion kinetics: modeling study for hydrogen-air mixtures in a non-thermal plasma reactor	337
S5_AII_04	High-pressure shock-tube study of the ignition and product formation of fuel-rich CH ₄ /dimethoxymethane/air mixtures	338
S5_AII_05	Testing several butanol combustion mechanisms against a large set of experimental data and investigating their thermochemical data inconsistency	339
S5_AII_06	Influence of pressure on H ₂ S conversion	340
S5_AII_07	ARAS study of ethanol, butanol and DME reactions with atomic oxygen behind shock waves	341
S5_AII_08	High temperature oxidation of 2,3-dimethyl-2-butene	342
S5_AII_09	Modeling of NO _x formation and consumption during oxidation of small alcohols	343

S5_AII_10	A novel approach for nitrogen flux accounting of NO_x formation pathways in 1D flames	344
S5_AII_11	Kinetic modeling of the destruction of organoarsenic toxics	345
S5_AII_12	CaRMeN: a novel software tool for the evaluation and development of reaction mechanisms	346
S5_AII_13	Thermochemical property estimation based on group additivity method: impact of groups on kinetic model predictions	347
S5_AII_14	On the reliability of Ab-Initio reaction rate constant estimations used for biofuel oxidation mechanisms on the example of CH₃OH + H	348
S5_AII_15	Reduction of NO_x in combustion of solid waste fuels by the SNCR process using ammonium sulfate as alternative additive	349
S5_AII_16	Experimental and modeling study of the oxidation of pentanones: 2-pentanone, 3-pentanone and 3-methyl-2-butanone	350
S5_AII_17	Formation of indene and naphthalene through C₆+C₃ and C₇+C₃ reaction pathways in low-pressure premixed flames	351
S5_AII_18	NO emission prediction using virtual optimized chemistry	352
S5_AII_19	Probing the low-temperature oxidation of tetrahydropyran and its effect on toluene ignition	353
S5_AII_20	Synthesized alternative kerosenes – characterization through experiments and modeling	354
S5_AII_21	Ethane/nitrous oxide mixtures as a green propellant to substitute hydrazine: validation of reaction mechanism	355
S5_AII_22	Mechanism comparison for PAH formation in pyrolysis and laminar premixed flames	356
S5_AII_23	Ammonia oxidation in a JSFR reactor. Towards a better understanding of ammonia chemistry	357
S5_AII_24	Degree centrality of combustion reaction networks for analyzing and modelling combustion processes	358
Soot and nanomaterials II		
S5_AII_25	High temperature synthesis of TiO₂ nanoparticles using TTIP-methane flat premixed flame	359
S5_AII_26	Comparative mass spectrometric study of gaseous key intermediates from tetramethylsilane and hexamethyldisiloxane in silica synthesis flames	360
S5_AII_27	Impact of the injector geometry on soot production in a model scale swirled combustor under perfectly premixed rich conditions	361
S5_AII_28	Experimental and numerical investigation of iron-oxide nanoparticles from flame assisted synthesis	362

S5_AII_29	Soot formation in laminar diffusion flames with population balance modelling and laser diagnostics	363
S5_AII_30	Absolute iron atom concentration imaging in nanoparticle flame-synthesis reactor using self-calibrating laser induced fluorescence	364
S5_AII_31	Newly-designed catalytic jet-stirred reactor for low-temperature oxidation of T135MB	365
Stationary combustion systems and environmental impacts		
S5_AIII_32	Dehydrogenation of a chemical hydrogen carrier using a porous media burner	366
S5_AIII_33	Chemiluminescence and structure characteristics of a H₂/O₂ downward inverse diffusion flame	367
S5_AIII_34	The impact fragmentation tendency of limestone particles in calcium looping systems: effect of steam and sulphur dioxide	368
S5_AIII_35	Sorption-enhanced methanation in a dual fluidized bed system: evaluation of two sorbents	370
S5_AIII_36	Emissions from combustion of fuels with oleoresin-based compounds as additives	372
S5_AIII_37	Implementation and validation of the discrete ordinates method for calculation of radiative heat transfer in the CFD software AVL FIRE™	373
S5_AIII_38	Effects of CO₂-H₂O dilution on characteristics of CH₄-air-O₂ flames	374
S5_AIII_39	Reliability of particulate matter sensor operation during uncomfortable weather conditions	375
S5_AIII_40	Effects of inner swirl on flow and combustion patterns from non-premixed oxygen enriched flames above coaxial injectors	376
S5_AIII_41	The influence of the combustion operation parameters in the process burners on the formation of NO_x and heat fluxes	377
S5_AIII_42	Cold flow analysis, flame stability and emission properties of blade-based premixed swirl burners at various blade angles	378
S5_AIII_43	Using high-speed multispectral infrared imaging for temperature calculation of composite materials under kerosene flame	379
Turbulent Combustion II		
S5_AIII_44	Natural gas replacement by syngas in Resource Energy Intensive Industries (REII) burners: numerical CFD evaluation	380
S5_AIII_45	Combustion-specific deep neural networks for modeling reactive flows	381
S5_AIII_46	Ignition and early stages of flame propagation in a non-premixed biogas planar turbulent jet	382
S5_AIII_47	Large eddy simulations of reacting spray jet with active control	383

S5_AIII_48	Determination of a correlation for predicting lean blow off limits of gaseous fueled, premixed turbulent jet flame arrays enclosed in a hexagonal dump combustor	385
S5_AIII_49	Large eddy simulation of a lab-scale 30 kW furnace operating in MILD combustion	386
S5_AIII_50	Fundamental analysis of DME pilot-ignited methane-air flame	387
S5_AIII_51	Turbulent bluff-body flames close to stability limits revealed by coupling of high speed optical diagnostics	388
S5_AIII_52	Mixing and entrainment of burned products in high Karlovitz number premixed jet flames	389
S5_AIII_53	Multi-scalar and velocity measurements in a turbulent bluff-body flame using spectral fitting of spontaneous Raman scattering and PIV	391
S5_AIII_54	Data-driven model development for CO emissions in stationary gas turbines	392
S5_AIII_55	The influence of the reactor model on EDC's mean reaction rate - a study on the relevance of choice	393
S5_AIII_56	Flame stabilization in a cavity based scramjet	395
S5_AIII_57	Modelling and simulation of high-pressure flows	396
S5_AIII_58	Mesh partitioning of reactive flow simulations – speed-up and other side effects	397
S5_AIII_59	Auto-ignition characteristics of transient methane, biogas and syngas jets at elevated pressure and temperature conditions: an axisymmetric DNS study	398

9TH EUROPEAN COMBUSTION MEETING 2019

14 - 17 April, 2019 | Lisboa | Portugal

Plenary Lectures



PL - 01

MILD combustion: from ignidiffusion to temperature tailored reactors

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Abstract

Variable Renewable Energies (VREs) are widely indicated as a very promising solution to the climate change issue. This is in principle true when looking at their positive impact on reduction emission in terms of greenhouses gases and it is assessed by thousands energy scenario published over the last years. On the other hand, an energy supply system entirely relying on VREs is far from satisfactorily meeting the pillars of the energy trilemma of equity, security and sustainability. Intermittency of the VREs, the need of appropriate electrification infrastructures, affordability of the sudden increase of metals and rare earths needs as well as consolidated and emerging geo-politics equilibria undermine the outlook to meet the emission targets foreseen by international agreements only with VREs. An unbiased analysis of VREs sustainability puts in evidence that it is not possible to have a low carbon society without the support of a relevant combustion based energy supply systems because their potential operational flexibility (in terms of fuel, load, load following and power intensity), together with the possibility of using chemical energy carriers to store VREs surplus, which actually is recognized as the best available means to guarantee a solid backup. MILD combustion processes and systems are among the few advanced combustion technologies which intrinsically satisfy the general criteria of sustainability, fuel flexibility and readiness level required. Because of inlet/local high diluted and preheated conditions in which the fuel conversion occurs, the process evolves through peculiar distributed spontaneous ignition based on local igni-diffusive structures, very different from the ones occurring in premixed and diffusion flames. Igni-diffusion will be described and discussed in relation to elementary configurations and different possible initial conditions highlighting its unique characteristics. Distributed spontaneous ignition also guarantees high resilience to the extinction as well as a solid fuel flexibility which will be analyzed in relation to a confined highly recirculated flow field, representing a scale bridging configuration between model reactors and real systems. By means of the stabilization of MILD combustion process for a wide palette of energy carriers, from standard carbon based fuels, to biogas, alcohols and ammonia it will be proved the possibility to tailor the operational temperature in a wide range of values provided that the attainment of the cross-over temperature of high temperature radical branching is locally achieved. This outstanding feature turns the concept of “combustion process” into those of “thermochemical conversion process” where the output conditions can be easily tuned based on end-use needs.

Keywords: Sustainable combustion technologies, MILD Combustion, Fuel flexibility

IL-02

The challenge of modelling aeronautical combustion chambers

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Abstract

The role of CFD in the design process of aeronautical combustors has increased significantly over the last 10 years, due to improved modelling of turbulence, chemistry and emissions, but also due to the increase of available computational resources. The introduction of tabulated chemistry models which include a description of the progress of combustion, like FGM (Flamelet Generated Manifold), FPI (Flame-Prolongation of ILDM) and FPV (Flame Progress Variable), have enabled the prediction of NO_x and soot emissions for both rich and lean burn combustors. The availability of high performance computers has made it possible to model entire combustion systems, so that boundary conditions could be placed more upstream of the combustion chamber. HPC also enabled the use of higher resolution meshes and more advanced turbulence models such as LES (Large Eddy Simulations).

Keywords: CFD, combustion modelling, emissions, LES, aeronautical combustors

IL-03

Recent advances in soot nucleation understanding

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Abstract

Combustion-generated soot particles are a significant pollutant affecting human health and environment. The soot nucleation, which delineates the transition from the gas phase to the solid phase, remains the least understood step in the process of soot formation, despite the great number of experimental, theoretical and numerical studies. The purpose of this lecture is to give an overview of the advances, recently achieved, which contribute to a much better understanding of the soot nucleation.

Keywords: soot, nucleation, flame, nascent

PL - 04

Laser-based flame structure visualization for quantitative interpretation of combustion in small scale turbulent flows

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Abstract

Combustion in most industrial devices takes place in turbulent flow fields. The interaction between turbulence and flame dictates the overall combustion and emission behavior. The current understanding of turbulent combustion is limited to low intensity and large-scale turbulence conditions, where the molecular diffusion and chemical reactions governs the structure of the reaction zone layers. For low intensity and large-scale turbulent flames, the wrinkled and corrugated flamelet models are frequently adopted. However, modelling and understanding of high-intensity and small-scale turbulent premixed flames remain a scientific challenge. Turbulent premixed combustion has been theoretically categorized into the thin reaction zone (TRZ) and the distributed reaction zone (DRZ) regimes depending on the interactions between turbulence and flame chemistry. Experimentally, the interactions between turbulence and combustion were investigated via instantaneous multi-scalars imaging measurements. Planar laser-induced fluorescence was employed to visualize the instantaneous distributions of combustion intermediate species as flame front markers, i.e. OH for production zone, CH for reaction zone and CH_2O for preheat zone. The instantaneous temperature field was recorded using laser-induced Rayleigh scattering, and velocity field was measured using laser Doppler velocimetry. Methane/air premixed flames at different turbulent intensity were prepared in a piloted jet flame burner with different Reynold numbers. By varying the stoichiometric ratio of the jet flame from slightly fuel rich to as lean as 0.4, Karlovitz number higher than 100 was achieved, where the flame conditions can well cover the TRZ and DRZ regimes. Experimental results of simultaneous multi-scalar imaging, i.e. CH/OH/ CH_2O , CH/OH/T and CH_2O /OH/T were recorded. Statistical analyses of the obtained instantaneous flame front structures shed light to the understanding of the interaction of turbulence and combustion at extreme conditions for a more accurate modelling. As a flame front reaction zone marker, CH_3 is better than CH, due to the fact that CH_3 has much higher concentration and more independent from local stoichiometric ratio. Some preliminary results of single-shot planar imaging measurement of CH_3 based photofragmentation planar laser-induced fluorescence measurements will be presented, for turbulent flame front structure visualization.

Keywords: turbulent combustion, laser diagnostics, flame front structures

PL - 05

Oxidation chemistry of oxygenated molecules

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Abstract

Given recent environmental concerns and a probable oil shortcut in the near future, there has been a growing need to find alternative feedstocks for the next generation biofuels. Second generation biofuels are lignocellulose derived, such as furans, butanol,...etc. These molecules are oxygenated and it is therefore of fundamental importance to understand their oxidation chemistry. Our efforts focus on detailed speciation (in jet-stirred reactor) and kinetic model development in order to reveal the relation between fuel structure, reactivity and pollutant formation. These studies of structure/reactivity concern many families such as ketones, alcohols, ethers, esters, and aldehydes. Although the initial motivation stems from new biofuels, we also focus our efforts on fundamentals such as detailing the oxidation chemistry of a molecule even if no potential biofuel use is known. Part of these show important reactivity at low temperatures, even a peculiar double negative temperature coefficient behavior as recently shown for long-chain ethers. On the other hand, evidence of highly oxygenated molecules came into light suggesting alternative oxidation pathways. Experimental results such as these put us beyond our comfort zone motivating us to investigate oxidation pathways and thermochemistry more in detail. This talk summarizes our recent studies and methodology with an emphasis on low-temperature chemistry.

Keywords: kinetics, oxidation, biofuels, jet-stirred reactor

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Poster Session 1



Abstract_S1_All_01

Exploring biofuel low-temperature chemistry with a hybrid reactive molecular-dynamics / quantum-chemistry scheme

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Abstract

Low-temperature ignition is a desired phenomenon in fuels for self-ignition engines and undesired in spark-ignition engines. A detailed understanding of the underlying chemistry is therefore important to design new (bio)fuels. Unfortunately, many of the involved reactions cannot be studied experimentally in an isolated way. Nevertheless, one can study such reactions with quantum-chemical computations or observe them in molecular dynamics simulations. Some drawbacks are, though, that quantum-chemical computations need good starting structures (and one needs to know the reactions that occur); reactions at the time scales of MD simulations, especially at low temperatures, are extremely rare events and will, in the worst case, not even occur. In this work, we show how we can overcome both drawbacks by a suitable combination of accelerated MD simulations and quantum-chemical computations. The complex process leading to ignition at low temperatures is composed of subsequent reactions like O_2 -addition, internal hydrogen abstraction and finally decomposition that releases two OH radicals and thereby leads to chain branching. Acceleration techniques are available for abstractions and decompositions. Most of them focus on energetic barriers by increasing the temperature, or altering the PES with a bias. Addition reactions show barriers resulting from translational entropy and no special acceleration technique for this has been designed to day. To accelerate also the two O_2 additions in the ignition chain, we design the pAD (pressure-accelerated dynamics) method. While increased temperature tends to hamper addition reactions, increased density (or pressure) can strongly accelerate addition reactions and stabilize the corresponding products. By increasing pressure, low-temperature chemistry tends to appear at higher temperature. Increased pressure thereby not only accelerates addition reactions strongly but also allows to increase the simulation temperature, thereby also accelerating subsequent abstraction and decomposition reactions. Accelerated simulations that start with a fuel radical and O_2 not only quickly unfold low-temperature chemistry known from present combustion mechanisms but also reveal side reactions and undergo isomerizations that allow to study also fuel isomer low-temperature chemistry from the same simulation run. The MD simulations evaluated by the ChemTraYzer 2.0 software yield first estimates for the reaction rate constants. This software also extracts reactant and transition state structures from the trajectory. This allows to start high-accuracy quantum chemical calculations. We also derive corrections for anharmonicity from the MD simulation. We apply the method to reveal the largely unknown ignition chemistry of new biofuel candidates like diocylether and complete well-investigated base mechanisms with the new fuel-specific reactions revealed and computed by the presented approach.

Detailed chemical modeling of biomass combustion in domestic heating appliances in order to reduce their polluting emissions

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Abstract

This paper presents a new kinetic model of wood combustion considering especially in details the gas-phase reactions related to the combustion of the tars produced by the biomass devolatilization. The tar production is predicted using a semi-detailed mechanism of the literature. The tar gas-phase combustion model has been built as a compilation of several literature mechanisms. The new detailed kinetic model of wood combustion, BioPOx (Biomass Pyrolysis and Oxidation), has been tested against a wide range of experimental devices and operating conditions.

Abstract_S1_All_03

Design and validation of single pulse shock tube for combustion chemistry investigations

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Abstract

Experimental validation plays an important role for the further development and improvement of chemical kinetic mechanisms. This work discusses the implementation of a well-established method of measuring species concentrations in a shock tube. An existing shock tube facility was converted to single-pulse mode and coupled to a gas chromatograph/mass spectrometry (GC-MS) system to facilitate gas-phase chemical kinetic experiments. Temperatures of up to 2000 K can be achieved. The test pressures are in the range of 1–3 atm. The details of the design and construction of this facility are described. The results obtained are compared with existing data in the literature and demonstrate that the new facility has been commissioned successfully and confirm the validity of the methodology.

The thermal degradation of nitro and nitrate compounds: a study of nitromethane and isopropyl nitrate pyrolysis

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Abstract

Soil remediation becomes more and more important for the preservation of the environment and human health and the reuse of polluted areas. Several strategies can be used according to the nature of organic pollutants. Thermal desorption followed by thermal decomposition can be used for the treatment of pollutants in soils such as hydrocarbon fuels, poly-aromatic hydrocarbons, or toxic gases containing heteroatoms (e.g. chlorine, nitrogen, sulphur...). Among them, nitro and nitrate compounds are widely used as pesticides or explosives and can cause environmental woes including pollutions of groundwater reservoirs or soils. That is why it is crucial to understand the chemistry of the thermal decomposition of these compounds to predict the influence of operating conditions on the reactant decomposition and on the nature and yields of reaction products. In this work, the nitromethane and the isopropyl nitrate were chosen as surrogates to model the thermal destruction of nitro and nitrate compounds. The pyrolysis of nitromethane was studied at temperatures from 500 to 1100 K using an alumina tubular reactor (TR) placed in a high temperature horizontal furnace. At 925 K, nitromethane was fully destroyed. The following products were detected and quantified: NO, CO, methane, CO₂, formaldehyde, H₂O, ethane, propene, and methanol. The main decomposition reaction of nitromethane is the unimolecular initiation by breaking the C-N bond (53 kcal/mol). The pyrolysis of isopropyl nitrate (IPN) was studied at temperatures between 373 and 773 K in the same tubular reactor. At 548 K, IPN was fully destroyed and the main reaction products are acetaldehyde, formaldehyde, methane, CO, NO, methanol and nitromethane. The O-NO₂ bond dissociation (38 kcal/mol) is the major way of decomposition of IPN. A detailed kinetic model has been developed and tested against both experimental set of data for the pyrolysis of nitromethane and isopropyl nitrate. A significant number of reactions parameters have been estimated. Overall, this model gives good predictions of the reactivity and of the major products but improvements is needed to better take into account the formation of minor products, especially for the kinetic parameters estimated.

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Abstract_S1_All_05

Temperature and pressure dependence of the C-O bond fission reactions of dimethoxymethane

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Abstract

The pyrolysis of dimethoxymethane (DMM) was investigated behind reflected shock waves at temperatures between 1100 and 1600 K at pressures between 0.4 and 4.5 bar with Ar as bath gas. H-atom concentrations were monitored by atom resonance absorption spectroscopy. Temperature-dependent rate coefficients for the C–O bond fission reactions of DMM were inferred from the recorded $[H](t)$ -profiles and found to exhibit a pronounced pressure dependence. To gain further information, we performed quantum chemical calculations at the coupled cluster level of theory to explore the relevant potential energy surface. On the basis of these data, statistical rate theory calculations with the simplified Statistical Adiabatic Channel Model were performed and preliminary results of these calculations are presented and discussed.

Abstract_S1_All_06

Byproduct formation in the thermolysis and hydrolysis of urea

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Abstract

We investigated elementary gas-phase reactions in the context of the thermolysis and hydrolysis of urea with high-level quantum-chemical calculations, putting the focus on byproduct formation in urea-SCR applications. Explicitly correlated coupled cluster and density functional theory calculations were performed to characterize stationary points on relevant potential energy surfaces and to provide molecular properties for statistical rate theories. In our contribution, we report on reaction pathways for this system and discuss implications of our findings. First results showed that a purely homogeneous mechanism is not able to explain the extent of byproduct formation, leading us to a more detailed study on the influence of water on the kinetics.

Abstract_S1_All_07

Low-temperature combustion of methylbutene isomers under engine-relevant conditions

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Abstract

Ignition delay times of the C₅ branched alkenes, i.e. 2-methyl-1-butene, 2-methyl-2-butene, and 3-methyl-1-butene, are measured under the engine-relevant thermodynamic conditions of 700–890 K and up to 20 bar with the ULille rapid compression machine. Results show that the ignition delay times as well as the deviation from Arrhenius behavior are determined by the molecular structure of these isomers. The H abstraction and O₂ addition, followed by the internal isomerization reaction scheme that leads to the low-temperature chain-branching pathway, is affected because of the C=C double bond. In detail, if the C–H bond is allylic, it hardly undergoes the O₂ addition pathway and relevant negative temperature coefficient behavior, which is confirmed with our experimental results.

Pyrolysis kinetics of n-propylcyclohexane and isopropylcyclohexane at various pressures

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Abstract

Cycloalkanes are an important class of chemicals in jet fuels. Pyrolysis and combustion of cycloalkanes tend to produce more aromatics than those of alkanes. In order to better understand effect of the fuel structure and pressure condition on reaction pathways, the pyrolysis experiments of n-propylcyclohexane (n-PCH) and isopropylcyclohexane (i-PCH) were conducted in a flow reactor at the pressures of 30 and 760 Torr. Pyrolysis species including C₁ – C₄ hydrocarbons, dialkene, cyclic hydrocarbons and aromatics were comprehensively detected and identified by using synchrotron vacuum ultraviolet photoionization mass spectrometry (SVUV-PIMS). The primary decomposition pathways of the two isomers were analyzed, including the initial unimolecular decomposition and H-abstraction reactions. The experimental and modeling results show that the pyrolysis behavior of the two isomers are influenced by the fuel structure. More branched hydrocarbons such as pentene and hexadiene were produced in the i-PCH pyrolysis. However, the pyrolysis of i-PCH produced less ethylene, propene, 1,3-butadiene and aromatics than that of n-PCH, which suggests that the branched alkyl substitute in alkylcycloalkanes might lead to more initial decomposition pathways and have an inhibiting effect on the formation of PAHs and soot precursors.

Abstract_S1_All_09

Study of the oxidation of the butanol isomers in a plug flow reactor

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Abstract

New experimental data on the oxidation of the four butanol isomers (n-butanol, 2-butanol, isobutanol and tert-butanol) in a plug flow reactor setup, in the temperature range from 800 to 1400 K, under different stoichiometry conditions, ranging from fuel-rich ($\lambda=0.7$) to fuel-lean ($\lambda=10$) conditions, are provided and the results are simulated with a reaction mechanism compiled from literature submechanisms. Results indicate that stoichiometry is found to slightly modify the onset temperature for the butanol isomers conversion, while it is more important once reaction has been initiated. Additionally, a similar behaviour of the conversion of 1-butanol, 2-butanol and isobutanol is seen, since those isomers exhibit a similar oxidation regime, while tert-butanol behaves differently. Simulation predictions agree quite well with experimental results.

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Thermochemical study for species and reactions occurring in the S-N-O system

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Abstract

Sulfur is a very cost-effective energy carrier and can be stored outdoor under ambient conditions. Besides its use for the production of sulfuric acid, sulfur combustion in oxygen or in air releases heat which may be used for generation of electricity in closed cycles where, e.g. solar heat is applied to recover elemental sulfur from the combustion products [1, 2]. In order to study the oxidation and combustion of sulfur with air, several sulfur- nitrogen-oxygen reactions are investigated with the objective of developing reaction mechanisms where the nitrogen from air is participating during combustion. The developed sub-mechanism will be then added to an existing mechanism for the oxidation of sulfur. Employing a number of computational chemistry methods, a detailed study of the thermochemistry of the species involved in the sulfur + air system is presented in this work. Structures and enthalpies of formation for a series of stable molecules, radicals as well as transition state structures resulting from the S-N-O association reactions are reported along with reaction paths and energy barriers. Enthalpies are calculated with the help of ab initio at CBS-QB3, G3B3, G4 and whenever possible at W1U levels of calculation. The calculations were combined with isodesmic reaction analysis, in order to cancel errors and to improve the accuracy of the calculations. Entropy and heat capacity contributions versus temperature are determined from structures, moment of inertia, vibrations and frequencies. The rate of reactions were calculated and compared with data from literature [3] when available. Kinetic parameters are determined as a function of temperature and pressure from the CBS-QB3 composite methods derived thermochemical parameters using bimolecular chemical activation analysis. High Pressure limit kinetic parameters are obtained from canonical Transition State Theory calculations and quantum Rice–Ramsperger–Kassel (QRRK) analysis to calculate $k(E)$ with master equation analysis to evaluate falloff in this reaction system. In a future study, the impact of the developed sub-mechanism on laminar burning velocities of sulfur combustion will be analysed.

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Abstract_S1_All_11

Pyrene + O₂: primary reactions, reaction pathways, and influence of functional groups

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Abstract

Graphene surfaces are layers of hexagonal carbon-based lattice and oxidation of graphene results in graphite oxide formation with different C:O ratios. Due to their advantageous properties, among others, thermal conductivity, graphene and graphite oxide on one hand are applied in fields such as solar cells, thermal interface materials or supercapacitors. They serve as energy storage alternative to traditional electrolytic batteries and have shown faster charging, longer life span and environmentally friendly production [1, 2, 3]. On the other hand, soot particles are composed of more or less ordered graphene layers which are oxidised during soot burn-out in flames or soot oxidation in particle filters. The present work is dedicated to the oxidation and decomposition of graphene and graphite oxide through molecular oxygen (O₂) addition using DFT calculations. To enable DFT calculations, graphene and graphite oxide are represented by four hexagonal rings assimilated to pyrene (C₁₆H₁₀ = A₄) and pyrene oxides. The goal of the study is to investigate the influence of oxygenated groups on the rate of oxidation reactions. The molecules considered in this work are Pyrene (A₄), 1-Hydroxypyrene (A₄OH), 1-Pyrenecarboxaldehyde (A₄-CH(=O)) and 1-pyrenecarboxylic acid (A₄-C(=O)OH). The attack of molecular oxygen on these molecules can occur on different sites. The primary reactions of O₂ on pyrene and pyrene oxide, is the abstraction of side-hydrogens to form a reactive radical plus OOH. The location of the hydrogen to the functional group is also considered. The direct addition of O₂ to a centered carbon resulting in the opening of the strong C=C double bond is also investigated. It is assumable that this last reaction requires higher activation energy than the H-abstraction. With the help of computational methods, using density functional theory (DFT), this study calculates and reports the species occurring in this systems, transition states and reaction pathways. The kinetics of the reactions as a function of temperature and pressure are determined using bimolecular chemical activation analysis. High Pressure limit kinetic parameters are obtained from canonical Transition State Theory calculations.

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The impacts of iso-butanol blending on the low temperature autoignition behaviour gasoline and its surrogate

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Abstract

This study investigates the impact of iso-butanol blending on the ignition delay times of gasoline (reference gasoline PR5801 – RON 95.4, MON 86.6) and a 5-component gasoline surrogate, at blends of 10%, and 50% by volume iso-butanol. Ignition delay time measurements were produced at compressed temperatures of 710-870 K and a compressed pressure of 20 bar, under stoichiometric fuel/air conditions ($\Phi = 1$). The 5-component surrogate provided a good representation of the reference gasoline's ignition behaviour, except under a high degree of iso-butanol blending, where the surrogate produced significantly longer ignition delay times, particularly at low temperatures. Kinetic simulations failed to represent the intensity of the NTC behaviour in both the 5-component surrogate and blends with 10% iso-butanol, which coincides with an over prediction of low temperature heat release rates.

Abstract_S1_All_13

Direct measurement of high-temperature rate constants and branching ratios on the pyrolysis of diethyl ether behind reflected shock waves

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Abstract

In the group of oxygen-containing organic compounds, ethanol is currently the most widely used biofuel. Besides alcohols, in particular ethers are used as additives and components of synthetic fuels. Diethyl ether (DEE) can be produced on large scale by vapour-phase dehydration of ethanol over heterogeneous catalysts. Recently, Yasunaga et al. [1] investigated the pyrolysis and oxidation of DEE behind reflected shock waves by measuring ignition delay times and by applying IR absorption and UV emission spectroscopy. They also measured product distributions behind reflected shock waves and based on these experimental results, a reaction mechanism on DEE combustion has been developed and validated [1, 2]. The aim of the present work is to directly determine rate constants and branching ratios of initial unimolecular DEE decomposition steps by combining three detection techniques: Time-dependent species concentrations during DEE pyrolysis were studied by high-repetition-rate time-of-flight mass-spectrometry (HRR-TOF-MS). Remaining reactants and stable reaction products were measured in the same shock tube operated in single-pulse mode by GC/MS after rapid quenching of the reaction through gas-dynamic processes. In addition, we measured the temporal variation of H-atom concentrations with highly sensitive atomic resonance absorption spectrometry (ARAS). The experiments span a temperature range of 1000–1400 K, and a pressure range of 1.2–2.5 bar. The initial concentrations of DEE range from 0.5 ppm (H-ARAS) up to 10000 ppm (HRR-TOF-MS). Additional single-pulse shock-tube experiments were performed with high excess of the radical trap toluene. The overall rate constant k_{total} of DEE decomposition [$k_{\text{total}} \rightarrow \text{products}$] consists of three channels: a molecular channel $\text{DEE} = \text{C}_2\text{H}_5\text{OH} + \text{C}_2\text{H}_4$, (k_1) and two bond-dissociation channels, $\text{DEE} = \text{C}_2\text{H}_5\text{O} + \text{C}_2\text{H}_5$ (k_2), and $\text{DEE} = \text{C}_2\text{H}_5\text{OCH}_2 + \text{CH}_3$ (k_3). Since secondary decomposition of C_2H_5 , $\text{C}_2\text{H}_5\text{OCH}_2$, and to a minor extent $\text{C}_2\text{H}_5\text{O}$ radicals yield H atoms, H-ARAS can be used to determine the sum of the rate constants $k_2 + k_3$. By HRR-TOF-MS and GC/MS, the present experiments permit to extract overall rate constant data k_{total} . Therefore, the combination of these detection techniques also allows to directly extract information on the branching ratio $(k_2 + k_3)/k_{\text{total}}$.

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Abstract_S1_All_14

Considerations in mechanism reduction applied to alcohol fuels

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Abstract

Analysis of the principal reactions subsets of methanol, ethanol, and n-propanol for reduced kinetics is presented. Three reduced mechanism, one for each fuel, was generated, consisting of 16 species and 44 reactions, 26 species and 84 reactions, and 36 species and 107 reactions respectively. The validity of the mechanisms was shown through species profiles and ignition delay times compared to reference mechanism by Gong et al. and AramcoMech 1.3. The analysis illustrates important chemistry for the reduced alcohol schemes, and highlights challenges with larger fuels. It was shown that the complexity of n-propanol is greater than for methanol and ethanol.

Abstract_S1_All_15

An experimental and modelling study of the oxidation of cyclopentanol at high pressures

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Abstract

In this study, experiments on the oxidation of cyclopentanol were performed at high-pressure and high-temperature in a jet-stirred reactor and a shock tube. Mole fraction measurements in JSR were obtained with an initial mole fraction of fuel of 1000 ppm, at 10 atm, for equivalence ratios of $\varphi = 0.35, 0.5, 1, 2$ and 4, temperatures ranging between 730 and 1180 K, and a residence time of 700 ms. Ignition delay times were measured for mixtures of 1% cyclopentanol/O₂/argon in a shock tube at 20 and 40 bar in a temperature range of 1000 - 1450 K and for equivalence ratios of $\varphi = 0.5, 1$ and 2. These experimental results were used as targets to develop and test a detailed kinetic mechanism allowing us to delineate the major pathways involved in the oxidation of cyclopentanol.

Abstract_S1_All_16

Study of the oxidation of ammonia as an alternative to carbon-based fuels

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Abstract

The present work is focused on the analysis of the ammonia oxidation process and the formation of main nitrogen oxides (NO, NO₂ and N₂O) over a wide range of temperatures and O₂ reaction environments. Experiments are performed at atmospheric pressure in a laboratory quartz tubular flow reactor, covering the temperature range of 800 to 1500 K and for different air excess ratios (from pyrolysis to very oxidizing conditions). The experimental results are simulated and interpreted in terms of a detailed chemical-kinetic mechanism. Reaction path and sensitivity analyses are used to delineate the NH₃ oxidation here.

Abstract_S1_All_17

Experimental and modeling study of the oxidation of benzaldehyde

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Abstract

The gas-phase oxidation of benzaldehyde has been investigated in a jet-stirred reactor at 107 kPa, temperatures between 700 and 1100 K, with a fixed residence time of 2 s, and an inlet fuel content of 0.5% in helium and for three equivalence ratios ($\varphi=0.5, 1$ and 2). Benzaldehyde is an aromatic aldehyde commonly considered in bio-oils surrogate formulation, and an important intermediate in the oxidation of other aromatic reference fuels such as toluene. However, its oxidation has never been previously investigated experimentally, and no product formation profiles were reported in the few studies performed under pyrolysis conditions available in the literature. In the present study 48 species, mainly carbon monoxide, carbon dioxide and phenol were detected using gas chromatography. These species indicate a rapid formation of phenyl radicals via the abstraction of the aldehydic H-atom and CO elimination. This was confirmed by the analysis performed using the current version of the CRECK kinetic model, in which the reactions of phenyl radicals and oxygenated aromatic compounds have been updated. The model analysis also showed up that phenoxy radicals are important intermediates in the decomposition of benzaldehyde.

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Experimental analysis and 1D modelling of counterflow ammonia-methane flames

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Abstract

To mitigate global warming, it became crucial to reduce our greenhouse gases emissions. Specifically, the reduction of emissions of carbon dioxide from combustion systems is a crucial issue. In this context, ammonia is considered as a promising alternative fuel. Ammonia is a carbon-free fuel, and theoretically, the end-products of its combustion consists only of nitrogen and water. Ammonia can be produced from renewable resources using water electrolysis for hydrogen production, combined with the Haber-Bosh process. It has the advantage to be transported and stored easily, at conditions similar to those of propane. These characteristics make ammonia a suitable candidate as an alternative fuel and an energy carrier for use in near future. However, ammonia presents low reactivity compared with other fuels. This makes the development of ammonia combustors for industrial applications challenging. In this study, mixtures of ammonia and methane have been considered. The combustion of ammonia/methane/air mixtures allows a reduction of carbon oxides emission compared with the case of pure methane/air combustion. In addition, the mixture has a higher reactivity compared with pure ammonia/air mixtures. Although there are a series of previous studies on ammonia oxidation, the characteristics of ammonia as a fuel remains partially unknown. Existing ammonia oxidation kinetics have been validated for some combustion characteristics of ammonia and at specific range of conditions. Hence kinetic mechanisms that can model over a wide range of conditions are scarce. Mixture of ammonia and methane have been essentially investigated for small amount of ammonia introduced. This is not representative of the case of applications considered in this study, where ammonia is used as a mean to reduce carbon emissions, and thus introduced in larger quantity. Hence, it is necessary to validate the mechanisms toward wide range of conditions, to understand the interactions between both fuel oxidation mechanisms, the formation/reduction of pollutant species such as carbon oxides as well as nitrogen oxides. In this study, flames were observed in a well-studied counterflow configuration, which can be easily modelled numerically and is thus suitable for chemistry validation. Both diffusion flames and premixed flames have been investigated, for fuel mixture going from pure ammonia to pure methane, and various stoichiometry. Mechanisms were validated based on the extinction stretch rate, as a global parameter of this type of flame, and the OH and NO radicals' distribution in the flame, as a local parameter essential in the understanding of NO_x formation. Extinction stretch rate was determined from the measurement of flow rate at flame extinction and corrected based on velocity flow field measurements using PIV method. OH and NO radicals' qualitative distribution was observed using PLIF imaging and then post-treated

for mechanism validation. Numerical simulations were performed on the opposed-flow commercial code from Chemkin-Pro software (ANSYS software). Experimental results were compared against several mechanisms available in the literature and an analysis of these chemistries has been performed.

Towards a better understanding of the combustion of oxygenated aromatic hydrocarbons. Comparing benzene, toluene, phenol and anisole with ignition delay times in a rapid compression machine

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Abstract

Ignition delay times (IDTs) of the oxygenated aromatic hydrocarbons (OAHCs) anisole ($C_6H_5OCH_3$) and phenol (C_6H_5OH) and the analogues non-oxygenated aromatic hydrocarbons (AHCs) toluene ($C_6H_5CH_3$) and benzene (C_6H_6) have been measured in the PCFC rapid compression machine (RCM) at stoichiometric, fuel-in-air conditions. With the two targeted compression pressures (p_c) of 1 and 2 MPa a temperature range of 870 to 1100 K was covered. The IDTs of all four molecules revealed an Arrhenius behavior. The different reactivity can be ranked as the following, starting with the lowest reactivity: benzene < toluene < phenol < anisole. Literature available models containing anisole and phenol have been used to simulate the IDTs of *this study* highlighting discrepancies in both, model to experiment and model to model accordance. Finally, the CRECK mechanism was used to conduct rate-of-production (ROP) and sensitivity analysis to gain insight into the combustion of OAHCs and highlight interconnections and shortcomings of OAHCs.

Abstract_S1_All_20

Global quasi-linearization (GQL) for methane-air MILD combustion

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Abstract

The moderate or intense low-oxygen dilution (MILD) combustion becomes more and more attracting because negligible soot formation and very low NO_x and CO emission can be achieved in this special combustion regime. Based on a simplified model, the phenomenon of MILD combustion can be studied by using homogeneous reaction systems, e.g. corresponding to auto-ignition processes, which are usually formulated by a set of ordinary differential equations (ODEs). Typically, for reliable results very detailed chemistry in terms of both dimensionality (as a number of species) and non-linearity (Arrhenius temperature and species concentration dependence) should be used to describe the process. This is usually computationally demanding. Thus, reduced modelling is needed to speed up computational time, decrease memory requirements and simplify analysis of the results. In this work, an automatic model reduction method for chemical kinetics, the so-called Global Quasi-Linearization (GQL) method, is implemented to reduce the homogeneous systems for MILD combustion. Unlike classical reduction methods such as quasi-steady state approximations (QSSA) that require a deep understanding/knowledge about chemical species, GQL is a suitable framework for automatic model reduction and decomposition of the system dynamics. It is based on an analysis of the characteristic time scales, and uses slow and fast low-dimensional manifolds defined in the system's thermo-chemical state space. In order to verify and present the approach in this special regime the methane/air system is chosen with the Warnatz mechanism (34 species, 147 reversible elementary reactions) used as chemical kinetics model. As a main outcome of the study a 14-dimensional (14D) GQL reduced chemistry can be considered in a wide range of system parameters and initial conditions for both the MILD combustion regime and for an auto-ignition process. It is shown that the 14D GQL reduced chemistry can predict both the ignition delay times and species concentrations very well, and agrees with detailed chemistry within less than 5% of relative error. For further validation the same 14D GQL reduced chemistry model is applied for N_2 - and CO_2 -diluted and H_2 -enriched MILD combustion. It is demonstrated that the effects of N_2 and CO_2 dilution and H_2 enrichment are captured very well by using this reduced chemistry.

Abstract_S1_All_21

Effects of radiation on premixed spherical flame propagation

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Abstract

For stretched propagating spherical flames, the flame propagation speed is affected by flame stretch as well as radiation. In this study, the effects of radiation on spherical flame propagation and radiation-induced uncertainty in laminar flame speed measurement are investigated. The radiation-induced thermal and flow effects are introduced, and their influence on laminar flame speed measurement is discussed. Furthermore, the radiation effects on small-scale and large-scale spherical flame propagation are compared.

Abstract_S1_All_22

Stability of buoyant laminar diffusion syngas flame: impacts of H₂:CO

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Abstract

A CFD model is generated based on the burner of [1] for studying the conditions of syngas laminar diffusion flames, in which stable flames naturally transform to flickering and tip-cutting flames. In the investigation, fuel flow rate of syngas, with the H₂:CO ratio as being 1:3, 1:1, and 3:1, is varied between 0.2 and 1.4 SLPM (standard litre per minute). Finite rate chemistry model is selected for computing the species production rate and this model is supplied with the DRM22 reaction mechanisms [2]. The critical Reynolds number obtained is relatively high when syngas contains a low H₂:CO concentration ratio. This finding is predicted at both the types of transformation; (i) stable/flickering, and (ii) flickering/tip-cutting. The fuel rate at which a stable flame transforms to flickering is found to be equal for all the studied flames. However, the syngas flame, with a low H₂:CO concentration ratio, has a lower critical fuel rate for the flickering/tip-cutting transition condition. In particular, at the stable/flickering critical condition, the stable flame of syngas, again with a low H₂:CO, provides higher heat from the chemistry reaction, thus resulting in the higher temperature and larger flame size. Furthermore, the flickering frequency of the unstable flames is predicted between 9.6 and 11.8 Hz for the hydrogen flame, while it is between 10.76 and 13.23 Hz for the syngas flame.

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Low dimensional chemistry manifolds applied to premixed methane/air flames under atmospheric conditions

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Abstract

Detailed simulations of turbulent reactive flows require high computational power, especially if hydrocarbons are involved. To reduce the chemistry mechanism, Intrinsic Low Dimensional Manifolds (ILDM) generated via dynamic perturbations of a reactor system are used in this work. A preliminary analysis of such manifolds is performed on methane/air premixed flames at ambient conditions. Autoignition times with the same order of magnitude of the finite rate calculation were predicted if a smooth transition between the ILDM subspaces was guaranteed. However, two reactive progress variables were not sufficient to correctly predict the laminar flame speed of 2D Bunsen flames. Future work aims to include an additional reactive progress variable and to remove the table interpolation routine by training an artificial neural network.

Effect of progress variable definition on the mass burning rate of premixed laminar flames in flamelet generated manifold methods

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Abstract

The Flamelet Generated Manifold (FGM) method is a well-known chemical reduction method which tabulates the combustion chemistry to speed up combustion simulations. In this study two-dimensional (2D) manifolds are used with reaction progress variable and enthalpy as first and second control variable, respectively. When two-dimensional burner-stabilized laminar flame simulations are carried out for premixed CH₄-air mixtures, it is found that the FGM flames are shorter than the direct numerical simulation (DNS) using the full mechanism. It is observed that the choice of species for the progress variable affects how long a particular FGM flame is. This is believed to be caused by the change in mass burning rates due to stretch and curvature effects. To study this in detail, 1D adiabatic flame simulations are carried out with different progress variable definitions for different stretch rates and curvature radii, which are extracted from the 2D flame calculations. It is shown that FGM is able to predict the main effect of stretch and curvature on the mass burning rate, but that certain progress variables predict changes in the mass burning rate closer to the detailed chemistry. This can help in deciding the best choice of progress variable for calculations where accurate prediction of the mass burning rate is important.

The effect of droplets on laminar propagation speed of an acetone-methane flame

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Abstract

We investigate the effect of acetone droplet size and concentration on the flame propagation rate of a methane/air laminar flame, and compare its behavior to the fully vaporized mixture, using a jet-wall stagnation flame configuration. A narrowly distributed polydisperse mist of acetone droplets are generated by an air blast atomizer and mixed with methane/air mixture for a total acetone concentration of 9% and 20% by mole of methane. We vary the Sauter Mean Diameter (SMD) of acetone droplets from 1.0 to 4.7 μm by carefully tuning the air flow rate passing through the atomizer. The droplet size distribution is characterized by a PDA system at the outlet of the burner. The flame propagation speed is measured using Particle Image Velocimetry for overall equivalence ratios ranging from 0.85 to 1.35 at various strain rates, and the result is compared with a reference case in which acetone was fully vaporized. Unlike the fully vaporized flame, a two-stage reaction flame structure is observed for all droplet cases: a blue premixed flame front followed by a sooty diffusion flame. The result shows that the mean burning velocity of the mixture is significantly enhanced by adding acetone droplets under rich cases, whereas for stoichiometric and lean cases, the presence of droplets appears to slow down the flame. The mean size also changes the measured Markstein length, especially for rich cases. The dual fuel study creates a systematic method for studying steady strained droplet-laden stabilized flames, which can be expanded to other fuels and conditions.

Abstract_S1_All_26

Experimental study of premixed ozone-seeded DME/O₂ cool flames on a stagnation plate burner

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Abstract

The Flamelet Generated Manifold (FGM) method is a well-known chemical reduction. The emergence of new low-emissions combustion strategies such as SACI (Spark Assisted Compression Ignition) or PPCI (Partially Premixed Compression Ignition) brings new challenges for the performance of kinetic models in the LTC (Low Temperature Combustion) parametric range. In this context, a novel stagnation plate burner is designed and developed at the PC2A Laboratory to study the LTC reactivity inside premixed cool flames. DiMethyl Ether (DME) is chosen as fuel for its strong low temperature reactivity. Ozone-seeding from 0 to 7.8 mol.% is used to enable LTC reactivity in these conditions. The plate is heated at 600K. The ozone mole fraction is monitored by means of absorption spectroscopy. CH₂O* chemiluminescence is used in conjunction with CH₂O Planar Laser Induced Fluorescence (PLIF) to locate the flame front and investigate the structure of the stabilized cool flames. Stability limits at low equivalence ratios (0.01 to 0.20 with a step of 0.01) and strain rate between 10 and 25 s⁻¹ are investigated.

Abstract_S1_All_27

1064 nm laser-induced grating spectroscopy (LIGS) measurements in flames at pressure

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Abstract

Laser-Induced Grating Spectroscopy (LIGS) using a 1064 nm pump laser is applied to premixed CH₄ air laminar flat flames under operating pressures of 1 to 6 bar. For the first time, temperature and water concentration are acquired simultaneously in a reacting flow environment using LIGS. The measured values of speed of sound, temperature, and water concentration in the flames examined compare favorably with flame simulations with Chemkin. These results confirm the potential for 1064 nm LIGS-based thermometry for high-precision temperature measurements of combustion processes.

Abstract_S1_All_28

An image processing routine to estimate the laminar flame speed of H₂-enriched biogas/air flames

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Abstract

This work aims at estimating the impact of hydrogen (H₂) content in the S_L of biogas (CH₄/CO₂/air) flames. CH₄/CO₂/H₂ blends are studied at lean conditions. Premixed laminar flames are produced experimentally to estimate SL using an in-house algorithm capable of identifying the flame front. Results are compared with data from CANTERA simulations in a freely propagating flame routine fed with the latest USC-Mech chemical kinetic mechanism. This approach detects the flame front of conical premixed flames and estimates the laminar flame speed (S_L) using the half apex cone angle (α), where $S_L = u_v \times \sin(\alpha)$, with u_v being the velocity of the reactants at the burner's outlet. Agreement with simulations was good, particularly for low CO₂ concentration.

Abstract_S1_All_29

Influence of DC electric fields on laminar pre-mixed propane/air flames

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Abstract

The present work evaluates the influence of Direct Current (DC) electric fields in small conical, laminar, premixed flames of propane/air, anchored in perforated plates. The electric field promoted a flame stability increase, characterized by an expression which estimates the blow-off Reynolds, Re as a function of the equivalence ratio, ϕ and electric field strength, E : $Re \cong m'_0 (1 + \kappa E)\phi - m'_0 (1 + \kappa E)LSL$, where m'_0 is the corrected slope of the blow-off line of the non-actuated flame, LSL is the lean stability limit and κ is an experimental constant. The electric field promoted a flame stability increase, allowing a burner power density increase up to 190% for $\phi = 0.8$.

Abstract_S1_All_30

Data consistency of the burning velocity measurements using the heat flux method: syngas flames

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Abstract

The present work is aimed at presenting detailed analysis and comparison of the existing experimental data of the laminar burning velocity obtained for syngas flames using the heat flux method. The core of the approach is the evaluation of any variability or inconsistency among data obtained under the same experimental conditions. Some questionable conditions have been experimentally revisited. The possible sources of uncertainty have been discussed and analyzed. Recommendations are given towards the reduction of experimental errors.

Propane/air flame impingement on a cylindrical surface: experimental investigation of heat transfer

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Abstract

Heat fluxes at the stagnation point were investigated for laminar, premixed propane/air flame impinging against a water-cooled ceramic tube by surface temperature measurement with phosphor thermometry. The temperatures in the gas phase were also measured with a thermocouple of type R. The evaluated heat fluxes for propane/air flames were compared to previously studied methane/air flames for stoichiometric condition. The results show change of flame stabilization mechanism, from burner stabilized to wall stabilized, with 2.3% higher heat fluxes for propane/air than methane/air flames at wall stabilized, and no noticeable change at burner-stabilized flames. Higher heat fluxes were obtained at smaller burner to impingement surface separation distances.

Abstract_S1_All_32

Study of laminar burning velocities and NO formation for methanol-air flames

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Abstract

Laminar burning velocities for methanol-air combustion were measured in flames stabilized on a heat flux burner. In addition, the quantitative NO concentration was measured in the product zone at height 10 mm above the burner surface by means of laser-induced fluorescence. Moreover, the method was verified by measurements of NO concentration in premixed methane-air flames for which results could be compared with previous probe-sampling measurements. The investigated flames were modelled with five kinetic mechanisms. While the thermal NO is well predicted by all the models, there is large variations between predictions of the prompt formation.

The H₂, H preferential diffusion effect on extinction behavior in SNG/air premixed symmetric flames

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Abstract

SNG which has complex component is generated by carrying out the methanation process to H₂ and CO generated through the gasification process of coal for making equality heat value with LNG. SNG-C11 (CH₄: 80%, C₃H₈: 9%, H₂: 11%) was used in counter flow burner in order to observe the effect of preferential diffusion of hydrogen in the flame extinction behavior. OPPDIF-code was used for numerical analysis which describing the counterflow burner. To confirm H₂, H Preferential diffusion effects, H₂ and H's mass diffusivity equalized with N₂' one. Effects of mass diffusivity was dramatically occurred in flames let, production of species, reaction path.

Abstract_S1_All_34

Laminar burning velocities of hydrocarbons with ethanol addition

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Abstract

Laminar burning velocities of n-decane, p-xylene and methylcyclohexane mixed with ethanol + air flames were determined using the heat flux method at atmospheric pressure and initial temperatures of 298–400 K. The experiments were conducted on two different experimental setups: at Samara University and Lund University. In the course of the study, the effect of ethanol addition on the burning velocities was investigated. Data consistency was assessed with the help of analysis of the temperature dependence of the laminar burning velocity, which was interpreted using an empirical expression $S_L = S_{L0}(T/T_0)^a$. The predictions of the PoliMi detailed mechanism were found in a good agreement with the experiments performed with n-decane, p-xylene and their blends with ethanol.

Nature and origin of O-PAH compounds in biomass combustion emissions and their destruction

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Abstract

There is considerable interest in the emission of oxygenated PAH species from the combustion of fossil fuels and from biomass; at present there is particular interest in wood combustion. This arises originally because of the importance in climate chemistry and in relation to the health aspects especially of the reactive oxygenated species (ROS). It has been suggested that an extension to the 'EPA sixteen list' to include O-PAH is necessary. The pyrolysis of biomass leads to two classes of O-compounds: firstly cellulose products form small PAH via HACA and together with CPDyl etc give the soot precursors, some of which have five-membered rings. The initial pyrolysis products of the lignin are phenols – for example 4-methyl-2-methoxyphenol from eugenol in our previous modelling experiments- which go on to form precursors of larger PAH species. The five-membered rings in these PAH compounds formed by both routes can lose an H by H-abstraction and react with an oxygen atom forming compounds such as 1-indanone, 9-fluorenone and peri-naphthalenone. The ratio of the O-PAH to the PAH present in the combustion products is determined by the thermodynamic stabilities of these compounds; these can act as precursors of the oxygenated involatile atmospheric PAH species observed. Five-membered rings in the precursors can then lead to pentagonal curved network regions and hence to bowl-shaped structures (so-called 'protofullerenes') and curved carbon atom sheets consistent with the observed morphology of the soot. Some of these O-PAH are the analogues of the 'protographene' PAH such as benzo[ghi]perylene which act as 'dead- end' PAH and terminate HACA reaction sequences. There is considerable interest in controlling the emissions of these pollutants from the combustion of wood whether they are formed in simple or more sophisticated wood stoves, Strategies are considered for the reactive removal of these species including catalytic means.

1. G. Shen, S. Tao, Y. Chen, Y. Zhang, S. Wei et al., Emission characteristics for polycyclic aromatic hydrocarbons from solid fuels burned in domestic stoves in rural China, *Environ. Sci. Technol.* 47 (2013) 14485–14494.

2 J.M. Jones, A.B. Ross, E.J.S. Mitchell, A.R. Lea-Langton, A. Williams, K.D. Bartle Organic carbon emissions from the co-firing of coal and wood in a fixed bed combustor, *Fuel* 195 (2017) 226-231

Experimental investigation and comparison of particle-laden flows in a gas-assisted oxy-coal combustion chamber for reacting and non-reacting conditions

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Abstract

The investigation of the coupling between fluid mechanics, particle dynamics and turbulent flames is essential to gain a more detailed knowledge in pulverized coal combustion processes. To evaluate the impact of the turbulent flame on the flow field of a 20 kWth gas-assisted coal flame in a oxy-coal combustion chamber, flow fields for non-reacting and reacting conditions are compared. The chamber is optically accessible and equipped with a swirl burner. A two-phase PIV/PTV approach is used to measure gas and particle velocity simultaneously. For the non-reacting conditions the slip velocity between large particles and the gas phase is determined. A systematic study of measurement errors is presented.

Char emissivity measurements for coal chars

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Abstract

Radiation - especially particle radiation - is dominant in pulverized fuel combustion systems. As the radiative heat flux from burning coal particles to the surroundings is linearly dependent on the particles surface emissivity, this value is of special importance. Several parameters affect the emissivity of fuel particles, as there are coal rank, mineral content and composition. During burnout, increasing mineral content and change in pore structure may also contribute to a change in emissivity. The current knowledge on the emissivity of burning coal particles is very limited due to the difficulties associated with measuring this property "in flight". Recently a wider data range on char emissivity of burning char particles determined in in-flight measurements has been created. It includes char emissivity of coal chars in the wavelength range 1.25-5.5 μm . This data set provides unique information on char emissivity, as it includes the first and only measurements of single particle emissivity at char particle temperatures in the range of 1800-2500 K. Although this data set covers a wide temperature range, the in-flight technique which was used restricted the measurement to the early char burnout phase, such that no information on char particles with lower carbon content and high ash at the very late stage of burnout is included. The next step in char emissivity measurements directly tackles the final phase of char combustion. As in-flight measurements have shown their limitation, the particles will be positioned in a levitator, where a laser is used to ignite the char and the burnout process can be monitored with a modified version of the spectrometer system that has previously been used. The new setup and initial results on coal and biomass char emissivity will be presented. The data will include temperature and thermal radiation of burning particles, demonstrating the working principle of the new setup and a forecast to the results which are expected to be the result of a wide measurement campaign.

Demonstration of laser-induced incandescence in single coal particle enveloping flames

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Abstract

Pulverized solid fuels, coal and biomass, are still of interest for worldwide energy supply. Their tendency to cause environmental pollution motivates the investigation of the combustion process with special emphasis on clean and efficient combustion. One aspect is the ignition phase, which is characterized by the release of volatile species. These species contain lighter components but also heavy tars, which burn in an enveloping flame around particles in oxidizing atmospheres when conditions are laminar. This is a very characteristic step in carbonaceous fuel particle combustion and thus deserves further attention. Especially the formation of soot in these flames is an interesting phenomenon which significantly contributes to heat transfer and thus requires deeper understanding. Laser-induced incandescence (LII) has been applied to flames of coal volatiles enveloping single pulverized coal particles for the first time. Measurements were carried out on burning particles of a Colombian high volatile bituminous coal in two atmospheres containing 2 and 10% of oxygen in a laminar flow reactor with optical access. These conditions were chosen to mimic the conditions in the near burner region of coal burners, where soot formation from volatiles is expected to be most relevant. Coal particles sieved to a size fraction of 106-125 μm were injected into the hot gas flow. The ignition process was monitored with time-resolved LII (TiRe-LII) and imaging pyrometry. Using a camera setup with a spatial resolution in the μm -range in the image plane, both LII and pyrometry signals resolve the volatile flame and soot cloud around single burning particles perpendicular to the line of sight and integrating in spatial depth. The results are of preliminary nature, but already indicate the potential of this technique to add valuable information and to supplement existing experimental methods which are already established for optical investigation of pulverized fuel particle ignition.

Heat transfer modeling using waste rubber as starting material in fluidized bed chamber

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Abstract

The lumped model of heat transfer in fluidized bed boiler was investigated to compare the total heat transfer coefficient between experimental and predicted calculation. Waste rubber was used in the combustion process, meanwhile, in the starting (heat up) process, the sand was used as the bed material. The mid-scale fluidized bed burner was 5000 mm in height and 158 mm in internal diameter, in Energy Department, Budapest University of Technology and Economics. Both convection and radiation heat transfer were taken into account in the calculation model. The method for estimating the total heat transfer coefficient was proposed by Golriz and Grace, 2002. The result in the expectation of heat loss and the total heat transfer coefficient reached a high agreement with the experimental calculation data. In the experimental period, the projected heat loss in free-wall and total heat transfer coefficient were about 50 kW and 55 kW/m²K, respectively.

Abstract_S1_AIII_40

Applicability investigation of a validated simulation method developed for a large scale grate incinerator for the case of a small scale pellet boiler

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Abstract

In order to study the applicability of an existing CFD method onto a small-scale pellet boiler, a simulation was conducted. The validated method was developed for the CFD simulation of a waste fuel fired incinerator with a moving grate combustor and is based on an empirical fuel bed model utilizing experimentally derived operating parameters to produce inlet conditions for the freeboard gas phase combustion simulation. It was found that the developed method is suitable for small-scale combustion appliances when freeboard modelling is the priority.

Experimental two stage gasification of Hungarian brown coal for increased H₂ and CO ratio in the produced synthesis gas

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Abstract

Coal is still one of the primary energy source used to fulfill the energy demand of the modern world. While combustion is the most widespread energy production solution, gasification can produce secondary raw materials for chemical processes as methanol production. However, controlling the process of different stages of gasification as pyrolysis can be challenging if the goal is to produce a synthesis gas with a specific requisite composition. The temperature control of the process on its own is not enough to alter the composition of the produced synthesis gas, especially if all reactions take place in a single stage. The main objective of our research is to separate the low temperature and high temperature pyrolysis and gain additional control over the whole process. Two separate reactors were connected through a still pipe that could allow gas flow between them, and they were inserted in two independent temperature-controlled furnaces. Even though synthesis gas produced at low temperatures has high methane quantity, this perhaps can be thermally decomposed by forcing it through the high temperature zone of the experiment setup. The prospects of this setup have been investigated detailing the gasifier setup and the results of experiments.

Gasification of miscanthus x giganteus grown on heavy metal contaminated land

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Abstract

Biomass is a low-carbon resource that is increasing being considered in place of fossil fuels both for energy and chemical feedstock. As such, demand for the supply of dedicated energy crops, such as *Miscanthus*, for the generation of sustainable energy is rising. Various routes for thermochemical conversion of biomass exist, and gasification of *Miscanthus* is highly promising; in part due to high process efficiency and also because of the many advantageous properties of this crop. Previous studies have shown that *Miscanthus* has a unique ability to thrive on land contaminated by heavy metals; land that covers a large expanse throughout Europe, often considered unsuitable for agriculture. This presents great opportunities, in terms of land utilization and remediation, but also poses interesting challenges with the production of a now contaminated biomass fuel. This work investigates the metal uptake and partitioning as well as the gasification potential of commercially available *Miscanthus x giganteus*, and two novel seed-based hybrids, GNT 34 and GNT41, grown on heavy metal contaminated land. Metal content in the stems (partitioned at three different heights), analysed with ICP and XRF, showed a high efficacy of metal uptake by all samples. A gradient in the concentration of metals with the highest values toward the top of the plants was observed. The fuels were analysed with TGA and gasified in CO₂. Pyrolysis activation energies for the samples were low, on the order of $E_a \cong 65$ kJ/mol and $\ln A \cong 8$ s⁻¹, indicating a strong metal catalytic effect on degradation though gasification rates seem independent of the content of the three metals studied and imply that char morphology may play a more significant role at this stage.

Pyrolysis of plastic wastes for the purpose of liquid fuel production

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Abstract

The pyrolysis process of HDPE, PP and PET plastic wastes was investigated in a batch reactor and the yield of pyrolysis oil and transportation fuel were determined. The collected liquids were further processed by atmospheric distillation to separate the gasoline range hydrocarbon molecules. The transportation fuel yields were 279 g/kg_{waste}, 624 g/kg_{waste}, and 0 g/kg_{waste} for HDPE, PP, and PET, respectively. The HDPE and PP fuels were successfully tested in a traditional spark-ignition engine. The results show that the thermal pyrolysis of different plastic wastes is a viable method to reduce the accumulation of plastics on landfills and provide value-added liquid transportation fuels.

Abstract_S1_AIII_44

Laboratory scale pyrolysis of organic fraction and RDF from municipal solid waste

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Abstract

The continuous increase in generated waste became one of the main problems of the 21st century. According to the waste management hierarchy, the primary goal is recycling the wastes we cannot reuse. Although recycling is preferable than energy recovery, its key criteria is selective waste collection. At the same time selective collection is not a guarantee that recycling is feasible. The utilization of this type of waste is the topic of several studies these days. Thermal decomposition is a remarkable solution to this problem. The main advantage of pyrolysis compared to combustion is that the products can be further used as secondary starting materials. The initial starting material and the process parameters have the greatest impact on the quality and quantity of our final products (synthesis gas), these are in the main focus of our research. In this work we studied the pyrolysis of organic fraction and RDF (refuse derived fuel) from MSW (municipal solid waste) in laboratory conditions. We also examined the mixture of these materials. During the experiments the amount and composition of the initial materials, products (synthesis gas) and residues (slags) have also been investigated.

Development of a vision-based monitoring system for optimizing industrial scale moving step grate biomass combustion

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Abstract

The main objective of this work was to minimize emission levels and optimize thermal efficiency of a 3 MW nominal capacity, moving step grate fired biomass boiler without an on-line fuel analysis system by applying novel combustion process control based on routinely measured operating parameters and real-time flame image processing and machine learning. Two important tasks of image-based combustion monitoring systems are providing alerts and predictions regarding the state of the system. The system issues alerts based on the location of the reaction zone and predicts boiler performance based on image and operating data.

Sewage sludge combustion in the rotary kiln

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Abstract

The importance of finding new ways of utilization of sewage sludge is momentous and it is gaining its importance every day. Moreover, every solution has to follow the given procedure given by legislative. The production of sewage sludge in the developed countries is without substantial differences but it is continuous. The mass of the sewage sludge is both difficult to handle and to transport to other facilities. Therefore, one of the ways how to deal with the incessant production of sewage sludge is the combustion. Sludge was combusted in the semi-industrial rotary kiln in this test. The main goal of the experiment was to verify the possibility of the utilization by the combustion. The material used for combustion was predried in the semi-industrial rotary drier. One of the problems with the combustion of sewage sludge is the number of incombustible components which lower the overall LHV, which is already very low. The amount of the water in the material used for combustion was around 30 %wt. LHV of the predried material was 7 MJ/kg on average. The dosage of solid fuel was 30 kg per hour and it was kept at the same level during the whole experiment. Combustion of the material had to be supported with the extra heat delivered by the natural gas burner. During the experiment the burner for the natural gas was operated at the three different heat outputs – 100 kW, 65 kW, and 42 kW. Presence of NO_x and SO_2 was measured in the flue gas. At some regimes the amount of these two components exceeded limits given by the law. In the end the samples of ashes were analyzed and tested for the water residues and elementary analysis has been performed. The experiment exposed some weak spots of the technology and of the process of the combustion of the sewage sludge itself. However, in the long term perspective it has proven that combustion is possible.

Detailed analysis of single biomass particle combustion by shadowgraphy

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Abstract

In the view of the environmental impact of current fossil fuels, the need to alternative resources is an issue for industrial combustion furnaces. Despite the increasing awareness of the polluting role of coal combustion in power plants, it is still the second source of primary energy. Incorporating a fraction of biomass into coal in pulverized burners can be an effective solution. However, this significantly modifies the behavior of the installations considering the different combustion behaviors of biomass at particle and flame levels. This work aims to investigate the physicochemical phenomena involved in pulverized biomass combustion, and to highlight the influences of biomass composition, especially volatile matter (VM), and the preparation techniques. An experimental study of single particle combustion is performed on a high temperature particle reactor. Once introduced to the hot zone on the tip of a thermocouple, the particle (<1mm) is continuously monitored by high magnification direct and shadowgraph imaging techniques. The latter eliminates the flame barrier which usually obstructs the visual imaging techniques to view the particle when enveloped by a flame. This allows tracing the time-resolved evolution of the particle volume in the course of its degradation as a function of its burnout. Superposing the data of both imaging techniques with the particle temperature for a series of experiments helps to identify the events corresponding to each involved phenomenon including the ignition delay, the volatile flame duration and the char oxidation duration. Moreover, this method provides the onset of the heterogeneous oxidation associated with the increase of the particle brightness even during the flame phase. The heterogeneous ignition occurs earlier for larger particles containing lower volatile content. This means higher overlap in addition to higher burnout duration. The timeline of events is determined by the volatile content of the particle, so is the volume evolution as well. The particle swell upon heating and the volume reduction during the flame phase are directly related to the volatile content. VM occupy around 40% of the initial particle shadow which decreases with devolatilisation progress following a power trend. The flame duration appears to be more influenced by the particle size than the particle composition. This leads to more intense combustion for higher VM particles given comparable duration and continuously more exposed char. The char appears to burn at the surface and then switch to internal combustion leaving an ash matrix behind. The particle shrinks to this moment where oxygen penetrates the surface and the shadow remains almost constant hereafter.

The results are validated in comparison to conclusions of other experimental methods and the volume evolution obtained by shadowgraphy will be integrated in a 1-D solid combustion model developed and validated for different compositions and preparations of biomass.

The energy aspects of biogas production from sheep manure

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Abstract

The result of the anaerobic degradation of organic material is a renewable energy source, called biogas. Due to its high methane content, biogas is primarily used for energy production. A beneficial method for energy production is cogeneration. Thus, heat and electricity can be produced at the same time. Sheep manure was used for biogas production in lab-scale experiments, using various reactor temperatures with and without the addition of inoculum. The recorded gas yield and gas composition was used to estimate the replaceable natural gas quantity. Furthermore, the necessary gas engine performance was also calculated.

Investigation of agriculture biomass for pyrolysis and gasification

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Abstract

The agriculture biomass has a broad energy potential. Unfortunately, because of its ultimate properties (high moisture content, low energy density) during the direct combustion some operational problems may appeared. Thus, processes like pyrolysis and gasification seem to be better and more environmentally profitable solutions. Pyrolysis is a process of a thermochemical decomposition of biomass into biochar, biotars and syngas going under non-oxidizing atmosphere in the range of temperatures: 300-600 °C. The yields of products formed strongly depends on the reaction temperature, time and heating rate. The formation of gas as a main product is promoted by high temperatures and long residence times, while low temperatures and long residence times promote the formation of biochar. Gasification is a process leading to obtain mainly gas as a product. Produced gas mainly consists of H₂, CO, CO₂, N₂, CH₄ and other hydrocarbons, as well as char, ash, tar and oil. Gasification is conducted under oxidizing atmosphere with an equivalence ratio between 0.2-0.4, depending on the process temperature (700-1200 °C). The main aim of this study was to investigate agriculture biomass (oat straw) under pyrolysis and gasification process. The main investigation of pyrolysis and gasification was done on laboratory scale semi-batch vertical reactor. The pyrolysis was done at 300, 400, 500 and 600 °C and gases were collected to analysis using gas chromatography method. The tars were collected, too and analysed with GC/MS. The pyrolysis process kinetics were studied using TGA. The gasification of straw was carried out at 700 and 800 °C. The main gaseous products in both processes were CO₂, H₂, CO, CH₄. Based on obtained results is can be concluded that for studied agriculture biomass pyrolysis process gave better products (more valuable gas and as well as biochar which can be next combusted). The gasification process at 700 and 800 °C is not so effective as it was assumed for studied biomass.

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Physical and chemical characteristics of ash deposits in a utility boiler firing an Indonesian lignite

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Abstract

Ash deposits were collected from several locations of superheaters in a utility boiler burning a pulverized Indonesian lignite in a fertilizer plant. Characterization of deposits were carried out in term of the chemistry and structure via Scanning Electron Microscope (SEM) and Energy Dispersive Spectroscopy (EDS). The ash deposits have three significant layer: initial layer, sintered layer and slag layer, with the boundary of each layer can be clearly determined. It is found that Ca and Fe are the main binding elements of deposit growth during boiler operation while Na only plays a minor role. The Ca species act as the fusing agent while the Fe species act as the fluxing agent. Calculations based on operational data taken from the plants suggests that ash deposit growth was fast in the beginning when first layer formed and the growth of second layer became slower and third layer was the slowest phase. The formation of the first layer of ash deposit took 4 weeks operations, followed by that of the second layer for a period of 21 weeks, after which the third layer started to form. The boiler was in operation for 32 weeks before shutdown for maintenance and cleaning of superheater tubes.

Biomass for energy: excess air ratio effects on combustion characteristics of pulverized olive cake

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Abstract

The aim of this work is to study effects of excess air ratio (λ) on combustion dynamics of pulverized olive cake (OC) in a vertical furnace. Four cases namely (a), (b), (c) and (d) with different excess air ratio (EAR) ($\lambda=1.3, 1.7, 2.3$ and 2.7 respectively) are also studied. The numerical approach is based on Reynolds Average Navier-Stokes (RANS) equations. The chosen turbulence closure model is the $k-\varepsilon$ model. For turbulence-chemistry interactions of the non-premixed combustion, a mixture fraction/PDF approach is used. A comparison is done between all cases for, flow topology, velocity contours, temperature distribution and species concentration profiles in several locations along the furnace. Results show that increasing excess air ratio dilutes the emission of CO and CO₂ inside to the furnace (figure below), lowered the temperature in the furnace exit and reduced the visible lengths flames L_{visible} .

Potassium release from single burning pulverized biomass char particle

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Abstract

Atomic chemiluminescence emission was used for a quantitative measurement of the potassium. Atomic chemiluminescence emission was used for a quantitative measurement of the potassium release from single pulverized wheat straw char particles in different combustion environments. The char particles were injected upwards into a hot gas flow and oxidized. Potassium was released and its K* chemiluminescence was captured by an ICCD camera with a band-pass filter at 766 nm. Measurements were conducted on the particles having a residence time from 20 ms to 50 ms in the hot gas flow. To achieve quantitative results, the correlation between the signal of the chemiluminescence of K* and the potassium concentration was obtained through the hot gas flow doped with known amounts of KOH. After the calibration, the amount of potassium released from the char particles was determined simply based on the captured signal of the K* chemiluminescence around the burning particles. The results showed that the release of potassium already occurred at residence times of 20 ms, and that potassium was continuously released at a constant release rate of about 1 µg/s from 20 ms to 50 ms. The release intensity was significantly enhanced as the oxygen concentration increased from 6.5% to 8.5%, and the temperature from 1580 K to 1670 K.

Study on the high load potential under natural gas/diesel dual-fuel combustion in a heavy-duty engine

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Abstract

After Paris Agreement, it becomes more important to reduce carbon dioxides (CO₂) emission. Especially, in South Korea, CO₂ emission should be reduced 37 % more than current level until 2030. However, in the transport part, it is challenging to reduce CO₂ emission without the improvement of internal combustion engines. Although diesel compression ignition (CI) engines have great potential to reduce CO₂ emission compared to that of gasoline spark ignition (SI) engines, diesel CI engines have gone tough time due to 'diesel gate' in these days. For these reasons, the supplementation of natural gas on diesel CI engine by using dual-fuel combustion method can be one of the effective approach to reduce CO₂ emissions. Since natural gas contains lower carbon compared to that of diesel under the same low heating value (LHV), the amount of CO₂ emission could be reduced. However, the limitation of high engine operating load extension is one of major challenging problem of dual-fuel combustion due to high the maximum in-cylinder pressure rise rate (PRR_{max}). As a result, in this research, the maximum power rate of natural gas/diesel dual-fuel combustion was evaluated with a 6 L heavy-duty CI engine. The restrictions were the maximum in-cylinder pressure (190 bar), PRR_{max} (15 bar), CoV of net indicated mean effective pressure (nIMEP) (3 %), brake specific nitrogen oxides (BNO_x) (0.4 g/kWh), BCO₂ (645 g/kWh) and Bsmoke (0.02 g/kWh) under 1,800 rpm condition. Main variables were diesel injection timing, the ratio between diesel and natural gas and intake pressure. The result showed that 81 kW could be achieved by dual-fuel combustion mode with the all satisfaction of above restrictions. In addition, further discussion to extend dual-fuel combustion operating range was described.

An analysis on the combustion and performance characteristics of a hydrogen spark ignition engine with boosting condition

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Abstract

Hydrogen has been shown to have many benefits in terms of emission and thermal efficiency in application of spark ignition engines. But, hydrogen gas engines have lower power and torque than conventional fuel engines due to low volumetric efficiency. This study systematically investigated the application of a boosting system to a hydrogen engine to get higher power and torque. The exhaust manifold of a commercial 2.4-liter natural aspiration spark ignition engine was modified by adopting a turbocharger system for the engine experimental work. Test engine speeds were 2,000 – 6,000 rpm at intervals of 1,000 rpm under maximum torque conditions. The quantity of hydrogen and spark timings were varied before the back-fire occurred. Engine performance results between natural aspiration and boosting conditions were compared. The results indicated that distinctly higher boosts with the turbocharging system helped to extend high load conditions and increase thermal efficiency, however, high speed performance with boosting showed disadvantages due to the high exhaust pressure.

Abstract_S1_AIII_55

1-methylnaphthalene LIF for the investigation of the mixture formation at diesel engine conditions and kHz repetition rates

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Abstract

This work presents the first high-speed tracer-LIF mixing study using 1-methylnaphthalene in a rapid compression machine (RCM). A burst mode Nd:YAG-laser at 266 nm was used to excite the tracer at a frequency of 7.5 kHz. A high-speed intensified CMOS camera equipped with an image doubler was utilized for two color detection. Both homogenous conditions during compression and fuel injection at TDC (top dead center) were investigated. Measurements were conducted in nitrogen atmosphere at maximal pressures of 4.4 MPa.

Highly resolved near-wall flame and flow measurements in an optically accessible SI engine using SO₂-PLIF and PTV

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Abstract

Understanding near-wall processes (e.g. flame propagation, flow field) is important to further improve efficiencies and decrease pollutant emissions of internal combustion (IC) engines. Near-wall processes affect heat transfer and pollutant formation and with continuously improving capabilities to model near-wall processes, the demand for corresponding measurements increases. In this study highly resolved flame position measurements are conducted in an optically accessible SI engine using high-speed planar laser induced fluorescence (PLIF) of sulfur dioxide (SO₂). SO₂ is added to the intake flow as an inert tracer and excited with a frequency quadrupled Nd:YAG laser at 8.0 kHz. The fluorescence of SO₂ is highly temperature sensitive and thus enables the measurement of burnt gas areas. Measurements are conducted in a 13x9 mm² region in the central symmetry plane at the piston surface. An optical resolution of <100 μm is achieved. The engine is operated at two engine speeds (800 rpm and 1500 rpm) and two different intake pressures (0.95 bar and 0.4 bar) using port fuel injection of iso-octane at stoichiometric mixture. Flame contours are extracted and statistical distributions of the burnt gas area determined. The burnt gas distributions are compared with simultaneously recorded high-speed flow field measurements in the unburnt gas. For this, particle tracking velocimetry (PTV) was utilized allowing for a highly resolved flow field which enables the determination of boundary layer profiles. A direct comparison with motored engine operation showed comparable boundary layer profiles until the flame approaches the wall. Flow acceleration, due to flame expansion, rapidly increases velocity gradients and the boundary layer development becomes highly transient. It is shown that the interaction of flame and flow depends on the operating conditions, which results in a different evolution of burnt gas positions within the field-of-view. This has additional implications on the development of the velocity boundary layer. Depending on the operating conditions, the flame strongly affects the velocity boundary layer profiles resulting in boundary layer thicknesses in the order of the flame thickness (50 - 150 μm).

Coupled experimental and numerical investigation of reactive spray processes in internal combustion engine

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Abstract

It is known that the injection strategy in the internal combustion engines has an impact on the combustion, pollutant formation and total energy efficiency. In the modern internal combustion engines, the multi-injection strategies are commonly used to reduce pollutant emissions and combustion noise. Furthermore, the combustion process as a result of the multi-injection strategy depends on numerous parameters that are commonly examined with the coupled Computational Fluid Dynamics (CFD) and experimental investigation. In the observed experimental direct injection diesel engine, the liquid fuel is injected through the separated pilot and main injections. The pilot injection is used to produce a small amount of vapour that ignites and increases the mean in-cylinder temperature before the main injection occurs. The special focus of this research is given to the numerical investigation of the spray influence on the combustion process, where two spray modelling approaches were applied. The Euler Lagrangian (EL) spray approach and the Euler Eulerian (EE) spray approach were investigated and compared with the experimental results. In both spray modelling approaches, the general gas phase reactions were used for describing the combustion process. The 3D results show that the evaporated fuel predicted with the EE approach has a better physical description in the dense spray region than with the conventional EL modelling approach that has the better physical description in the near wall region. Additionally, the difference between spray models in the fuel disintegration and evaporation process modelling resulted in the lower temperature values of the gas phase in the near the nozzle region for the EE spray approach. Finally, the results from both spray modelling approaches, such as the mean pressure and rate of heat release are found to be in good agreement with the experimental results.

Experimental and modeling study of 2-ethylhexyl nitrate promoting effect on a low octane gasoline surrogate

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Abstract

Reactivity control of lean combustion by using additives is an efficient method to get better internal engine performances. 2-ethylhexyl nitrate (EHN) promoting effect (0.1 - 1% mol.) on combustion is investigated experimentally and numerically. The targeted fuel is mixture of toluene and n-heptane. Experiments were carried out in a rapid compression machine at equivalence ratio of 0.5, at 10 bar, from 675 to 995 K. A kinetic model is developed from literature data assembly. At the experimental condition, it is found that the EHN enhance the fuel reactivity in the whole temperature range. Numerical analyses reveal that the EHN effect is linked to a NO₂-NO loop which enhances fuel reactivity.

Abstract_S1_AIII_59

A modeling study of a partial oxidation polygeneration process of fuel-rich ethanol/ozone mixtures in an HCCI engine

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Abstract

A fuel-rich homogeneous compression ignition (HCCI) engine combustion fueled with ethanol is analyzed and parameter studies are carried out in a modeling study. It is found that ethanol ignites at an intake temperature range between 505 K and 701 K, at equivalence ratios (Φ) of 2 to 10, increasing with Φ and an addition of 1000 ppm ozone decreases these values by up to 58 K. Maximum mole fractions for different species are found for different conditions, for H_2 , CO, C_2H_2 and C_2H_4 values of 15.8 %, 18.0 %, 2.4 % and 5.8 % can be achieved at $\Phi = 3, 8, 4$ and 10, respectively. The maximum exergetic efficiency is found at $\Phi = 2$ with a value of 83.7 %, making ethanol a promising biofuel for polygeneration processes.

CFD model of a spark-ignition engine fueled with several oxygenated compounds

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Abstract

A Computational Fluid Dynamics model of an ASTM-CFR engine was implemented with the aim of comparing the Indicated Mean Effective Pressure and pollutant formation of neat gasoline with gasoline + ethanol / dimethyl carbonate / diethyl carbonate blends. The model showed good agreement with experimental in-cylinder pressure data. Comparison of the simulated blends evidences the differences in flame evolution and allows establishing a relationship to IMEP and pollutant formation. Furthermore, the results underline the advantages of CFD modeling for assessment of new fuels, allowing faster and cheaper comparison to standard fuels.

Abstract_S1_AIII_61

Experimental study on the knock phenomena in the individual cycles of direct-injected spark ignition engine with various stroke-to-bore ratios

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Abstract

In this study, knock phenomena occurred in each individual cycle was comprehensively investigated, with varying the main engine geometry – stroke-to-bore ratio (S/B ratio). The single-cylinder, direct-injected, spark ignition engine was used with constant compression ratio and displacement volume with varying S/B ratios. From the experimental data, it was shown that with similar number of knock incidence, faster burning speed and unburned zone geometry attributed to higher S/B ratio resulted in increased knock intensity, which would cause further ignition retard and resultant loss in gross work.

Numerical simulation of the prechamber processes in a lean-burn gas engine

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Abstract

Gas engines are a promising alternative for the future of sustainable electrical power production in the form of stationary power plants or combined heat and power (CHP) units. Furthermore, they are more flexible and lower in cost compared to gas turbines and the possibility to use biogas from agricultural waste or sustainable sources allows a carbon neutral operation. A favorable engine concept is the lean-burn strategy due to their higher efficiency and low nitrogen oxides (NO_x) emissions without the need of complex exhaust gas aftertreatment. One challenge is the stable ignition of lean mixtures. With biogases as fuel, which have lower specific heat values, this problem is even more prevalent. For such operating points, a scavenged prechamber is considered necessary. In this work, Reynolds-averaged Navier-Stokes (RANS) and scale-resolved simulations (SRS) are conducted to investigate the scavenged prechamber processes in lean-burn gas engines by means of computational fluid dynamics (CFD). SRS models allow the investigation of cycle-to-cycle variations and determine the source of misfiring in the prechamber. Therefore, different hybrid SRS models were evaluated for a simple cylinder-valve arrangement. The results of the hybrid models correspond well with experimental measurements and are on the same level as the Large-Eddy-Simulations (LES) with a reduced calculation time. Furthermore, studies regarding geometry and injection timings for the prechamber are investigated with the SRS model to evaluate the cyclic dependencies. By tilting the nozzles of the prechamber, a controlled swirl motion could reduce the fluctuations, but at the same time hinder mixing processes with high tilt angles, leading to unfavorable ignition conditions. Finally, an extended combustion model, based on a progress variable approach, is proposed. The model showed for RANS simulations a good agreement with the experimental data of the optical single-cylinder research engine. The hot prechamber jets produce very high turbulence degrees in the main chamber and allow wider operating conditions.

Time-resolved chemiluminescence spectroscopy of diesel and alternative fuel flames at engine relevant ambient conditions

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Abstract

To understand the ignition and reaction processes of (oxygenic) fuels without aromatic compounds, often optical experiments are conducted. A common method, is the imaging of OH radical chemiluminescence around a wavelength of 308 nm. The separation of signals of specific species can be difficult due to various overlapping signal sources. In this study, we focus on the influence of aromatic compounds on the OH* signal at engine relevant ambient conditions. Flame spectroscopy is executed simultaneously with OH* chemiluminescence imaging for various fuels. A clear influence of soot and soot precursors on the flame signal spectrum around 308 nm is shown.

A power-to-gas process in a piston engine: exergy storage through pyrolysis of methane and ethane

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Abstract

The conversion of mechanical energy and simple hydrocarbons like methane and ethane to storable higher energy fluids in a motored piston engine is investigated in a modeling study. The time-dependent engine model simulates as a compression-expansion cycle with detailed chemical reaction kinetics. The fuel is diluted with argon to increase the temperature at the end of compression stroke and to improve the fuel conversion in endothermal reactions. Inlet pressure and temperature as well as argon dilution are varied and the storable energy with regard to the specific chemical and physical exergy of the product gas mixture and efficiency are analyzed to determine the limits of the process. The main products are hydrogen, benzene and acetylene. The storable chemical energy per cycle is 258 J for a 400 ccm cylinder, thus a storage power of 10.9 kW and an energetic efficiency of 51% could be achieved with methane as fuel and inlet parameters of 473 K, 10 bar and 91 % argon dilution. Using ethane as fuel, the storage power increases to 14.4 kW with the same efficiency and inlet parameters of 373 K, 10 bar and 95 % argon dilution. The separation of the higher hydrocarbons and recirculation of argon in a process concept reduces both, the maximum storage power and the efficiency.

Investigation of the chemical stability of the laser-induced fluorescence tracer 1-methylnaphthalene at IC engine relevant conditions by supercontinuum absorption spectroscopy

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Abstract

1-methylnaphthalene (1-MN) is a common laser-induced fluorescence (LIF) tracer for planar imaging of mixture formation in terms of fuel concentration and temperature distributions in internal combustion (IC) engines. However, the tracer may start to react during LIF-calibration at high temperature and pressure. In this context, the oxidation of 1-MN and the base fuel isooctane is examined within a calibration flow cell using broadband supercontinuum absorption spectroscopy (SC-AS). The fuel and tracer conversion is correlated to the produced H₂O mole fraction. Pressure- and air-fuel ratio dependencies are presented at pressures up to 2.5 MPa and temperatures up to 850 K.

Comparison of fuel additives for syngas production by fuel-rich methane HCCI combustion

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Abstract

Internal combustion engines can be used as reactors for partial oxidation of methane (or natural gas) to produce syngas together with mechanical work. Such a “polygeneration” process could provide a load-flexible solution for energy and species conversion in the chemical industry. In our previous work, it was shown that HCCI operation can extend stable engine operation from a maximum of equivalence ratio of 1.5 with spark ignition to much higher equivalence ratios that are more favorable for syngas production. Exergetic efficiencies of 80% could be achieved using this process. Since the auto-ignition characteristics of methane are unfavorable for compression ignition, more reactive additives are necessary. In this work, n-heptane, dimethylether (DME), diethylether (DEE), and ozone are compared as ignition-promoting additives for fuel-rich HCCI operation. DME and DEE have been investigated widely as diesel-fuel alternatives. Ozone was recently investigated as a very promising additive in lean HCCI combustion by a group at the University of Orléans (France). Our experiments were performed in a single-cylinder engine with a compression ratio of 10 at 150°C intake temperature. The engine was operated with variable fractions of DME, DEE, and n-heptane added to the methane/air mixture in the intake. Also, experiments with ozone fractions from 30 to 1700 ppm and DME as a second additive were conducted. Operating limits, additive demand, and syngas yields were compared for equivalence ratios from 1.6 to 2.4. While the demand for the hydrocarbon additives was almost constant at about 25 mass% of the overall fuel mixture, independent of equivalence ratio or additive, the addition of 75 ppm ozone to the overall mixture led to a decrease in DME demand of about 50%. It was found that the syngas yield is mostly unaffected by the choice of additive but shows a dependency on combustion phasing. Consistent with results in lean HCCI, ozone in small amounts already strongly promotes ignition, with exponentially decreasing efficacy for increasing ozone fractions. Also, ozone appears to stabilize very late combustion for high equivalence ratios.

Exploration of the high load limits in dual-fuel combustion operation

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Abstract

Internal combustion engines have to deliver the required performance while satisfying regulations regarding harmful pollutants and at the same time having fuel consumption and CO₂ emissions as small as possible. Standard compression ignition combustion mode achieves good overall efficiency, but the pollutant emissions are lately debated. To enable further improvements of the compression ignition engine and to enhance the use of natural gas, dual-fuel type of combustion is introduced. The potential of the dual-fuel type of combustion is based on the lower CO₂ emission, lower fuel costs and usage of alternative fuels. Further on the dual-fuel operation at high load under ambient conditions shows significant improvement of engine efficiency and soot emissions, compared to normal diesel operation. Due to limited data given in the literature that shows how the performance of the dual fuel engine changes at high load with various operating conditions this research presents a comprehensive set of experimental results obtained with the conventional dual fuel operation (diesel/natural gas) at boosted intake conditions. Experimental setup on which this research is performed consists of the internal combustion engine, AC dynamometer, software for control of the engine and dyno, and various measurement devices including the indicating equipment. The original single cylinder compression-ignition engine (Hatz 1D81) was modified so that it can operate with common rail direct injection of diesel and port fuel injection of the natural gas. The experimental setup is located at the Laboratory of IC Engines and Motor Vehicles at the Faculty of Mechanical Engineering and Naval Architecture, Zagreb, Croatia. In this research the challenge was to obtain load as high as possible while simultaneously satisfying the limiting values such as pressure rise rate and in-cylinder peak pressure. Such operation contributed to better understanding of the control parameters for the dual-fuel operation at high load. During the tests compression ratio and engine speed were kept constant, while some other operating parameters of the engine were varied, such as air to fuel ratio, intake pressure, natural gas to diesel ratio and injection timing. By recording multiple engine operating parameters, e.g. engine load, pressure rise rate, oil temperature, engine head temperature, in-cylinder pressure, emission of nitrogen oxides and hydrocarbons the analysis of the pathways for achieving high load while satisfying constraints and optimizing other performance data is made.

Operating parameters of the biogas-diesel dual-fuel engine

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Abstract

In order to reduce air pollution from internal combustion (IC) engines, new types of combustion processes are constantly developed. One of these processes is named dual-fuel (DF) where small amount of diesel ignites the primary fuel. If this primary fuel is produced from renewable energy sources, such as biogas which consist mostly of methane (CH_4) and carbon dioxide (CO_2), benefits to the environment protection are even higher. An additional benefit of a dual-fuel engine is lower CO_2 emissions and lower fuel costs with main disadvantage presented as the increase in carbon monoxide (CO) and hydrocarbon (HC) emissions. On the other side, the main disadvantage of the biogas as the IC engine fuel is relatively high auto ignition temperature, especially when its CO_2 ratio is increased. To enable research of these new combustion processes and usage of alternative fuels an experimental setup for IC engine testing is developed in the Laboratory for IC Engines and Motor Vehicles of the Faculty of Mechanical Engineering and Naval Architecture in Zagreb. Core of the setup is experimental engine made by modification of single cylinder diesel engine Hatz 1D81Z. After required modifications the experimental engine can operate in spark ignition (SI), compression ignition (CI), homogeneous charge compression ignition (HCCI) and in dual-fuel mode of operation. Diesel fuel is injected in the cylinder using fully flexible common rail system while biogas is injected into the intake manifold. Biogas is premixed in two different volumetric ratios of CH_4 and CO_2 . First blend is in ratio $\text{CH}_4:\text{CO}_2 = 80:20$ and second one is in ratio $\text{CH}_4:\text{CO}_2 = 60:40$. Both blends are stored in pressurized cylinder tanks. The goal of this research is to determine the influence of different biogas composition, (different ratio of CH_4 and CO_2) used as a primary fuel in the dual-fuel mode of operation, on the performance of the same engine at similar operating conditions. Similar operating conditions mean that the engine tests were performed at the same indicated mean effective pressure (IMEP) in all ratios of biogas composition at the same engine speed. Engine speed in this research is set to 1600 rpm. Predefined IMEP level is measured in DF mode of operation with pure methane as primary fuel. Each of the comparative operating points is optimized to satisfy the limits for coefficient of variation of IMEP (CoV IMEP), maximum pressure rise rate (MPPR) and to obtain the highest engine efficiency. A result of this research presents a comparison of indicated efficiency, excess air ratio, energy of fuel and combustion duration obtained in NDO and in DF mode with different fuel combinations. Also, this research presents a comparison of the emissions levels of HC, CO, CO_2 and NO_x .

Abstract_S1_AIII_69

Active pre-chamber ignition systems: an enabler for new ICE combustion concepts

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Abstract

Pre-chamber ignition systems can increase the ignition energy in internal combustion engines. Instead of a spark plug, a small chamber with multiple orifices is installed. Inside this pre-chamber, a spark starts the combustion and thus generates hot and reactive gases, which penetrate the main chamber, increase the turbulence and ignite the mixture on multiple sites. This leads to an increased turbulent flame speed and extended operation limits, especially for diluted (lean or high EGR) mixtures.

Ignition characteristics of plasma reformed n-heptane in a homogeneous combustion compression ignition engine: a modeling study

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Abstract

The effects of a plasma reformed charge on ignition timing of n-heptane is investigated using zero-dimensional time dependent models. A small charge of air-fuel mixture is subjected to a plasma discharge and then mixed with a main charge in order to modify ignition characteristics. Ignition delay was shortened significantly using a small amount of reformed fuel, especially at low temperatures of 600 to 800K. The results show potential as a method to control ignition timing in advanced engine technologies.

Abstract_S1_AIII_71

Ignition delay times of diluted mixtures of ammonia/methane at elevated pressures

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Abstract

Mixtures of $\text{NH}_3/\text{CH}_4/\text{O}_2$ have been studied in a rapid compression machine in order to assess its auto-ignition properties. Ignition delay times were measured at pressures of 20 and 40 bar, temperatures between 920 and 1100 K, and equivalence ratios ranging from 0.5 to 2. The results show that an increase in the content of ammonia in the fuel mixture delays the ignition onset and narrows the temperature range where ignition occurs, hindering the flammability of the mixture. In addition, a decrease in equivalence ratio shortens the ignition delay, thereby increasing the mixture reactivity. Finally, it was found that higher pressures lead to considerably lower ignition delay times.

Abstract_S1_R1_72

Study of a gasoline surrogate blended with pentanol isomers: sooting tendency and flame structure analysis

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Abstract

E10 fuel (gasoline with 10% of ethanol) represents today 43% of the French gasoline market. However, heavier alcohols have a higher energetic density. Pentanol can be produced on an industrial scale and its properties make it a potential additive to both gasoline and diesel. Despite extensive investigations over the last decade, there is still a lack of information with respect to pentanol sooting tendency. The present work focuses on this issue through two experimental analyses: Yield Sooting Index (YSI) on a Santoro burner and flame structure on a McKenna burner. Thus, 1-pentanol exhibits a lower sooting tendency than 2- and 3-pentanol. This observation suggests different decomposition pathways depending on the molecular structure of the isomer considered.

Abstract_S1_R1_73

Spray and particle characterization of a spray flame synthesis process using wide-angle light scattering (WALS)

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Abstract

Spray Flame Synthesis (SFS) is a promising technology to produce nanomaterials with well-defined functional properties. Since particle size and morphology have a significant influence on the properties of the synthesized nanoparticles, correlations between these parameters, the droplet size of the spray and process conditions are required. For this reason, Wide-Angle Light Scattering (WALS) is applied to a flame of a standardized SFS burner, which allows for both droplet and particle size evaluation. For the aggregate size $R_{g,eff}$, no significant influence of different dispersion gas flow rates on particle morphology is measured, while the droplet size d decreases with increasing dispersion gas flow rates.

Measurement of the sooting propensity of aviation fuel mixtures

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Abstract

The combustion of a fuel in a jet engine of an aircraft in cruising altitude is connected with the direct emissions of different pollutants such as nitrogen oxide (NO_x), sulfur dioxide (SO_2), and soot particles in the upper troposphere and lower stratosphere. Here, the soot particles are acting as a nucleus for the condensation of water vapor leading to cloud formation, which eventually influences the radiation balance of the earth's atmosphere and increases the radiative forcing. It is already well-known that aromatic components in fuels promote the soot formation, but a minimum content of 8.0 vol-% of aromatics is required for jet fuels containing synthetic components. Therefore, for the development of alternative fuels a better understanding of the influence of aromatics on soot formation is necessary. For this reason, the sooting propensity of different jet fuels and blends of synthetic paraffinic kerosene (SPK) with aromatic compounds was determined experimentally to investigate the dependency of soot formation on the kind and concentration of the specific aromatic compounds contained. To this end, an aromatic free surrogate consisting of ndodecane, isooctane and npropylcyclohexane was derived from jet fuel-GCxGC-MS analysis as an initial SPK mixture. Using this surrogate six different mixtures containing aromatic compounds were prepared with five selected aromatic compounds and one aromatic mixture prepared out of them. In subsequent measurements, the concentration of the aromatics was increased from initially 8.0 vol-%, to about 16.5 vol-%, and 25.0 vol-%. The aromatics used were toluene, npropylbenzene, indane, 1methylnaphthalene, and biphenyl. Furthermore, the sooting propensities of a crude-oil based Jet A-1 and four different alternative aviation fuels (two SPK fuels and two synthetic kerosenes with aromatics (SKA)) were also investigated. The results indicate that the influence of the aromatic compounds' molecular structure on the sooting propensity is more significant than their concentration. Finally, these experimental findings will be compared to modeling results. The modeling includes besides the investigation of the dependency on aromatic type and content also the influence of temperature, pressure, fuel stoichiometry, and residence time on sooting propensity.

Raman spectroscopy of soot sampled from high-pressure diffusion flames

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Abstract

Fuel-rich hydrocarbon flames produce carbonaceous by-products, including soot nanoparticles, which are currently of environmental and health concerns. Although the majority of existing combustion devices operate at high pressure conditions, most of our understanding of the soot formation process and soot physicochemical properties rely on studies performed at atmospheric pressure. Pressure is known to have nonlinear effects on combustion processes and a significant influence on soot formation; soot loading increases with increasing combustion pressure. Due to scarcity of information on soot primary particles, aggregate morphology and soot nanostructure relevant to high-pressure combustion, there are challenges in handling the soot oxidation and radiation. These soot characteristics directly affect soot oxidation and optical/radiative properties and to have a better insight into these characteristics under high-pressure conditions is desirable. Raman spectroscopy has emerged as one of the most powerful analytical tools in recent years for providing chemical and structural information on carbon-based materials including soot. In this study, we perform Raman spectroscopy measurements on soot sampled from a set of laminar diffusion flames of ethylene at various pressures, from atmospheric to 12 bar. Within the range of investigated pressures our results show an increase in soot maturity as the pressure increases. However, pressure does not seem to have a direct influence on soot nanostructure. Indeed, the increased pressure condition might turn on a faster and earlier inception of soot in the co-flow flame leading to a longer residence time of the carbon soot particles in the hot and reactive flame environment. The longer residence time could be the reason behind the higher degree of graphitization observed as well as contributing to a higher soot loading as pressure increases.

Production and characterization of superhydrophilic TiO₂ nanoparticle coatings via flame aerosol synthesis and thermophoretic deposition

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Abstract

This paper reports a method based on a highly controllable and tunable technique for the production of thin coating layers made of TiO₂ nanoparticles via aerosol flame synthesis and direct thermophoretic deposition. A flame reactor was designed and operated in different conditions in order to study the effect of particle size and film properties on coating performances. Particle dimension and crystal structure, coating morphology and optical properties were characterized using Scanning Mobility Particle Sizer, Raman spectroscopy and UV-Vis Absorption. Water contact angle analysis was performed and the wetting behavior was investigated, showing that titania coating layers possess a photoinduced superhydrophilic character, which is activated by normal solar radiation in standard room illumination conditions. Hydrophilicity was found to be dependent on the dimension of primary particles composing the coating layers. Moreover, measurements of microbial biofilm formation inhibition showed a high antibacterial activity from TiO₂ nanoparticle films. The optimal synthesis conditions have been identified to produce a coating material with the best performances.

Abstract_S1_R1_77

Numerical modelling of detailed soot radiative properties of a laminar coflow sooting flame

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Abstract

The effect of soot radiation on a laminar ethylene-air diffusion jet flame at atmospheric pressure is investigated. A spectral analysis is first performed using a Monte-Carlo method to solve the radiative heat transfer equation (RTE) on a preliminary field assuming unitary Lewis numbers for species. Soot particles appear to have a negligible impact on the overall radiative budget due to their strong localization comparing to hot gases. However, locally, where the soot volume fraction is maximum, soot dominate the radiative processes. Then, a model is derived and validated to additionally consider differential diffusion effects, which will be applied to the ethylene-air diffusion flame in future work.

Modelling soot particle inception and soot particle probe sampling

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Abstract

A sectional aerosol model is used to simulate soot particle inception via the polymerization of hydrocarbons (HACA mechanism). The model includes 50 bins, 11 of which are reserved to light (gas phase) species in the mass range 26 – 2860 amu with variable species density. The particle coagulation rates are calculated using the Fuchs interpolation of the collision kernel from the free molecule regime into the transition regime. Realistic adjustments for bimolecular reaction rate constants of gas phase species and for heterogeneous gas particle reaction rate constants are made [1]. The model input is the amount of acetylene to be converted into particulate soot by polymerization and heterogeneous surface growth at a given temperature (e.g. $1.25 \cdot 10^{15} \text{ cm}^{-3}$ acetylene molecules are converted to soot with a volume fraction of $3 \cdot 10^{-8}$ at 1700 K). The developing soot particle size distribution is calculated as function of time. The following parameters were varied: flame temperature, initial acetylene, rates of gas phase reactions, of heterogeneous surface growth and of particle coagulation. During the inception phase, no bimodality of the particle size distribution was found. This seems to be in agreement with previous modelling studies [2,3]. At the end and after the inception phase, a trough develops between the primary particle mode and the coagulation mode. At this stage, the contribution of the primary particles to the total soot mass is already negligible, however. These results appear to be consistent with a variety of experimental results obtained via dilution probing and SMPS measurements. Recent experimental results on incipient soot formation showed also that the bimodality in the size distribution can be due to sampling artefacts [4]. Since horizontal tube dilution sampling probes may not be able to quench gas phase reactions, heterogeneous surface growth and particle coagulation kinetics rapidly and simultaneously, CFD calculations were carried out to study their performances. The sampled gas flow is found to remain close to the tube wall and, no homogeneous dilution across the tube diameter is achieved. This may require a thorough consideration during data evaluation and result interpretation. CFD may also help to improve the sampling procedure.

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Abstract_S1_R1_79

Formation of soot precursors in benzene-laden producer gas combustion: experimental and computational study

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Abstract

Experimental results of temperature and concentration profiles of 4 non-premixed flames—1 neat PG and 3 benzene-doped (0.2, 1 and 2 vol.%)—collected in a counterflow burner were compared with CHEMKIN simulations using 3 kinetic mechanisms of PAHs formation: ABF_GRI3 and two mechanisms of the Institute of Combustion Technology of the German Aerospace Center (DLR2012 and DLR2018). The three mechanisms accurately capture the concentrations of major species, unaffected by benzene addition, while DLR2018 predictions are in closer agreement with the experimental results of small-chain hydrocarbons and aromatics. Nonetheless, a significant mismatch is found between measured and predicted naphthalene. Further analysis will focus on this disagreement, aiming at contributing to the DLR2018 upgrade on PAH-formation.

Abstract_S1_R1_80

Pathways of soot precursors formation in combustion of producer gas in presence of benzene

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Abstract

This study focuses on the pathways of soot precursors formation in flames of model PG, representative of wood gasifiers, in the presence of benzene as a tar surrogate. The analysis is based on the chemical kinetic mechanism of PAH formation and growth, DLR2018, developed by the Institute of Combustion Technology of the German Aerospace Center (DLR). Results are compared with experimental concentration profiles of 1 neat PG and 3 benzene-doped flames, finding a fair reproduction of the concentration magnitudes for most of the measured compounds. However, notable discrepancies are found for naphthalene. Reaction-path and sensitivity analyses of DLR2018 are used to identify the factors underlying the observed disagreements. The obtained insights should be included in the next iteration of PAH reaction model development.

Abstract_S1_R1_81

Characterization of soot volume fraction and particle size inside premixed kerosene flames

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Abstract

Soot particles from combustion processes pose a severe health risk and current and future emission legislations focus on reducing particle emissions from combustion systems. In order to predict correctly the emissions from real combustion systems, soot models need to be developed and tested on simple model flames. Since soot emissions depend on the fuel, studies with different fuels are needed. Many of these studies exist for a variety of different gaseous and some liquid fuels. In the case of liquid fuels, most data is available for one-component fuels (e.g. Octane) and very little results for more complex fuels can be found. In order to extend the available data for complex fuels, this study presents results of soot measurements on one dimensional, premixed kerosene (Jet-A1) flames. The kerosene is diluted with argon, in order to lower the required temperature for evaporation and evaporated at 150°C. The kerosene/argon mixture is mixed with oxygen and burned using a McKenna type flat flame burner. The fuel lines and the burner system are temperature controlled in order to prevent fuel condensation. Soot volume fractions were measured via laser extinction using a 638nm diode laser. Primary particle and aggregate diameters were determined by measuring the light scattering of the same laser at two different angles using photomultiplier tubes together with a lock-in amplifier. Additionally, temperature profiles were recorded using a coated thermocouple and the results are corrected for radiative heat losses. The sooting behavior was determined at different fuel-air equivalence ratios and data was recorded at different heights above the burner plate. The results are compared to measurements of a two component kerosene surrogate comprising of 80% n-decane and 10% 1,2,4-trimethylbenzene.

Experimental investigation of hydrogen impact on atmospheric sooting premixed methane flames

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Abstract

The effect of hydrogen on aliphatic and aromatic species formation has been experimentally investigated in a methane "nucleation flame". The nucleation flame conditions were identified by laser induced incandescence (LII) at equivalent ratio $\Phi=1.82$. The approach and the definition of the "nucleation flame" have been previously reported in our recent work [1,2]. Various stable species (C_1 - C_6) were measured by gas chromatography while polycyclic aromatic hydrocarbons (PAHs) such as naphthalene and pyrene were measured by jet-cooled laser induced fluorescence (JCLIF). To keep the C/O ratio and temperature values constants in the sooting flame region, all H_2 -flames have been studied by replacing or adding the equivalent of 1.8% N_2 . The Pt/Rh thermocouple measurements confirmed similar temperature values in the post flame region of methane/ O_2 / N_2 and methane/ H_2 / O_2 / N_2 flames. Moreover, additional experiments carried out in similar conditions with helium allowed to exclude the diluent affect. The new experimental results demonstrated that hydrogen can enhance significantly soot precursors (benzene, naphthalene, pyrene) even it is added at low amounts (lower than 2%). However, these aromatic compounds peak mole fraction can significantly be reduced if the experiments proceed via a low N_2 - amount substitution(1.8%).The soot volume mole fraction measurements and the modeling work which are in progress should confirm the importance of H atoms in the chemical growth process of PAHs and soot formation.

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Abstract_S1_R1_83

Particle size distribution measurements in ethylene/toluene premixed flames

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Abstract

Combustion generated particle formation was studied in a series of laminar premixed flames fueled with binary ethylene-toluene mixtures varying from pure ethylene to pure toluene. A very similar maximum temperature (T_{max} around 1750K) was obtained for all the flames keeping constant the equivalence ratio ($\phi=2$), the cold gas velocity and the total carbon flow rate, changing accordingly the diluents (N_2/O_2). It was possible to follow the influence of the aliphatic-aromatic ratio in the fuel mixture composition on combustion generated particle formation in comparable combustion conditions. Particle size distribution (PSD) measured at the end of the flame showed that particles with sizes less than 10 nm decrease as toluene percentage in the feed mixture increases, disappearing for toluene percentages above 40%, whereas aggregates with sizes larger than 100 nm increase when toluene concentration is increased. This behaviour has been previously observed with a simpler aromatic fuel (benzene). Toluene with respect to benzene has showed a different threshold in concentration in the fuel mixture at which the particles with sizes smaller than 10 nm disappear. The enhancement of PAHs and high-molecular mass aromatics precursors due to toluene presence in the fuel mixture combustion is hence quite important, especially at concentration relevant for the commercial fuel application. In fact, the results found for benzene and confirmed for toluene can suggest a difference fuel strategy for the future use of highly-aromatic natural and synthetic fuels, especially looking to the forthcoming soot emission regulations

Soot measurements over a series of laminar pool flames of biofuels, methyl esters and blends with diesel

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Abstract

Biofuel combustion results in lower soot compared with petroleum fuels. There have been several studies of soot formation measurement in flames of biodiesel surrogates (methyl esters), but few quantitative measurements from real biodiesels. In this study, we use laser induced incandescence and extinction measurements to obtain soot volume fraction in co-flow stabilised pool flames fueled with four different real biodiesels and two methyl esters. The results show that the degree of unsaturation plays an important role in the soot yield of fuels. A SEM analysis shows that the biofuels with lower degree of unsaturation produce a lower amount and smaller soot particles comparing the more saturated fuel.

Abstract_S1_R1_85

Quantification of the evolution of mean gaseous species concentrations across the sooting limit in turbulent premixed opposed jet flames

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Abstract

The soot particle inception process is not well understood (particularly) for turbulent flames. A back-to-burnt opposed jet configuration, featuring fractal grid generated turbulence, is used to investigate fuel-rich premixed ethylene/air flames close to the soot inception point and under heavily sooting conditions. Counterflowing hot combustion products at 1500 K were used to provide aerodynamic flame stabilisation. A probe sampling process was used to analyse the distribution of gaseous species within the PAH containing layer and combined with CH₂O/PAH PLIF. The axial sample positions along the stagnation point streamline featured 2 mm steps (i.e. half of an integral length scale of turbulence) to include the location of the PAH layer with GC/MS used to identify a range of gaseous species. Comparisons of measured concentrations with laminar flame calculations using detailed chemistry suggest a potential underlying flamelet-like structure for major non-aromatic gaseous species under the studied conditions.

Numerical prediction of soot particle size distribution in a turbulent flame using the LES-PBE-PDF method

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Abstract

In this paper we present a joint LES-PBE-PDF scheme for modelling soot formation in a turbulent non-premixed flame. A detailed population balance model including nucleation, surface growth and coagulation is combined with LES-PDF scheme in order to predict the time and spatial evolution of soot particle size distribution. To solve the PDF efficiently, statistically equivalent Eulerian stochastic equations are employed. The soot kinetics includes acetylene-based nucleation, surface growth and oxidation, all of which have been validated in the context of laminar diffusion flames. The numerical results are compared with experimental data. Overall, the paper demonstrates the computational viability of the LES-PBE-PDF method and its potential for modelling soot in turbulent combustion processes.

Abstract_S1_R1_87

A reduced virtual chemistry model for soot precursors prediction in hydrocarbon-air flames

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Abstract

A novel reduced chemistry approach, named virtual chemistry, has been recently developed to predict pollutant formation. The methodology consists in designing a mechanism made of virtual reactions and virtual species whose thermodynamics and chemical properties are optimized to capture user-specified target flames quantities. The present work aims at extending this technique to predict soot production. A virtual scheme is optimized by targeting a set of reference 1-D premixed and counterflow non-premixed ethylene-air flames including detailed soot formation chemistry.

Influence of surrogate biofuels admixture on soot characteristics in isooctane counterflow non-premixed flames

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Abstract

The legislation for particle emissions from combustion processes and especially in the transportation sector has become stricter in the last years, by limiting not only the mass but also the total number of particles. At the same time, the use of biofuels in gasoline engines is of increasing importance to reduce the global CO₂ emissions from vehicles [1]. In order to undertake these new challenges concerning soot particle emissions simplified investigations in model flames with well-defined boundary condition, where the motor complexity is decoupled from combustion chemistry, are essential.

In this context, counterflow non-premixed flames of iso-octane, iso-octane/ethanol and iso-octane/butanol are examined focusing on soot formation characteristics. The examined flames are laminar and one-dimensional. The oxidizer in all investigated flames is air and the fuel mixture is diluted with nitrogen. Soot formation limits in non-premixed iso-octane flames are examined under the influence of strain rate and fuel concentration (mass fraction) in the fuel stream. Moreover the influence of adding biogenic components in iso-octane is examined for different percentages of ethanol and n-butanol, up to 85 % in the fuel volume. The sooting limits were determined for all investigated mixtures, as the critical fuel mass fraction at which soot started to appear, using a scanning mobility particle sizer (SMPS). The data obtained under well-defined experimental conditions hold particular interest for the development and validation of combustion chemistry models. The results of this study show a strong dependency between the fuel structure and the sooting limit. Furthermore, it is observed that with addition of both alkanols, the sooting tendency of the fuel-mixture decreased and the limits are shifted to higher fuel mass fractions. An increase in the strain rate reduced the sooting tendency of all the fuels tested. The sensitivity of the sooting limit to the strain rate was more pronounced for less sooting fuels.

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Abstract_S1_R1_89

Impact of spray nozzle k-factor on spray characteristics, flame propagation, and soot formation under engine-relevant conditions

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Abstract

In direct injection (DI) engines, the fuel injection process is the dominating mechanism for mixture preparation, and thus is essential for the combustion process, the heat release rate, and emission formation. In this context, the inner spray nozzle design has substantial impact on atomization and spray break-up. In order to study the effect of nozzle design on the spray formation and combustion, two Bosch piezo 8-hole injectors with different k-factors were investigated. The measurements were performed under engine relevant conditions in a high-pressure constant flow chamber. First, LPL, LCA, and LOL are compared for both injectors. It is demonstrated that the LOL is similar for both injectors, whereas the LPL reduces with increasing k-factor. This observation suggests an improved spray break-up for the nozzle with larger k-factor. Statistics of the soot mass are used to compare the soot formation tendencies of the two injector nozzles. An increased k-factor slightly reduces the soot formation. A further analysis of the dependence of soot formation on flame lift-off length revealed a strong reduction of the soot formation with increasing flame lift-off.

Soot particle nanostructure from HRTEM Images and reactivity towards oxidation

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Abstract

This paper presents a HRTEM image analysis method for quantitative and reproducible analysis of the carbon nanostructure in soot and Carbon Black nanoparticles. The method applies top-hat transformation and Gaussian low-pass filtering and eliminates the negative impacts of both methods by image comparison. The subsequent binarization uses a threshold derived from the region of lowest sensitivity of size structures against the shape of the distribution of pixel intensities. Image analysis is completed by skeletonization and a modification of the objects, in which branches within the structures are resolved. Coding this procedure with MATLAB, a fully automated calculation of length, tortuosity and separation distance of graphene like layers is performed. The analysis shows an excellent correlation between the carbon nanostructure of the investigated soot and Carbon Black samples, in terms of fringe length, tortuosity and separation distance, and its reactivity towards oxidation.

9TH EUROPEAN COMBUSTION MEETING 2019

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Poster Session 2



Simulation of flameless combustion in Delft lab-scale furnace using EDC model

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Abstract

Flameless combustion has been developed with the aim of reducing NO_x pollutant emissions. Its application in industrial combustion systems, such as, high temperature furnaces and gas turbine combustors is in progress. It uses dilution of fuel and air stream by aerodynamic recirculation of flue gas leading to uniform mean temperature heat flux profiles. This work aims at accurate simulation of Delft-Lab-scale furnace by an improved simple model. The furnace consists of a burner with a central fuel nozzle surrounded by four air nozzles and a rectangular furnace box cooled via the top wall (avoiding cooling pipes inside the box, which would create more complex and more difficult to simulated flow patterns). The outflow is via a slit in the bottom wall. The simulation model comprises the realizable two-equation k-ε turbulence model, the Eddy Dissipation Concept (EDC) model for turbulence chemistry interaction and a Discrete Ordinate (DO) model and weighted-sum-of-gray-gases model (WSGGM) for radiation. The implementation is made on ANSYS Fluent, release 18.2. The role of model parameters of the EDC model is investigated. The chemical mechanism is DRM19, having 19 species and 84 reactions. The Standard Eddy Dissipation Concept (EDC) model assumes reactions to be fast (Damköhler number much larger than one) and reactions to occur in small reaction zones, that are modelled using well-stirred reactors. In flameless combustion, the Damköhler number is not large in the reaction region ($Da \approx 1$) and the temperature fluctuations are significantly lower than in conventional combustion. These differences lead to bad performance of the EDC model with standard values of the model constants C_ξ (finite structure constant) and C_τ (residence time constant). It is known that the values of these constants directly affect the predictions of temperature in the furnaces. In this work, as C_τ has almost no influence on flameless simulations in contrast to the influence of C_ξ , C_ξ is given different values in order to analyse its influence on combustion gases temperature prediction. The combustion results for six different values of finite structure constant are compared: $C_\xi = 2.1317$ (original), $C_\xi = 2.4$, $C_\xi = 2.9$, $C_\xi = 3.7$, $C_\xi = 4.5$, and $C_\xi = 5$ and the best value is identified. Also a new Extended EDC (NE-EDC) model where model constants are space dependent and calculated directly based on local Reynolds number and Kolmogorov scale Damköhler number is formulated and applied. The simulation results show that both modified models predict a more homogeneous temperature distribution in agreement with experiments. But flameless combustion conditions are better predicted with the NE-EDC model than by changing the finite structure to a new constant value. The former predicts homogeneous temperature along the full height of the furnace while the latter gives accurate results only in the lower

part, close to the burner. It is a significant advantage of NE-EDC model that calibration of the model using experimental data is not necessary, in contrast with the EDC model with globally modified C_{ξ} value were the optimal value of C_{ξ} is case dependent. In contrast, the standard EDC model predicts temperature peaks in disagreement with flameless combustion characteristics.

Reaction-diffusion manifolds (REDIMs) simplified chemistry for the simulation of laminar and turbulent CH₄ diffusion flame

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Abstract

Numerical modelling of laminar and turbulent combustion is based on the solution of the governing conservation equations for mass, species, momentum and energy. However, detailed chemical kinetics consist of more than hundred species and reaction steps, corresponding to a large number of species conservation equations to be solved. Therefore, reduction methods for the simplification of chemical kinetics are necessary. Typically for a given fuel different detailed kinetic schemes exist from different groups, and they also differ in the quantitative results for flame structures, ignition properties, etc.. Sophisticated model reduction methods for chemical kinetics must be able to reproduce these differences, if the same reduction method is used for different detailed chemical kinetics. In other words, if one detailed mechanism predicts the concentration of one species higher than another mechanism, then the simplified chemistry built for these two mechanisms must also reproduce this phenomenon. In this work, the Reaction-Diffusion Manifolds (REDIM) method is applied to reduce the chemical kinetics and to reduce the computational time in the numerical simulation. The REDIM reduction method takes into account the molecular transport processes. As a test for different detailed mechanisms, the GRI 2.11 and GRI 3.0 are selected. Both mechanisms predict a similar behavior for most thermo-kinetic quantities (e.g. temperatures, O₂, H₂O etc.), but large differences (up to a factor of 2) for NO concentration. Two REDIM simplified chemistries are built, one for GRI 2.11 and the other for GRI 3.0. Then both REDIM simplified schemes are applied to laminar and turbulent test cases. It is shown that in laminar diffusion flames, temperature and species concentration profiles based on detailed chemistry and REDIM simplified chemistry agree with each other very well for both test cases, meaning that the different behavior the different detailed schemes is reproduced by the REDIM-reduced scheme. simplified chemistry can be represented. As a turbulent test case, the well-known Sandia Flame D is used, and the REDIM simplified chemistry is coupled with a probability density function (PDF) method. Again, it is shown that the reduced schemes can capture the differences in the detailed reaction mechanisms.

Application of the shadow-position mixing model to large eddy simulation with the Eulerian subgrid probability density function approach

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Abstract

The Shadow-Position Mixing Model (SPMM) accounts for scalar-localness of molecular mixing in transported Probability Density Function (PDF) simulations of turbulent flow, while maintaining correct turbulent dispersion behaviour. The SPMM was originally formulated in the context of the Lagrangian PDF implementation. Here, the SPMM is developed for use with the Eulerian PDF approach. After confirming consistency of behavior between the Lagrangian and Eulerian formulations in idealized one-dimensional test cases, we provide the first validation of any SPMM implementation against experimental measurements of a turbulent flame, in this case through Large Eddy Simulation of the Sandia D piloted turbulent jet flame. Compared to the less-sophisticated interaction by exchange with the mean mixing model, the SPMM model improves predictions of minor species and the scattering of composition in mixture fraction space, which is a measure of the localized extinction occurring in Sandia D.

Abstract_S2_All_04

The behavior of flame with the increase of turbulence intensity on low swirl combustor

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Abstract

This study is intended to identify the effect of changes in flow fields on turbulent generator plates used in a low-swirl combustor. The turbulent generator in this study is not a circular perforation but bar. The width of bars changed. The turbulent is formed by the effect of the bar, and turbulent of various scales is generated by different width of bars. As a result of the various widths of the bars, the turbulent has intensified. The mean velocity doesn't exist in the inner circulation zone. Further, the flame's base is closer to the nozzle due to the increase in turbulent burning velocity due to the increased turbulent intensity.

Abstract_S2_All_05

LES modelling of nanoparticle synthesis in the SpraySyn burner

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Abstract

LES is conducted to obtain the combustion regimes and the conditions experienced by the synthesised nanoparticles within the SpraySyn burner. The subgrid effect of the small scale turbulence is described by Nicoud's Sigma Turbulence Model. The liquid phase droplets are modelled with a Lagrangian approach considering momentum and mass transfer between the liquid and the gas phase. The nanoparticle dynamics of growth and coagulation are modelled by a sectional model resolving the particle size distribution in time and space, but so far, without considering their subgrid distribution and the sub-filter effects on aggregation. The combustion chemistry is parametrised by precalculated tables, following the Flamelet Generated Manifold (FGM) approach. Two mixture fractions and a progress variable are chosen as controlling parameters.

Abstract_S2_All_06

Comparison of LES combustion models for turbulent premixed flames at atmospheric pressures

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Abstract

Multiple combustion models are available to simulate premixed turbulent combustion cases. Here we compare three combustion models: a flame surface density (FSD), an artificially thickened flame (ATF) and a transported PDF Eulerian stochastic fields (ESF) model. Simple laminar finite-rate chemistry is performed as a reference. A turbulent premixed Bunsen flame with methane-air is evaluated using the same mesh with similar numerical schemes and time steps for each model. Relatively coarse meshes yield good results for the FSD and the ATF model. To describe the flame in the ESF model and finite rate chemistry, a finer mesh resolution is needed.

Eulerian stochastic fields method and model free finite rate chemistry applied to Sydney partially premixed flame

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Abstract

Large-eddy simulations (LES) of a piloted methane/air jet flame with inhomogeneous inlets are conducted using finite rate chemistry and a 19 species mechanism. The jet flame configuration studied here can smoothly transition from a fully premixed flame mode fully non-premixed mode by retracting central fuel pipe. Finite rate chemistry in combination with the Eulerian Stochastic Fields (ESF) transported PDF method seems to be a promising approach to cope with partially premixed combustion and the associated extinction and re-ignition events. In this study, the effect of the ESF sub-grid scale (SGS) model is investigated by a direct comparison with results of a model free laminar finite rate simulation (assuming no SGS turbulence–chemistry interaction) applied to the Sydney partially premixed flame (case FJ200-5GP-L175-57). The simulation results are in good agreement with the experimental data and the mayor flame structures are well reproduced.

Abstract_S2_All_08

Machine learning for sub-grid scale turbulent combustion modeling

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Abstract

In the context of sub-grid scale (SGS) modeling of premixed turbulent flames, the estimation of unresolved scalar sources and transport terms from Convolutional Neural Network (CNN) is discussed. A Direct Numerical Simulation (DNS) imbedded in a Large Eddy Simulation (LES) of a premixed turbulent jet flame is coupled with machine learning, to propose a self-consistent modeling with tabulated detailed chemistry. Mining the DNS database, specific features are observed connecting filtered non-linear chemical sources and the divergence of the unresolved fluxes, respectively, to the burning rates and the divergence of the diffusive fluxes computed from the resolved LES fields. These features suggest that image-type machine learning can be readily applied to dynamically determine two mapping functions from CNN, so that all unknown terms in the progress variable equation are dynamically reconstructed from a neural network. A priori tests are then conducted varying the LES filter size between 0.3 mm and 0.9 mm. The capability of CNN to provide a reliable approximation of the two mapping functions (chemical source and divergence of fluxes) is confirmed for all filter sizes. It is also observed that blurring the data in the training phase, improves reliability with cases not initially learned by the CNN.

Abstract_S2_All_09

Turbulent premixed flames in a hele-shaw cell

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Abstract

We study a propane-air premixed flame propagating downwards against a turbulent flow in a Hele-Shaw cell with variable width. We analyze the modification of the flame shape with the turbulent intensity. In particular, the asymmetry in the curvature statistics is shown to decrease when the turbulence is increased. In addition, we measure the turbulent flame speed increase with the turbulent intensity. For this weakly turbulent regime, the Darrieus-Landau influence is highlighted and a bending effect of the turbulent flame speed is observed.

Effects of fuel composition on the minimum ignition energy and its transition on homogeneous biogas-air mixtures

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Abstract

Localised forced ignition (laser, spark) plays a vital role in the design of modern Spark ignition and Direct Injection engines, in which misfire causes ineffective combustion. Several experimental and numerical investigations of the forced ignition of turbulent homogeneous mixtures can be found in the existing literature. In particular, the Minimum Ignition Energy (MIE), which is defined as the minimum energy deposited in the flow to obtain a successful ignition of the mixture and subsequent flame propagation has been extensively investigated for single component fuels in air, and in particular methane. Both experimental and numerical studies have been carried out on this phenomenon, but only stoichiometric methane-air mixtures have been investigated numerically. As compound alternative fuels, e.g. biogas ($\text{CH}_4 + \text{CO}_2$), syngas ($\text{H}_2 + \text{CO}$), etc. are increasingly used in power generation and transportation applications to address the challenges of diminishing fossil fuel supplies, it is necessary that their localised forced ignition be investigated. Carrying on from previous studies on methane-air mixtures, three-dimensional compressible Direct Numerical Simulations (DNS) have been used to investigate the MIE of homogeneous premixed stoichiometric biogas/air mixtures for a range of turbulence intensities and different biogas compositions. The biogas is represented by a $\text{CH}_4 + \text{CO}_2$ mixture and a two-step mechanism involving incomplete oxidation of CH_4 to CO and H_2O and an equilibrium between the CO oxidation and the CO_2 dissociation has been used. This two-step mechanism captures the variation of the unstrained laminar flame speed with equivalence ratio and CO_2 dilution with sufficient accuracy when compared with detailed chemistry results. The primary goals of the present study are to investigate the effects that CO_2 dilution has on (1) the MIE and its transition characteristics (i.e. critical turbulence intensity (u_c'/s_l°) and dependence of the MIE with the turbulence intensity) (2) the kernel development after successful ignition (e.g. growth rate, etc.). It will be shown that a transition in the increase of the MIE with increasing u'/s_l° is observed and for $u'/s_l^\circ > u_c'/s_l^\circ$ the MIE requirement increases significantly faster than that for $u'/s_l^\circ < u_c'/s_l^\circ$, which is consistent with the literature. It was also found that regardless of CO_2 dilution, the variations of the normalised MIE (MIE normalised by its laminar value), with normalised turbulence intensity are qualitatively and quantitatively similar to those obtained for the undiluted mixture. However the MIE increases as the dilution with CO_2 increases, and this is explained by the detrimental effect of the CO_2 dilution on the laminar flame speed and heat release. This in turn leads to more energy being required for the kernel to reach the critical radius required to obtain self-sustained combustion.

Visualization of turbulent inverse diffusion flames at elevated pressure using OH-PLIF and OH* chemiluminescence imaging

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Abstract

A co-axial inverse jet burner was installed and tested in the high-pressure combustion rig (HPCR) at Lund University to investigate the characteristics of methane/air inverse diffusion flames (IDF) at elevated pressure. OH-PLIF and OH* chemiluminescence imaging were employed to capture the instantaneous flame image. Flames were stabilized with a fixed fuel velocity (V_f) of 0.3m/s and flow rate of the co-flow air, while varying either the air to fuel velocity ratio (V_r) from 200 to 600, increase the inner air jet velocity or the pressure in the combustion chamber from 2bar to 5bar. The effect of pressure on the flame front structure and flame lift-off height are analyzed from single-shot and averaged OH-PLIF image. Results indicate that the inner flame structure changed with pressure. With same V_f and V_r , more wrinkles and larger curvature of the flame front were found in the inner flame structure at higher pressure. This could be explained by the flame intrinsic instability or smaller scale turbulence eddy interacting with the flame front. In addition, the flame lift-off height increased with an increase of pressure. The effect of V_r on the flame front structure and overall flame shape were also observed. Wrinkles and flame front area were found to increase as V_r increased, by increasing the air jet velocity with a fixed V_f corresponding to a higher turbulence intensity. Moreover, the flame shape became narrower as V_r increased for a constant pressure, which can be explained by the enhanced shear-layer effect leading to inward inclination to the centerline of the flame.

Abstract_S2_All_12

Turbulent burning characteristics of hydrogen/air premixed flames in different combustion regimes

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Abstract

A direct numerical simulation (DNS) study has been conducted to understand turbulent combustion behavior at different combustion modes that are mainly characterized by the Karlovitz number (Ka). Particular interest is on the extreme conditions where Ka exceeds $O(100)$, exhibiting strong turbulence-flame interaction. Two cases are considered which are representative of the thin reaction zone and distributed combustion regime. It is found that the cellular structure of the lean hydrogen flame is enhanced by turbulence at a moderate turbulence level ($Ka = O(10)$), while it is attenuated at strong turbulent conditions ($Ka = O(100)$). Turbulent flame structures, based on averaged solution quantities, show that the temperature and species profiles of the flame in the thin reaction zone fluctuate significantly, while those corresponding to the distributed combustion regime resemble the laminar ones more.

Abstract_S2_All_13

Flame front detection in combustion imagery based on ridges in two and three dimensions

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Abstract

A generic description of combustion structures as Ridges is proposed. These are low-dimensional structures where scalar field has restricted local maxima along a eigen-directions of the Hessian. Important spatial structures arising in combustion (like laminar and turbulent flame fronts, or also objects like combustion islands, broken reaction zones, isolated or merging auto-ignition centers) can very naturally be represented by ridges. DNS examples are shown which demonstrate methods to identify ridges in given combustion data. Ridge analysis identified a novel type of reaction front structure of essentially filamentary shape.

Abstract_S2_All_14

Study of an opposed jet turbulent flame using the sub-grid PDF method

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Abstract

A numerical simulation of turbulent premixed flames generated by a counter-flow burner under different operating conditions is performed in the context of Large Eddy Simulation (LES). The simulation aims at investigating the reactant stoichiometry and mixing with combustion products on the performance of turbulent counter-flow flames. The probability density function (pdf) approach is adopted to simulate sub-grid scale (sgs) turbulence-chemistry interaction. The solution of the evolution equation of the joint sgs-pdf of the scalars is obtained by the Eulerian stochastic field method. The methane-air reaction is modeled by means of a simplified chemical reaction mechanism with 15 reaction steps and 19 species. The perturbation at the inflow planes are prescribed using a digital generator for artificial turbulence to trigger jet break-up in reality. The flow field of both the reacting and the non-reacting flows are investigated, with averaged axial, radial velocities and the RMS velocity fluctuations along the reactor simulated. The velocity field in the relative frame of the gas mixing layer interface (GMLI) is also presented and compared with experimental data. Overall, the computed results for both the unconditional and conditional velocity field are in good agreement with the experimental data.

Near-wall behaviour of turbulence in flame-wall interaction of premixed turbulent combustion in boundary layers

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Abstract

Wall-bounded turbulent combustion occurs in many flows of engineering interest [e.g. spark ignition (SI) engines and gas turbines], and modelling these flames remains challenging. The treatment of near-wall turbulence for non-reacting flows is still a difficult problem and quite often the limiting factor in flow prediction of practical applications. In the case of reacting flows, this problem becomes more challenging as combustion is strongly influenced by the presence of walls which may lead to flame quenching. The flame also has a significant effect on the flow near the wall as well as on the heat flux to the wall. Consequently, the turbulence structure is altered by the walls and the interaction of flame elements with walls leads to modifications of the underlying combustion process. In the case of flame-wall interaction (FWI), the spatial and temporal fluctuations of wall temperature induce thermal stresses and strongly affect combustor lifetimes. These fluctuations are directly related to the fluid mechanical effects generated in the boundary layer near combustor walls. In practice, very little is known about the effects and behaviour of turbulence during flame-wall interaction. In this spirit, direct numerical simulation (DNS) data has been interrogated to understand the behaviour of wall heat fluxes, quenching distances, non-dimensional velocity, non-dimensional temperature, turbulent kinetic energy and its dissipation in FWI of two flame configurations. The first configuration considered is a V-flame interacting with an inert isothermal wall in a fully developed turbulent channel flow at $Re_{\tau}=110$. The second configuration is representative of a head-on quenching (HOQ) of a flame in a fully developed turbulent boundary layer. In this configuration, a planar flame propagates normal to the wall and interacts with the fully developed boundary layer near the wall. In both cases a unity Lewis number stoichiometric methane-air premixed flame is simulated under low Mach number conditions. It is found that the log-layer region of the flow along with the friction velocity are significantly altered by the flame. Furthermore, the behaviour of velocity, temperature, turbulent kinetic energy and its dissipation are considerably altered in the near-wall region during FWI. These results along with the influence of the flame configuration are presented in the paper.

Abstract_S2_All_16

Studies on the lean flammability limits of hydrogen/methane/air turbulent flames in a combustion bomb

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Abstract

Lean flammability limits are an important characteristic of a given fuel, with applications in combustion engine and safety technology. In our work, we present comparative studies on the initiation and flame propagation (or the lack of it) in mixtures of methane and methane/hydrogen air mixtures under idealized conditions in a constant volume combustion bomb with turbulence generation. Experiments show that hydrogen addition widens the flammable range under both laminar and turbulent conditions. The addition of hydrogen to lean methane/air mixture strongly widens the flammable range. Also, visual studies of flame development are presented.

Abstract_S2_All_17

Effect of equivalence ratio on turbulent premixed stratified methane-air flames

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Abstract

The equivalence ratio effect on methane/air lifted flames structure, dynamics and on several key flame properties are investigated. High frame rate (3 kHz) combined PIV/PLIF measurements were performed to in detail study the flame front structure (OH) and distribution and transport of CH₂O reflecting the properties of the flame preheat zone and its interaction with the turbulent flow field. Detailed statistical data are obtained of the velocity field, the mean flame location, flame brush thickness, the flame surface density, wrinkling factor and thickness of the preheat layer.

Abstract_S2_All_18

Combined PIV/SO₂-PLIF experiments for multi-mode combustion

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Abstract

A novel burner was designed to provide a canonical configuration with well-defined boundary conditions for the investigation of multi-mode combustion processes and to offer validation data for numerical simulation models. A combination of particle imaging velocimetry (PIV) and planar laser induced fluorescence (PLIF) of SO₂ was applied to measure the flow field and the location of flame fronts in this configuration. Mean and rms axial and radial velocities as well as mean and instantaneous PLIF data as a marker for the reaction zone have been evaluated. A flame front tracking algorithm was applied to the fluorescence images and will enable a detailed investigation of flame-turbulence interaction.

Statistical dependence of mixture fraction and progress variable in partially-premixed combustion

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Abstract

The statistical dependence between mixture fraction and progress variable is investigated and modelled across three different classes of partially-premixed flow: (1) flame propagation through equivalence ratio-stratified reactants; (2) extinction and re-ignition in a non-premixed system; and (3) autoignition in a lifted jet flame. A mathematical transformation is developed in order to visualise the underlying structure of the statistical dependence of mixture fraction and progress variable, as distinct from the contributions of the respective marginal distributions, revealing qualitatively different dependence structures in each case. Flame propagation through equivalence ratio-stratified mixture leads to a diagonal dependence structure, with the sign of the correlation depending on the mean alignment in the mixture fraction and progress variable fields. Extinction of a diffusion flame leads to a 'v'-shaped dependence because, during extinction, the progress variable falls fastest in the stoichiometric mixture. Autoignition produces an 'n'-shaped dependence due to ignition at a preferred 'most reactive' mixture fraction. The common assumption of statistical independence is not justified in any of the three classes of partially-premixed combustion, leading to significant errors in regions with significant mixture fraction-progress variable covariance. The diagonal dependence of the joint distribution observed in the stratified flame can be modelled using a Plackett-family copula, at the expense of modelling additional moments of the joint distribution. In order to reduce the number of moments needed to accurately model the joint pdf, we use the physical insight that flamelets evolve temporally to obtain a model for the statistical dependence by referring to the residence time distribution in mixture fraction-progress variable double-conditional moment closure solutions. The new approach represents a generalization of the Lagrangian non-premixed flamelet approach to account for partially-premixed and perfectly-premixed conditions.

Abstract_S2_All_20

Assessing heat release and chemical mode manifold in multi-regime combustion under experimental conditions

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Abstract

Obtaining information about burning characteristics and flame structures by assessing experimental data only, are important issues for analyzing combustion processes. Based on a constrained approximation procedure, the chemical mode (CM) and the local heat release rate (HRR) are assessed using variables involved in experimental measurements only. The objective of this study is to analyze and characterize the CM and local HRR of multi-regime combustion processes using experimental data from a novel multi-regime burner configuration. Tabulated manifolds of HRR and the CM are compared to flamelet look-up tables. Building on this, similarities and differences of the manifold are discussed.

Artificial neural network prediction of emissions from primary reference fuel combustion in jet stirred reactor

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Abstract

Strict regulations on air pollution motivates clean combustion research for fossil fuels. To numerically mimic real gasoline fuel reactivity, surrogates are proposed to facilitate advanced engine design and predict emissions by chemical kinetic modelling. However, chemical kinetic models have difficulty predicting minor compounds, e.g. aldehydes, ketones and unsaturated hydrocarbons, which are important air pollutants. In this work, we propose a machine learning method to achieve better predictions. Combustion chemistry of two gasoline components; n-heptane and iso-octane, and six primary reference fuels (binary mixtures of n-heptane and iso-octane) were tested in a jet stirred reactor. Experimental data were collected in the same setup to maintain data uniformity and consistency under following conditions: residence time at 1.0 second, fuel concentration at 0.25%, equivalence ratio at 1.0, and temperature range from 750 to 1100K. Measured species profiles of methane, ethylene, propylene, hydrogen, carbon monoxide and carbon dioxide are used for artificial neural network model development. The model considers both chemical effects and physical conditions. Chemical effects are described as different functional groups, e.g. primary, secondary, tertiary, and quaternary carbons in molecular structures, and physical conditions as temperature. Artificial neural networks exhibits good prediction accuracy for primary reference fuels. This finding shows the potential of machine learning application on combustion chemistry. By expanding the experimental database and hybridizing with chemical kinetic simulations, artificial neural networks can be further applied to other hydrocarbons.

Abstract_S2_All_22

CO-concentration and temperature measurements of fuel-rich CH₄/O₂ mixtures doped with diethyl ether behind reflected shock waves

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Abstract

CO is one of the main products during partial oxidation of many hydrocarbons. This work uses shock tube and laser absorption spectroscopy to measure time-resolved temperature and CO concentration during oxidation of CH₄/diethyl ether mixtures ($\phi=2$) highly diluted in He/Ar at 1500–2100 K and 1.7 bar. Two mid-IR quantum cascade lasers were used for measuring time-resolved temperature and CO concentration by using the fundamental vibrational of CO at the transition lines P20 and R21 near 4.8546 and 4.5631 μm . This paper compares the experimental data with numerical predictions from two mechanisms (Fikri et al., ICDERS 2017 and Yasunaga et al., JPC 2010). The mechanism of Fikri et al. showed very good agreement with the experiments (CO and temperature) whereas the mechanism of Yasunaga et al. showed too fast CO formation and temperature increase.

Experimental study of the autoignition of isooctane/anisole mixtures at low to intermediate temperatures

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Abstract

Anisole (methoxybenzene) is investigated due to its potential octane booster properties and interest as a lignin pyrolysis and oxidation surrogate. The autoignition of isooctane/O₂/inert and isooctane/anisole/O₂/inert mixtures has been studied in a Rapid Compression Machine (RCM) in order to validate a co-oxidation detailed chemical kinetic mechanism. The experimental data for autoignition of isooctane/anisole in a Rapid Compression Machine at low to intermediate temperature bridges the gap of previous studies. The results for isooctane/O₂/inert ignition delays, at 20 bar and $\Phi = 1$, match very well with similar conditions found in the literature [1]. Stoichiometric isooctane/anisole/O₂/inert mixtures were compressed at pressures between $p_c = 14$ and $p_c = 20$ bar and temperatures from $T_c = 683$ to $T_c = 850$ K. A non-Arrhenius behavior with negative temperature coefficient (NTC) was observed for mixtures with 40 % anisole, at $p_c = 20$ bar. Furthermore, these anisole mixtures have shown to be less reactive than pure isooctane, in agreement with the RON values of the pure fuels. The effect of anisole mole fraction in the mixture has also been investigated at two separate temperatures. Finally, the pressure effect was analyzed for all considered anisole compositions.

Abstract_S2_All_24

Experimental speciation study during oxidation of n-butane in a rapid compression machine

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Abstract

The importance of understanding the chemical kinetics of n-butane is vital because it serves in understanding the kinetics of higher order hydrocarbons and it is one of the components found in liquefied petroleum gas (LPG) and compressed natural gas (CNG). Experimental speciation study has been carried out for a stoichiometric n-butane/air mixture at a compressed pressure and temperature of 20 bar and 749 K, respectively. Additionally, ignition delay time measurements have been performed in the temperature range from 650 – 950 K. A mechanism is chosen based on its ability to predict these experimental targets and used for analyzing the important reaction pathways and the sensitive reactions influencing the reactivity of the fuel.

High pressure ignition delay time measurements and consistent kinetic modeling of C4 - C7 ethyl esters

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Abstract

Biodiesel from renewable resources have emerged as a significant sustainable fuel source and are considered an important factor in overcoming fossil energy shortcomings and decreasing harmful emission of internal combustion engines at the same time [1]. The use of renewable electricity to further process and refine biomass-based fuel components represents a promising concept for a sustainable production system of future liquid fuels. Lange et al. [2] showed that ethyl valerate (EV) is synthesizable from alternative carbon feedstock by several catalytic supported reaction steps. Besides lignocellulosic platform molecules, this process requires hydrogen and heat, which both can be acquired from renewable power plants. They also proved the usability of EV as a beneficial blending component to fossil gasoline fuel. Due to the hierarchic nature of combustion processes and hence kinetic mechanisms, a fundamental understanding of the class of ethyl esters is mandatory when studying EV or higher ethyl esters. In this study, a high-pressure shock tube (ST) was used to measure ignition delay times of four different ethyl esters, namely ethyl acetate, ethyl propionate, ethyl butyrate and ethyl valerate. Experiments were conducted with non-diluted stoichiometric mixtures in order to investigate the ignition behavior of different ethyl esters under engine relevant high-pressure conditions. A consistent high-temperature kinetic model was designed for all ethyl esters up to EV based on existing mechanisms reported in literature. Great care has been taken to use the same rates and analogies for all ethyl esters whenever possible. Zero-dimensional simulations considering the facility effects were performed and compared to the experimental results of this study. Sensitivity analysis and rate of production evaluation were applied to isolate the most important reaction pathways during auto ignition. The kinetic mechanism developed in this work is able to predict the measured ignition delay times well for all ethyl ester except ethyl propionate for which the reactivity is underestimated. According to previous studies, the unimolecular decomposition forming ethylene and a carboxylic acid was found to be the major fuel consumption pathways in the high-temperature regime.

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A chemical functionality approach towards the formulation of a high-fidelity surrogate fuel for FACE gasoline F

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Abstract

¹H and ¹³C nuclear magnetic resonance spectroscopy are used to determine an accurate, quantitative description of the atom type population of FACE-F, a research-grade gasoline. On this basis, a surrogate palette of seventeen components is proposed. Two surrogate fuels are formulated; a seven-component mixture (FGF-TCD₁), and a nine-component mixture (FGF-TCD₂). The autoignition behavior of FGF-TCD₁ and FGF-TCD₂ is investigated. Measurements are compared to tests with FACE-F, and blends of FACE-F with ethanol. Conditions at the transition from low-temperature to NTC chemistry are targeted such that first-stage, main ignition times, and exothermicity can be monitored. From the same manner, perturbed ignition characteristics due to the ethanol addition can be quantified. The results of this study demonstrate that although the atom type populations of both surrogate fuels are consistent with FACE-F and each other, the observed reactivity is different. This is may be attributed to atom type descriptors alone being insufficient to capture the combustion behavior of FACE-F. Interestingly, however, similar degree of reactivity differences in response to ethanol blending is observed.

Experimental and modeling study of the pyrolysis and combustion of di-tert-butyl peroxide

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Abstract

The replacement of conventional fuels by biofuels is a promising solution for the independence from fossil energy sources within a reasonable period. To control the kinetics and emissions of these novel fuels, cetane enhancers such as di-*tert*-butyl peroxide (DTBP) might be important to increase the reactivity after the injection into the cylinder. DTBP consists of two *tert*-butyl groups bonded by a weak peroxide bond with a bond dissociation energy of about 40 kcal/mol that cleaves at temperatures above 400 K [1]. It rapidly provides radicals to the system, which accelerate the consumption of the base fuel. Its suitability as a cetane booster has already been investigated in internal combustion engines [2–5]. Fundamental experiments in a mechanically stirred closed vessel [6] as well as RCM-Experiments [7] were already carried out. In addition, Iizuka *et al.* [8] studied the decomposition behavior of DTBP in an accelerating rate calorimeter in combination with GC-MS species measurements. Nevertheless, further fundamental investigations are still necessary to determine the details of the DTBP kinetics, especially the combustion behavior. In this study, the pyrolysis and oxidation of di-*tert*-butyl peroxide (DTBP) were investigated. A rapid compression machine (RCM) and a shock tube (ST) were used to measure ignition delay times (IDTs) over a temperature range from 540 K – 650 K at different pressures (10 – 30 bar). Zero-dimensional simulations including the facility effects of RCM and ST were applied to understand the complex multi-stage ignition behavior of DTBP. Within this work, the most important reaction for the energy release at pyrolysis conditions was identified as the DTBP dissociation reaction and its Arrhenius parameters were determined according to these experiments. Subsequently, the affiliation of the consumption of the following intermediate subspecies like acetone, methyl hydroperoxide, and methanol was assigned to the multiple stages within the DTBP combustion. The results of this work help not only to understand the combustion of the promising cetane booster DTBP but also to examine methyl reactions in more detail.

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Abstract_S2_All_28

Influence of CO₂ dilution on shock tube ignition delay times of dimethyl ether/air mixtures at high pressures

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Abstract

For oxy-fuel combustion concepts or those involving exhaust gas recirculation, CO₂ diluted combustion mixtures play an important role. Nevertheless, there is very limited number of studies on ignition delay times of mixtures containing high amounts of CO₂ at technically relevant high pressures. Therefore, high-pressure shock tube study has been performed to measure first-stage and overall ignition delay times of DME/air mixtures diluted with CO₂ at different dilution ratios. The data have been collected for various equivalence ratios ($\varphi = 0.5, 1.0, 2.0$) and pressure of 35 bar. Experimental ignition delay times for CO₂ diluted mixtures have also been compared with those for nitrogen diluted mixtures at given dilution ratio as well as for undiluted mixtures. A prolonging effect of CO₂ on ignition delay times of DME/air mixtures is observed, being specifically pronounced for the conditions exhibiting two-stage ignition. Finally, all experimental data are compared with the predictions from zero-dimensional simulations using several common chemical kinetic mechanisms in order to assess their predictive ability.

Multi-dimensional transport phenomena of flame-wall-interactions and the REDIM method

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Abstract

The increasingly stringent guidelines regarding exhaust values leads to a trend towards downsizing e.g. in internal combustion engines. In this respect, questions of heat loss and surface reactions of reacting flows near boundaries, i.e. flame-wall-interactions (FWI), become very important. Besides experimental investigations, computations of FWI are performed to study and to improve the combustion processes in these configurations. For the modeling of the chemical kinetics for the computation of combustion processes, reaction mechanisms with hundreds of species are developed. Furthermore, the Arrhenius law used for modelling rates of the elementary reactions leads to an exponential dependence on the temperature. Therefore, even today with modern computational facilities, the detailed simulation of complex combustion processes is very time-consuming due to the high dimension and stiffness of these systems. In order to run simulations in a reasonable CPU time, reduced kinetic models are needed and have been developed recently. The Reaction-Diffusion-Manifold (REDIM), which accounts for both chemical kinetics as well as for diffusion processes, performs a model reduction in a very generic way. There are two major difficulties complicating standard model reduction methods based e.g. on the flamelet assumption which need to be considered and addressed for the FWI configuration. The gradients of the different species do not everywhere point into the same direction. Thus, multi-dimensional transport phenomena are observed. In addition, there is a heat loss towards the wall that needs to be accounted for. In this work, we show how multi-dimensional transport phenomena and heat losses during flame-wall-interactions can be addressed within the REDIM method. The so-called Side-Wall-Quenching (SWQ) flame configuration is considered as representative model system. In order to investigate the phenomenon in detail, the gradients of a Direct Numerical Simulation (DNS) are studied and used as gradient estimates for the REDIM. In order to convert the gradients of the SWQ DNS and treat them in the REDIM method, the gradients are filtered and a Singular-Value Decomposition (SVD) is performed to study geometrical properties of the gradients fields in the system's thermo-chemical state space. The transformed gradient estimate is used to generate the REDIM with multi-dimensional transport phenomena and the influence of this gradient estimate on the REDIM is investigated. The study confirms the assumption that in many cases multi-dimensional transport phenomena have only minor influence on the REDIM.

Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Projektnummer 237267381 –TRR 150[8] Y. Iizuka, M. Surianarayanan, Ind. Eng. Chem. Res. 42 (2003) 2987–2995.

Abstract_S2_All_30

The role of chemical structure in the thermal decomposition of xylan

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Abstract

Xylan is one of the most abundant polysaccharides found in hemicellulose from hardwoods and herbaceous plants. Thus, a strong understanding of its chemical reactivity will greatly aid in the utilization of biomass as an energy source. Towards this goal, thermal conversion processes, such as pyrolysis, are implemented as valorisation pathways for biomass sources. Consequently, significant attention has been devoted to modelling the pyrolysis behaviour of hemicellulose. Typically, this is achieved through the use of lumped kinetic models. In such models, a generic chemical composition is attributed to the xylan component. This work uses thermogravimetric analysis (TGA) to investigate the pyrolysis of xylan from corncob and beech wood. It is shown that xylans from different biomass sources exhibit markedly different pyrolysis behaviours. Significantly, it is demonstrated that the reactivity of xylans from the same biomass source, also exhibit notably different pyrolysis behaviours. Toward understanding this variability, and computational modelling of the pyrolysis of the highly complex xylan structure, the pyrolysis of several “model molecules” of xylan; xylose, xylobiose and xylotriose are investigated. It is shown that while the TGA obtained reactivity obtained for xylose and xylobiose are comparable, that observed for xylotriose is markedly different.

Isomerisation and decomposition of alkylperoxy and hydroperoxy alkylperoxy radicals of three heptane isomers

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Abstract

Reaction enthalpies and transition state enthalpies are computed for a number of important process of the alkyl peroxy and peroxy alkyl hydroperoxide radicals of three heptane isomers (*n*-heptane, 3-methylhexane and 2,3-dimethylpentane) with the complete basis set method, CBS-QB3. The transition state enthalpies defining the competition between peroxy radical isomerization and peroxy radical elimination to olefin and HO₂ radical are first investigated. The transition state enthalpies for isomerization are shown to be dependent on both the dissociation energy of the C-H bond, and the transition-state ring size, scales as; tertiary C-H < Secondary C-H < Primary C-H and 6 membered ≈ 7 membered << 5 membered. Peroxy radical elimination is shown to be independent of C-H bond dissociation energy, and to have a transition state enthalpy of ~ 30.5 kcal/mol regardless of the molecular structure of the initial alkyl radical. The fate of the hydroperoxy alkylperoxy radical is also investigated by computed transition state and reaction enthalpies of its decomposition to ketohydroperoxide and its isomerization to dihydroperoxy alkyl radicals. Finally, it is shown that all of the isomerizations of the peroxy radicals follow quite a strict relationship between transition state enthalpy and reaction enthalpy dependent on the type of isomerization.

Abstract_S2_All_32

Autoignition properties of liquefied natural gas (LNG): an experimental and modeling study

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Abstract

Liquefied natural gas (LNG) is an important world energy resource and gains increasing attention. This study aims to aid in developing an experimental validation program for the calculation of the methane number (MN) from the LNG composition by detailed understanding its autoignition kinetics. Experiments were performed in rapid compression machine (RCM). The ignition delay times of selected LNG type mixtures containing the species $\text{CH}_4/\text{C}_2\text{H}_6/\text{C}_3\text{H}_8/\text{n-C}_4\text{H}_{10}/\text{i-C}_4\text{H}_{10}/\text{n-C}_5\text{H}_{12}/\text{i-C}_5\text{H}_{12}/\text{N}_2$ were studied in the temperature range between 850 and 1100 K. The experimental results were validated with literature mechanisms to get deeper insights of combustion chemistry.

An experimental and theoretical comparison of the novel e-fuel class oxymethylene ethers

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Abstract

In order to meet future stringent emission regulations without increasing technical exhaust aftertreatment efforts in modern combustion engines, the combustion process might be improved by the use of alternative fuels. Oxymethylene ethers (OME_x , $\text{CH}_3\text{-O-}[\text{CH}_2\text{O}]_x\text{-CH}_3$) have been recently identified as potential future fuel candidates, which can be used pure or as fuel-blending agents. OME_x as neat fuels or as diesel additives are efficient in reducing of soot emissions [1, 2]. The results of these investigations show that OME_x can improve the trade-off between nitrogen oxides (NO_x) and particulate matter (PM). The suppression of soot formation is assumed to be due to their C-O moieties imbedded in their saturated molecular structure, as a result their lack of carbon-carbon bonds, and their high amount of oxygen mass content [3, 4]. Diesel-like properties become more prominent with increasing of the chain length of OME_x [3]. Consequently, previous investigations have shown that the optimal chain length is $x = 3\text{-}4$ [2] or $x = 3\text{-}5$ [5], and as such these OME_x have the potential to be used in existing compression ignition (CI) engines. In this study, the auto-ignition behavior of neat $\text{OME}_{1,2,3,4}$ were investigated. The experimental study contains ignition delay measurements of premixed OME_x /air mixtures in a shock tube and a rapid compression machine. The new experiments for the higher OME_x were carried out at pressures of 10 and 20 bar, at temperatures in the range of 565-1087 K, and under stoichiometric conditions in air. The experimental investigation showed that the derived cetane number (DCN) is not a characteristic number to identify chemical reactivity in general. In addition, the experimental results were compared to the predictions of available published literature models [6-9] in order to investigate the fundamental processes of the oxidation chemistry of OME_x . At engine relevant conditions, the prediction performances of the different literature models for long-chain OME_x vary widely, or do not currently exist, indicating the need for further work on the development of kinetic models for these promising fuels.

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Abstract_S2_All_34

Reaction kinetics studies of unsaturated methyl ester: methyl crotonate

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Abstract

This study examines the effect of unsaturation on the combustion of fatty acid methyl ester (FAME). Methyl crotonate, a biodiesel surrogate fuel with short chain lengths and known physical chemical properties was chosen for this chemical kinetic study. Methyl crotonate oxidation initiated by ozone addition (ozonolysis) was carried out in a jet-stirred reactor to explore the kinetic pathways relevant to low-temperature oxidation. Also, ignition delay experiments were performed in a rapid compression machine (RCM) facility at pressures of 20 and 40 bar under diluted conditions over a temperature range between 870 and 1080 K, and at different equivalence ratios ($\phi = 0.25, 0.5, 0.75$ and 1.0). Furthermore, the obtained experimental data were compared to preliminary modeling results in order to get a deeper insight into the combustion chemistry of methyl crotonate in the intermediate temperature regime.

A new camera-based flame stability measure for non-oscillating and oscillating combustion

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Abstract

With an increasing share of fluctuating wind and solar power in the future energy system, conventional combustion power plants have to enable a high load-flexibility. In addition, a high load-flexibility aiming at the partial substitution of coal with biogenic fuels is desired. Especially in low load conditions, a total shutdown of combustion plants has to be prevented. Instead, in such situations, a stable low load operation should be realized, e.g. by increasing the share of biogenic fuels with a lower calorific value, and thus decreasing the total power. Unfortunately, this low load operation with a high share of biogenic fuels usually leads to a destabilization of the flame, which can (up to a certain degree) be circumvented by online adapting fuel-, air- and swirl settings of the burner system or by using plasma supported burners. A necessary precondition for these adaptations is the availability of a quantitative real-time measurement of the flame stability, e.g. using camera systems. Some approaches for the flame stability measure already exist for continuous, non-oscillating combustion systems based on flame flicker analysis. So far, existing approaches for the flame stability measurement are rather empirical and give no defined value range and interpretation for a stable flame. Thus, they have to be adapted to the specific burner and fuel system. For forced oscillating combustion systems with a pulsed fuel flow rate, aiming at reducing the NO_x -formation, no flame stability measurement systems exist at all. In this paper, we present a new image processing based measurement system for the quantitative online flame stability monitoring for non-oscillating as well as for oscillating (pulsed) low NO_x combustion systems. The new flame stability measure has a clear geometric interpretation and can thus be directly applied to different burner-, fuel- and camera configurations. We demonstrate the new flame stability measure at a 1 MW pilot-scale power plant with co-combustion of torrefied coal with hard coal using cameras in the visible and near-infrared spectral range with a standard framerates of 25 fps.

Image-based analysis of flames in industrial afterburner chambers using geometric constraints

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Abstract

In the industrial sector of chemical and process engineering, many processes require a thermal treatment of emissions in afterburner chambers to reduce atmospheric pollution. Typical afterburner chambers have a circular ground plan and multiple burners evenly arranged on one or more levels. In particular, waste incineration plants apply the burners in afterburner chambers to burn further residues. For this purpose, multi-fuel burners are used which allow the burning of liquid, paste-like or solid fuels. However, varying fuel properties such as calorific value or humidity can lead to unstable flames and hence reduce the efficiency of the overall thermal treatment. Moreover, burner flames can hit and damage the refractory of the opposite wall inside the afterburner chamber, which may cause frequent maintenances. A fast adaption of process parameters in the process control system is necessary to prevent both situations. For this reason, continuous monitoring and characterization of the states of the burner flames are required. In this paper, we present a camera-based approach combined with an image processing system, which calculates various flame characteristics. A near-infrared camera installed at the ceiling of the afterburner chamber with a top-down view, acquires the images. Due to overlapping and turbulent flames a robust image segmentation and an allocation of flame regions to burners is difficult. In the presented approach, geometric prior information about the flames' possible manifestations in the acquired images is used to improve the robustness of the image processing system. Two combined parabolas parameterize each flame, which allows a good approximation of various flame manifestations. The segmentation step incorporates the geometric prior information and the intensity values in the images. Based on the segmented flame regions, flame characteristics can be calculated individually for each burner, including the distance of the flame tip to the refractory. First results of our method are presented based on image data of an industrial afterburner chamber where multiple burners can be activated.

Application of image-based process parameters for analyzing multi-fuel burners

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Abstract

Minimizing energy costs and reducing environmental pollution is a major challenge for plant operators in the energy-intensive industrial sector of combustion processes. An important step in overcoming these challenges especially at cement clinker production in rotary kilns is the substitution of primary fossil fuels, such as coal, with so-called alternative fuels, such as plastic waste or scrap tires. Therefore, multi-fuel burners allow the use of both fuels in adjustable proportions. Due to the varying fuel composition and quality of the alternative fuels, an optimal combustion with a high fraction of alternative fuel can only be ensured by a proper process control that permanently adjusts the burner parameters. For this purpose, a detailed monitoring of the current state of combustion is necessary, which existing measurement systems do not provide. Previous work presented a camera-based measurement system that uses image-based parameters to analyze online the flight and combustion behavior of alternative fuel at multi-fuel burners even under difficult industrial environmental conditions. The implementation of these methods in an industrial prototype and the use of this prototype in 24/7 operation under real process conditions is focus of this paper. The results of a long-term use at an industrial rotary kiln for cement production are presented. Based on the information of the long-term industrial use it is demonstrated how the newly acquired image-based information allows conclusions about the current combustion process. Thus, the developed measurement system provides information about the alternative fuel currently being used at the burner. In this context, a major advantage of the camera-based measurement system compared to the existing systems on cement plants is the rapid availability of the measurement values, which describe the current combustion state. Furthermore, a proposal for a control concept for multi-fuel burners on the basis of the image-based parameters and a model for describing the clinker quality can be developed. The newly developed measuring system and the control concept makes it possible to ensure less variation in combustion conditions, even with high proportions of alternative fuels or highly fluctuating quality of the fuels. Thus, the CO₂ balance and the cement clinker quality can be optimized.

Abstract_S2_AIII_38

In situ LIF and ex situ CRDS applied to NO measurement in flames: probe perturbation and absolute quantification

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Abstract

Flame-sampling experiments allow describing the species profiles as function of the height above the burner. However, the so-measured species profiles are perturbed by the heat losses due to the probe, and/or species losses inside the probe. In order to attempt to clarify the perturbations induced by a microprobe, NO species profiles were obtained in a stoichiometric low-pressure flame by using in situ and ex situ measurements. An unperturbed NO species profiles was measured locally by LIF. Two shapes of microprobes were used to perform ex situ measurements by CRDS after gas probe sampling. The comparison of the profiles shows that the profiles obtained after probe sampling are shifted downstream, and that the absolute mole fraction of NO may be drastically affected during the sampling.

Abstract_S2_AIII_39

MZI measurements on an oxidant-diluted N_2O/CH_4 inverse diffusion flame

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Abstract

Mach-Zehnder interferometer (MZI) was used to capture an instantaneous two-dimensional temperature profile of an inverse diffusion flame (IDF) produced by a triple port burner. The results not only confirmed with the bare-eye observation of the intricate flame structure, which constituted multiple flame fronts but also revealed the non-uniformity of the temperature distribution near the soot region. The flame front transition varied by changing the oxidant/ fuel velocity ratio R from 2 to 5 was observed in the MZI measurements. The results of the temperature measured by MZI system were verified by using a B-type thermocouple at some selected positions.

Abstract_S2_AIII_40

Absolute SiO concentration imaging in low-pressure nanoparticle-synthesis flames via laser-induced fluorescence

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Abstract

In this work we present a strategy for imaging measurements of absolute concentration values of gas-phase SiO in the combustion synthesis of silica, generated from the reaction of hexamethyldisiloxane (HMDSO) precursor in a lean ($\Phi = 0.6$) hydrogen/oxygen/argon flame at a total pressure of 30 mbar. The method is based on laser-induced fluorescence (LIF) exciting the Q(42) rotational transition within the $A^1\Pi-X^1\Sigma(1,0)$ electronic band system of SiO at 231 nm. Corrections for temperature-dependent population of the related ground state are based on multi-line SiO-LIF thermometry. Corrections for local collisional quenching are based on measured effective fluorescence lifetimes from the temporal signal decay using a short camera gate stepped with respect to the laser pulse. This fluorescence lifetime measurement was confirmed with additional measurements using a fast photomultiplier. The resulting semi-quantitative LIF signal was photometrically calibrated using Rayleigh scattering from known gas samples at various pressures and laser energies, as well as with nitric oxide LIF. The obtained absolute SiO concentration values in the HMDSO-doped flames will serve as a stringent test case for recently developed kinetics mechanisms for this class of gas-borne silica nanoparticle synthesis.

Investigation of the time-resolved luminescence spectra of thermographic phosphors for combustion applications

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Abstract

This study characterizes the luminescent properties of the thermographic phosphor particles YAG:Dy,Er as a bulk powder and coated onto a metallic surface, which was studied under increased temperature and pressure conditions in a calibration cell. The phosphor particles were excited by a picosecond Nd:YLF laser at 351 nm, and the time-resolved luminescent signal was recorded using a streak camera. The effects of a temperature variation from room temperature up to 900 K and pressure effects on the luminescence properties were investigated. Additionally, the luminescence properties of the thermographic phosphor BAM:Eu were evaluated.

Abstract_S2_AIII_42

High-speed OH* imaging in a twin piston rapid compression machine

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Abstract

Rapid compression machines (RCMs) are key instruments in studies of fuel oxidation and in the development and improvement of chemical kinetic models. This relevance mandates good quality data, which needs to be obtained in the ideal conditions of homogeneous ignition after the compression stroke. However, there have been some previous reports of inhomogeneous ignition in RCMs. This study examines the combustion processes inside a twin piston RCM using high-speed OH* imaging. A new optical chamber was designed and manufactured for the KAUST RCM which allows complete the visualization of the test section. High-speed camera coupled with a bandpass filter was used to visualize the oxidation of mixtures of ethanol/air, isooctane/air and diethyl ether (DEE)/air at a rate up to 100,000 fps. Preliminary results show the existence of pre-ignition events in ethanol combustion and a tendency of isooctane mixtures for starting ignition close to the surface of the pistons.

The application of Raman crystals as narrowband light sources for shifted vibrational CARS thermometry in sooting flames

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Abstract

Coherent anti-Stokes Raman scattering (CARS), as a laser-based measurement technique is a powerful tool for combustion diagnostics, even in harsh combustion systems (see e.g. [1, 2]). However, for sooting flames well known problems are interferences from C_2 -radical absorption/emission lines at a wavelength of around 473 nm. This is the usual case for N_2 vibrational CARS signal-wavelength when a frequency-doubled Nd:YAG laser is applied. The interaction of the C_2 Swan bands and the vibrational CARS signal leads to significant errors in vibrational CARS thermometry [3]. Different approaches have been proposed in the past to overcome this problem. One option is to use a rather complex dual-pump vibrational CARS setup [3]. Another approach is called shifted vibrational CARS [4]. Both approaches require an additional expensive narrowband dye laser. In this work, we propose a novel method using a Nd:YAG laser-pumped Raman crystal as narrowband light source. Two Raman crystals, a Barium Nitrate ($Ba(NO_3)_2$) and an undoped potassium gadolinium tungstate ($KGd(WO_4)_2$) are investigated in respect of their suitability for their application in a vibrational CARS system for sooting flames. Such Raman crystals have been investigated in the past for several applications [5] even for combustion diagnostics [6]. Nevertheless, this is the first application for CARS thermometry. Temperature measurements were performed in laminar sooting ethylene/air flames established on a McKenna burner. The results were compared to standard vibrational CARS and pure rotational CARS temperature measurements.

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Abstract_S2_AIII_44

Automatic defect detection in a model combustion chamber using support vector machine

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Abstract

A disturbed combustion process in an aircraft engine has an impact on the internal flow and leads to specific irregularities in the species distribution in the exhaust jet. The distribution provides information about the status of the combustion and the measurement of it offers the possibility to reduce the engine down-time during inspection. The approach has the potential to improve the resource management as well as the availability and safety of the system. Aim of the research project is to evaluate the state of an aircraft engine by analyzing the emission field in the exhaust jet and using a support vector machine algorithm for automatic defect recognition. The current work demonstrates the combination of an exhaust gas analyzer and machine learning algorithms in order to recognize the pattern in the exhaust jet automatically. The present paper consists of two parts: In a first step, a generic study on a model combustion chamber will be done. The setup features the flexible variation of the operating point or the alignment of one burner of eight premixed swirl burners to simulate a defect in the combustor. The influence on the distribution and concentration of the species field for different exemplary defects are investigated experimentally. In a second step, the measurement data is used to implement and test a support vector machine for pattern recognition at this given setup. The results demonstrate the potential of the approach and support the feasibility of an automatic defect detection in a combustion chamber of a real aircraft engine.

Femtosecond two-photon laser-induced fluorescence imaging of atomic hydrogen in a laminar methane/air flame stimulated by nanosecond repetitively pulsed discharges

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Abstract

In this work, femtosecond two-photon absorption laser-induced fluorescence (fs-TALIF) 2D-imaging has been used to investigate atomic hydrogen distribution in a plasma assisted combustion (PAC) burner at atmospheric pressure. Nanosecond Repetitively Pulsed (NRP) discharges acting on a laminar methane air flame are shown to affect the atomic hydrogen distribution in the flame. Results are presented in terms of atomic hydrogen fluorescence images and trends of fluorescence signal with forcing condition (voltage and repetition frequency).

Towards non-intrusive diagnostics of ethanol and hydrocarbons formed as intermediates in its flames by Raman scattering

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Abstract

Spontaneous Raman/Rayleigh scattering has been used as a non-intrusive diagnostics to quantify major species concentrations and temperatures for various flame configurations fueled by hydrogen, methane or DME. To allow for the investigation of the thermochemical state in flames of more complex fuels like alcohols the extension of this diagnostic method is required. Ethanol was selected as a first target for this extension for two reasons: First, it makes up for a significant share of the global biofuel market. Second, alcohol flames are in general less prone to the formation of C₂ and polycyclic aromatic hydrocarbons (PAHs) as soot precursors compared for instance to alkanes. Laser induced fluorescences of C₂ and PAHs excited by the laser light of the Raman system do strongly interfere with Raman scattering and would thereby impede quantitative main species concentration measurements. Accordingly, flames with larger mole fractions of C₂ and PAHs are not accessible by Raman scattering. In ethanol flames the number of (partially-oxygenated) hydrocarbon (HC) intermediates with mole fractions within the limits that can be quantified by Raman scattering increases substantially compared to methane flames. The most prominent ones in terms of their mole fraction are the alkane's methane and ethane as well as the aldehyde's formaldehyde and acetaldehyde. Raman scattering is a temperature dependent process. Changes in temperature result in the variation of the spectral shape as well as the Raman cross-section. Accordingly, the temperature dependent Raman response function of each of the main species is required to convert the measured Raman signal into concentrations. For di- and triatomic molecules these response functions are computed based on the transitions up to high ro-vibrational levels using quantum mechanical methods implemented in the RAMSES code [1]. However, such simulation methods are still not available up to flame relevant temperatures for the more complex (partially-oxygenated) hydrocarbon molecules like ethanol and the HC intermediates in ethanol flames. To overcome this limitation, an experimental approach [2] was applied to characterize temperature dependent Raman spectra of various HCs in the C-H stretch and C-H bending wavenumber region based on a CW Raman spectrometer in combination with a novel gas heater system. Highly heated helium (90 vol. %) as a carrier gas was mixed with the respective HC (5 vol. %) to avoid thermal decomposition of the latter near electrical heater elements. The large diffusivity of helium ensures rapid mixing, while at the same time the helium as a single atom species is not Raman active and does therefore not interfere with the Raman signal of the investigated HC. Additionally, nitrogen (5 vol %) was added to

obtain a reference for the HC species since the temperature dependent spectra of N_2 can be computed with a high accuracy. Temperature dependent Raman spectra of the most important HC intermediates for ethanol combustion were measured. A custom designed dual-resolution Raman spectrometer [3], based on a split of the wavenumber range of C-H stretching Raman signal from the wavenumber region of CO_2 , O_2 , CO , N_2 , H_2O and H_2 by an optical element, will be employed to quantify these intermediates. The purpose of this dual-resolution spectrometer is to increase the spectral resolution in the C-H stretching region substantially and thereby allow for a separation and quantification of the spectrally closely spaced Raman spectra of the intermediate HCs.

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Abstract_S2_AIII_47

Investigation of flame propagation enhancement by a ultrashort nanosecond discharge pulse using the advanced laser-based diagnostics

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Abstract

This work aims at investigating the direct impacts of a single-pulse nanosecond (NS) discharge on a lifted methane-air flame. The lifted flat flame is sustained by a McKenna burner together with a round brass stabilizing plate. A diffusive plasma discharge, which is powered by a NS-pulsed high voltage generator with a duration of 3 ns, goes through the lifted flame directly. The temperature profile around the flame front is measured by the planar Rayleigh scattering thermometry. The upstream propagation of flame front is detected after the discharge pulse even though the gas temperature increment due to discharge is less than 30 K. By tracking the trajectory of the flame front, the enhanced propagation speed is determined to be 5 cm/s, which is around 55% of the local flame speed. This flame propagation enhancement is speculated to be a result of the discharge-induced long-lived radicals, besides the thermal effect.

Phantom studies on a new evolutionary reconstruction technique applied to 3D scalar fields in the gas-phase

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Abstract

We present extensive studies on our recently developed evolutionary reconstruction technique (ERT), using a scalar 3-dimensional phantom (exactly known) field. The ERT method has been successfully demonstrated to reconstruct the chemiluminescence intensity field of different flames, including a Bunsen, a highly turbulent swirl and the turbulent Cambridge-Sandia stratified flames. Here we present results for the stratified flames. A direct numerical simulation (DNS) of the Cambridge-Sandia flame (available from the literature) was used as a phantom. We investigated the dependency of the reconstruction quality on the number of cameras, and the effect of noise in the phantom projection data that was obtained using a pin-hole camera model. Furthermore, we implemented a multi-grid reconstruction scheme which produced results very close to the single grid reconstruction. The ERT reconstructions were also compared to those based on the conventional algebraic reconstruction technique (ART).

Alternative soot detection strategies for application in aero-engine test-beds: assessment of the performance and uncertainties of time-integrated LII

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Abstract

The requirement for methods to accurately measure soot volume fraction in challenging environments such as aero-engine exhausts has become increasingly important due to progressively tighter emission standards and regulations. Extractive sampling systems are the current approved methods for measuring exhaust gas and fine particle emissions from various types of aircraft engines under actual operating conditions. Emerging non-intrusive techniques offer alternatives to extractive methods, with some significant advantages. Laser induced incandescence (LII) in open path is one of the methods which can be used to measure soot concentration; it has high sensitivity and is essentially non-intrusive in nature. The demands of industrial test-bed environments necessitate rugged and compact equipment for use in engine exhaust measurements. For a measurement system to be widely used, it should also be relatively low cost. These factors have led to the consideration of non-intensified cameras for LII signal collection. The consequence is that signal collection is not 'prompt' but is instead temporally integrated. Modelling of LII signals has been performed to assess the applicability and uncertainty in measuring soot volume fraction in this time-integrated mode. Specifically, simulation allows us to quantify the sensitivity of the measurement to variation in physical properties such as primary particle size, over a range of laser fluences. Since fluence varies radially across the beam, as well as axially as it propagates through the plume, these models are essential to LII signal interpretation. We discuss the implications of our results for optimisation and calibration of soot imaging in exhaust streams.

Abstract_S2_AIII_50

A novel approach to high-speed 1D Raman-scattering for combustion dynamics

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Abstract

A novel approach to extend 1D Raman scattering to sampling rates up to 10 kHz, with precision and accuracy comparable to conventional 5 Hz system is here presented. The new instruments features a 10 kHz optical shutter to suppress flame luminosity, and a system of dichroic mirrors and bandpass filters to spectrally separate the Raman signal of up to seven species. Seven EMCCD cameras, operated in kinetic mode are used for signal acquisition. Design of the system, and preliminary results are here presented.

Characterization of UV endoscopic imaging systems for combustion applications

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Abstract

Compared to internal combustion engines with large optical access, endoscopic optical diagnostics offer the advantage of retaining the full operating range and thermal properties of the production engine. However, most endoscopes are only transparent in visible range. In previous work, a two-component UV-transparent modular endoscope system had been developed. The relay stage incorporates a diffractive optical element (DOE), which provides a large aperture but is expensive and has a narrow operating wavelength range. Here, to make this endoscopic imaging system more universally usable, the relay-stage DOE was replaced by commercial UV camera lenses often available in combustion laboratories. Several combinations were compared in terms of resolution, brightness, and chromatic aberration. A back-lit knife-edge target was used and the modulation transfer function (MTF) was determined via the slanted-edge method as specified in ISO 12233. MTF was determined at various wavelengths in UV from 280 to 385 nm. The value of MTF₅₀ (the spatial frequency at 50% MTF) was used as a metric for a quantitative comparison of resolution. Endoscope systems using a Cerco 45 mm f/1.8 UV lens or a LaVision 85 mm f/2.8 UV lens for the relay had better resolution and limited the chromatic aberration over larger wavelength range. Systems with the DOE had lower resolution and a narrower useful wavelength range, but –similarly to the 45/1.8 lens system– were approximately three times brighter than those with the 85/2.8 lens. The addition of UV achromats as “close-up lenses” (common practice in visible-light macro photography) did not improve system performance. Finally, a selection of the imaging systems investigated on the optical bench were used in a near-production endoscopic spark-ignition engine. OH* chemiluminescence were imaged to benchmark performance in realistic application examples.

Rayleigh temperature measurements in a non-premixed, swirl stabilized burner with iCCD and sCMOS camera systems

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Abstract

This study investigates the suitability of two different camera systems – a conventional intensified CCD system (iCCD) and a recent non-intensified scientific CMOS system (sCMOS) – for quantitative Rayleigh thermometry. The test object is a novel non-premixed lean methane/air swirl burner. Despite their different advantages and disadvantages, their results coincide within the uncertainties. The derived maximum temperatures in the recirculation zone of the burner are of the order of 2000 ± 100 K for global equivalence ratios from 0.3 up to 1.0.

Abstract_S2_AIII_53

Lagrangian approach to GCH₄/LOX axisymmetric spray combustion of movable pintle injector

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Abstract

Axisymmetric spray combustion of the movable pintle injector is simulated using the Lagrangian approach. Since, the pintle injector has a movable pintle rod, which can easily change the movement of propellant and cause the combustion characteristics. Therefore, two cases with two different pintle opening are considered to perform at the subcritical condition. In the 2D-simulation model, the liquid oxygen as a thin hollow sheet is from the center gap and broken by the gaseous methane from annular gap. Finally, the spray combustion is modeled using Lagrangian approach by the assumption and theoretical expressions from literature to calculate the initial droplet size for liquid oxygen.

Analysis of LIF and Mie signals from single micrometric droplets for instantaneous droplet sizing in gasoline sprays

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Abstract

The paper investigates the suitability of the tracer nilered for LIF/Mie droplet sizing (LIF-laser-induced fluorescence) for the gasoline surrogate fuel Toliso (which consists of 65 vol% isooctane, 35 vol% toluene). The investigations were split into two parts. The temperature dependence of the spectral fluorescence of nilered was investigated in a test cell. The measurements showed an almost negligible temperature sensitivity at moderate temperatures. Afterwards, the individual microscopic LIF and Mie scattering signals of monodisperse droplets generated by a droplet generator were investigated and a calibration curve was determined. The droplet investigations showed an almost linear dependence of the intensity ratio on the droplet diameter.

Abstract_S2_AIII_55

VOF method: numerical analysis of single droplets impinging upon liquid films

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Abstract

Numerical simulations of the vertical impact of a single droplet upon a liquid surface are performed. The numerical model consists of solving the Navier-Stokes equations using the explicit VOF method for a 2D axisymmetric assumption. The results are compared with available experimental data regarding the initial impact and crown expansion. Three different phenomena were simulated: crown splash, jetting and bubbling. The first two outcomes are in good agreement with the experimental results, whereas bubbling requires more research to understand the crown development and bubble formation, as the current model is not capable of accurately predicting its progress.

Experimental study of a droplet impact on oblique dry surface

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Abstract

The aeronautical sector significantly contributes to greenhouse gas emissions. It is essential to introduce biofuels in the fuel mixture of aircraft engines with the purpose of reducing the negative impact on the environment. The main goal of this study is to compare the dynamic behavior of a droplet impinging onto a sloped surface and a droplet impinging onto a surface with the influence of crossflow. Four different fluids were used: H₂O, 100% Jet A-1 and 75%/25% and 50%/50% of Jet A-1 and HVO, respectively. Through this study, only the mixtures presented similar phenomena for both oblique impacts. The results show that the gravity and the variation of the incident angle promotes an asymmetric splash.

Abstract_S2_AIII_57

Numerical simulation of sulfur combustors with high-power-density

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Abstract

Highly-resolved numerical simulations have been carried out to assess a preliminary burner design for combustion of liquid sulfur. The computational method resolves adequately prevailing physical-chemical processes such as turbulent flow, spray dispersion, evaporation, ignition of the fuel-air mixture and flame stabilization, yielding a detailed insight into the complex phenomena of combustion of sulfur. Calculations of two nozzle configurations with different swirl intensities (SI) have been conducted, reproducing appropriately the main characteristics for the spray distribution and flame stabilization behaviors observed in previous experiments using similar nozzle designs. An intensive inner recirculation zone was observed for the nozzle configuration with a higher SI of the airflow, which leads to a strong radial spray dispersion and a compact flame attached to the burner nozzle. However, sulfur droplets hitting the wall of the combustion chamber have been detected, leading to incomplete combustion of sulfur. Compared with the high SI configuration, the burner concept with a smaller SI leads to a narrower spray cone angle and a longer flame lifted from the burner with only a negligible small amount of droplets hitting the wall.

SpraySyn – standard burner for the collaborative investigation of spray-flame synthesis of nanoparticles: droplet velocity and size of the non-reactive ethanol spray

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Abstract

In many scientific communities, the definition of standardized experiments has enabled major progress in process understanding. The investigation of the spray-flame synthesis of nanoparticles at a well-defined standard burner by experiment and simulation makes it possible to produce a comprehensive data set with various established and novel measuring methods. In this work, we briefly introduce the design of the SpraySyn burner as a new standard that offers well-defined and simulation-friendly boundary conditions and geometries as well as accessibility for optical diagnostics. To verify correct burner operation, we characterized the ethanol spray flame according to the unified procedure proposed in the SpraySyn concept. Subsequently, the non-reactive ethanol spray is investigated by LDA/PDA measurements finding axial droplet velocities in the range of 83 m/s and droplet sizes around 14 μm . Thus, this study offers a first step towards a comprehensive characterization of the two-fluid nozzle of the SpraySyn burner.

Abstract_S2_AIII_59

Liquid fuel MILD combustion with two stage combustion structure in a closed combustion chamber

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Abstract

The MILD combustion has been considered as one of the promising combustion technology for high thermal efficiency and reducing nitrogen oxides and carbon dioxide emissions. Recently, many studies have revealed the potential of MILD combustion in various power systems but most studies have been focused on gas phase fuel MILD combustion. Therefore further study on MILD combustion using liquid fuel is needed for some applications like liquid fueled gas turbine especially. In this work, a possibility of formation of the liquid fuel MILD combustion was investigated under the low oxygen concentration and the temperature above auto-ignition temperature in a closed combustion chamber like real combustion system. A series of numerical simulations using Ansys fluent 19.2 have been carried out in order to investigate the details of the flow field in the closed combustion chamber and the spray patterns on the formation of MILD combustion. Also, the experimental study has been carried out to validate the numerical simulation results. A two-stage combustion structure similar to 'Deft jet in hot co-flow' configuration was designed to study the formation of liquid fuel MILD combustion. The operating conditions were fixed at heat intensity of 1.28 MW/m³atm and various global equivalence ratio changed by the first stage burner condition. The experimental results represent that the length of the flame became shorter and the pale blue flame like MILD reaction region was formed in the case of the burnt gas velocity of 45.5 m/s and 65 m/s, respectively. In the combustion chamber, even the wall temperature approached to 1150 K, the NO_x emission showed still low emission of less than 10 ppm. The numerical results show that the high temperature region was decreased and the flame temperature was uniformly distributed due to the high velocity of ejected diluted burnt gas from the velocity control nozzle, which can be confirmed from experimental results as well. It was also found that the maximum temperature in the main reaction zone became lower than 1700 K and the average temperature was lower than 1600 K such that thermal NO formation was suppressed.

Numerical modeling of the secondary droplet break-up in spray flows

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Abstract

The break-up and evaporation of liquid jets is crucial to the efficiency of the combustion process in direct injection engines. Despite its importance, no final consensus concerning the mathematical framework to compute sprays has been reached yet. In the current study we perform simulations of n-dodecane jets with three different models and make comparisons of their predictive capacities. These are the Taylor Analogy Breakup, Reitz-Diwakar and Pilch Erdman models. The values of the model parameters that we use for our simulations are those typically used in the studies of fuel injection in diesel engines. The numerical setup is based on the Engine Combustion Network "Spray A" operating conditions. Due to the high Reynolds numbers of the flow, the motion of the surrounding air is treated numerically via Large Eddy Simulations (LES), whereas the motion of the droplets is tracked in the Lagrangian framework, assuming two-way coupling between the two phases.

Abstract_S2_AIII_61

Analysis of multiphase MMC coupling using DNS of a reacting double shear layer

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Abstract

A sparse particle implementation of the multiple mapping conditioning / large-eddy simulation (MMC-LES) model for two-phase flows is compared against carrier-phase direct numerical simulation (CP-DNS) of a droplet-laden temporally evolving double shear layer with combustion. A consistent multiphase MMC-LES model for turbulent spray combustion has already been formulated by Khan et al. (2018 CNF). Here we extend this work by conducting a detailed analysis and validation of the coupling between the stochastic particles representing the gas phase and the liquid fuel droplets. We do not perform a separate LES for our model analysis but calculate LES-filtered values that are required as inputs to the MMC-LES model by explicitly post-filtering the DNS results. This allows us to isolate the specific modeling issues that are under investigation here from other modeling errors associated with LES-type closures of the flow and mixing fields. In addition, the DNS provides validation data for the MMC solution. In contrast to dense particle methods, the correct coupling between the stochastic particles and the liquid phase is more challenging in a sparse particle method, due to the added difficulty of finding a suitable partner for heat and mass transfer when only a small number of stochastic particles is present. Here the mass and energy transfer from the droplets to the stochastic particles is realized by a one-by-one coupling, where each droplet is paired with a single stochastic particle. In analogy to the pure gas-phase MMC mixing model we apply a minimization of the effective square distance between the droplets and the stochastic particles, which is the weighted sum of squared distances in physical and reference space. The introduction of a reference space enables a conditioning of the particle selection, where the weighting factor is used to control the strength of conditioning. This weighting factor is a parameter that is still unknown and its detailed investigation is focus of this study. Once a droplet is assigned to a stochastic particle, the evaporation is calculated based on the properties of the stochastic particle, and heat and mass are returned to the stochastic particle via source terms. Our simulations show a good agreement between the MMC model and the CP-DNS. We find that a conditioning in reference space is not necessary, and that a conditioning in pure reference space leads to discrepancies to the CP-DNS. We also point out that MMC compensates potential problems with small cell sizes and high evaporation rates related to CP-DNS and better represents the infinity condition required for the evaporation model. Finally it is shown that variance increase due to evaporation is implicitly taken into account in the multiphase MMC-LES model.

Abstract_S2_AIII_62

Quantifying the effect of the turbulence and break-up modelling for spray simulations through a dimensionless number analysis

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Abstract

A comparison between the standard k-epsilon model (RANS) and the dynamic k-equation (LES) has been made using the Eulerian-Lagrangian approach in order to simulate the spray injection, for ECN spray A, in inert condition. Here they're outlined the difference between the two turbulence models, depending on the grid sizes and the break-up sub-model parameters, comparing the results with the experimental data. A dimensionless analysis based on the droplets Stokes number have been carried out in order to get a physical characterization of the coupling between the grid and the spray, depending on the turbulence model. Results' discrepancies between the two numerical approaches are due to dynamic viscosity characteristic. The droplets Reynolds and Weber number have been measured too, providing useful information for modeling strategies.

Abstract_S2_AIII_63

Investigation of the sulfur dioxide absorption in water droplets

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Abstract

Flue gas desulfurization in spray towers is an efficient sulfur dioxide removal method for the combustion flue gases. It is based on the absorption mechanism of sulfur dioxide in droplets falling in the stream of flue gases, removing the pollutants due to concentration differences. To describe all the relevant phenomena, a lumped-parameter absorption model for the falling pure water droplet has been implemented. The main factors limiting the absorption are the mass transfer of pollutants through the gas-droplet interface and the aqueous phase chemistry in droplet. Mass transfer coefficient modeling is the most significant parameter regulating the absorption dynamic into the droplet, while the in-droplet chemistry regulates the maximum quantity of dissolved pollutants. The implemented model was used on the single droplet and compared with the available literature data. With the stricter legislation regulating the allowed emissions for marine and stationary applications, the model can be used for prediction of sulfur dioxide uptake on a single droplet scale, and as a basis for further development of the more complex sulfur dioxide absorption models.

A direct numerical simulation analysis of turbulent V-flames propagating into droplet-laden mixtures with an overall equivalence ratio of unity

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Abstract

Combustion in droplet-laden mixtures has applications in automotive engines and gas turbines and can potentially play important roles in the case of explosions. Combustion of droplet-laden mixtures depends on the complex interactions between flame, flow field and liquid fuel droplets. Thus, a detailed understanding of combustion of droplet-laden mixtures remains a challenging task considering its wide range of applications. In this study, flame propagation into droplet-laden mixtures in a rod-stabilised V-flame configuration has been investigated using three-dimensional Direct Numerical Simulations (DNS) with a modified single-step Arrhenius chemistry. The simulations have been performed for different initially mono-sized droplet diameters a_d (i.e. $a_d/\delta_{th} = 0.04, 0.05$ and 0.06 where δ_{th} is the thermal flame thickness of the laminar stoichiometric premixed flame) for an overall (liquid+gaseous) equivalence ratio of unity. The V-flame is subjected to a moderate level of inlet turbulence (i.e. $u'/S_{b,st} = 2.0$), with a mean inlet velocity of $u_{mean}/S_{b,st} = 5.0$. The flame holder is placed at approximately $10\delta_{th}$ from the inlet plane and the computational domain is taken to be a cube of $(30\delta_{th})^3$. The radius of the flame holder is $0.3\delta_{th}$ and flame statistics are obtained at three different axial distances from the flame holder (e.g. $9\delta_{th}$, $13\delta_{th}$ and $17\delta_{th}$). It has been found that combustion mainly takes place under fuel-lean mode and the probability of finding fuel-lean burning increases with increasing droplet diameter. However, the distribution of gaseous equivalence ratio within the flame has been found to exhibit smaller likelihood of obtaining fuel-lean mixtures with increasing axial distance from the flame holder. The presence of droplets has been found to give rise to dimples on the reaction progress variable isosurface, but the effects of droplet-induced flame wrinkling on curvature distributions are masked by the turbulent flow field. The heat release has been found to arise mainly from premixed-mode of combustion. Detailed analysis of reaction progress variable transport has been used to explain the mean variations of consumption speed and density-weighted displacement speed with the axial distance from the flame holder. The mean values of both consumption speed and density-weighted displacement speed have been found to decrease with increasing droplet diameter. Detailed physical explanations have been provided for the observed behaviour.

Abstract_S2_AIII_65

The effect of atomizing media on the flame characteristics

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Abstract

The impact of different atomizing media on the combustion of liquid fuels is tested in this article. As atomizing media the compressed air and the superheated steam were chosen. The tests were performed in the horizontal water-cooled combustion chamber. The Methyl-ester of rapeseed oil was chosen for tests. The atomization of liquid fuel was realized using the effervescent atomizer. The gas-to-liquid (GLR) ratio was held at 15, 20 and 25 %. The observed characteristics were the inflame temperature, NO_x and CO emissions, heat transfer and the quality and the stability of the combustion. The results revealed the atomizing media has a significant effect on combustion characteristics. The combustion using the compressed air showed higher heat transfer for about 6 % and higher NO_x emission for about 13 % (compared to atomization using superheated steam). The effect of atomizing media on inflame temperature was likewise substantial.

Droplets autoignition simulations of ethanol mixtures with a reduced kinetic mechanism

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Abstract

Droplet ignition and combustion is a very relevant problem in combustion applications. Many studies have been conducted in the past, both theoretical [1, 2] and experimental [3, 4]. In view of the increasing use of biofuels, either as pure fuels or mixed with hydrocarbons, accurate modelling of vaporization and chemistry of such fuels is needed in order to optimize the systems to be used with biofuels and thus, facilitate their introduction. Ethanol is, by large, the most used biofuel, because it is easy to produce and because it is adequate to be used with present-day systems, considering both engine technology and fuel storage aspects. In typical combustion applications involving liquid fuels, the fuel is injected, in the form of a spray, in the combustion chamber, where the prevailing conditions include recirculated exhaust gases at high temperatures. In these conditions, heat transfer from the produces fuel vaporization and a fuel mixture evolves in the gas phase until either ignition is forced or autoignition is achieved. In this work we will focus on the vaporization and autoignition of a single multi-component droplet in realistic high temperature ambient conditions, in the absence of microgravity. With the aim of obtaining realistic autoignition times, accurate submodels for the different inter-coupled physical phenomena are required. Especial attention is given to the chemistry, where a multipurpose 14-steps chemical model, previously developed [5] is used, while adequate models are used for molecular transport, thermodynamics and phase change. Numerical results are obtained using an unsteady finite volume discretization. Effects of droplet size, ambient temperature and humidity content -both in the ambient and in the liquid fuel- on autoignition times are analyzed.

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Abstract_S2_AIII_67

Uncertainty of droplet evaporation measurements and its effect on model validation

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Abstract

Measurement of droplet evaporation is challenging since the average practical droplet size is too small, thus single droplets with a larger diameter are usually investigated. However, measurement data often bears notable uncertainty or bias, encumbering model validation. Therefore, typical conditions of evaporation measurements are evaluated by numerical modeling, and the results are compared to experimental data of n-heptane droplets. Vaporization rate of millimeter-scale droplets is considerably enhanced at high temperature due to thermal radiation. Heat balance of droplet is dominated by convective heat transfer at the early, and heat conduction through the suspension fiber in the late vaporization period. However, fiber conduction has no significant impact on vaporization below a certain fiber-to-droplet initial diameter ratio.

Abstract_S2_AIII_68

Temporal and spectral correlation of acoustic and chemiluminescent signal of a liquid-fueled turbulent swirl burner

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Abstract

Real-time diagnostics and control of modern combustion chambers are required in order to fulfill pollutant emission standards and ensure high-efficiency operation. If the acoustic disturbances are in phase with heat release disturbances, the resulting fluctuation will have positive feedback and lead to combustion failure or structural damage. Presently, combustion in a 15 kW liquid fueled burner was analyzed by using a microphone and a photomultiplier tube. The synchronously acquired data were evaluated by two spectral techniques, Fast Fourier Transform, and Continuous Wavelet Transform. Finally, the temporal signal is analyzed by correlation functions at several window sizes. The comparison of the spectral data of the two sensors showed no correlation, unlike the temporal data.

Abstract_S2_AIII_69

Determination of the minimal acoustic signal length for fast-acting control of a liquid-fueled turbulent swirl burner by Wavelet and Fourier transform

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Abstract

The acoustical signal of combustion noise is often analyzed spectrally by Fourier or Wavelet transform. The present paper focused on the measurement data of a 15 kW diesel oil-fueled swirl burner at various combustion air flow rates and atomizing air pressures, evaluating straight, transitory, and V-shaped flames. It was concluded that the smallest applicable window size is 64 samples which enables the statistical characterization of the combustion noise. Probability density functions were fitted to the spectrally filtered to analyze stable operating points. In addition, a scale parameter filtering performed to evaluate the representativeness of the data gathered by using different window sizes.

High-fidelity simulations and experiments of oxymethylene ether spray ignition

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Abstract

Today and in the foreseeable future, internal combustion engines burning liquid fuels will provide a large fraction of transportation energy. With a quickly growing share of electrical power from renewable sources, “Power-to-X” technologies, such as producing tailor-made CO₂-neutral liquid fuels using renewable energy, are a promising way to both improve utilization of volatile green power and drive the decarbonization of the transport sector. One possible synthetic fuel group is that of oxymethylene ethers (OME_x) with short chain length, i.e. CH₃O(CH₂O)_xCH₃ with 1<x<5, which can substitute fossil fuel in diesel engines. Due to the lack of carbon-carbon bonds, formation of soot during the combustion of these oxygenated fuels is suppressed. Thus, the soot/NO_x tradeoff of classical diesel engines is eliminated and exhaust gas recirculation can be raised significantly, also leading to a sizeable reduction in NO_x-emissions. Especially OME_x of short chain length have, however, significantly different fuel properties such as higher vapor pressure, lower viscosity, and lower cetane number compared to conventional diesel fuel. As these properties are known to have considerable impact on injection and ignition behavior, predictive and affordable simulations of spray injection and combustion are required to optimize existing engines with respect to engine design and control for OME_x fuels. Within this work, real liquid fuel properties and newly developed chemical reaction mechanisms are combined in high-fidelity large-eddy simulations (LES) of spray injection and combustion of OME_x under engine-relevant conditions. Simulation results are presented for both OME₁ and OME₄, as well as *n*-dodecane as a reference fuel. Global mixing and combustion quantities, such as spray penetration, ignition delay time, and flame lift-off length, as well as instantaneous flow fields are compared with experimental results obtained in a high-pressure spray chamber and acceptable agreement is found. Similarities and differences in mixing and ignition behavior between OME_x of different chain lengths and *n*-dodecane representing conventional diesel fuel are analyzed. Discrepancies between fuel cetane numbers and homogeneous chemical ignition delay times are discussed and attributed to significantly higher stoichiometric mixture fractions for the oxygenated OME_x fuels compared to conventional alkanes such as *n*-dodecane.

Abstract_S2_R1_71

The influence of film cooling flow over turbine blades from different shaped holes

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Abstract

The influence of different shaped holes on the film cooling performance of gas turbine blades was numerically investigated. The hot stream of exhaust gasses from the combustion chamber enters the turbine section of gas turbine engines at high velocity and temperature. The combustion efficiency highly depends on the temperature, but currently used turbine blades materials are not capable to withstand such conditions, therefore utilising the film cooling system is necessary. In this work, CFD simulations were performed to describe the interaction between the hot stream gas from the combustion chamber and the coolant jet from a shaped hole. The computational domain consisted of a hot gas channel and a cooling shaped hole. The validation case with the cylindrical hole was compared to the experimental results and results from LES simulations available in the literature. Temperature distributions were analysed and compared to the case with a cylindrical hole to investigate the influence of different shaped holes on cooling performance. The results showed the possibility of improving the film cooling performance through different design of cooling holes which allows the increase of the temperature in the combustion chamber, and consequently overall combustion efficiency.

How far can we go? Stability limit assessment of micro gas turbine combustion in diluted condition using LES.

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Abstract

To fully satisfy the needs of future small-scale electricity production, the mGT has to become more operational and fuel flexible and in addition, carbon clean. Applying advanced mGT cycle modifications, such as humidification and Exhaust Gas Recirculation (EGR), offers a solution. However, the advanced mGT cycle development is still limited by the rather small operating range of the mGT combustion chamber. To improve the mGT performance further, stable and complete combustion also has to be achieved under unconventional, CO₂ and water diluted conditions. In this framework, a comparison between four different water and CO₂ diluted cases of the natural gas combustion process in a generic mGT combustion chamber using Large Eddy Simulations (LES), is established. Results show that water dilution leads to lower combustion temperatures while a lower and delayed reactivity is observed with CO₂ dilution, leading to a reduced combustion efficiency and increased CO emissions.

Abstract_S2_R1_73

Detection of high-frequency thermoacoustic combustion oscillations in a model rocket combustor

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Abstract

We numerically investigate the transition and the subsequent well-developed high-frequency combustion oscillations in a model rocket combustor from a viewpoint of information theory. The directionality index is useful for capturing the onset of high-frequency combustion oscillations, allowing us to reveal the directional dependency between pressure and heat release rate fluctuations.

Abstract_S2_R1_74

Early detection and prevention of blowout in a laboratory-scale gas-turbine model combustor using complex networks

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Abstract

We experimentally conduct an early detection and prevention of blowout in a swirl-stabilized-type combustor using time series analysis based on complex networks. We use the ordinal partition transition networks (OPTN) constructing from both pressure and OH* chemiluminescence emission intensity fluctuations. The probability of the dominant patterns in OPTN has potential use for detecting the onset of blowout.

Abstract_S2_R1_75

Quantifying acoustic damping in a multi-injector annular combustor

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Abstract

The present study is concerned with the evaluation of acoustic damping rate in a model scale annular combustor (MICCA-Spray). The operating point under consideration features thermoacoustic oscillations coupled by a longitudinal acoustic mode. The acoustic damping is estimated using two methods from simultaneous chemiluminescence and pressure records. As the oscillation is in a stochastic limit cycle with a mean amplitude and random fluctuations, an acoustic energy balance is employed, and the damping is deduced by noting that the system is in equilibrium. A second method relies on system identification of the acoustic transfer function. Both methods are in good agreement.

Emission estimation for lean premixed methane - air flame at high pressure

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Abstract

The main motivation of current study is to investigate detailed NO_x and CO formation in lean premixed methane-air flame at high pressure using CFD-CRN hybrid method. Three-dimensional steady RANS CFD simulations for high-pressure dump combustor are performed for three premixed lean methane-air mixture equivalence ratios, $\phi=0.43$, 0.50 and 0.55 in Simcenter STAR-CCM+ V 13.06. The Flamelet generated manifold (FGM) model is used for combustion modelling. The chemical reactor network from CFD data is modelled and solved in recently developed reactor network capabilities in Simcenter STAR-CCM+ V 14.02. In this study, the method for CRN generation in Simcenter STAR-CCM+, is briefly discussed and used to validate the emission formation at the exit of combustor. The NO_x prediction from hybrid CFD-CRN tool closely matches with experiments. However, exit CO trends are different in CFD as well as CFD-CRN from experiments. In the later section, detailed NO_x formation pathway study inside the combustor is performed for all the equivalence ratios test case. It is found that two pathways thermal NO_x and N₂O intermediate contributes significantly in the above lean conditions, with the thermal NO_x pathway contribution is more for $\phi=0.55$ and N₂O intermediate pathway contribution is more for $\phi=0.43$.

Abstract_S2_R1_77

LES-pdf of combustion dynamics in a partially premixed swirl combustor

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Abstract

The dynamic behaviour of the partially premixed, swirl-stabilised PRECCINSTA gas turbine model combustor is studied using a fully compressible large eddy simulation solver with a 15-step and 19 species reduced methane mechanism. The solver applies a transported sub-grid probability density function approach solved by the Eulerian stochastic fields method to allow for a burning regime independent description of turbulent flames. A specific operating condition prone to self-excited thermo-acoustic and hydrodynamic instabilities is targeted to evaluate the predictive capabilities of the computational method. Excellent agreement with experimental data is obtained for the predicted thermo-acoustic mode representing a pronounced limit-cycle oscillation at the correct frequency and amplitude. Moreover, the periodic formation and suppression of a precessing vortex core is identified as well as periodic shedding of toroidal vortices at the burner nozzle rim. Both phenomena are shown to be directly coupled to the dominant thermo-acoustic mode and their respective interaction with the flame is investigated in further detail.

A tabulated chemistry method for the LES of diluted, non-adiabatic, premixed flames including auto ignition

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Abstract

The chemistry tabulation for a non-adiabatic premixed flamelet generated manifold (PFGM) combustion model is extended to diluted configurations, where reactants are mixed with recirculating hot products, promoting auto ignition events. For the generation of the chemistry tables, Cantera is used applying GRI-Mech 3.0. Heat losses are accounted for using burner-stabilized flames. A mixing parameter ζ is introduced to determine the mixing state between pure fresh gas ($\zeta = 0$) and burnt products ($\zeta = 1$). The flame stabilization mechanism of a mixture composed of fresh and burnt gases is not unique. Multiple flame solutions are generated following the approach of Schulz et al. (Combust. Flame, 2018), where auto ignition in 1D flames is induced by varying the length of the computational domain. Consequently, different states can exist for one single mixture ranging from flame propagation to auto ignition. To distinguish between the different flame solutions, the scalar dissipation rate of the normalized combustion progress variable is used in a first attempt.

Abstract_S2_R1_79

Suppression of instabilities of swirled premixed flames with minimal secondary hydrogen injection

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Abstract

In this experimental study, the effect of an additional axial jet of hydrogen injected near the exit plane of a swirled injector on the flame dynamics of a methane-air premixed flame is explored. Keeping the air flow rate and thermal power constant, it is shown that even for very small flow rates of hydrogen of the order of one percent of the main fuel flow rate, flames become shorter and their stabilization more robust. The dynamic stability of the combustor is studied and it is shown that hydrogen injection also changes the flame response to flow perturbations, reducing its susceptibility to thermo-acoustic instabilities for a wide range of operating conditions. This proves that minor hydrogen injection may be used as an efficient passive control system to mitigate combustion instabilities.

Abstract_S2_R1_80

Large-eddy simulation of flame dynamics during the ignition of a swirling injector unit and comparison with experiments

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Abstract

During the ignition of a swirled single-injector combustor, two stages are observed experimentally which may be of importance in the design of gas turbines: (1) Penetration of the injection unit and (2) Lift-off and stabilization downstream of the injector after a substantial delay. These dynamics are investigated using LES based on an Eulerian description of the liquid spray in combination with the TFLES combustion model. The injector mass flow rate decreases rapidly in response to the positive pressure excursion associated with the burnt gas expansion (1), whereas the heat transfer of recirculating burnt gases in the vicinity of the injector exhaust section (2) is linked to the flame lift-off.

Effects of mixture stratification on thermo-acoustic instabilities in a dual-swirl gas turbine model combustor

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Abstract

Modern gas turbine (GT) combustors are typically operated in the lean-premixed regime. However, in order to avoid flashback, the premixing section in such combustors is often short, leading to imperfect premixing (or mixture stratification) of the fuel/air mixture entering the combustion chamber, which is often termed as “technical premixing”. The goal of the current study is to assess the influence of the stratification level on flame stabilization and thermo-acoustic instabilities in a technically relevant geometry. Therefore, an optically accessible GT dual-swirl model combustor was operated at atmospheric pressure and studied using optical and laser-based measurement techniques. The gas streams to each swirler could be controlled individually and were supplied with premixed methane/air mixtures at different equivalence ratios. The global thermal power and global equivalence ratio were kept constant at $P_{th} = 25$ kW and $\phi = 0.75$, respectively. The equivalence ratios of the two gas streams were varied, thus resulting in three flames with different stratification levels $S = 1$, $S = 1.38$ and $S = 1.67$ (defined as the ratio of the equivalence ratios in the inner and outer swirler). Acoustic oscillations in the combustion chamber and in the two plenum chambers were measured using calibrated microphone probes. One intensified high speed CMOS camera was used to image both flame shape and heat release oscillations via OH* chemiluminescence (CL) and as well as the reaction zone via OH planar laser-induced fluorescence (PLIF) at a frame rate of 10 kHz. This was achieved by running the camera at 20 kHz and alternating short (300 ns) and long (15 μ s) intensifier gates. The short intensifier gates were temporally overlapped with the laser pulses (10 kHz pulse repetition rate) and the long intensifier gates were temporally placed in between two consecutive laser pulses. Consequently, every other camera frames correspond to OH PLIF and OH* CL, respectively, resulting in a perfect, calibration-free spatial overlap between OH* CL and OH PLIF. Additionally, the experimental cost and complexity is reduced. The flow field was simultaneously measured using high speed stereoscopic particle image velocimetry (PIV) at a frame rate of 10 kHz. All three flames featured a V-shape and were lifted from the nozzle, the integrated OH* CL intensity was similar for all flames. The stratification level had only a slight influence on the overall flame shape and the flame lift-off height. The flow field showed slight differences in the velocity magnitudes in the inflow and within the recirculation zone. All flames showed a strong acoustic mode at approximately 700 Hz as well as several other modes with smaller amplitude. Here, the stratification level showed a clear influence on the thermo-acoustic properties of the flames.

Systematic CFD-CRN study of exit NO_x emission in a methane/air diffusion flame

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Abstract

Hybrid CFD- chemical reactor network (CRN) methods have been extensively used in the literature to predict emissions for combustion systems. In this approach, CFD is used to characterize a flow-field, and then detailed chemistry is modelled using a CRN to calculate emissions accurately. Although some algorithms have been developed for systematic construction of CRNs using CFD, the focus of studies is on user expertise to adjust important factors in CRN modelling for practical applications. The algorithms are still under development, and there is no universal approach to generate CRNs from CFD systematically. Most available algorithms are suitable for a single analysis only, and hundreds or thousands of reactors are required to calculate emissions, which cannot be fitted for probabilistic modelling and uncertainty quantification (UQ) studies. Therefore, the goal of this study is (1) to develop a method for systematic construction of CRN from a CFD database and (2) to propose an integrated framework in Python to implement the method and run the CRN for calculation of exit NO_x emission in a benchmark flame. The developed framework is a computationally-efficient approach that can be used in a UQ study. The method is implemented on a RANS CFD database for Sandia flame D as the benchmark case. A set of homogeneous zones is constructed for the CFD database in Python using K-means clustering method. A CRN consisting of several perfectly stirred reactors (PSRs) is then mapped on the zones and solved by Cantera to calculate exit NO_x emission. The results show reasonable performance for the developed method as a computationally-efficient approach to predict exit NO_x emission. Future work will see the implementation of the method for a practical combustion system and integration with a UQ study as well.

Abstract_S2_R1_83

Analysis of ignition processes at combustors for aero engines at high altitude conditions

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Abstract

The ability to re-ignite at high altitude after a flame out event is critical for flight safety. For this research work a rectangular, one sector combustion chamber was utilized for experimental investigations at high altitude conditions. The investigation focuses on the characterization of the ignition process, in terms of probability, minimum fuel to air ratio and ignition timing for a successful ignition event. In addition, the flame kernel generation and propagation has been analyzed by high speed imaging recording. Results show that pressure is the dominant parameter, which affects the ignition process. Moreover, numerical simulations were performed to better understand the prediction capabilities of the employed computational tool. The comparison against experiments was carried out in terms of propagation of the flame kernel and minimum fuel to air ratio.

Abstract_S2_R1_84

The effects of compressibility on the response of a flame to acoustic forcing

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Abstract

This paper demonstrates that compressible simulations must be used to accurately capture the effects of acoustic forcing on realistic fuel injector geometries for gas turbines. Several important interactions between the acoustic and flow fields are shown using a compressible CFD methodology which cannot be reproduced with an incompressible method using bulk mass flow forcing. A new novel method for reproducing these effects using an incompressible method is then tested against fully compressible simulations and experimental data to derive the flame transfer function of an injector geometry with promising results.

Abstract_S2_R1_85

Prediction of combustion instability by using a feedback transfer function approach in a model chamber

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Abstract

A closed-loop feedback system consists of flame transfer function (FTF) and acoustic transfer function (ATF) for a gas turbine combustor to analyze the combustion instability. The FTF is fitted by three methods based on experimental results. After comparing the results, two FTF fitting methods, which can be applied to more general models, are adopted in this work. The ATF is obtained by using Laplace transform for the system expression which describe the acoustic wave propagation in the combustor. The combustion stability in the combustor is judged by checking the stability of the combustor system transfer function composed of FTF and ATF. The prediction results show a good agreement with the experimental results, indicating that the feedback transfer function approach can provide acceptable accuracy in predicting combustion instabilities.

Simultaneous measurement of 2D mixture fraction and flame structure in a non-premixed, swirl stabilized burner

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Abstract

Simultaneous 2D fuel mixture fraction (acetone-PLIF) and flame structure (OH-PLIF) measurements in a non-premixed model gas turbine (GT) burner are reported. The burner, consisting of a large bluff body base with an annular swirl region produced a non-sooty lifted flame with varying global equivalence ratios (Φ_{glob}). Two modes - swirl influenced conical shaped and bluff-body influenced toroidal shaped - of flame stabilization are observed in OH* measurements. The mixture composition in the region beyond 1 mm upstream of the flame front is within the flammability limit indicating premixed flame propagation. The time averaged 2D mixture fraction distributions show that the variation of the flame stabilization location with Φ_{glob} is closely related to the development or movement of the stoichiometric surface.

Abstract_S2_R1_87

Assessing emission characteristics of multiphase fuel combustion under gas turbine conditions

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Abstract

The search for greener energy generation processes has led down several pathways including the use of renewables and multiphase combustion. In this study, the emissions from a swirl-stabilized gas turbine burner operating in diesel/biodiesel-natural gas dual fuel mode has been numerically investigated. In the case of neat liquid fuel combustion, NO_x and CO emissions are lower in instances involving biodiesel compared to those involving diesel. In the multiphase cases, CO emissions diminish as the mass fraction of natural gas in the fuel increases but only up to about a 70:30 liquid:gas fuel ratio. However, in all simulated cases, multiphase fuel combustion appears to elevate NO_x emissions. Overall, there is a good potential of combating certain emissions in the gas turbine engine using multiphase fuel combustion.

Assessment of subgrid-scale turbulence-radiation interaction on the filtered mean radiative emission in large-scale pool fire simulations

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Abstract

Subgrid-scale turbulence-radiation interaction (SGS-TRI) is studied for a large-scale ethanol pool fire by comparing the results of large eddy simulations to those obtained with a model that accounts for SGS-TRI in the filtered radiative emission. Spatial grids with different resolutions are employed to assess how the filter width contributes to SGS-TRI. The simulations are fully coupled and the participating medium is assumed to be non-gray. The results indicate that SGS-TRI has a very small impact on the predicted temperature and a slightly larger one for the species concentrations. Nevertheless, considering SGS-TRI only marginally affects the radiative heat source and the radiative emission and absorption.

Abstract_S2_R1_89

Experimental and numerical study on the interaction between sprinkler water spray, fire plume and smoke layer

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Abstract

An important aspect of the sprinkler protection process is the interaction between water spray (droplets), smoke layer and the fire plume itself. In order to investigate these interactions, numerical simulations and experiments have been carried out in a specially designed 36 m² compartment. Measurements were taken of the fuel mass loss rate, smoke density, gas temperature profile, oxygen, carbon monoxide and carbon dioxide concentrations in the compartment. The gas temperatures were measured at three different places in the compartment – along the flame centerline, in the middle of the compartment, where the sprinkler had been installed and in the room corner opposite the fire location. The flame behaviors and fire propagation were also recorded by different video cameras. The experimental results show the main phenomena during the fire and smoke propagation in the compartment before sprinkler activation and additionally the interaction between the hot flue gases in the smoke layer and water spray. The obtained results were used for the validation of numerical CFD methods, which extend the measurements regarding the understanding of the physics behind the fire and smoke propagation and behind the interaction with the sprinkler water spray. The ANSYS CFX solver, based on the concept of detached eddy simulation, is adopted in the present simulation. The simulation results were compared with the experimental data and show good agreement with respect to temperature profiles, smoke layer density and position. The numerical simulation was also able to reproduce the main effects after the sprinkler activation, namely the cooling effect by the water spray and the drag force produced by the water droplets. These two phenomena can lead to the loss of stability of the stratified smoke layer and also to an increased smoke propagation in the regions of the escape routes.

Laboratory investigation of the ignition of wood structural materials under the influence of spot fires

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Abstract

The main factors affecting the ignition of building materials and the spread of fires in the wildland–urban interface are the radiative and convective flame heat transfer and the firebrands, which may accumulate on the roof, in the corners of buildings, near fences or indoors and ignite the structures. One of the ways to reduce the flammability of artificial and natural polymer materials (including wood) are the use of flame retardants that can be introduced into polymer during the production of materials or deposited on polymer during the surface treatment of finished products. Thus, the purpose of the work is to study the ignition of wood samples treated with a flame retardant exposed to firebrands under the laboratory conditions, and to obtain data on fire resistance of wood samples exposed to heat. In the series of experiments was used a one glowing firebrand, then two firebrands and so on up to 10 firebrands to model the ignition of wood beginning from one firebrand and finishing with "fire rain". Three repetitions were performed for each experiment. The wood sample was considered ignited if the ignition occurred at least in one of the three experiments. The samples of spruce, plywood and standard oriented board (OSB) were used as the samples which imitated the wood used in constructions. It may be concluded that the presence of a high amount of an oxidizer in the combustion zone leads to the flame combustion of the firebrands. Surface combustion of the sample was observed in the combustion zone of the firebrands. After the influx of the oxidizer was stopped, the surface combustion of the sample continued for some time, but it was not stable. It is worth noting that for the selected range of the number of firebrands, their thermal energy was not sufficient to ignite the wood. Usually, a wood sample charred (sometimes locally ignited) only in the combustion zone of the firebrands which scattered before the flame combustion was started due to the influx of the oxidizer from the thermal dryer. Flame combustion of wood samples was not observed, in contrast to the experiments with the wood untreated with a fire retardant. With increasing the wind speed, the probability of wood ignition by firebrands of the same size increases, but stable combustion of wood subjected to the heat of falling firebrands is not observed. Usually, all wood samples treated with flame retardants react during the heating as follows: charring takes place in the heating zone, thereby creating a protective layer that improves the fire resistance of wood. For the selected parameters the wood samples treated with flame retardants were resistant to firebrand attack. Combustion was observed on the surface of the wood sample during the flame combustion of the firebrands. The experimental

results show that fire retardants significantly increase the protective properties of wood exposed to firebrands.

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Poster Session 3



Abstract_S3_All_01

Activation effect of diethyl ether on the partial oxidation of methane

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Abstract

Homogenous partial oxidation of methane (CH_4) within piston engines is an interesting approach to obtain useful chemicals, work and heat, simultaneously or depending on demand. In view of the low reactivity of methane below 1000 K, the addition of small amounts of higher reactive species like diethyl ether (DEE) to the gas mixture is a viable way to initiate CH_4 conversion at lower temperatures and control the product composition. To assess the effect of DEE onto the partial oxidation process, a plug-flow reactor study of fuel-rich diluted $\text{CH}_4/\text{DEE}/\text{O}_2$ mixtures is performed at temperatures between 423 – 973 K, a pressure of 6 bar and residence times ranging from 5 – 10 s. The product composition is evaluated by gas chromatography and compared with predictions from kinetic simulations using a literature reaction mechanism.

Estimation of sticking coefficients using mobile and immobile transition states for catalytic platinum systems

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Abstract

The estimation of rate data suitable for microkinetic analysis of reaction pathways in heterogeneous catalytic systems typically requires sticking coefficients. These can be derived experimentally or, at major computational expense, using *ab initio* quantum mechanical methods. The current work explores an alternative theoretical framework based on Variational Transition State Theory (VTST) for estimating Arrhenius parameters. The gas-phase vibrational frequencies are determined using the Mo6-2X density functional with adsorbed species modelled as attached to a plane of metal atoms using the Mo6 functional. The 6-311 G(d,p) basis set was used for C, O, H and the Stuttgart-Dresden (SDD) and Los Alamos National Laboratory 2-double-z (LANL2DZ) effective core potential methods used for surface atoms. A total of 31 adsorption reactions were considered with sticking coefficients derived for mobile and immobile transition state over a wide range of temperatures. The ability of the developed method to reproduce experimental tubular reactor data is also explored and compared to the collision theory approach.

Evaluation of polycyclic aromatic hydrocarbon formation in counterflow diffusion flames

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Abstract

There is an increased concern about the occurrence of polycyclic aromatic hydrocarbons (PAHs) in the environment as they are amongst the strongest known carcinogens. These pollutants are associated with particulate carbonaceous materials resulting from the incomplete combustion of transportation fuels. A considerable amount of effort has been put into the mode of formation of PAHs in burner stabilized premixed flames. However, for numerical simulations, boundary conditions for burner-stabilized flames are difficult to determine. As a result, temperature profiles are usually specified rather than being computed. On the contrary, counterflow diffusion flames are excellent candidates to mimic the non-premixed combustion mode in diesel engines, fire, and furnaces. Moreover, the flames stay away from any walls or surfaces, hence uncertainties resulting from boundary conditions are minimized. Prompted by this insight, this work first presents a short review of the available PAH relevant counterflow diffusion flames. Then, available data for various hydrocarbon fuels are used to critically assess the performance of the existing PAH models. As part of a broad investigation on the chemical behavior of diffusion flames, the present study includes the formation of PAHs in ethylene (Carbone et al., 2017 and Figura et al., 2014), acetylene (Baroncelli et al., 2018), methane doped acetylene (Baroncelli et al., 2018), toluene doped methane (Carbone and Gomez, 2012), toluene doped ethylene (Carbone and Gomez, 2012), and toluene doped n-heptane (Hamins and Seshadri, 1987) flames. The performance of four different literature models, namely, the ITV model (Blanquart et al., 2009), the CRECK model (Pejpichestakul et al., 2018), the KAUST model (Wang et al., 2013), and the ABF model (Appel et al., 2000), has been evaluated against these experimental data sets. Overall, the predictive capability of the ITV model and the CRECK model is found to be satisfactory. The main formation pathways for PAH precursors and main PAH species have been analyzed. Particular attention has been given to the formation of the first PAH ring and its growth in ITV and CRECK mechanisms. For instance, propargyl and 1,3-butadiene-yl radicals are observed to be important precursors for the formation of the first ring in an atmospheric acetylene flame. These precursors are mainly formed by methylene radical, acetylene, allene, propyne, and vinyl radical. The present work serves as a base for the modification and revision of the existing kinetic models in order to further our understanding of PAH formation and growth under non-premixed combustion mode.

Combustion study of a 3-components surrogate fuel

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Abstract

This study reports on the experimental and numerical investigation of the oxidation of a three-component jet fuel surrogate, here 66.2% n-dodecane 15.8% n-propylbenzene, and 18.0% 1,3,5-trimethylcyclohexane, in mol. The experiments were performed within a wide range of temperature, fuel equivalence ratio, and pressure by referring to measured data of species profiles from a jet stirred reactor JSR ($T = 550\text{--}1100\text{ K}$, $\phi = 2.0$, $p = 1\text{ bar}$), ignition delay times measured in a shock tube ($T = 700\text{--}1500\text{ K}$, $\phi = 1.0$, $p = 16\text{ bar}$), and laminar burning velocities obtained in a burner by using the cone angle method ($T = 473\text{ K}$, $p = 1\text{ bar}$, $\phi = 0.5\text{--}2.0$). As a result obtained from this broad experimental data base, a negative temperature coefficient (NTC) behavior was observed in the JSR and shock tube experiments, due to n-dodecane, a long-chain alkane. Based on the experimental studies, an updated detailed chemical-kinetic mechanism involving 401 species and 2838 reactions was developed, for allowing a more detailed understanding of the oxidation of the surrogate. In addition, quantum chemical methods have been applied for the determination of important initiation reactions by using Gaussian and ChemRate. Furthermore, rate-of-production and sensitivity analyses were done at 900 K. For example, 1,3,5-trimethylcyclohexane was found to be mainly consumed through H-abstraction reactions; then, the formed C_9H_{17} radicals mostly isomerize to iso-alkane radicals and further on, decompose to light hydrocarbons. The comparison of predicted data for ignition delay time and laminar burning velocity with measured ones shows that the mechanism for the surrogate is able to reproduce the combustion behaviour of a typical crude-oil stemming jet fuel. The surrogate fuel mechanism as well as the experimental data are considered as a valuable contribution towards a better understanding of the combustion behaviour of aviation fuels as well.

This work is supported by the Ministry of Science and Technology of China (2017YFA0402800), the Natural Science Foundation of China (No. 51476168/91541102), *Recruitment Program of Global Youth Experts and AvH Research Linkage Group*.

Mechanism and kinetic study on the pyridine low-temperature oxidation under fuel-rich condition

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Abstract

The low-temperature oxidation (LTO) of pyridine was investigated in a jet-stirred reactor over the temperature range of 700-1000 K at 1 atm and equivalence ratio of 2.0. Mole fraction profiles of the reaction products were obtained based on molecular beam mass spectrometry and tunable vacuum ultraviolet synchrotron photoionization techniques. Based on Photoionization efficiency spectra, hydrogen peroxide, methanamine, acetylenamine, ethenamine, acetaldimine, ethylamine, allyamine, and methylformamide were newly identified compared with previous pyridine flame and pyrolysis studies. HCN was the dominant N-containing species of pyridine LTO, which accounts for accounts for 92.5% selectivity at 1000 K. Pyrrole, acrylonitrile, acetonitrile, and ammonia were also found at the same level of N₂O and NO. Based on the new measurements and the updated rate constants of several reactions including the H-abstractions of pyridine and the oxidation of ortho-pyridyl using density functional theory calculations, a new pyridine LTO kinetic model consisting of 588 species and 3516 reactions was developed with a reasonable agreement with the experimental results. In general, the predictions of the predominant species have been improved compared with the existed model. Rate-of-production analysis indicates that pyridine mainly consumes via $C_5H_5N \rightarrow C_5H_5N \rightarrow C_5H_4NO_2 \rightarrow HCN + CO + CH_2CHCO$, and $C_5H_5N \rightarrow C_5H_5NO \rightarrow C_2H_2 + HCN + CH_2CO$. Sensitivity analysis shows that $C_5H_5N + O_2 \Rightarrow C_5H_4NO_2$, and $C_5H_5N + OH = C_5H_4N + H_2O$ have significant promoting effect, while $C_5H_4N + HO_2 = C_5H_4NO + OH$ has strong inhibiting effect. The results of this work will enrich the understanding of pyridine low-temperature oxidation mechanism, which can be applied to the fields of coal pretreatment, staged combustion, mild combustion, etc.

This work is supported by the Ministry of Science and Technology of China (2017YFA0402800), the Natural Science Foundation of China (No. 51476168/91541102) and Recruitment Program of Global Youth Experts.

Abstract_S3_All_06

Reduction of methane-air combustion kinetic model through flux analysis and optimized with adaptive Monte Carlo optimization for chemical kinetics

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Abstract

A method of systematic kinetic model reduction by path flux analysis and optimized with the Adaptive Monte Carlo Optimization for Chemical Kinetics (AMOCK) algorithm is presented for the reduction of large chemical kinetic models. The objective of this reduction method is the construction of highly reduced models capable of numerically reproducing the combustion behavior of natural gas, targeting the concentration changes of target species as predicted by the detailed model. This reduction and optimization process is applied to the NUIG_18_17_C3 FLAME detailed natural gas model with methane as fuel. A 24 species compact model obtained shows high fidelity against the detailed model performance and improved performance against a 24 species PFA reduced model. The methods presented here are numerically simple and flexible for potential applications in the production of highly reduced mechanisms for computationally efficient numerical modelling of combustion.

An experimental and theoretical kinetic study of the reaction of hydroxyl radicals with 1,4-Pentadiene

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Abstract

It seems quite unlikely for the renewable sources of energy to surpass the petroleum-based fuels in the foreseeable future. For the few decades to come, internal combustion engines will still continue to power the transportation sector burning fossil fuels. Therefore, the strategy for curbing environmental pollution and greenhouse gas emissions remains a big challenge. One of the strategies to mitigate the environmental effects of transport sectors is to significantly improve the combustion technology, e.g., fuel-engine co-optimization for the best performance in advanced low-temperature combustion modes. Recently, the development of more efficient spark ignition (SI) engines is shifting towards increasing the compression ratios and implementing turbocharging. As olefins are high-octane sensitive fuels, they may provide the desired antiknock quality for internal combustion engines operating at high pressures. Therefore, understanding of the detailed kinetics of the olefinic fuels is crucial for developing combustion models. In this work, we investigated the reaction of OH radicals with 1,4-pentadiene (14PTDN + OH) over a wide range of experimental conditions ($T = 881\text{--}1314$ K and $p \sim 1150$ Torr) using a shock tube. The progress of the reaction was monitored by detecting OH radicals near 307 nm using a UV laser-absorption technique. OH radicals were generated by fast thermal decomposition of *tert*-butyl hydroperoxide (TBHP). To discriminate among various reaction pathways, high-level QCISD(T)/cc-pVTZ//BH&HLYP/6-31G(d) *ab initio* methods were employed to explore the various reaction pathways for the 1,4-pentadiene + OH reaction system. Kinetic analyses, using both the *deterministic* and *stochastic* ME/RRKM models, were carried out with the help of the Multi-Species Multi-Channels (MSMC) code. Interestingly, unlike conjugated dienes + OH reaction, it was found that the abstraction reaction dominates over the addition pathways throughout the finite temperature and pressure range of our study ($T = 200 - 2000$ K and $p = 0.1 - 10000$ Torr). Beyond 1000 K, the addition channel contributes negligibly small for all pressures. To our knowledge, this is the first direct experimental and detailed theoretical kinetic study of the reaction of 1,4-pentadiene with OH radicals at high temperatures.

Combustion behaviour of ammonia blended with dimethyl ether

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Abstract

Ammonia is recognized as a carbon-free and hydrogen carrier fuel with a high content of hydrogen atoms per unit volume. Recently, ammonia has received increasing attention as a promising alternative fuel for transport sectors. The viability of ammonia fueling internal combustion engines (ICEs) has several barriers to overcome. One feasible way to alleviate these barriers is to go for a dual-fuel component to enhance the combustion properties of ammonia. Therefore, we have investigated the ignition characteristics of NH_3 /DME blends using rapid compression machine over a temperature range of 650 to 714 K, pressures near 20 bar and equivalence ratios of $\Phi = 1$ and $\Phi = 0.5$. The fuel blends of various composition were employed, viz. 75% NH_3 /25% DME, 60% NH_3 /40% DME and 50% NH_3 /50% DME. Our results indicate that dimethyl ether promotes the reactivity of the fuel blends resulting into significant shortening of the ignition delay times of ammonia under RCM conditions. The last two fuel blends containing 40% and 60% of DME exhibited very similar reactivity behavior as compared to pure DME suggesting a higher percentage of ammonia in fuel blends might be attractive for transport sectors with the development of modern NH_3 -engine technology.

Exploring the combustion chemistry of a novel lignocellulose-derived biofuel: cyclopentanol

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Abstract

Biomass derived chemicals may offer sustainable alternatives to petroleum derived hydrocarbons, while also enhancing engine combustion performance with co-optimization of fuels and engines. This paper presents a numerical study on the oxidation and combustion of a novel biofuel compound, cyclopentanol. Its reaction kinetics is first explored using quantum chemistry methods. C-H bond dissociation energies of cyclopentanol are computed for different carbon sites. To understand the oxidation kinetics of cyclopentanol at low and intermediate temperatures, the potential energy surfaces of the oxidation reactions of fuel radicals are calculated. Based on the theoretical results, a chemical kinetic mechanism is then developed to describe the oxidation of cyclopentanol. The model matches the data obtained from a shock tube and a rapid compression machine over a range of initial conditions with respect to temperature, pressure, and composition. It is found that the alcohol functional group introduces two major features into the reaction pathways, compared to those of cyclopentane. First, it facilitates an alcohol-specific HO₂ elimination reaction for the α -hydroxycyclopentyl radical, which decreases the fuel reactivity at low temperatures strongly. Second, it reduces the C-H BDE at the α -carbon site and consequently the barrier height of the intramolecular H-migration from this site, thus promoting the chain-branching channel of the γ -peroxy radical in the low temperature range slightly. The major reaction pathways of β - and γ -radicals are similar to those of cyclopentyl radicals that are the sequential and formally direct reactions of fuel radicals with O₂ to form cyclopentenols and HO₂ radicals.

Comparison of methane combustion mechanisms based on shock tube and RCM ignition delay time measurements

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Abstract

Methane as the main component of natural gas is in the focus of interest for many years. One of the most important characteristic features of methane containing gas mixtures is the ignition delay time. Majority of such experiments were carried out in shock tubes, but there are some also in rapid compression machines (RCMs). In this work we utilized both types of experiments and 13 methane combustion mechanisms were tested against them. The method developed by Olm *et al.* [1,2] was used for the comparison of mechanisms. Ignition delay time measurements at a wide range of experimental conditions were collected; data points were measured in the range of 870–2800 K and 0.1–260 atm, equivalence ratios were varied between 0.04–8.00 and diluent concentration was varied between 0.00–0.997, using various diluents. Altogether about 4500 data points in more than 500 datasets were used for the comparison of thirteen methane combustion mechanisms. The simulations were carried out using computer program FlameMaster [3] called from framework code *Optima++* [4]. Based on the simulation results, the performance of the mechanisms was determined by taking into account also the estimated experimental scatter error of the measurements. Based on the comparison carried out using the whole dataset, the mechanisms which reproduced the measurements the most and the least efficiently were identified. The investigations related to subsets of the experimental data allowed the determination of the shortcomings of several mechanisms. Experimental conditions were identified, at which additional measurements are needed for the further development of the methane combustion mechanisms.

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Comparison of detailed reaction mechanisms for nitrogen chemistry in syngas combustion systems

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Abstract

In the recent years, there has been an increased interest in studying the combustion of fuel mixtures consisting of carbon monoxide and hydrogen, referred to as syngas or “wet CO”. These fuels can be produced from coal or biomass via gasification, and are considered to be a promising option towards cleaner combustion technologies for power generation. The formation of nitrogen oxides (NO_x) during combustion processes are also of high interest due to their environmental hazards. In the last two years, three comprehensive reaction mechanisms [1-3] were published, which can be used to simulate NO_x formation during syngas combustion. The aim of this work is to investigate the performances of these mechanisms at various experimental conditions. Shock tube ignition delay times, laminar burning velocities, and shock tube, flow reactor and jet stirred reactor concentration measurements were collected from 23 publications and encoded in 298 RKD 2.0 format [4] datasets. These datasets consist of about 4000 data points covering a wide range of conditions ($p = 0.20\text{--}98.7$ atm, $\varphi = 0\text{--}5$, cold side temperatures of flames $T_c = 294\text{--}304$ K; initial temperatures of shock tube, flow and jet stirred reactor experiments $T_{in} = 702\text{--}2712$ K). The method developed by Olm et al. [5, 6] was used for the comparison of the mechanisms. The simulations were performed using the Optima++ simulation environment [7] with code FlameMaster [8]. The comparison revealed that a minor part of the experiments is problematic and their reliability is questionable. The mechanisms of Zhang et al. [1] and Glarborg et al. [2] provided somewhat better results than the POLIMI mechanism [3]. The chemistry of species HOCO and the importance of reaction $\text{N}_2\text{O} + \text{H}_2 = \text{N}_2 + \text{H}_2\text{O}$ were investigated in details.

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Modelling study of ignition delay time characteristics of ultra-rich C1/C2 mixtures in a constant volume reactor at low-pressure

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Abstract

In this work we study the ignition delay time characteristics of an ultra-rich mixtures of C1/C2 gaseous hydrocarbons, at temperatures ranging from 590-790K, at atmospheric pressure, at equivalence ratios from $\varphi \approx 13$, and at very long residence times (>10s). The ratio of CH₄/C₂H₄ was 3:4, and was simulated with an oxygen concentration of 16%. These conditions are typical of those present in the certain industrial process. Previous experimental studies in a constant volume reactor observed a negative temperature coefficient (NTC)-like behavior, which is unusual for low molecular weight components such as methane, and unsaturated species such as ethylene. It was unclear at the time of the experiments measurements whether the NTC behavior was the result of facility effects, such as heat loss to the walls, or gas motion due to natural convection, or whether it was due to the underlying chemistry. In order to isolate the chemical kinetic effects, and to ascertain whether and NTC-like behaviour is plausible under these conditions, three chemical mechanisms were used to interpret the experimental data based on zero-dimensional (0-D) modelling.

An updated chemical kinetic model for the simulation of laminar burning velocities of premixed hydrogen-, methane-, and n-heptane/air flames

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Abstract

The laminar burning velocity is one of the most important characteristics of a fuel describing the progress of chemical reactions, diffusion, and heat conduction. It is one of the key parameters for the simulation of combustion processes in gasoline engines determining the expansion of the early flame kernel. Although the importance of laminar burning velocities as a validation target for kinetic models is well-recognized, it still plays a secondary role compared to ignition delay times, which are solely driven by chemical kinetics. The objective of the present study is to compile a compact model specifically for the prediction of laminar burning velocities of n-heptane flame, e.g. for investigation of physical effects in outwardly propagating flames or simulation of combustion processes in engines. For the simulation of n-alkane combustion processes a large amount of chemical kinetic models are available. The choice of a suitable model would be significantly reduced if a compact model is required which is able to predict laminar burning velocities at conditions similar to combustion engines. In the present study, ongoing work is presented on the update and extension of a skeletal mechanism for n-heptane based on the model by Pitsch and Peters [SAE Technical Paper. No. 982464, 1998]. In its original state, the model substantially over-predicts laminar burning velocities for n-heptane/air flames. Therefore, the hydrogen chemistry has been replaced by the Hong model [Combust. Flame 158(4), 2011] and outdated rate constants for the hydrocarbon base chemistry have been updated. It was ensured that the model retains its ignition behavior by capturing the first and second stage of ignition. Sensitive reactions for laminar burning velocities at atmospheric and elevated pressure have been identified and successfully included in the model. Especially, the H-abstraction reaction of HCO by a hydrogen radical was found to have a large impact on the overall pressure dependency of the laminar burning velocity. Validation targets for hydrogen-, methane-, and n-heptane/air flames were measured in an optical high-speed setup utilizing the closed-vessel method. The predictability of the updated model, comprising 45 species and 124 reactions, was found to be promising for all three fuels. In comparison with the comprehensive model by Cai and Pitsch [Combust. Flame 162(5), 2015] the updated model showed a similar and overall good agreement.

A jet-stirred reactor study of the oxidation and pyrolysis of di-n-propyl-ether

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Abstract

Ethers are renewable green fuels that have been used as additives in spark ignition engines in order to minimize the soot formation as well as enhancing the gasoline octane number [1]. One of the most famous, methyl tert-butyl ether (MTBE), has been used as a gasoline additive since the 70's. Among symmetric ethers, dimethyl ether, the smallest, has been intensively studied. On the other hand, studies on larger symmetric ether are scarce. We have recently reported speciation data [2, 3] on diethyl and dibutyl ethers, however no such data are available in the literature for the dipropyl ether (DPE). This study reports the oxidation and pyrolysis of DPE in a jet-stirred reactor. Oxidation experiments were performed at 10 atm. Fuel-lean, stoichiometric and fuel-rich mixtures were oxidized at a constant fuel mole fraction (1000 ppm), between 450 and 1300 K with constant residence time of 700 ms. Four mixtures were tested in total. In addition, a pyrolysis experiment was conducted, keeping the residence time and the initial fuel mole fraction constant. The evolution of the mole fraction profiles of the main species with the temperature were monitored with on-line Fourier transform infrared (FTIR) spectrometry and off-line gas chromatography (GC). These profiles indicated a strong low-temperature reactivity. Besides, the fuel mole fraction profiles show an unusual behavior similar to dibutyl ether: two negative temperature coefficient regions were observed for the fuel-lean and stoichiometric conditions, however less pronounced than in the case of DBE. A kinetic model was developed and tested against the current measurements, based on recently published parameters from the literature and analogies with our previous studies on diethyl ether and dibutyl ether. The proposed detailed mechanism shows good performances for representing the present experimental data.

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Abstract_S3_All_15

Determination of the rate parameters of N/H/O elementary reactions based on H₂/O₂/NO_x combustion experiments

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Abstract

A mechanism for the description of the H₂/O₂/NO_x combustion systems was optimized via the method developed in our laboratory using computer framework code *Optima++*. In total, 5073 experimental data points (ignition delay times, concentration profiles and burning velocity measurements) were collected from the literature and were reproduced using 17 recent NO_x mechanisms. The performance of the Glarborg-2018 mechanism was the best. Ten elementary reactions were selected based on local sensitivity analysis and the Arrhenius parameters of them were fitted to indirect experimental data, and direct experimental and theoretical determinations of the rate coefficients. This way more accurate rate parameters of these reactions were obtained and the temperature dependent uncertainties of the rate coefficients were calculated.

Experimental and modelling study of the oxidation of methane doped with ammonia

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Abstract

Biogas is a mixture of different gases produced by the breakdown of organic matter in the absence of oxygen. It primarily consists of methane and carbon dioxide, but it also contains smaller amount of nitrogen, oxygen, water, hydrogen sulfide and ammonia. The composition of biogas depends on the biomass source. The oxidation of methane doped with ammonia was experimentally and theoretically studied to better understand the interactions between these two molecules in combustion processes fed with biogas. Neat ammonia oxidation was also investigated during this study. Experiments were carried out in a jet-stirred reactor operated at steady state, at a residence time of 1.5 s, a pressure to 800 Torr and over the temperature range 500-1200 K. The inlet flow composition was 10000 ppm of methane and 500 ppm of ammonia. Three equivalence ratios were investigated: 0.5, 1 and 2, with dilution into helium. Several diagnostics were used to quantify reaction products. Gas chromatography for the quantification of carbon containing species. A NO_x analyzer was used for the detection of NO and NO₂. Ammonia quantification was performed using an advanced spectroscopic technique: continuous-wave cavity ring-down spectroscopy, which was successfully used for the detection of species like hydrogen peroxide [1] and HONO. Particular phenomena were observed during this study, making the oxidation study of ammonia tricky. The first was the occurrence of oscillation regimes under some conditions. This phenomenon has already been reported in literature before for the oxidation of neat methane [2]. The second phenomenon was the occurrence of wall reactions strongly enhancing the ammonia consumption in the case of neat ammonia oxidation. The addition of NH₃ did not show any significant effect on the reactivity. This is in agreement with the N-H bond in ammonia stronger than the C-H bond in methane. Small amount of NO and NO₂ were detected but did not allow to close the N-atom balance. Further investigations shew that nitrogen was the main reaction products. The oxidation of neat ammonia was also carried out to highlight the specificities of the chemistry of this fuel alone. All these data were satisfactorily compared with data computed using a model developed by Politecnico di Milano. The model catches well the reactivity of methane and ammonia, as well as the effect of the equivalence ratio on the reactivity temperature window.

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An experimental and kinetic modeling study on the reactivity of 1,3-dioxolane under engine relevant conditions

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Abstract

A severe problem of our time is the use of fossil fuels due to their impact on the greenhouse gases, and their potential harm as particle emission or nitrogen oxides (NO_x). Therefore, more sustainable alternative fuels must be found. One option is the usage of 1,3-dioxolane, which is prepared by the reaction of ethylene oxide and formaldehyde catalysed by Brønsted-acids [1]. Ethylene oxide can be produced by the conversion of ethanol [2] obtained from biomass in the form of corn grain or sugar cane [3]. Formaldehyde can be obtained from methanol, itself obtained from gasification of biomass [4]. Literature regarding the reaction kinetics of 1,3-dioxolane is scarce. Due to its use as chemical solvent the kinetics of the oxidation of 1,3-dioxolane by OH-radicals has been studied under atmospheric conditions [5]. Also the impact of 1,3-dioxolane/diesel blends on soot reduction in diesel combustion has been examined. It was observed, that 1,3-dioxolane does reduce the soot formation while showing only a modest effect on NO_x emission. The reduction is based most likely on a later ignition of 1,3-dioxolane/diesel blends in an engine due to its low cetane number of 30 [6]. The kinetics of the oxidation of pure 1,3-dioxolane under engine-relevant conditions has not been investigated yet. In this study, the ignition delay times of 1,3-dioxolane/air mixtures are measured in a rapid compression machine and a shock tube. The experimental conditions are a temperature range of 600-1200 K, pressures from 10 bar to 40 bar and various equivalence ratios ($\varphi = 0.5, 1.0, 2.0$). For both the high and the low temperature range a detailed kinetic sub-model is designed considering the specific decomposition reactions of 1,3-dioxolane as well as the oxidation process of the sub-species. For the reaction rate parameters suitable analogies from literature were used. The model is validated on the experimental data, and used to further investigate the oxidation process of 1,3-dioxolane through reaction pathways analysis. The most sensitive reactions on the ignition delay times are identified.

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An experimental and modelling study of diisobutylene oxidation

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Abstract

The development of surrogate fuels to represent the combustion characteristics of commercial fuels is important to enable multi-dimensional simulations of IC engine combustion. A reliable multi-component surrogate model usually contains one or more components of each class of hydrocarbon in the real fuel that it attempts to represent. 2,4,4 trimethyl-1-pentene (*iso*-octene) is one of the isomers of di-isobutylene (DIB), which gained significant attention in the recent past as a representative of branched alkenes in commercial gasoline [1-5]. However, there is very limited experimental ignition delay time (IDT) data available in the literature for neat DIB at engine-like conditions, and hence most existing DIB models have not been extensively validated. In *this study*, we provide extensive and reliable experimental database for a DIB oxidation study conducted in both high-pressure shock tube (HPST) and rapid compression machine (RCM) facilities at NUI Galway. The IDT experiments are performed at pressures (15 and 30 bar) and equivalence ratios ($\varphi = 0.5-2.0$) in the temperature range (650–1350 K). Moreover, all available DIB and multi-component gasoline surrogate kinetic models are tested to compare their predictions against the experimental data recorded in *this study*. To understand DIB kinetics further, sensitivity and flux analyses were performed using the Metcalfe et al. [6] model. Modifications to the existing model [6] were made to improve high temperature predictions.

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Response-surface and group-additivity methodology for estimation of thermodynamics properties of oxygen-containing organosilanes

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Abstract

In this study, we provide thermochemical data of 32 stable oxygen-containing organosilanes, required for studying the kinetics of oxygen-containing precursors such as hexamethyldisiloxane (HMDSO) and tetraethoxysilane (TEOS). These data are based on quantum-chemical calculations performed using the G4 composite method. Based on molecular properties obtained from the G4 calculations, data for heat capacities, enthalpies of formation, and entropies are derived. A combinatorial approach is used to build all possible groups that contain Si, C, H, and O atoms. This leads to 73 Si-, C-, and O-atom-centered groups. We are interested in 33 groups that contain Si and O. The group-additivity values (GAV) for other 40 groups are already known as hydrocarbon groups in the literature or calculated as part of the Si-C-H system. In order to calculate the GAVs from the compounds in the training set, a multivariate linear regression model is defined. The thermodynamics properties recalculated via group additivity are compared with few available experimental data sets and ab initio calculated values.

Abstract_S3_All_20

Global quasi-linearization (GQL) method for high dimensional detailed reaction mechanisms

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Abstract

Reliable chemical kinetics is crucial for an accurate description of combustion and fuel oxidation processes. In order to improve the predictions of e.g. ignition delay times and species time-profiles reaction mechanisms have steadily been developed and improved leading to a considerable increase of the dimensionality and non-linearity of the mathematical model. Therefore, the complexity of the system significantly increases and makes the numerical treatment very demanding. Large kinetic models require sophisticated integration software and an enormous computational effort (e.g., in terms of CPU time and memory storage) making them unviable for parametric studies and for reacting flow computations in technical applications. This has motivated the development of reduced modelling concepts able to describe combustion process with a reasonable/acceptable accuracy but with a significantly lower computational cost. In this study, an automatic reduction method based on the computation of the Global Quasi-Linearization (GQL) matrix is implemented to reduce a detailed mechanism for methane (CH_4) / dimethyl ether (DME) oxidation (558 reactions among 83 species) at extremely rich fuel mixture compositions. The GQL is a method based on an analysis of the characteristic timescales. It is a robust and scaling invariant approach able to automatically identify combinations of chemical reactions that can be assumed partially equilibrated as well as species linear combinations which can be assumed to be in quasi-steady states. The study shows how technical difficulties to define the GQL matrix for large mechanisms are overcome. The problem with ill-conditioned matrices of the state space vectors and the selection of appropriate reference states is in the focus of the study. The obtained information about linear combinations between species is implemented to reduce the reaction mechanism and define the optimal dimension of its reduced form. The reduced model is presented in an implicit form but, it can also be represented in form of a skeletal mechanism by using an entropy production analysis. The results of species profiles and ignition delay time computations are compared against those carried out with the detailed reactions mechanism. Additionally, the reduced model dimension implementing the GQL approach presented in this work is compared with results obtained by applying a local timescale analysis for the same initial conditions and reaction mechanism. A dimension of 32 was found to be enough to describe the ignition process with an acceptable accuracy implementing the local analysis. The global analysis predicts a dimension with a factor 1.18 higher as the latter one.

Prediction of non-premixed combustion regimes in a DI diesel engine in various operation points

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Abstract

In turbulent combustion, various regimes exist posing different implications to the accompanying modelling procedure. In essence, turbulent scales are compared to different scales of the flame to determine the turbulence-flame interaction. Most conventional operation points of Diesel engines fall into the flamelet regime, where an ensemble of thin laminar flame structures is attached to the flame surface, which is wrinkled by turbulence. However, in certain operation points, the separation of scales between turbulence and combustions ceases to exist due to the low temperatures and the consequently longer chemical time scales or high local turbulence intensities. A method for evaluating local turbulent scales in scalar fields is the so-called Dissipation Element (DE) analysis. DEs are ensembles of grid points whose gradient trajectories reach the same extremal points. In this fashion, scalar fields are compartmentalized into regions in which the scalar profile is monotonic. The Euclidian distance between its extremal points l and the scalar difference in these points $\Delta\phi$ can then be used to parameterize a DE and the region of the flow occupied by it. The characteristic distance l is used as a measure of the local turbulent length scale. The space filling nature of the DEs guarantees that all scale interactions are considered. The correlation between DE parameters and the dynamics of reacting scalars is demonstrated in a series of 3D direct numerical simulations (DNS) of planar temporally evolving jet flames. The Jet Reynolds number of the DNS ranges from 4,500 to 6,000. Scaling laws of the mean DE parameters and a stochastic transport equation for the joint probability density function the DE parameters are employed for the modeling of the statistics of DE parameters in the framework of computational fluid dynamics (CFD) of a passenger car direct injection (DI) Diesel engine. These statistics are used for a spatial and temporal classification of the combustion regimes in the 3D CFD. The CFD simulations feature a wide range of operation points, including injection timings, intake temperatures and exhaust gas recirculation. The results of the classification are presented and potential critical points in the CFD simulations are addressed.

Methodology for knock investigation in spark ignition engines

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Abstract

In spark ignition engines, many developments are focused on downsizing techniques in order to reduce fuel consumption and to increase engine efficiency. However, this technology promotes knock occurrence. As knock is related to fuel physical and chemical characteristics, the objective of this work is to use 3D simulations capabilities to through mono-parametric variations of fuel characteristics, impossible to achieve in real try-out. A specific numerical methodology consisting in combining detailed kinetic mechanisms and CFD simulations is used. First, chemical kinetic simulations of a ternary reference fuel of interest, a binary mixture of Toluene / 1-hexene, are conducted using three different mechanisms from POLIMI, IFP Energies Nouvelles and KAUST. These three mechanisms are evaluated and their limitations are highlighted, thus, potential chemical and physical behaviors of interest are identified. In this context, the present results deal with the description of the numerical methodology focusing on the chemical inputs validation. The implementation of these inputs is done through the generation of tabulated kinetics for ignition and laminar flame speeds that arise from detailed kinetic modeling and associated experimental validation. The chemical validation is based the surrogate fuel reactivity in a shock tube as well as in a spherical bomb respectively for simulating existing ignition data and laminar flame speeds. These simulations are validated with original data in shock tube ranging from 60 to 190 atm and 750 to 1200K, which coincide with engine thermodynamic conditions. However, the measurement of laminar flame speeds for these conditions is not yet feasible. But in order to verify the mechanism performance regarding flame speeds, an experimental study, using expanding spherical flames, was conducted at less stringent conditions: 1 atm and 375-475K. Finally, the several fuel parameter variations that will be addressed in 3D will be discussed by analyzing different molecule behaviors in order to characterize their relative effect regarding knock phenomenon. The next step will be to perform 3D combustion simulations in an engine configuration available using the RANS (Reynolds Average Navier-Stokes) approach. The numerical configuration chosen for this work is based on the ECFM (Extended Coherent Flame Model), ISSIM (Imposed Stretch Spark Ignition Model) and TKI (Tabulated Kinetics for Ignition) models to respectively represent premixed flame propagation, spark ignition and auto-ignition. These models have been widely validated in the past, and are available in the CONVERGE software that is chosen to perform these numerical simulations.

Abstract_S3_All_23

Toward direct numerical simulations of a gas engine pre-chamber

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Abstract

The present study aims at investigating with direct numerical simulations mixing quality, key aerodynamic features, ignition and flame flash-back in a pre-chamber geometry provided by industrial partners. The real, highly complex pre-chamber geometry is described in an efficient manner by an in-house, higher-order ghost-cell immersed boundary method. All necessary steps have been developed and – as far as possible – tested against references. Due to migration problems concerning the employed HPC system, the full-scale full-resolution benchmark is still in the queue. Final results will be presented at the Conference.

Development of a phenomenological blending rule for the assessment of the antiknock quality of hydrocarbon fuel mixtures

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Abstract

The knocking phenomenon occurs in the end-gas region of the combustion chamber of a spark-ignition engine when the temperature of the unburned fuel-air mixture remains above certain value during a time enough for ignition to take place before the arrival of the flame front, thus triggering spontaneous combustion in multiple spots within this region. The occurrence of knock is influenced by fuel and engine factors, and the assessment of the fuel antiknock quality is carried out in such a way that the engine factors are kept unchanged. The Octane Number (ON) is used to express this fuel quality. The ON determination follows a trial-and-error experimental procedure in which a standardized apparatus (the CFR engine) is operated at conditions corresponding either to Motor ON (MON) or Research ON (RON) standard test specifications. One of the many intermediate steps included in this procedure is the determination of a compression ratio that produces standard knock intensity when the CFR is fed with the investigated fuel – this is the Critical Compression Ratio (CCR). After a first successful determination of the ON, the entire procedure should be completed twice again and the average of the three values so obtained is then taken as the sought ON. This way, the experimental ON rating is a task intensive in time, labor and money, and a methodology that would enable computing instead of measuring the fuel ON is a practical necessity. This is particularly true in the case of an oil refinery plant, where demands for ON determination are frequent for purposes such as mixing refinery streams, formulating a new gasoline, and designing gasoline surrogates or special fuels. A thorough review of the antiknock quality blending rules reported in literature shows that all of them are essentially empirical and do not draw upon the underlying physics of the knocking phenomenon. The present work aimed the development of an ON blending rule capable of overcoming this issue. Such a rule was derived considering a single-step kinetics for pre-flame reactions occurring within the cylinder of a CFR engine, and employing both single- and two-zone representations for the working fluid experiencing combustion. In order to validate the proposed rule, Motor ONs (MONs) of paraffinic fuels; and Research ONs (RONs) of Liquefied Petroleum Gas (LPG) fuels were computed and compared with experimental data reported in literature. It was found that the proposed model performed outstandingly well.

Combustion characteristics of diesel blended with sludge-derived hydrothermal liquefaction oil and its application

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Abstract

In general, hydrothermal liquefaction oil (HLO) has the characteristics of high heating value, low oxygen and water content. If hydrothermal liquefaction oil is added to commercial diesel oil and applied to diesel engines, it can increase industrial fuel diversification and reduce CO₂ emissions. In this study, a spray combustion experiment was employed with a small-scale atomizer for pure diesel and diesel blended 5% sludge-derived HLO spray combustion. In order to compare the pure diesel and 5% HLO blended diesel spray combustion, flame feature, flame temperature distribution of the central axis as well as exhaust emission were detected and discussed. The experimental result indicates that hydrothermal liquefaction oil can yield volatile gas in upstream of diffusion spray flame and facilitate diesel combustion in downstream. However, it leads to increasing NO_x concentration in the case of diesel blended with 5% HLO. For a practical application, a commercial diesel engine was employed the operating test with a full throttle condition for pure diesel and 3% HLO blended diesel. Exhaust gas emission (UHC, NO_x, CO) and fuel consumption rate were measured. The results display that diesel blended with 3% HLO did not influence the performance of diesel engine in terms of gas emission, but fuel consumption rate. Furthermore, applying 3% HLO blended diesel in diesel engine has no serious impact on the combustion phenomenon and pollution emission of commercial diesel engine.

A computationally efficient combustion progress variable (CPV) approach for engine applications

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Abstract

Modern Computational Fluid Dynamic (CFD) simulations are used to support the engine development and to deepen the understanding of complex chemical and physical processes as the formation of soot particles and other emissions based on detailed reaction schemes. The high number of species leads to more accurate and predictive simulation results, but at the same time to unacceptable high calculation times. For practical applications, users often need to choose between accuracy and computational costs. One solution to overcome this drawback of huge CPU times is to solve the chemical progress prior the CFD run and store it in look-up tables. This methodology enables to use detailed reaction mechanism of any size without affecting the CPU time of the CFD run. In this work, we present a tabulated chemistry approach based on a Combustion Progress Variable (CPV) and well-stirred reactors. The model is based on the assumption that the chemical reaction trajectory can be parametrized using chemical enthalpy as progress variable. The tables are generated through the calculation of a wide range of adiabatic constant pressure reactors, and species, thermo-properties and source-terms are stored in a look-up library. The CFD code retrieves source-terms for mixture fraction, mixture fraction variance and chemical enthalpy from the table. The tabulated chemistry model is implemented in the 3D CFD code CONVERGE 2.4. The capabilities of the model are demonstrated using engine and spray applications. For the spray application, the Spray A from the (Engine Combustion Network) ECN is used.

Cycle variation analysis of the partially premixed combustion (PPC) using natural flame luminosity and planar laser-induced fluorescence imaging

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Abstract

We studied the evaluation method for cycle variation of PPC based on natural flame luminosity (NFL) imaging and UHC planar laser-induced fluorescence (PLIF) imaging. Two-dimensional probability distribution index (PDI) and coefficient of variation (COV) of the line-of-sight NFL imaging and UHC PLIF imaging were used to analyze the flame structure and combustion stability. Results indicated that the PDI distributions of NFL intensity and UHC LIF intensity were complementary to each other in space. The overall COVs of NFL and UHC PLIF intensity could predict the combustion stability trends properly. But they were one order magnitude higher than the COV of net indicated mean effective pressure.

Modelling of auto-ignition to premixed flame transition in a context of Dual-Fuel engine combustion

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Abstract

Finding alternative internal combustion engine (ICE) technologies has become a challenge of primary importance as emission regulations are getting increasingly stringent. In particular, conventional applications such as Diesel and spark-ignition (SI) engines see their efficiencies reaching their limits, and extending the potential of ICE needs their operating principle to be rethought. For this purpose, Dual-Fuel (DF) engine combining characteristics relied to SI and Diesel aims at taking the advantages of both technologies while limiting their adverse aspects. Thus, DF engine principle relies on the Diesel spray injection ignition of a lean, high octane number, homogeneous compressed mixture. It allows reducing soot, NO_x , and CO_2 emissions, while maintaining comparable efficiency to conventional Diesel engines. However, auto-ignition (AI) events occurring inside a premixed chamber may lead to various phenomena. They strongly depend on the reactivity stratification encountered around these hot spots and the whole phenomenology following their onset has to be thoroughly investigated in order to avoid any deteriorating effect, such as knock. A numerical study is proposed here to shed light on the combustion process emerging from an AI event. The simulations consist in the examination of the reaction front propagation induced by the spontaneous ignition of hot fresh gases in a reactivity stratified medium. A one-dimensional regular mesh was used to run a set of simulations covering a wide range of reactivity gradients. The cell size of $10\mu\text{m}$ allows a sufficient resolution of the reaction front in the horizontal direction, and symmetrical conditions were imposed at the top and bottom of the domain. The left and right ends of the domain use respectively an adiabatic wall, and an outlet imposed pressure boundary condition. The reaction front evolves in an adiabatic, constant pressure environment. To study a reactivity stratification, a linear variation of the initial temperature was imposed in the domain. The reaction front displacement speed calculated in the fresh gases $S_d(GF)$ was compared to the one of an AI propagation in non-uniform conditions predicted by the Zeldovich theory (S_{AI}) and to the one of a canonical 1D laminar flame (S_L), all at the same pressure-temperature-enthalpy level. Multiple amplitude and spatial extent of thermal stratification were tested, and one consistent trend was identified: At early instants, $S_d(GF)$ matches well with S_{AI} whereas later instants see $S_d(GF)$ reaching close to S_L values, after a transition time. This time also shows a similar trend for the evolution of the reaction thickness δ_{reac} , which reduces until permitting the laminar flame characteristic diffusion-reaction balance to take place. As a result, the transition from one regime to another seems intrinsically connected to the reaction front thickness dynamics and not only to its displacement speed.

Reactivity controlled compression ignition combustion using renewable fuels

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Abstract

To reduce environmental impact of combustion based technologies in terms of greenhouse gas emissions and emissions of directly health hazardous emissions, in the presented study, Reactivity Controlled Compression Ignition (RCCI) was established with a combination of two renewable fuels being Hydrotreated Vegetable Oil (HVO) and Methane. The main combustion, performance and emission indicators of the engine operation depending on start of injection timing and energy share supplied by natural gas have been deeply investigated and presented in the results. The study thus establishes interrelations between different engine control strategies, including direct injection timing, engine thermodynamic parameters and engine-out emissions. The general goal of engine operation under RCCI operating conditions being simultaneous reduction of NO_x and PM was achieved with appropriate combination of engine control parameters and utilization of alternative fuels featuring low CO_2 footprint.

Experimental investigation of the impact of advanced injection strategies on a LTC concept for a single cylinder CI engine

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Abstract

In the foreseeable future, the transportation sector will continue to rely on internal combustion engines. Therefore, reduction of engine-out emissions and an increase in engine efficiency are important goals to meet future legislative regulations. One viable option, which provides lower peak temperatures and increased mixture homogeneity and thus simultaneously reduces nitric oxides as well as soot, is a low-temperature combustion (LTC) concept. However, LTC might result in an increase of unburnt hydrocarbon, carbon monoxide, and combustion noise due to early combustion phasing and lower engine efficiency. Various studies show that these drawbacks can be compensated by advanced injection strategies, e.g. employing multiple injections. The aim of this work is to identify the optimum injection strategy, which enables a wide range of engine operating points in LTC mode with reduced engine-out emissions. To achieve this goal, experiments with variations in the number of injections, injection timings of each injection, injected amount of fuel, and EGR-rate are carried out and analyzed.

Comparison of two velocity-pressure coupling algorithms for laminar non-premixed combustion

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Abstract

The investigation of laminar combustion by computational fluid dynamics has been improved for years, and the pressure-velocity coupling is one of main difficulty. Because of this, a comparison of two segregated algorithms with SIMPLE-type pressure-velocity coupling for laminar non-premixed combustion is presented in this work. In the simulations the laminar flow field was obtained solving the Navier-Stokes equations and the non-premixed combustion was treated with the flame sheet model. Velocity fields and computation times are compared for two different pressure-velocity coupling algorithms and the results indicated the same predictions for both algorithms and quite different computation times.

Effect of burner diameter and diluents on structure and stability of co-flow laminar diffusion flames of diluted methane fuel

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Abstract

The present research work has been carried out to study the flame structure and stability of nitrogen and helium-diluted methane flames in a laminar non-premixed oxygen-enhanced co-flow configuration. A wide range of experiments for all four varying parameters (i.e. oxygen and fuel percentage, jet and co-flow velocity) are performed using nitrogen and helium as diluents in methane with two different burners of 4 and 9-mm diameter, respectively. The general approach for analyzing the variation of oxygen enrichment level is to reduce the oxygen percentage from 100 % to the blow-off limit in the oxidizer stream for a fixed diluted fuel composition, jet and co-flow velocity. The other parameters are also varied in similar fashion. The jet flow rates are maintained at 0.5 liter per minute (LPM) and 1 LPM. The co-flow rate is kept at 10 LPM for all the cases. The flame length and lift-off height are measured under the influence of oxygen enrichment level, fuel dilution, jet and co-flow rate. It is observed that the flame length in case of the 4-mm burner diameter is higher than the 9-mm burner flame and usually the 9-mm burner flames can sustain up to a lower oxygen percentage compared to the 4-mm burner. This is arguably because the same jet flow rate would cause a lower jet velocity in case of the higher burner diameter. The effect of different diluents is also found to be significant. For helium flames, it is observed that the flame length initially increases as the oxygen content decreases and then it starts to drop beyond certain oxygen percentage, whereas flames of nitrogen-diluted mixtures exhibited a continuously increasing flame length trend. The lift-off height dependence on burner diameter is observed to be opposite, in sense, to the flame length dependence, as the 9-mm burner flames get lifted higher than their 4-mm counterparts. This can be attributed to an increased effect of buoyancy in case of the higher burner diameter and that can, in turn, be explained in terms of the Richardson number. Stable lifted flames are observed for helium flames, whereas all the nitrogen flames were almost anchored in spite of less than unity Schmidt number for both the cases.

Analysis of $\text{CH}_2\text{O}_x\text{OH}$ as marker for fuel-rich air to pure oxy-fuel flames under higher preheat temperature and elevated pressure

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Abstract

The scope of the present work is a numerical and experimental investigation about the range of validity in terms of applicability of $\text{CH}_2\text{O}_x\text{OH}$ as a marker for the heat release rate (HRR) for fuel-rich air to pure oxy-fuel flames including preheating and elevated pressure. Therefore, laminar, freely propagating 1d CH_4 flames were calculated, where oxygen content in the oxidizer (from air to pure oxy-fuel combustion), inlet temperature and pressure were varied for a wide range of the equivalence ratios. The preheat temperature and pressure were parametrically changed from 300 K to 573 K and 1 bar to 5 bar, respectively. Different reaction mechanisms were used, namely GRI30, DLR, USC/II, Caltech2.3 and ABF. The performance of the $\text{CH}_2\text{O}_x\text{OH}$ as a marker for HRR is assessed in terms of correlation coefficients of their profiles in laminar flames. The comparison of the obtained correlations of CH_4/air and CH_4/O_2 flames shows that in case of air combustion, the HRR can be accurately estimated by the product of $\text{CH}_2\text{O}_x\text{OH}$ for slightly rich flames ($\Phi = 1.5$), whereas the quality of the correlation degrades with increasing equivalence ratio. In contrary, the correlation coefficient increases with higher equivalence ratios in the fuel-rich domain for enhanced oxygen contents in the oxidizer. For pure oxy-fuel combustion, the best correlation is found at an equivalence ratio of approximately $\Phi = 3.0$. Elevated pressure leads in all flames to better correlations at lower equivalence ratios compared to standard inlet conditions, whereas preheating induces the opposite trend and expands the valid regime. A series of CH_4/air flames were also investigated experimentally in a range of the equivalence ratio between $1 < \Phi < 2$ at standard inlet conditions. The qualitative CH_2O (excitation at 355 nm) and OH (excitation at 283 nm) concentration were resolved applying two-dimensional LIF for flames stabilized at a McKenna burner. Comparisons show similar trends for measurements and numerical simulations.

Numerical simulation of flames in narrow combustion chambers

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Abstract

Small-scale combustion is currently studied as a potential technology for embedded low power sources [1]. The high energy density of hydrocarbon fuels, about 60 times larger than that of most efficient lithium-ion electrical batteries, motivates the development of these small-scale combustion devices. In small-scale combustion, the flame sits in a narrow channel leading to a specific interaction between the flame and combustion chamber, whose understanding is a keystone for engineering design in this field. A two-dimensional flame stabilised in a planar channel, of internal height $L_i = 5$ mm and of external height $L_e = 7$ mm, with 1 mm thick walls made of quartz, is simulated with a fully compressible solver as in [2]. A stoichiometric mixture of methane-air at the ambient air temperature $T_o = 300$ K and atmospheric pressure is considered in a laminar flow regime. A two-way flow/solid coupling is organised to solve heat transfers between the gas and the wall and the alternate direction implicit Douglas-Gunn method [3] is adopted to solve for the temperature in the solid. The exterior wall surface exchanges energy with the surrounding air at 300 K with a coefficient $h_o = 30$ W·m⁻²·K⁻¹. Radiative heat loss of the solid to the ambient air is also accounted for through a gray body hypothesis. The response of the premixed flame shape to various operating conditions is analysed in terms of flame propagation velocity and flow topology in the vicinity of the reactive front. A focus is made on the interrelations between the flame speed, the configuration taken by the flame surface, the flow deviation induced by the heat released and the fluxes at the wall. Compared to an adiabatic flame, the flame speed increases with edge-flame quenching at an isothermal cold wall in the absence of a boundary layer, decreases with a boundary layer, to increase again with heat transfer coupling within the wall. A regime diagram is proposed to delineate between flame shapes in order to build a classification versus heat transfer properties. Finally, upstream reaction zone propagation in a narrow channel after introducing heat upstream of a premixed flame front has been studied numerically, along with the role of gravity in the symmetry breaking of lean premixed flames.

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Features of cellular flames propagating between closely spaced parallel plates

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Abstract

Laminar premixed flames exhibit instabilities of hydrodynamic and thermal-diffusive types, leading to growth of perturbations, wrinkling of flame front and formation of cells. In this work, results of an experimental study on cellular flame propagation are presented in the configuration where combustion occurs in a gap between two parallel plates, with the separation distance (few millimeters) much smaller than the lateral sizes of the plates (60 cm diameter). Such a quasi-2D setup allows one to perform visualization of flame front propagation features, including the instantaneous shape of the leading edge, and overall flame propagation pattern obtained by the long-exposure photography. Results of experiments on stoichiometric and fuel-rich propane flames are presented, including those obtained upon ignition at one or two points. Fractal dimension of flame front is evaluated at different distances from the ignition point. The results presented in the current paper confirm that Hele-Shaw cell has many advantageous features for studying the instability of flame propagation, including the unique possibilities for flow visualization. In particular, the technique of long-exposure photography allowed us to observe not only the local behavior of unstable flame (inception and merging of cells), but also enables the global flame behavior to be revealed. For example, it has been shown here that some cells in the flame form stable pairs which are long-living and propagate all the way from the ignition source to the boundaries of combustion chamber. The fractal dimensions of premixed flames in Hele-Shaw cell are estimated to be between 1 and 1.1, with the fractal dimension increasing with the distance travelled by flame and, accordingly, flame length. The experimental results presented in this paper provide important qualitative and quantitative data for validation of analytical and numerical models of flame instability and behaviour in microchannels.

Investigation of NO_x emission for different laminar premixed CH₄-fuel blends stabilized on a flat-flame burner

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Abstract

To preserve resources and reduce pollutant emissions, the demand of various efficient and climate friendly technologies to be implemented in industrial and domestic appliances emerged. In this context, the condensing gas boiler embodies a promising technology. It allows to recover the latent heat of the flue gas and thereby increases the energy efficiency significantly. Nonetheless, the further development of condensing boilers is still a relevant issue, since emission levels are and will be further restricted by legal regulations. Great importance is given to nitrogen oxides (NO_x). The aim of this study was to experimentally investigate the NO_x emission for different laminar premixed CH₄-fuel blends stabilized on a flat-flame burner, since previous work indicated that the majority of NO_x formation occurs within the flame zone. The burner was designed to closely match the properties of the burner used in the cylindrical heating unit of a condensing gas boiler, but also allowing optical access in addition to probe measurements. A planar flame structure was chosen over a cylindrical flame, since it is easier to investigate (no curvature effects). Additionally, a control or determination of boundary conditions is technically feasible in this setup. Local measurements of the temperature and NO_x concentration were performed at different heights above the burner surface. By means of qualitative OH-LIPF measurements, flame front location and OH radical distribution were evaluated. The CH₄+H₂-flame showed the lowest NO_x emissions of all fuel blends, although it produced the second hottest flame. The origin was assumed to be caused by the very short residence time in the flame zone and the relatively low radical concentration in the post flame zone. The high content of H₂ in the CH₄-fuel blend was linked to inhibit NO_x formation through the prompt NO pathway due to less CH radicals in the flame when comparing it with a pure CH₄-flame. The CH₄+C₃H₈-flame produced the highest temperatures, which consequently lead to the highest NO_x concentrations of all investigated CH₄-fuel blends. Additionally, NO_x formation was promoted by the longest residence time for this fuel blend.

Laminar burning velocity and extinction strain rates of $\text{H}_2/\text{CH}_4/\text{O}_2/\text{N}_2$ in flat flames

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Abstract

In this paper the extinction behavior of laminar non-premixed and the laminar burning velocity (LBV) of premixed methane and hydrogen flames are evaluated. The aim of the work is a better understanding of fuel components in interaction with inert gases and oxygen reduced air. For these gas mixtures, the extinction rates and LBV as two important physical-chemical properties were investigated. These properties are basic values for validation of reaction mechanisms and the specific design of burner systems. For this purpose, an experimental setup with a counter-flow and a Heatflux burner was used. The extinction limits and strain rates of the counter-flow for non-premixed $\text{H}_2/\text{CH}_4/\text{O}_2/\text{N}_2$ flames at atmospheric pressure are experimentally determined. Furthermore, the detailed flame structure and the extinction limits are visualized by using a high-speed- and an OH^* -chemiluminescence camera system. The results pointed out that the blow-off limits are enhanced with higher fuel substitution in the flames. In addition, it could be shown that more distance between the nozzles have a dramatic impact on the strain rate whereas the OH^* detection allows for the detection of the flame position relative to the nozzles. Furthermore, the Heatflux burner method was applied to measure LBV of hydrogen containing fuel blends. Therefore, different hydrogen containing fuels were tested within a range of equivalence ratios between 0.7 and 1.6 and for a gas mixture with lower and higher oxygen partial pressure from $Y_{\text{O}_2}=0.14$ to $Y_{\text{O}_2}=0.21$. Initial temperatures of 298 K up to 378 K were tested for atmospheric conditions. In addition, it could be shown that the LBV reduction is significantly influenced by the oxygen content. With these results, the lack of data for hydrogen containing gases could be partly closed and helps to validate reaction mechanisms for better simulation of internal combustion with exhaust gas recirculation (EGR) or oxygen enriched atmosphere for special combustion systems.

Numerical generation of multidimensional flamelet databases using an adaptive wavelet method

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Abstract

Many physical problems are characterized by phenomena having wide ranges of spatial and temporal scales. When a system of partial differential equations (PDEs) is employed to model such phenomena, high resolution discretization is required for solving the finest spatial and temporal scales. Accurate numerical simulations of unsteady, compressible and reactive flows on a fixed computational grid is particularly challenging in terms of computational resources. The wavelet-based adaptive methods are able to provide a direct measure of the local error at each grid point, this feature allows to control spatial grid adaption, simply removing grid points in regions having smooth fields. A Wavelet Adaptive Multiresolution Representation (WAMR) code is used for the numerical integration of the one-dimensional laminar diffusion flames equations. Taking advantage of the method capability to generate accurate databases with compact size allocating the data only where needed, accurate chemical kinetic mechanisms involving a large number of chemical species and reactions can be used to solve flamelet problems. Furthermore, more complex Equations of State (EoS) can be adopted to better describe the fluid behaviour in non-ideal conditions. This allows the generation of detailed multidimensional flamelet databases for flows which usually operate under supercritical and near-critical conditions. In such conditions, the thermodynamic and transport properties exhibit large changes in the phase space of the thermodynamic variables. These steep gradients are accurately and efficiently captured by the WAMR algorithm, with an associated reduction of the number of DOFs, allowing a highly efficient flamelet database generation. The capability of the wavelet method to well capture strong variations of the solutions with high compression degree is shown by integrating the flamelet equations for different values of pressure p scalar dissipation rate χ_{max}^0 and wavelet threshold parameter ε . For example, by fixing $p = 60$ bar, $\chi_{max}^0 = 200 \text{ s}^{-1}$ and $\varepsilon = 10^{-4}$ a compression ratio of $\pi = 99\%$ is reached since the selected low error requires a high refinement around the steep c_p variation and a course grid is used elsewhere. Furthermore, it is shown that smaller solution variations are well captured with small threshold parameters, while if lower accuracy is requested WAMR automatically ignore these by using a coarser grid. The computational cost associated with the evaluation of the thermodynamic properties in near-critical and supercritical conditions is extremely reduced when dynamically adaptive grids are used, because it represents approximatively the 95% of the total computational time associated with the evaluation of the right hand side of the flamelet equations for a single point. These results represent the preliminary work to build a compressed multidimensional tabulated flamelets through WAMR.

Influence of natural gas composition and hydrogen addition on fundamental flame characteristics

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Abstract

With increasing fuel variability and the prospect of hydrogen addition, detailed understanding of physical and thermo-diffusive properties of methane-higher-hydrocarbon-hydrogen mixtures at lean conditions is required. An outwardly propagating spherical flame has been studied for CH_4 and C_3H_8 with H_2 addition, alongside blends of $\text{CH}_4/\text{C}_3\text{H}_8$, and $\text{CH}_4/\text{C}_3\text{H}_8/\text{H}_2$ to characterise changes in the thermo-diffusive flame response. Analysis of the blends show hybrid response relating to the sensitivity of individual fuel components to flame stretch and corresponding Lewis number trend.

Abstract_S3_AIII_40

A DNS study of the impact of gravity on spherically expanding premixed flames

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Abstract

Direct Numerical Simulations (DNS) of spherically expanding laminar premixed flames have been conducted employing detailed finite rate chemistry. For all flames, the fresh mixture conditions are set to yield a small flame speed such that the flame dynamics are strongly affected by buoyancy. This leads to a strong deformation of the originally spherical flames such that the flame stretch, the strain rate, and the curvature vary along the flame front significantly. The simulations feature large domain sizes to avoid confinement effects on the flame dynamics and long integration times to investigate the long-term behavior of the flames. A lean methane/air and a rich hydrogen/air flame diluted with molecular nitrogen are considered, so the influence of buoyancy on flames with different Markstein numbers can be assessed. Additionally, a DNS of the rich hydrogen/air flame with unity Lewis number for all species is conducted to assess the Lewis number effects on the buoyant flame dynamics. In all simulations, the flames initially expand spherically, and eventually buoyancy leads to the deformation of the flames such that a mushroom-shaped flame is formed. The effect of buoyancy on the flame dynamics is found to be governed by the Richardson number, which describes the relative importance of buoyancy with respect to the flame expansion, unless significant variations of the flame propagation speed due to strain rate and curvature occur as for the hydrogen/air flame with non-unity Lewis numbers. In contrast to spherical flames, no linear dependence of the flame's displacement speed on stretch is observed. However, the displacement speed is found to be proportional to strain rate and curvature, which both vary independently along the flame front of a buoyant flame. This correlation enables a linear extrapolation to zero curvature and strain rate, which is in reasonable agreement with the laminar burning velocity of an unstretched premixed flame with extrapolation errors smaller than 5%.

Laminar premixed flames of ethanol-water-air mixtures

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Abstract

Next to the use of fossil fuels, other fuels are increasingly becoming the focus of public discussion. Reasons for the search for alternatives are the limited crude oil reserves, but also the environmental pollution and emissions that occur during the combustion of mineral oil products and their additives. An alternative to diesel or gasoline offer bio-alcohols such as ethanol. An important property is the adiabatic laminar burning speed. To understand the impact of water content in ethanol, either due to long term storage or due to water injection strategies during combustions, an extensive measurement campaign was carried out. The determination of the laminar burning velocity of ethanol-water-air was performed with the heat flux method. This method is well established for the determination of the adiabatic laminar burning velocity [1,2]. The mixture containing 0 to 40 % water by mole. The flames were investigated with the initial temperature of 358 K and the equivalence ratio (ϕ) range was varied from 0.7 to 1.4 at atmospheric pressure. The laminar burning velocities obtained in this study, along with their uncertainties, are compared against with the predictions of three models: the reaction scheme developed by Moshhammer et al. [3], Shrestha et al. [4] and a model derived from the group of Konnov [5]. The experimental laminar flame speed (SL) for ethanol-water-air mixtures decrease with increasing the water content 10 - 40%. General the experimental data for SL show a better agreement with the model of Konnov et al. [5], which contains updated methanol sub-mechanism agrees best with present data. The model of Konnov et al. [5] leads to a slight underestimation of the SL in particular at rich conditions by below 2 cm/s. The experimental results for ethanol-water-air flames, which are good agreement with the model [3] at lean conditions with a underprediction of around 3 cm/s. For the dilution of 10 % water the model tends to underpredict the experimental SL by around 10 cm/s. For equivalence ratio above 0.9 the deviation increase between the model of Moshhammer et al. [3] and experimental data. The model of Shrestha et al. [4] predicts the experimental results very well at rich mixtures with the difference in SL being around 2 cm/s. At lean- and stoichiometric conditions this model shows larger deviations than the model of Konnov et al. [5]. All models show an underprediction of SL at stoichiometric conditions.

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Abstract_S3_AIII_42

Laminar flame speed simulations of methane-air and n-heptane-air mixtures by using an adapted mechanism

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Abstract

In the dual fuel combustion process, various types of fuel inhomogeneously distributed within the combustor interact in complex ways with each other. For simulating these processes, a mechanism is necessary that correctly reproduces the interactions of the fuels. Based on the Complete San Diego mechanism with the n-heptane extension, a mechanism for the simulation of dual fuel combustion processes is currently under development. The evaluation of the adapted mechanism is performed by comparing calculated and measured ignition delay times of methane-propane-n heptane mixtures at up to 100 bar. Furthermore, the simulated laminar flame speed of methane-air and n-heptane-air mixtures between 1 and 25 bar is compared with experimental values. It should be noted that the development is not yet completed, the paper reports on the actual status of the adaption process.

Propagating edge flames in nonpremixed coflow jets under electric fields

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Abstract

To investigate the effect of the electric field on propagating edge flames, we employed numerical and experimental methods in an axisymmetric coflow jet system. In general, when electric fields applied to a flame, charged species, which are generated in a flame zone via chemi-ionization, are separated according to their polarity and move to each corresponding electrode (a cathode pulls positive ions and an anode attracts electrons and negative ions). Such breakdown of neutrality creates the electric body force resulting in a bulk flow modification—ionic wind. Recent studies experimentally showed that the ionic wind blows bi-directionally from a flame to both an anode and a cathode, and experimental results supported a hypothesis that applied electric fields have significant effects to a flame mostly through a flow modification due to ionic wind rather than altering chemistry or thermal heating. In order to further understand the previous observation, two-dimensional numerical simulations for hydrocarbon lifted flames were conducted. The results of simulation reproduced the previous experimental study and it has a good agreement. The flame propagated toward the nozzle in voltage charged condition because of the negative velocity zone near the nozzle caused by ionic wind.

Effect of diluent addition on methane/nitrous oxide inverse diffusion flame

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Abstract

In this study, the effect of adding dilution gas on the combustion characteristics of N_2O/CH_4 inverse diffusion flame (IDF) was conducted experimentally and numerically. The purpose of this study was to examine the combustion characteristics of CH_4/N_2O IDF with different diluents, namely He, CO_2 and Ar, respectively. A coaxial burner with three ports is used in the experiment. A mixture of nitrous oxide and different diluents (Ar, He, CO_2) was introduced through the central tube, the annular port was introduced with methane, and the outer port was introduced with a mixture of 33% O_2 and 67% N_2 . It attempted to investigate the effect of adding different concentrations of diluent and flow rate on the flame feature, and meantime the transition of flame feature and inception of IDF can be theoretically and mathematically predicted. Eventually, some important contaminants (O_2 , CO_2 , NO_x , CO) were measured and discussed with regard to various dilution effect. After understanding the effect of the initial addition of dilution gas on the combustion characteristics, CHEMKIN PRO was used to employ more in-depth discussion on the flame structure, temperature, pollutant emission and pollutant forming mechanism for the addition of diluents. The influence of diluent addition on combustion characteristics attributes to three effects, inert effect, thermal/diffusion effect and chemical effect, respectively. Preliminary experimental results showed that in the flame phenomenon, with the addition of different concentrations of diluent gas, there are several different flame features, that is, normal diffusion flame, closed-tip inverse diffusion flame, opened-tip inverse diffusion flame, liftoff flame. In the theoretical analysis, the formation of the inverse diffusion flame can be divided into several stages: (1) the formation of a normal diffusion flame, and (2) the appearance of the rich-branch, the equivalent condition, and the lean branch of the inner flame sequentially, forming an inverse diffusion flame, (3) the rich, equivalent conditions and lean branches of inner and outer flame form an closed-tip flame in sequence, and finally an opened-tip inverse diffusion flame is formed. In the numerical simulation part, the thermal/diffusion effect dominates the increase of flame temperature with the Ar addition, while the inert effect and chemical effect dominate the reduction of flame temperature with Ar and CO_2 addition. Furthermore, for the pollutant emission, when Ar is added as a diluent gas, the inert effect dominates the formation of NO_x before the concentration is 40%, and after 40%, it is dominated by the thermal/diffusion effect, and the CO generation part is mainly dominated by the thermal/diffusion effect.

Determination of temperature and water-concentration in fuel-rich oxy-fuel methane flames applying TDLAS

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Abstract

Combustion processes with pure oxygen (oxy-fuel) instead of air as an oxidant are attractive for e.g. high temperature thermal or thermochemical and gasification processes. The absence of nitrogen as an inert gas leads in such combustion processes to an increase in temperature and species concentrations. The scope of this study was the determination of axial temperature profiles of flat fuel-rich methane-oxygen flames (equivalence ratios from $2.5 \leq \phi \leq 2.9$). A Heat-Flux-burner was used to stabilize a quasi-adiabatic one-dimensional flame. The inlet temperature of the gas mixture was kept constant at $T_p = 300$ K and the inlet velocity equals the laminar burning velocity, which was determined in a preliminary experimental study. The in-situ temperature and H_2O -concentration measurements were performed using Tunable Diode Laser Absorption Spectroscopy (TDLAS). Laser measurements were carried out for three different diode lasers at center wavelengths $\lambda_{cw} = 1344.5$ nm, 1392.3 nm and 1853.5 nm, respectively, where multiple absorption peaks of the water molecule were investigated. Additionally, one-dimensional calculations with detailed chemistry were performed using the PREMIX code together with the GRI3.0 and CalTec2.3 mechanisms and compared to the experimental results. The results of the temperature measurements showed temperature peaks in the flame zone and a temperature decrease in the endothermic post flame zone, where the synthesis gas is formed. The measured peak temperatures exceed calculated equilibrium temperatures by approximately 100 K to 400 K, which indicate the phenomenon of super adiabatic flame temperatures (SAFT). Both reaction mechanisms showed a similar trend in the decrease of the temperature in the post flame zone and were in good agreement with the measured temperature. In contrary, the decomposition of the water concentration in the post flame zone depends highly on the applied chemistry scheme. Here, the CalTech2.3 showed excellent performance in the comparison with the experimental data for $\phi > 2.5$. For $\phi = 2.5$ the GRI3.0 was better performing.

Experimental investigation of synthesis gas production in fuel-rich oxy-fuel methane flames

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Abstract

Combustion processes with pure oxygen (oxy-fuel) instead of air as an oxidant are attractive for e.g. high temperature thermal or thermochemical and gasification processes. The absence of nitrogen as an inert gas leads in such combustion processes to an increase in temperature and species concentrations. The scope of this study is the determination of axial profiles of major educts (CH_4 , O_2) and the development of the syngas products such as H_2 , CO and CO_2 in flat fuel-rich methane-oxygen flames ($2.5 \leq$ equivalence ratio $\phi < 3.0$). A Heat-Flux-burner was used to stabilize a quasi-adiabatic one-dimensional flame. The inlet temperature of the gas mixture was kept constant at $T_P = 300$ K and the inlet velocity equals the laminar burning velocity, which has been determined in a preliminary experimental study. Gas samples were taken at different heights above the burner (HAB) using a fused silica and a ceramic probe and analyzed by a GC/MSD. First, the influence of inlet diameter of the probe on the experimental results was investigated in a parametric study, resulting in a minimum inlet diameter of 1 mm for measurements downstream of the flame. Additionally, one-dimensional calculations with detailed chemistry were performed using the PREMIX code together with the GRI3.0 and CalTech2.3 mechanisms and compared to the experimental results. The results of the analyzed gas samples show a rapid reduction and rapid increase in the flame zone of the educts (CH_4 , O_2) and products (H_2 , CO and CO_2), respectively. Both mechanisms show a too sharp gradient of the synthesis gas production in comparison with the experimental results, nevertheless a tendency towards the CalTech2.3 scheme is observed. In the post flame zone the experimental determined species concentrations of H_2 fit the GRI3.0 and CO the CalTech2.3, for all investigated flames.

2D and 3D numerical simulation of chemiluminescent radical concentrations during side-wall quenching of premixed methane and propane flames

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Abstract

Side-wall quenching (SWQ) is investigated with 2D and 3D simulations of an experimentally measured flame setup. Quenching distances are identified by different markers, based on OH, OH* and CH* concentration profiles as well as temperature, which show qualitatively good agreement with measurements for two flames at different equivalence ratios. 3D simulations are necessary to reproduce the velocity field from experiments but do not affect the quenching distances. 1D simulations demonstrate the influence of different reaction mechanisms on quenching distances.

Experimental analysis of lean hydrogen premixed flames propagating in a confined vertical channel

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Abstract

An experimental study of lean hydrogen-air premixed flames propagating in a confined combustion chamber is presented in this paper. The combustion chamber has a rectangular prismatic shape of 900 x 200 x 10 mm (length x width x thickness). The thickness of the channel can be varied from 10 to 1 mm in order to study the effect of the gap size on the flame propagation. The hydrogen flames travel vertically from the top of the chamber, which is open to the ambient, to its closed bottom. First, the dependency on the mixture thermofluid properties related to the equivalence ratio is analyzed by keeping constant a 10-mm thickness of the combustion chamber. Two main regimes were found for the range of lean hydrogen-air mixtures analyzed (10% to 15% in volume of hydrogen). For mixtures up to 13% of hydrogen, the flame propagates with a violent oscillatory motion of a frequency around 80 Hz, driven by the acoustic pressure waves present in the chamber. For this case, the flame is almost planar and shows an unstable finger-like front shape, characteristic of the secondary thermoacoustic regime. In richer flames, the sound-flame interaction is much weaker and the reaction front remains almost unperturbed. Second, the effect of the channel thickness is addressed. In narrower channels up to 4 mm, only a decrease of the maximum pressure within the chamber was reported. In very narrow channels (< 2 mm), the heat losses are dominant, leaving unburned areas and controlling the dynamic of the reaction front. In these channels, the flame propagates either as a fractal making it look like a snowflake or as a two-headed hemispherical flame that travels with a steady propagation velocity.

Laminar burning velocity measurements of ethanol-air and methanol-air mixtures at atmospheric and elevated pressures on a novel heat flux method setup

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Abstract

To implement as well as analyze fuels in new and existing burner systems, detailed knowledge of the combustion behavior is required. The laminar burning velocity is a fundamental property of reactive fuel-oxidizer mixtures. It has a high importance for the validation and improvement of chemical reaction mechanisms and the design of combustion systems, because it gives information about flame behavior and stability. Thus, laminar burning velocity data aids to improve, test and develop fuels as well as new and efficient combustion systems. Several methods are most commonly used to measure the laminar burning velocity, including spherically expanding flame method, stagnation flame method, Bunsen flame method and the Heat Flux method. In this study the Heat Flux method was applied, because it allows direct measurement of laminar burning velocity, without the need to compensate for heat losses or flame stretch, by stabilizing a nearly adiabatic planar flame. This leads to a decrease in uncertainties and scatter compared to other methods. Several candidates from the group of alcohols are of interest as additive or replacement for fossil-based fuels. This study focuses on ethanol, which can be produced through fermentation of biomass, and methanol, which can be produced through chemical reaction of carbon dioxide and hydrogen, potentially with the use of solar-energy. A recent comprehensive review has shown that even for simple alcohols such as ethanol and methanol there are still gaps and scatter in available data for laminar burning velocities, requiring further investigation [1]. The Heat Flux method itself has typically been used so far for gaseous fuels in moderate pressure ranges and for liquid fuels at atmospheric pressure. In order to extend the method to a higher range of pressures for a larger variety of fuels, a new Heat Flux method setup has been designed and built, which is suited for gaseous and liquid fuels at both atmospheric and elevated pressure. Measurements were performed for ethanol-air and methanol-air mixtures over a range of conditions including equivalence ratio (0.8 to 1.3), inlet gas temperature (318 to 338 K) and pressure (1 to 5 bar). The results were compared to experimental data found in literature, detailed chemical reaction mechanisms and an empirical correlation for pressure, and discussed subsequently. [1] A.A. Konnov et al., Prog. Energy Combust. Sci. 68 (2018) 197-267.

Abstract_S3_AIII_50

Flames interaction under velocity and equivalence ratio gradients

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Abstract

The current work aims to explore the behavior of laminar V-shaped flames under different stratification regimes. Direct numerical simulations were performed with a two-dimensional numerical model, including detailed chemical kinetics, species transport and conjugated heat transfer between the fluid and the burner was used in the simulations. Results show clear differences between homogeneous and stratified flames. While velocity gradients change the flow field at the wake of the burner, equivalence ratio gradients create a flux of heat and radicals. When combined, these two strategies lead to a considerable increase of the heat release rate at the flame base, promoting flame stabilization.

Abstract_S3_AIII_51

Modeling the smoldering of a static bed of biomass with inert solids

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Abstract

This work presents a Multiphysics model to simulate experimental data of smoldering propagation in a mix of biomass and silica sand, in a static packed bed. The packed bed has been modelled as a variable density, porous media, in a tubular flow reactor. The main purpose is to formulate a simplified kinetic model to describe the global evolution of solid particle packed bed. Finally, the flexible, theoretical structure of the model allows further extension to processes involving the oxygen-controlled, thermal degradation of other unconventional solid fuels.

Abstract_S3_AIII_52

A detailed investigation on a novel combustion heat exchanger design for heating applications**B. Yadollahi, N. Karimi, M.C. Paul****Systems, Power and Energy Research Division, School of Engineering, University of Glasgow, Glasgow*

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Abstract

A novel Combustion Heat Exchanger (CHE) designed for household heating applications is investigated numerically. A lean-burn porous burner is in the heart of CHE providing hot gases for heat exchangers of the system. A model is developed in STAR-CCM+ and burner configuration, air-to-fuel ratio and power range effects on the combustion performance are investigated using a step-by-step approach. Results show that the burner can operate in a wide range of power and lean air-to-fuel ratios, enabling high flexibility in the operating range and lowering CO₂ and emissions. The design also shows strong potentials for applications of renewable fuels such as biosyngas and biogas. Clean combustion performance, with lower CO₂ emissions and improved thermal efficiency, therefore, indicates the promising design of CHE for future heating applications.

Development of a porous burner for low calorific gaseous fuels offering a wide operating range

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Abstract

In a process for the production of high purity hydrogen (H_2) from biogas, an offgas is generated within the H_2 purification. Approximately 25 %-vol of the offgas consists of combustible components, most of which is H_2 . The offgas is stated as a low calorific gas, since it has a heating value lower than natural gas. In order to enhance the efficiency of the H_2 production process, a combustion system combined with heat exchangers for reutilization of sensible heat is integrated into the process. By this measure, the process efficiency increases from 70 % to 80 %, based on higher heating values. Besides a nominal operation of the plant, further operation modes have to be considered in the development of the burner: Partial load operation under reduced offgas supply and a start-up procedure where biogas serves as a start-up fuel for the burner. Additionally, varying offgas compositions have to be taken into account. These requirements define the objectives for the capabilities of the combustor: flexibility regarding the fuel and a wide range of thermal power modulation. In order to account for these challenges, premixed combustion within a porous inert medium (PIM) featuring a kinematic flame stabilization mechanism is applied in the present work. Heating values of the fuels are 2 MJ/kg and 18 MJ/kg for offgas and biogas according to their nominal composition. The process requires an adiabatic flame temperature of 1400 °C, leading to preheating temperatures T_0 for premixed fuel-air mixtures of 550 °C for offgas and 180 °C for biogas. The effective flame speed in PIM for high T_0 was calculated using an extended version of Chemkin PREMIX. The calculated effective flame speeds range from 1.6 m/s to 14.2 m/s, under nominal conditions, depending on the fuel. While ensuring a modulation range in thermal power from 3-34 kW for a kinematic flame stabilization the cross-section area within the burner has to vary significantly. Therefore, a conical shaped structure of 10 PPI random foam Si-SiC with an inlet diameter of 12 mm and outlet diameter of 120 mm at a length of 150 mm was designed. In an experiment the temperature profile along the central axis was resolved using S-type, ceramic coated thermocouples. From these profiles and corresponding mass flows the effective flame speed was determined. The experimental results are in excellent agreement with numerical predictions.

Abstract_S3_AIII_54

Experimental study on the application of the water tube in porous media burners

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Abstract

The objectives of this study are the comparison of combustion characteristics in conditions with and without a water tube and the investigation of thermal efficiency in a two section porous media burner. The experiments are conducted with the variation of equivalence ratio and mixture velocity. As a results, the SIC foam of 10 ppi and 40 mm is used to experiments because the stable flame zone is most widen. The stable flame zone in the condition with the water tube is broader and shift to the regime of lower mixture velocity than in the condition without the water tube. In the condition with the water tube, the NO_x emission is lower markedly than the condition without water tube.

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Poster Session 4



Abstract_S4_All_01

The study of combustion in gas generator with a charge of solid propellant enriched by metal

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Abstract

The features of combustion of the solid propellant enriched by metal in the gas generator have been investigated. It is shown that the solid propellant enriched by metal burns in the mode of preferential heat release in the condensed phase. It is found that the metal fuel in a condensed phase is not a simple heat sink, and it is active in combustion. Oxidation of the metal in the condensed phase ensures the maintenance of heat balance during the combustion of solid propellant.

Abstract_S4_All_02

Development of a variable thrust water breathing engine

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Abstract

In the present study a hydro reactive fuel with a high ejection efficiency was developed and tested for a water breathing engine and, the variation of chamber pressure with oxidizer to fuel ratio was analyzed. In addition to this, analysis was carried out on different insulation materials available, to choose the best possible insulation for the engine. In the tests, change in the chamber pressure trend was observed when water was injected implying a change in thrust. Also, it has been observed that the combustion efficiency of the engine needs to be improved in future.

Abstract_S4_All_03

Development of cost effective high aluminum based fuel rich propellant

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Abstract

Metals are added to the fuel to increase the density of the fuel as well as to increase the combustion temperature. Boron has been traditionally used, however it is very expensive. The use of aluminum instead of boron has been explored. A zero residue fuel was developed and pressure index was calculated using port burning configuration. Also, the characteristic velocity was determined and the combustion efficiency was calculated.

Abstract_S4_All_04

Development of controllable lab-scale hybrid motor thruster

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Abstract

In the current study, a wax-aluminum based hybrid fuel is tested with air to understand the controllable nature of the propellant configuration. A ball valve actuated with servo motor is used to control the oxidiser mass flow rate. Polytetrafluoroethylene (PTFE) is used to mechanically activate the metal aluminum powder in the fuel. The Burn rate law that govern the fuel regression rate is obtained and the throttling capability of the proposed fuel is demonstrated in this article.

Experimental determination of ignition and combustion characteristics of two insensitive propellants

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Abstract

Safety improvements in the field of energetic materials led to the development of insensitive propellants. These materials belong to the family of LOw-Vulnerability Ammunition (LOVA). Security in the logistic phases (storage, transport) is much better with such insensitive propellants since they are expected to be insensitive to accidental ignition stimuli such as electrostatic discharge, heat, shock, friction or mechanical impact. Nevertheless, due to this insensitivity, their use in operational conditions remains a challenge. The study of their ignition behaviour is therefore fundamental. Present article deals with laser ignition of two insensitive propellants. Ignition is obtained thanks to thermal energy deposition on the material surface using a laser diode. This technique is a promising alternative to the classical pyrotechnic ignition devices, allowing the deposition of sufficient energy to compensate for sensitivity loss. Two insensitive propellants have been studied in this work. The first one is mainly composed of nitrocellulose (~98%) and the second one of RDX (1,3,5-trinitrohexahydro-s-triazine, ~84%). They are commercial propellants provided by ArianeGroup and used as received. Experiments are performed in a cylindrical closed-volume vessel (internal volume of 55 cm³), using a laser diode (Coherent, 808 nm). Two gaseous atmospheres are studied, nitrogen and argon, with initial pressures between 10 and 70 bars. Five laser powers have been studied, between 1.43 and 9.95 W. Ignition delays and maximal overpressures are given for the different initial conditions using the pressure signals. Ignition probabilities for different laser powers are investigated using the Langlie method. As already noticed, it is found that argon is a combustion enhancer for this kind of propellant. Gaseous atmosphere plays a great role on obtained overpressures, but not on ignition delays that are very sensitive to laser powers. It is also found that nitrocellulose-based propellant is more reactive than the RDX-based one: ignition delays are lower; overpressures and propagation rates are higher. Ignition energy results show the existence of a critical power around 3 W for the two studied atmospheres: RDX-based propellant needs more energy to be ignited above this power, and nitrocellulose-based one below it.

Thermal analysis and kinetics of biomass combustion

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Abstract

Three general types of thermal processes (pyrolysis, gasification and combustion) are usually applied for converting biomass to a useful energy form. Recent literature sources provide extensive research on thermal analysis and kinetics of biomass pyrolysis and gasification. These processes are mainly used for producing valuable products including fuels. When combustion is applied, significant concern must be drawn on the emissions and the ambient air quality, whatever technical appliance is chosen. Typical examples are the small- and medium-scale devices, operating with solid biomass-based fuels that are widely used in Europe for residential heating. The problem is significant in settlements, where centralized heating or alternative energy sources are not available or inaccessible due to different socio-economic factors. This work is focused on the combustion behavior of biofuels that are currently available at the Bulgarian biomass and biofuel market. For that purpose simultaneous thermal analysis was carried out with STA PT 1600 TG-DTA/DSC analyzer in a dynamic heating mode and static air gas environment. Generally, the effect on weight loss, thermal stability and energy was analyzed together with a few key kinetic parameters for three biofuel blends (pelletized sunflower husks, wheat straw and lucerne) and two type of biomass residue (cherry stones and coffee residue). The thermal decomposition analysis has shown four stage process in all samples: *a) water vaporization* (room temperature ÷ 458 K); *b) devolatilization and dehydrolysis of Ca(OH)₂* (420 ÷ 756 K); *c) biochar combustion and decarburization* (615 ÷ 986 K), and *d) residual combustion* (865 ÷ 1370 K). However, significant mass loss and energy effects during stage d) were observed only for the cherry stone samples. The higher heating value (HHV) was obtained in a calorimetric bomb, while the chemical characterization involves proximate, ultimate and ash analyses. In addition, the influence of the ash composition on the combustion reactivity and the overall exothermic effect occurring during stage c) was considered.

Abstract_S4_All_07

Thermal treatment of lignin rich residue from bioethanol production: preliminary study on char properties

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Abstract

Steam explosion is the most applied pre-treatment for the delignification of the biomass for bioethanol production. Only about 40% of the lignin rich residue (LRR) is used for the internal energy requirements. Pyrolysis can be explored as a thermal treatment capable of valorizing the LRR through char production. In this study the thermal behavior of the LRR was analyzed through thermogravimetric analysis and lab scale slow pyrolysis tests were conducted at different final temperatures in the range 400-700 °C for the evaluation of char yields and characteristics. The high char yields and the chemical characteristics suggested that the obtained chars are good candidates as carbon sink and soil fertilizers.

Hydrogen rich syngas from updraft gasification of lignocellulosic feedstock

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Abstract

Syngas is a mixture of carbon monoxide, hydrogen, carbon dioxide and lower percentages of incondensable hydrocarbons, like methane. It is a flexible energetic and chemical vector, and the process of its generation is flexible towards feedstock. Namely, any kind of material containing carbon can virtually be gasified: coal, biomass, organic urban waste. Fixed bed gasification is one of the most suitable process to exploit lignocellulosics because it can be carried out at small scale (<1 MWth) with a relatively simple and robust technology. From fixed bed gasifier syngas can be draft from the bottom (downdraft type) or from the top (updraft type). The latter is characterized by higher energy efficiency conversion and enhanced flexibility of feedstock, as regard moisture content, size and composition. One of the most important parameter for the syngas use is the ratio H_2/CO . In the reported work the focus is placed onto tuning syngas composition as a desirable feature of biomass gasification. Such process flexibility can be achieved by introducing steam in the system, by using oxygen or enriched air by a special reactor design (indirect gasification); by adding a catalytic step of water gas shift (WGS) or a CO_2 adsorption step. Gasification was carried out in a pilot facility able to treat 20-30 kg/g of lignocellulosic feedstock. In the reported tests almond shells were used that maintain a good gas permeation when loaded as bulk. Main system component is a fixed bed, autothermal, updraft gasifier, operated slightly above atmospheric conditions. The gasifier has a cylindrical basic shape with a height of 2.4 m and diameter of 0.5 m. Air, oxygen, steam or mixtures of these can be used as the gasifying means; the flow of gas is introduced into the lower part of the gasifier below the grate. Novelty of this work can be seen in the measuring evolution of gasification at different heights of the reactive biomass bed. This was achieved by probing syngas streams directly from the core and analyzing it onsite to measure the content of H_2 , CO_2 , CO , CH_4 , C_nH_m , N_2 , O_2 . The chemical composition was correlated to the thermal profile provided by in bed measurements of 7 thermocouples, plus 4 in freeboard. The plant is also equipped with section based on Water Gas Shift to increase the H_2 yield. The use of steam increased the hydrogen content and positively affected the molar ratio H_2/CO that reached the steady value of 1 by using air and steam as gasifying medium. In the tests, the biomass was completely converted in gaseous and liquid energy carriers with cold gas efficiency (CGE) ranging from 61% to 75%. With WGS the level of H_2 in gas reached 37 vol % (53 vol % on nitrogen free basis) corresponding to a new increased H_2/CO ratio of 9.

The co-oxidation study of coal and corn residue as a representative of biomass with photoionization mass spectrometry

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Abstract

Biomass captures increasing attracting attention due to low cost, renewability, low NO_x emissions, as well as zero-carbon production. However, the disadvantages of biomass, such as difficult to collect and transport, seasonal, low energy density and etc., limit its wide application. The most promising solution to figure out these drawbacks is to co-utilize with coal, such as co-combustion, co-gasification, and co-pyrolysis. In general, pyrolysis and low-temperature oxidation are the initial two important steps in combustion process, the study on oxidation mechanism will help to optimize the product distribution and improve efficiency of co-combustion of coal and biomass. Compared to the macroscopic physical and chemical parameters, the information of the products during co-oxidation is a key issue to reveal the co-combustion mechanisms at molecular level. The present work aims at performing the real-time and on-line detection of oxidation products, providing better understanding oxidation mechanisms during co-oxidation of coal and corn residue. A homemade pyrolysis vacuum ultraviolet photoionization mass spectrometry (py-VUV-PIMS) was applied for the product analysis. A krypton discharge lamp with 10.6 eV was used to ionize pyrolysis products. The fragment-free mass spectra of coal, corn residue, and blends oxidation products at different reaction temperatures from 300 to 800 °C were measured. The time-dependent profiles of major species were also measured during the oxidation processes. A series of peaks with m/z 15–300 were observed and products included alkanes, alkenes, dienes, nitrogen-and sulfur-containing compounds, and species derived from cellulose, hemicellulose, and lignin. The results reveal that cellulose and lignin in corn residue is faster to oxidize than hemicellulose. Coal have a influence on the lignin rather than cellulose and hemicellulose of corn residue in blend. Coal has no effect on the production of furfuryl alcohol obtained from coal-corn residue blend. According to this study, the potential for process control to get desired products is possible by monitoring reaction parameters, such as temperature and reaction time, during the co-combustion of coal and biomass. The current study on the oxidation mechanism is beneficial to optimize the product distribution and improve combustion efficiency.

PAH distribution in pig manure pyrolysis products

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Abstract

The abstract is prepared for inclusion in the Book of Abstracts of the ECM2019 and follows the format established in previous European Combustion Meetings. The purpose of this document is to provide rules for obtaining a high-quality proceedings volume. We urge you to submit your abstracts in the described format. The paper should begin with a four-to-six line one-column abstract as illustrated here. Pig manure is a waste generated in livestock farms and due to its high production, it is necessary to control and carry out an appropriate treatment to reduce its high pollutant potential for air, water and soil. Pyrolysis is a potential option to reduce the pollutant potential of this waste. Three products are obtained in the pig manure pyrolysis: gas, liquid and solid or biochar. While gas and liquid can be used for energy or value-added chemicals production, biochar can be potentially used as soil amendment product in a comparatively improved manner with respect to its direct application in agriculture soils. An aspect of relevance for the use of biochar in soils is related to the content of harmful pollutants, such as polycyclic aromatic hydrocarbons (PAH), which could be formed under pyrolysis conditions due to the high temperature used in this process. Not only their formation is relevant, but also their distribution among the three pyrolysis products. In the present work the formation and distribution of the sixteen EPA-PAH priority pollutants, classified, because of their toxic characteristics by the Environmental Protection Agency (EPA), were analyzed in the pyrolysis products. The effect of the pyrolysis temperature (350-550 °C) on the EPA-PAH formation and distribution has been analyzed experimentally in a fixed bed reactor. The experimental system consists of two different zones: reaction zone and condensation zone. In the reaction zone there is the fixed bed batch reactor, a vertical cylinder of stainless steel heated by an electric oven. In the experiments carried out, 300 g of pig manure were loaded inside the reactor. The condensation zone consists of two condensers refrigerated at 0 °C by a chiller and an electrostatic precipitator, where the condensable vapors and water are collected. Next, there is a cotton filter, whose purpose is to eliminate the traces of organic compounds that could have escaped with the outlet gas product from the condensation system. The PAH present in the outlet gas are collected in a thin tube of 300 mm in length and 10 mm of external diameter packaged with XAD-2 resin. Finally, the composition of the non-condensable gases is analyzed by a microgas chromatograph connected online (Agilent MicroGC 3000A). The main results show that there is an important effect of the pyrolysis temperature in the formation of EPA-PAH. A maximum in the total EPA-PAH formation (in gas, liquid and solid) was obtained at 450 °C, 122 mg/g of manure. The major concentration of EPA-PAH

was found in the liquid product in all the experiments carried out. Also, 15 of 16 EPA-PAH were found in this product. The amount of EPA-PAH in the gas product of the pig manure pyrolysis was almost negligible. In the case of biochar, the ones produced at 450 °C contained the lowest amount of EPA-PAH, 102 mg/kg of biochar, accomplishing the International Biochar Initiative (IBI) recommendations for its use as soil enhancer.

Innovative 3D CFD sewage sludge combustion modeling for furnace design optimization

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Abstract

Valid 3D CFD combustion simulations are crucial for successful furnace design optimization. With increasing interest for sewage sludge (SS) thermal treatment, a need for valid modelling of SS combustion has been noted. This is particularly true for small scale systems due to their relatively high public acceptance and manageable investment cases. The main obstacle in developing credible simulation models at low and medium thermal power outputs is recognized to be SS composition. Sludge namely includes high ash and moisture mass fractions, with ash present in matrix form entrapping combustible matter [1]. Additionally, vast amount of different volatiles is emitted upon thermal degradation, making SS different from other solid fuels [2]. In order to build a valid SS combustion model, which could accurately describe freeboard conditions the use of a rather simple surrogate fuel model, supported with a oD external bed model was taken as a starting point. The reasons for this lies in complexity of volatile composition, related importance of correct spatial distribution of surrogates in simulated domain and also legislation, which constraints flue gas temperatures and residence time [3]. The developed models are validated with data obtained from batch SS combustion in a small scale laboratory furnace. The basis of the proposed surrogate model is set at the short steady state interval during peak combustion of the batch, where majority of volatiles is emitted. As intention is to obtain accurate gas phase description, the main characteristic and advantage of the model is its capability to propose and test various surrogates. These are, following the literature, mainly composed of syngas components with an arbitrary heavier hydrocarbon is added to introduce and estimate its effects [4]. In the presented case, oD bed model is then used to obtain additional data on appropriate fuel bed conditions. Defined surrogate and bed conditions are then used in 3D CFD combustion simulations of a mentioned laboratory furnace, since it is small enough to allow detailed reaction mechanisms use. In this way, various surrogate compositions can be tested and compared with validation data, leading to definition of important effects caused by different volatiles and finally appropriate and validated surrogate composition. The presented model, with its innovative approach, enables considerable frontloading in the development process of more complex 1D or 3D fuel models, as these can be built with higher accuracy. This is a key step in obtaining legislatively imposed residence times and temperatures in small scale waste thermal treatment plants.

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Abstract_S4_All_12

Multi-phase reactive systems – analysis of involved time scales

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Abstract

The reaction progress of heterogeneous gas-solid reactions consists of several sub processes. Analysis of them by means of characteristic time scales provides insight to the on-going processes for process optimization. For this purpose, a generic reactive two fluid model has been implemented in OpenFOAM® and is validated with a gasification reactor from literature. An analysis of the gasification process based on the extracted time scales and the identification of possible optimization measures follow.

Dust explosion characteristics of corn starch at elevated temperature and pressure and reduced oxygen concentrations

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Abstract

Dust explosion characteristics are important parameters to assess the explosion risk in industrial installations. These explosion characteristics are determined in standardized set-ups according European or international standards. A disadvantage of these standardized set-ups is that they make use of small volumes, ambient temperature and pressure, and air atmospheres which do not always correspond with the industrial process conditions. It is well known that fine corn starch poses a dust explosion risk. Recently in June 2015 a large dust explosion occurred in Taiwan with colored corn starch powder at a festival. Colored corn starch powder was sprayed from the stage with high-pressure bottles and a dust explosion occurred. Almost five hundred victims suffered from second- to third-degree burns and 15 victims died. Corn starch is widely used e.g. as a food ingredient for thickening sauces, as an anti-sticking agent or in adhesives. There is a clear dust explosion hazard within the industrial production of corn starch. In this study the dust explosion characteristics, such as the minimum ignition energy (MIE) and the maximum explosion pressure (P_{\max}) and the maximum rate of pressure rise (K_{st}), are first determined at ambient conditions, i.e. in air and at room temperature and atmospheric pressure. Thereafter these characteristics are determined in oxygen poor mixtures in order to research the influence of the oxygen concentration. The minimum ignition energy lies between 3 mJ and 10 mJ in air and increases to a value between 300 mJ and 1000 mJ at 14% oxygen in nitrogen. The limiting oxygen concentration (LOC) of corn starch is equal to 12 vol% O_2 in N_2 . The P_{\max} in air is equal to 7.6 barg and decreases slightly to 5.5 barg at 13 vol% O_2 in N_2 . The K_{st} decreases rather linearly from 187 bar m/s in air to 39 bar m/s in 13 vol% O_2 in N_2 . A Kuhner 20L-sphere was adapted in order to perform experiments at elevated temperature and elevated pressure. At atmospheric pressure the P_{\max} decreases slightly with increasing temperature while the K_{st} has a maximum of 210 bar m/s at a temperature of 40°C and decreases again to 185 bar m/s at a temperature of 60°C. At an initial pressure of 2 bar absolute and at room temperature, the maximum recorded explosion pressure was 17.0 barg and the K_{st} -value was equal to 378 bar m/s. These values are about twice the values obtained at atmospheric pressure. It is clear that the safety measures should take into account the effect of the elevated pressure.

Combustion behavior of torrefied biochar with different constitutions of cellulose, hemicellulose, and lignin

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Abstract

Structural components differences of the biomass have impact on the chemical reactivity. Different constitution of cellulose, hemicellulose, and lignin of the biomass will react differently towards thermal treatment. Torrefaction, considered as one of thermal degradation process, can effectively improve the grindability, hydrophobicity and heating value of solid fuel. From previous research, temperature is the dominant factor regarding combustion behavior. However, the conversion of each fiber fraction remains unknown. The aim of this research is to study the influence of thermal pretreatment of biomass with different constitution of cellulose, hemicellulose, and lignin. Two biomass with different fiber components are chosen: ale tree (AT) and palm empty fruit bunch (EFB). Thermogravimetric Analyzer is used to investigate the complex transitions that occurs at different temperature. Proximate analysis and Ultimate analysis are discussed. Ultimately, the devolatilizing time, volatile burning time and char combustion time are determined through single pellet experiment. Those data are appropriate and informative to tailor the biochar-firing furnace.

Abstract_S4_All_15

Effect of CH₄ injection method on combustion and gasification efficiency of pulverized coal in the tuyere part of blast furnace

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Abstract

Reducing the amount of CO₂ generated in the ironmaking process has become a pressing issue from the viewpoint of preventing global warming. Low reducing agent rate operation of the blast furnace is one of effective measures for mitigating CO₂ emission. Injection of hydrogenous reducing agents (HRA) from the tuyere where is the lower part of blast furnace is also effective measure. In this study, the effect of HRA injection method on combustion and gasification efficiency of pulverized coal in the case of simultaneous injection of HRA and pulverized coal from co-axial lance was examined by experimental combustion furnace and three-dimensional numerical simulation.

Abstract_S4_All_16

Experimental study on reaction front propagation during biomass packed bed smouldering combustion

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Abstract

In this work, experiments about the smouldering combustion of biomass packed bed were conducted. The influence of ignition temperature and air flow rate on the smouldering reaction front was investigated in detail. The results show that, the smouldering reaction front keeps stable at lower ignition temperature and smaller air flow rate conditions, and the instabilities appear when the ignition temperature and air flow rate exceed a certain value. Further, increases in ignition temperature and air flow rate lead to the increases in the speed of the reaction front speed.

Abstract_S4_All_17

Numerical simulation of raceway zone in small-scale combustion equipment for blast furnace

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Abstract

The reduction of carbon dioxide has been focused on in the iron and steel making process. In this study, a numerical simulation of raceway zone in a small-scale combustion equipment for blast furnace was conducted to investigate the behavior of gas, pulverized coal, and cokes. Two cases of simulation were conducted: with coke oven gas (COG) and without COG, and they were compared with the experiments. The simulation succeeded in capturing the trend in the axial direction of the burner.

Direct numerical simulations of spontaneous ignition of biomass in turbulent, high temperature particle-laden mixtures

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Abstract

The spontaneous ignition of mono-disperse pulverized biomass in turbulent, high temperature particle-laden mixtures is investigated based on three-dimensional Direct Numerical Simulations of the carrier phase with Lagrangian point particles. Reduced mechanisms for devolatilization and gas-phase combustion were calibrated with data obtained with detailed mechanisms for the studied conditions. A highly volatile biomass is considered and surface reactions are neglected, as the focus of this study is on gas-phase ignition. The focus is on the calibration of reduced models to reproduce the characteristics of interest of existing detailed models, including devolatilization rate, volatile composition and laminar flame speed. Both the devolatilization model and the gas-phase reaction mechanism are calibrated using detailed mechanisms for biomass pyrolysis and combustion. The initial conditions for the DNS simulations and the biomass properties are selected to resemble those observed in industrial boilers. The preliminary results show that ignition occurs in multiple spots within the domain, leading to the formation of hot pockets that grow and coalesce with time. Most of the particles burn in single particle mode, as typified by a circular reaction front with a small diameter, while some particles burn in particle group mode, as typified by elongated reaction fronts that span across more than one particle. Finally, for the same simulated time, the particles do not exhibit identical temperatures, and consequently do not experience identical devolatilization rates and progress of devolatilization, as a consequence of variations of heat transfer between the gas and the particle phase owing to the turbulent fluctuations.

Abstract_S4_All_19

Kinetic modeling of the effects of Na⁺ and K⁺ on the slow pyrolysis of hemicellulose

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Abstract

The main objective of this work is to propose an extension of the Bio-PoliMi sub-mechanism of hemicellulose that can capture the effect of Na⁺ and K⁺ during the slow pyrolysis of hemicellulose. To this end, a large experimental database of the effects of the presence of Na⁺ and K⁺ on the slow pyrolysis of hemicellulose, previously obtained, is analyzed comparatively to the decomposition paths of the Bio-PoliMi sub-mechanism of hemicellulose. In order to clarify on inhibition/promotion effects, a sensitivity analysis is performed. Based on the analysis of the experimental results and the sensitivity analysis, two catalytic reactions are proposed to be incorporated in the Bio-PoliMi sub-mechanism of hemicellulose that capture the effects of alkali metals on the slow pyrolysis of hemicellulose.

Abstract_S4_All_20

Modelling of particulate matter emissions from non-woody biomass combustion

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Abstract

Woody biomass has been largely used for energy purposes but its intensive use has created pressure on forests. The use of agriculture residues can provide a good alternative owing to their high availability and worldwide distribution. However, the combustion of these residues is still associated to operational problems since they contain a high amount of inorganic matter. In the present study, a simplified ash vaporization model and a coarse ash particle size distribution model are implemented and used to predict the formation and emission of particulate matter resulting from the combustion of raw and torrefied pine shells and olive stones in a drop tube furnace. The predicted results are compared with available experimental data. Both simplified models can predict reasonably the biomass ash particles behavior, namely when the coarse particle size distribution has a unimodal form.

Abstract_S4_AIII_21

Influence of the cobalt oxide coated flame holder in stabilization of inverted-methane lean flames

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Abstract

In this work, the stabilization mechanism operation and the morphology characterization of a single inverted flame stabilized downstream of two different flame holders (AISI 316 stainless steel (SS) and cobalt oxide coated stainless steel flame holder (SSCo)) in a lamella type burner was investigated. Stability analysis, suggest that, for higher Reynolds number (Re), the SSCo flame holder presents lower equivalence ratio (ϕ) for blow-off conditions when compared with the SS flame holder.

Feasibility of natural gas pyrolysis for production of unsaturated hydrocarbons: an RCM study

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Abstract

Nowadays, there is a change in the types of power plants wherefore the whole grid needs more flexibility in energy demand, supply and storage. In this context, the reversion of the heat engine process, converting an input of mechanical energy and low-grade substance into an output of high-grade substance, is of special interest. In this paper, we investigate such a process experimentally in a Rapid Compression Machine (RCM). In particular, the pyrolysis of C₁ – C₃ alkanes and its capability to produce hydrogen (H₂) and several valuable hydrocarbons such as acetylene (C₂H₂) and ethylene (C₂H₄) is studied. H₂ is a key for energy storage and becomes increasingly important as a fuel; and C₂H₂ and C₂H₄ are highly relevant for the chemical industry. In the RCM experiment, the thermal decomposition of a highly diluted natural gas surrogate (C₁ – C₃ alkanes) under compression engine conditions is investigated, and the production of H₂, C₂H₂ and C₂H₄ (target species) is measured. A RCM run proceeds like a single stroke piston engine; with the piston at bottom dead center, the combustion chamber is evacuated and then filled with the premixed test gas at the desired initial pressure and temperature. The piston is then pushed into the combustion chamber, resulting in a near-adiabatic compression with the corresponding pressure and temperature rise. High temperature and pressure at top dead center can initiate chemical reaction in the mixture. The mixture is then allowed to cool down by heat losses, which slows down and eventually stops chemical reactions. In this time period, the mixture is also homogenized by diffusion. A gas sample is taken from the combustion chamber and admitted to a micro gas chromatograph for chemical analysis. In comparison to conventional piston engines, this procedure offers well-controlled initial conditions and time for leveling out any thermal and mixture stratification. The conversion of natural gas to the target species is investigated for variable pressure (21.4 – 30.6 bar) and temperature (1378 – 1733 K) conditions. A strong influence of temperature is seen, especially for the species H₂ and C₂H₂. The higher the temperature, the more C₂H₂ and H₂ are formed as products. The formation of these two species is also pressure dependent, the lower the pressure, the more H₂ and C₂H₂ is formed. The yield of C₃H₄ decreases with increasing temperature, however, there is no strong influence of pressure on C₂H₄. The conversion rate of natural gas reaches 38 %, whereby C₂H₆ and C₃H₈ have a conversion rate up to almost 80 %.

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Abstract_S4_AIII_23

Plasma-assisted super-equilibrium radical generation and its effect on ignition

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Abstract

This work explores ignition in flowing mixtures of methane and air using a nanosecond-pulsed high-frequency discharge ignition source. OH planar laser induced fluorescence is utilized at a frequency of 50 kHz to examine the time dependent radical generation in and after the plasma discharge. The results indicate that a super-equilibrium concentration of OH is generated in the discharge and may last up to 1 ms after the discharge. The degree of this super equilibrium concentration is dependent on the pulse repetition frequency of the NPHFD source.

Abstract_S4_AIII_24

Designing a cooking burner using biogas as fuel

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Abstract

The use of biogas has been increasing in recent years. As clean renewable energy, the number of biogas burners is increasing especially in kitchens. The aim of this work is developing a special burner designed especially for biogas as one of the locally available energy sources and effective combustion process for cooking. Parametric study on pressures, various compositions and burner hole diameters are examined to obtain an optimum design for a biogas burner. As a result of the simulations, the optimum configuration were obtained to be used in our industrial kitchen appliances.

Partial methane oxidation via MILD combustion

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Abstract

The main source for hydrogen production is natural gas, which consists predominantly of methane. Two main methods of hydrogen production from natural gas - are endothermic steam reforming and exothermic partial oxidation of methane. The second method can be conducted both with and without a catalyst. In this study we have analyzed the feasibility of the non-catalytic conversion. The so-called MILD combustion conditions were chosen. Under these conditions the mixture is strongly diluted, so that combustion is ignited by preheating the inlet gas mixture and the resulting, combustion-induced, temperature jump is relatively weak. The mixture of methane and oxygen diluted by nitrogen by 70 - 95% was heated in the quartz flow cell placed in the tubular oven heated to about 1200 K. The exhaust gases were analyzed by gas chromatograph. The temperature increase was observed by thermocouples mounted along the tube, and found to be in the range of 50-100 K. It was found that non-coated thermocouples produce strong catalytic effect which results in the enhancement of the methane conversion and in the increase of the H₂/CO ratio in reaction products. It was found that without catalytic effect the conversion of the methane and the increase of the H₂/CO ratio can be obtained by increasing of the extent of dilution. The increase of the temperature and of the equivalence ratio also leads to the similar changes in the final products. However, strong soot formation is observed at temperatures above 1250 K and equivalence ratios $\varphi > 3$.

Abstract_S4_AIII_26

Experimental and numerical studies on CO₂ reforming in piston engines

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Abstract

We investigate the conversion of CO₂/CH₄ mixtures to syngas (CO and H₂) under compression-ignition engine conditions. Numerical optimization based on detailed chemistry is used to identify conditions which theoretically yield maximal CO₂ conversions for given boundary conditions. The optimization results are used to guide experiments in a rapid compression machine (RCM) setup that is used in place of a real compression engine. The optimization predicts, and RCM experiments confirm, that CO₂ conversion of 50% is possible under engine-like conditions. The conversion is supported by adding oxygen to the initial mixture; this also renders the process exothermal. An engine can therefore both delete CO₂ and deliver useful work as output.

Abstract_S4_AIII_27

Autothermal and steam reforming of liquid synthetic fuels

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Abstract

For the first time worldwide, the production of synthesis gas using a catalytic reforming process was studied using several different synthetic liquid fuels. The autothermal and steam reforming of four liquid synthetic fuels, with origins of biomass and full synthetic, is compared to diesel as reference. The study was performed with a reformer equipped with a commercial catalyst coated with precious metal. The results show that especially the ratios of the educt components are essential, for the composition of the product gas. This paper presents a pathway of the reforming of liquid synthetic fuels that can support the diversification of the energy supply. It is shown that diesel can be directly substituted by different liquid synthetic fuels.

Key modeling aspects in the simulation of a cyclonic burner operated in MILD combustion conditions through flamelet generated manifold model

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Abstract

Thermal efficiency and reduction of pollutants are key drivers for the design of innovative combustion systems and their development. For a given process, several operating solutions may involve the enhancement of mixture dilution and preheating, result in reaching very peculiar combustion regimes. Diluted combustion concepts, such as the moderate or intense low-oxygen dilution (MILD) combustion, needs high preheating and internal exhausts recirculation, leading to a local self-ignition process between burned gas and fresh reactant mixtures, with a distributed ignition. The development of MILD Combustion systems on a global scale, especially in industrial applications is limited by the unlimited knowledge concerning the underpinning physics behind such a regime. Moreover, several modeling issues related to diluted mixtures must be properly investigated, to allow the development of this concept through a computationally driven design. In this background, CFD optimization appears essential for a successful assessment of such combustion regime in new combustion systems. A major issue in the modeling of MILD combustion is the pronounced sensitivity of the reactive structure to the reaction chemistry and therefore detailed kinetic schemes are necessary when a gas mixture is subjected to dilution by hot reaction products. In order to include detailed chemistry in fluid-dynamics simulations, the tabulated chemistry models can be a reasonable choice. Specifically, the goal of this work is to prove the reliability of the Flamelet Generated Manifold (FGM) in modeling a MILD combustion system with respect to a cyclonic burner used as a test case, in order to identify the main parameters that determine the MILD specific characteristics. Reynolds-averaged Navier-Stokes simulations were realized. The role of the heat loss in the combustor and the relative importance of each controlling variable was discussed. To conclude, an assessment of the heat transfer mode and the heat loss at walls was carried out by emphasizing the important role of radiative heat transfer on the stabilization of the reactive structure. The numerical results were compared with the measured temperature inside the chamber. Results point out that, for a small-scale configuration operating under MILD combustion regime, the heat transfer plays a dominant role in MILD stabilization and the radiative heat transfer is crucial to reaching the homogeneous thermal field experimentally observed.

Abstract_S4_AIII_29

Investigation of heterogeneous kinetic combustion of propene using novel CJSR

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Abstract

Efficient mixing and thermal control are important in the flow reactor for obtaining a high product yield and selectivity. Here, we report a heterogeneous chemical kinetic study of propene oxidation over thin CuO films within a newly designed catalytic jet-stirred reactor (CJSR). To better understand the interplay between the catalytic performances and catalyst properties, the prepared catalysts have been comprehensively characterized and the adsorbed energies of propene on the adsorbed and lattice oxygen were theoretically calculated using DFT method. Structure and morphology analyses revealed a monoclinic structure with nano-crystallite size and porous microstructure, which is responsible for holding an important quantity of adsorbed oxygen as also revealed by surface composition analysis. The catalytic tests demonstrated that CuO within the newly designed CJSR is very active for the complete propene oxidation at low temperature with good reproducibility and reusability. The residence time inside the flow CJSR is calculated to be in the range of 1.12-7.84 seconds, which is suitable for the kinetic study and could give good guidance for scale-up. The kinetic study revealed that using CJSR the reaction rate increases with O₂ concentration in the gas phase that is commonly not achievable for catalytic flow tube reactor, whereas the reaction rate tends to increase slightly above 30% of O₂ due to the catalyst surface saturation. The apparent activation energy also exhibited a strong correlation with the catalytic activity and the lower activation energy leads to higher catalytic activity. Moreover, DFT calculations of the reaction over CuO surface catalyst demonstrated that adsorbed oxygen is the most involved oxygen in the catalytic reaction. Accordingly, these findings revealed that CJSR combined with theoretical calculation is suitable for kinetic study, which can pave the way to investigate the kinetic study of other exhaust gases at low temperature.

This work is supported by the Ministry of Science and Technology of China (2017YFA0402800), the Natural Science Foundation of China (No. 51476168/91541102) and Recruitment Program of Global Youth Experts.

Abatement of toluene by non-thermal plasma coupled with Cu-Co-O thin film coated on stainless steel mesh

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Abstract

Toluene abatement has been investigated in the non-thermal plasma technique at room temperature. In order to increase the efficiency, a Cu-Co-O film, with the thickness of 160 nm, was used to assist the toluene removal. The thin film of the Cu-Co binary oxide was coated on a round piece of stainless steel mesh (SSM), with the diameter of 60 mm, via pulsed spray evaporation chemical vapor deposition method and characterized using XRD, SEM and EDS. Two annular dielectric barrier discharge (DBD) reactors with different plasma region length, 60 and 200 mm, were self-designed and used to generate the non-thermal plasma. The Cu-Co-O/SSM was respectively located in the DBD reactors fully and partially. In the 60-mm DBD reactor, toluene removal process could be divided into two stages as the discharge power increasing. In the first stage, fully locating the round SSM, no matter coating Cu-Co-O thin film or not, could equally improve the toluene removal significantly. Cu-Co-O thin film has little effect on the toluene conversion in this stage. It indicates that SSM dominates the catalytic role by its influence on the plasma discharge. In the second stage, fully locating Cu-Co-O/SSM could improve the toluene conversion to achieve 100% and increase CO₂ selectivity as large as 80%, as the specific energy density being above 153 J/L. Cu-Co-O thin film presents a prominent catalytic effect by providing a surface for the chemical reaction selectivity. In the 200-mm DBD reactor, partially locating SSM, with or without Cu-Co-O thin film, in the center of the plasma region, could equally improve the toluene conversion to achieve 100% as the specific energy density being above 8 J/L. Similar to the first stage in the fully locating plasma-Cu-Co-O/SSM configuration, Cu-Co-O thin film has little effect on the toluene conversion. Although the binary oxide film could increase the concentrations of CO₂ and CO, it has little effect on the CO₂ selectivity. The gas and surface reaction mechanism has been proposed. Specific energy density and locating pattern would influence the effect of Cu-Co-O thin film coated on SSM.

This work is supported by the Ministry of Science and Technology of China (2017YFA0402800), the Natural Science Foundation of China (No. 51476168/91541102) and Recruitment Program of Global Youth Experts.

Abstract_S4_AIII_31

Investigation of support effect of Fe-Cu-Co thin film catalyst on the catalytic activity and stability for CO oxidation

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Abstract

The effective valuation of catalyst supports in the catalytic oxidation makes the contribution to understanding the support effect of great interest. Here, the effect of inert and active supports on the catalytic activity and stability of non-crystal Fe-Cu-Co ternary thin film oxides deposited on stainless steel grid mesh (SSGM) and copper grid mesh (CUGM) by pulsed-spray evaporation chemical vapor deposition (PSE-CVD) technique, was investigated for catalytic abatement of CO at low temperature. The catalytic activity and stability depended on the nature of the interphase between the metal substrate and the deposited thin film ternary oxides. The physicochemical properties disclosed the formation of needle-like shaped morphology with amorphous structure of ternary oxides, which provided abundant sites for oxygen evolution. Moreover, metallic species (Fe^{3+} , Co^{3+} , Co^{2+} and Cu^{2+}) and oxygenated species were confirmed to co-exist at the surface and offered effectual synergetic effects on oxidation reaction. The open porosity of nano-grains, abundance of surface metallic and oxygen species, high reducibility at low temperature owing to low optical bandgap energies played together a crucial role in the catalytic oxidation reaction. The ternary oxides exhibited excellent performance towards the total oxidation of CO with a high gas hourly space velocity. Therefore, the doping strategy is used to adapt highly active transition-metal ternary oxides at low temperature.

This work is supported by the Ministry of Science and Technology of China (2017YFA0402800), the Natural Science Foundation of China (No. 51476168/91541102) and Recruitment Program of Global Youth Experts.

Experimental investigation of stabilization and emission characteristics of ammonia combustion in a cyclonic burner

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Abstract

The utilization of ammonia as a fuel seems to be a promising concept in the context of chemical storage for future energy systems. Its high hydrogen density and the possibility of being employed as a fuel for combustion systems without requiring a hydrogen extraction process, or as a fuel in other applications make such molecule very important in the future energy system scenario. Nevertheless, a significant gap exists between the growing interest in ammonia-based power applications, current knowledge and understanding required to obtain good designs. Hence, this work helps to fill the gap between research, development and implementation for new technologies which has the potential to provide a sustainable energy system. The combination of reactants dilution and preheating may greatly increase system energy efficiency and lower pollutants production producing very peculiar combustion regime (MILD Combustion). Hence, the aim of this work is to provide an insight into these practical issues, utilizing a cyclonic flow combustor under MILD Combustion conditions, investigating ammonia-firing conditions. An investigation into the influence of operative parameters (preheating temperature, equivalence ratio and thermal power) is also explored for stationary applications. The study aims at exploiting the performance of a small-size cyclonic burner for a carbon-free fuel (NH_3) through the characterization of the process stabilization and pollutant emissions as a function of the mixture equivalence ratio and the nominal thermal power of the inlet mixture (from 2 to 10 kW), with the aim of identifying the optimal operating condition of the system. The process was monitored through temperature measurements and flue gas analysis at the exit of the combustion chamber. Results suggest that for ammonia/air mixtures the burner has to operate under slightly rich conditions to minimize NO_x emissions. Furthermore, the burner temperatures have to be higher than a certain value to ensure combustion process stabilization. Therefore, the burner can be exercised also with ammonia-based fuels for higher thermal powers according to the low LHV. However, it results that an efficient recirculation of the exhausts produces a robust MILD combustion condition also when low calorific or alternative fuels are used. Despite that, the use of pure ammonia as fuels decreased the operability range of the burner in terms of temperatures and equivalence ratio ranges.

Abstract_S4_AIII_33

Experimental study of MILD combustion in a cyclonic burner using prevaporized liquid fuels

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Abstract

MILD combustion applications were reported in the literature for gaseous fuels as a function of operative parameters and fuel type. In general, the establishment of MILD combustion depends on maintaining a hot and diluted environment, leading to a delayed, but spontaneous and homogeneous ignition. Few studies have explored the benefits of extending MILD combustion technology to liquid fuels for stationary applications such as gas turbine and boilers. In several cases, visible flames and high NO_x emissions were found in MILD combustion of oil, and the contributing factors for this are not clear. In this background, the present study reports an experimental study on moderate or intense low oxygen dilution (MILD) combustion of prevaporized liquid fuels burning in a cyclonic-flow combustor under atmospheric pressures. The influence of fuel type, equivalence ratio, carrier gas, inlet temperature and thermal power on the combustion stability and emissions are investigated. Ethanol, methanol and butanol are vaporized and carried to the combustor using nitrogen and air as oxidizer. The cyclonic-flow configuration applied in the present study has been proven to be effective in the establishment of MILD combustion of gaseous fuel (methane, propane, biogas), and is well described in previous publications of the same group. The mixing of reactants and hot combustion products is essentially similar to that of gaseous fuels in previous studies. The prevaporization of liquid fuels allows the current study to ignore the complexity of spray development and focus on the impact of chemical kinetics, fluid-dynamics and fuel type on the stabilization of the process. In particular, the combustion process was monitored through a set of thermocouples placed inside the reactor and by means of flue gas analyzers to monitor the main species concentrations. Results show that the combustion stability is highly dependent on fuel type, with ethanol being the most unstable due to its fast ignition under all conditions studied. Measured CO emissions emitted from all fuels are very low except when the equivalence ratio approaches the lean extinction limit, and this effect is slightly dependent on the fuel type. The joint regime of low CO and NO_x emission strongly depends on the fuel nature and molecule complexity. The NO_x formation rate via the nitrous oxide mechanism, the mixing rate, the reactor temperature and residence times are believed to strongly influence NO_x levels by changing the operative conditions.

New method of refinery gas processing into valuable petrochemicals

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Abstract

A new effective method of refinery gas processing based on its selective oxidative cracking (oxycracking) with the production of ethylene, CO and hydrogen with the subsequent involvement of these products in catalytic hydroformylation or carbonylation with the production of valuable petrochemicals is proposed [1-3]. Non-catalytic gas phase oxycracking of light alkanes is realized at a pressure of 1-10 atm and allows obtaining a gas mixture containing ethylene, CO and hydrogen in regulated proportions. The principal possibility of obtaining ethylene, CO and hydrogen in the ratios suitable for their further catalytic treatment has been shown experimentally [4]. This opens up real prospects for the production of valuable petrochemicals from a mixture of reaction products without the stage of their separation. The sequence of the process steps is shown in the Figure. The catalytic hydroformylation or carbonylation [5, 6] allows obtaining petrochemicals with high added value, including aldehydes, diethyl ketone, polyketones, etc. [7]. These products can also be used for subsequent condensation with an acid catalyst and subsequent hydrogenation to produce higher alcohols – high-octane components of motor fuels. It should be noted that dry fuel gas purified from heavier hydrocarbons and having a high methane index is obtained as an additional result of this process [8]. The possible schemes of the process of obtaining liquid petrochemicals from olefins, hydrogen and CO were analyzed and the optimal parameters (composition, ratio of components) of catalytic systems for the production propanal, propyl alcohol, propionic acid from the product mixture obtained by oxidative cracking of refinery gases were selected.

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Abstract_S4_AIII_35

A preliminary assessment of alternative fuels for marine engines using combustion chemistry tools

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Abstract

The de-carbonization of the shipping industry is critical in the context of low-carbon economy and the mitigation of the adverse effects of GHG emissions. Reducing GHG emissions from shipping is a challenging task that requires the use of energy efficiency measures and the increased penetration of alternative renewable fuels. The introduction of alternative fuels will also have a positive effect on local air quality in ports, harbours and coastal areas as it will lead to significant reductions in sulphur emissions. However, the effect of fuel substitution on pollutants, including nitrogen oxides and unburned hydrocarbons, cannot be readily quantified and dependent not only on fuel/fuel mixture properties but also on engine operating conditions.

Abstract_S4_AIII_36

Evaluation of gas turbine concepts for ammonia combustion

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Abstract

This work reports on the performance evaluation of three modern gas turbine concepts fuelled with ammonia. Flame speeds, temperatures and NO_x and NH_3 emissions were evaluated. Zero-dimensional reactor networks combined with one-dimensional premixed flame models were used to simulate the concepts of lean-burn dry-low emissions (DLE); rich-burn, quick-quench and lean-burn (RQL); and moderate or intense low oxygen dilution (MILD) combustion. A recently-developed detailed chemical kinetic mechanism was employed. Results showed that the lowest emissions come from the RQL and MILD concepts, while the DLE concept only presents values below legislation limits in conditions deemed unstable.

Unsteady pure straining effects on lean premixed flames of different Lewis numbers

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Abstract

The present work investigates numerically the effects of unsteady straining on lean premixed flames. In order to obtain a purely strained flame front with time dependent strain rate, the present work introduces a new numerical setup. This setup uses the laminar Couette-flow velocity field to control the strain rate at the flame front which remains laminar and curvature-free during the whole simulation. According to the setup, the Couette velocity field is initially imposed on the planar flame front and drives further the time-dependent pure straining. Thus, the strain rate at the flame front initially increases and after reaching a certain maximum, it starts decreasing. Three different lean flames are considered in the investigation: hydrogen-air with Lewis number $Le < 1$, methane-air with $Le \approx 1$ and propane-air with $Le > 1$. The Lewis number is defined as the ratio of thermal diffusivity of the gas mixture and the diffusivity of the deficient species (here: the fuel) into the unburned gas mixture: $Le = D_{TH}/D_{Fu}$. The simulations use a detailed modelling for the transport coefficients of the multicomponent gas mixture. A detailed chemical kinetic mechanism was used for the hydrogen flame (9 species and 38 reactions) and reduced mechanisms for the methane (16 species and 50 reactions) and the propane (28 species and 143 reactions) flames. The numerical method uses 6th order central differencing in space and a 4th order Runge-Kutta scheme for the explicit time advancement. The spatial resolution of the numerical domain (with dimensions 180x10 mm) is 0.020 mm. The present work focuses on the unsteady interaction between the flame and the Couette-flow. The results show that the three flames (fuels) investigated react in quite a different way to the pure unsteady straining introduced with the present setup: the methane flame remains almost unaffected by straining, while the hydrogen and the propane flames are subject to considerable changes of the heat release rate. At the straining conditions of the present study, the heat release rate for the hydrogen-air flame reaches values which are 6.9 times larger than that of the unstrained flame at $t=1.0$ ms (a time at which all three flames become quasi-steady-state). Also at $t=1.0$ ms, the heat release rate of the strained propane-air flame becomes smaller by a factor of 1/2.4 than the corresponding unstrained propane-air flame. A time delay was observed in the response of all three flames. This delay, called 'relaxation time' of the flame was defined using a criterion based on the (3%) relative deviation of the heat release rate from its initial unstrained value. For all three flames the relaxation time is found to be one to two orders of magnitude smaller than the characteristic time of the flame, defined with the flame speed and the thickness of the unstrained flame.

Abstract_S4_AIII_38

Laminar burning velocities and laser-induced fluorescence measurements of nitric oxide formation in propyl alcohols+air flames

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Abstract

The use of short aliphatic alcohols as additives in transportation fuels has been proven to sensibly reduce harmful pollutants, such as CO, HC and soot derived from anthropogenic activities, while some inconsistencies among researchers were found for NO emissions. To this end, it would be of particular interest to analyze the effect of alcohol structure on nitric oxide (NO) formation. In this study, the laser-induced fluorescence (LIF) technique was applied to measure NO production of n-propanol and i-propanol; new burning velocity measurements performed with heat flux method were also provided. In addition, new detailed kinetic mechanism for propyl alcohols combustion was presented. Flames were stabilized on a heat-flux burner at the initial gas conditions of 323 K, 1 atm over the equivalence ratio range 0.7-1.4. Measurements were performed in the production zone at 10 mm above the burner plate. The laser power used resulted in fluorescence measurements in the so-called saturated regime to minimize quenching effects. No appreciable differences were observed between the two isomers for the NO formation. Numerical simulations showed qualitative agreement with experimental data.

Flame structures and local heat release rates during side-wall quenching of atmospheric methane and DME flames

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Abstract

This paper is focused on the characterization of local heat release rate and its correlation with flame structures within atmospheric flames in a side-wall quenching geometry. The influence of different wall temperatures ranging from 330 K to 670 K is compared for stoichiometric and lean ($\phi = 1.0$ and 0.83) methane/air as well as dimethyl ether (DME)/air flames. Simultaneous formaldehyde (CH_2O) and hydroxyl radical (OH) planar laser-induced fluorescence (PLIF) are used to determine relative local heat release rates (HRRs). In the laminar flame configuration, the relative CH_2O - and OH-signal distributions indicate a change in the flame structure within the flame-wall interaction (FWI) zone. In the turbulent flame configuration, fluctuations prevail in the FWI zone and are analysed statistically regarding flame curvature.

Abstract_S4_AIII_40

Influence of iron and phosphor containing additives on the laminar flame speed

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Abstract

Polymers are highly combustible. To ensure safe handling of polymeric materials, flame retardants (FR) are commonly used. Due to environmental impact. FRs of the past, such as Halon1301 have been banned. In order to find a replacement of halogenated FRs, new methods are needed to test the mode of action of various FRs. In this study, a new arrangement is tested to prove the gas phase activity of FRs by determining the laminar flame speed of a premixed CH₄/air flame doped with FRs, which are already known for their effectiveness in the gas phase, such as ferrocene (FEC) and triethyl phosphate (TEP). A small content of FEC has been found to drastically reduce the flame speed of CH₄, while TEP requires significantly higher levels to achieve the same results as FEC.

Abstract_S4_AIII_41

Measurement of laminar burning velocity of SNG fuel with various hydrogen content

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Abstract

The present work investigates to obtain unstretched laminar burning velocity using spherical propagating flame method for SNG fuel based on result of combustor verification with CH₄/air mixture. The smoothed flame was observed for C₃, C₇ and C₁₁ regardless of equivalence ratio. As hydrogen contents increase from 3 to 11% in SNG fuel, S_u^0 also increases. Markstein length is positive in all conditions and when hydrogen contents rise, its values are declined, therefore, it is considered that the rise of hydrogen contents could lead to diffusional-thermal instability.

Experimental study of the maximum upstream location of premixed CH₄/air and CH₄/O₂-He flames with repetitive extinction and ignition in a quartz micro flow reactor

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Abstract

Portable power generation devices exploiting the high-density energy of hydrocarbon fuels have led to a growing interest of research in the field of microscale combustion [1]. Reactors used in micro combustion have an inner diameter that is typically smaller than the quenching diameter. At this scale, characteristic flame behaviors are experimentally [2] and numerically [3] observed such as flames with repetitive extinction and ignition (FREI), weak flames and hot flames. The experimental set-up presented here consists of a cylindrical quartz micro flow reactor (1.85 mm inner diameter) externally heated by three H₂/O₂ blowtorches. An infrared camera continuously monitors the external temperature of the reactor. The flame position is determined based on the CH* emission from the flame using an intensified high speed camera. Experimental data used to characterize the dynamics of FREI in such a micro flow reactor in previous studies were ignition and extinction points [4]. We considered that extinction occurs when the signal-to-noise ratio of CH* is too low to get the location of the flame. By definition, the location of this point strongly depends on the sensitivity of the measurement method and is difficult to compare with numerical studies. A better choice would be to extract the flame location at its maximum upstream propagation. There are two main reasons to choose this point for experimental measurements. One is that at this point, the flame propagation speed becomes smaller than the local flow velocity, inducing little variations of flame position in the reactor which facilitates its spatial determination. The other is due to the high signal-to-noise ratio of the CH* signal at this position. In the present work, the impact of the inlet velocity in the micro flow reactor on this position is studied for a stoichiometric CH₄/air flame and compared with previous numerical and experimental studies. In order to point out physico-chemical properties that play an important role in microscale combustion, a stoichiometric CH₄/(21% O₂-79% He) flame is also experimentally investigated. Hence, it allows to experimentally study the effect of an increase of laminar flame speed and adiabatic flame temperature on the FREI.

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Abstract_S4_AIII_43

Thermoacoustic instabilities: flame-flame interaction and boundary conditions

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Abstract

Thermoacoustic instabilities are the result of positive feedback between pressure and heat release rate fluctuations. Annular combustors in particular can suffer from complex thermoacoustic modes, partly due to the presence of multiple flames. By considering the effects of acoustic forcing on two neighboring flames, this paper attempts to isolate the effects of each reactive front on its neighbor. The forcing was in the non-linear regime, where flame pinch off was observed across several orders of magnitudes and shown to be an additional source of noise that helped destabilize the remainder of the flame.

Numerical analysis of characteristics of biogas and syngas combustion

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Abstract

In the present work characteristics of biogas and syngas flames are studied numerically. Numerical calculations are performed using the COSILAB code for one-dimensional premixed flames. Three cases of flames are analyzed: CH₄-air, biogas (CO₂-CH₄-air) and syngas (CO-H₂-air and CO-H₂-CO₂-air). Calculations include laminar flame velocity, flame temperature and CO-NO_x emissions with different parameters, such as temperature and pressure of fresh gases, equivalence ratio and gas composition. Temperature varies from 298 K to 500 K, pressure from 1 bar to 5 bar, equivalence ratio from 0.8 to 1.3 for flame biogas and 0.5 to 5 for flame syngas, composition 90-10%, 80-20% and 70-30 for CH₄-CO₂ mixture and 90-10%, 75-25% and 50-50% for CO-H₂ mixture. Several mechanisms of chemical reactions as GRI-Mech3.0, GRI Skeletal, San Diego mechanism, NIU GALWAY, CRECK Modeling Group, S. Davis et al. mechanism are used and compared to the results from the literature. Results show that calculations with some of these mechanisms reproduce well experimental results of the literature. In the biogas case, the increase of CO₂ rate induces a decrease in laminar flame velocity and flame temperature. For the syngas flame, calculations show that H₂ enrichment increases significantly the flame velocity and shift the maximum value ($S_{L,max}$) towards the equivalence ratio of 2.5, compared to the methane which is around 1.

Abstract_S4_AIII_45

Laminar burning velocity of CH₄/O₂/N₂/CO₂ flames measured by heat flux method under elevated pressure

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Abstract

A new high pressure rig was built to stabilize the planar adiabatic stretchless flames on a specially designed heat flux burner under elevated pressures up to 5 bar. Laminar burning velocities of CH₄/O₂/N₂/CO₂ mixtures were measured at equivalence ratios between 0.6 and 1.6. Reaction orders of CH₄/O₂/N₂ and CH₄/O₂/CO₂ are compared for same initial S_L or same T_{ad} conditions. Correlations between S_L and radical mole fraction $[H+O+OH]_{max}$ give good agreement especially for lean and stoichiometric flames. Radical mole fraction profiles combined with reaction path analyses indicate the OH radical plays important role in CO₂ dilution flames. As pressure increases, lower decrease (increase) rate of H, O and OH contribution to positive (negative) sensitivity reactions leads to higher reaction orders of CO₂ dilution flames than that of N₂ dilution flames.

Abstract_S4_AIII_46

High-temperature laminar flame speed experiments in a shock tube: laminar flame speed, temperature, and species measurements

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Abstract

Laminar flame speed, temperature, and species (CO_2 and H_2O) measurements were conducted in high-temperature, spherically expanding ethane-air ($\Phi = 1.0$) flames. The experiments were conducted in a shock tube, which allowed access to previously unexplored, high-temperature unburned gas conditions of 449-537 K, 1 atm. An Nd:YAG laser was used to spark-ignite the heated gas mixtures and initiate laminar flame propagation. OH^* endwall imaging was used to record the propagation of the spherically expanding flames and the images were analyzed to determine the unburned, unstretched laminar flame speed. Single line-of-sight laser absorption diagnostics were simultaneously used to measure burned gas temperature and CO_2 and H_2O species concentrations. The flame speed, temperature, and species measurements showed excellent agreement with modeled results.

9TH EUROPEAN COMBUSTION MEETING 2019

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Poster Session 5



Abstract_S5_All_01

Non-ideal effects in shock tubes: experiments, modeling, and simulations

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Abstract

This work examines shock-tube experiments by measurements and simulation. The computational work aims for a deeper understanding of the processes inside a shock tube and to develop an efficient method for the accurate prediction of the experiment, including non-ideal effects that hamper the use of experimental data for improving the chemical reaction mechanisms. Facility-dependent effects on temperature and pressure were studied with non-reactive mixtures (N_2 and Ar) for Mach numbers between 2.67 and 2.93 and pressures between 1.2 and 2.0 bar. The time-dependent temperature was measured via two-line absorption thermometry near 4.5 and 4.8 μm addressing fundamental vibrations of CO with two continuous-wave quantum-cascade lasers. For this purpose, 1 mol% CO was added as target species and 4 mol% H_2 was also added for accelerating the vibrational relaxation of CO. The two selected transitions are $v'' = 0$, P(20) and $v'' = 1$, R(21) at 4.8546 and 4.5631 μm , respectively. The measurements are compared to highly-resolved 2D simulations, using the in-house code PsiPhi with an approximate Riemann solver and a high-order discretization scheme. The inflow is modeled according to the theory of Mirels to account for shock attenuation outside of the computational domain and the evolution of a laminar boundary layer at the inlet.

An ignition delay time and kinetic modeling study of 1- and 2-pentene

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Abstract

It is necessary to understand the combustion chemistry of 1- and 2-pentene as they are components of real gasoline fuels and can also be important representative alkene components in gasoline surrogate fuels. Several previous studies were performed to develop a chemical kinetic model based on experimental ignition delay times recorded in shock tubes. However, most of the available ignition delay data for these fuels are limited to low pressures, high temperatures and highly diluted conditions. Therefore, ignition delay times under engine-like conditions are needed to provide target data to understand the low-temperature fuel chemistry and extend the model development to lower temperatures and higher pressures for fuel-air mixtures. In this study, both a high-pressure shock tube and a rapid compression machine have been employed to measure ignition delay times of 1- and 2-pentene at equivalence ratios of 0.5, 1.0 and 2.0 in 'air', at pressures of 15 and 30 atm. At high-temperatures (> 1100 K), the experimental results show that the fuel reactivity of 1- and 2-pentene are very similar at all equivalence ratios and pressures. However, at low-temperatures 1-pentene shows two-stage ignition and higher fuel reactivity compared with 2-pentene. Starting from a published pentane mechanism, modifications have been made to the 1- and 2-pentene sub-mechanism resulting in good predictions of ignition delay times under the engine-like conditions studied. Moreover, flux and sensitivity analyses were also performed to determine the important reactions involved in the oxidation process.

Abstract_S5_All_03

Plasma assisted combustion kinetics: modeling study for hydrogen-air mixtures in a non-thermal plasma reactor

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Abstract

Non-equilibrium plasma discharges can enhance both reforming and combustion processes through the generation of reactive species, *in situ*, almost independent of temperature or location. Plasmas can influence existing combustion processes and applications in several ways, which led to the emerging field of plasma assisted combustion (PAC). Studying the plasma chemistry and its kinetics will be key to understand the observed effects. To date most kinetic studies on PAC are performed either in Argon environments or at low pressures. Here we present a plasmachemical kinetics study of undiluted hydrogen-air at atmospheric pressure and room temperature.

High-pressure shock-tube study of the ignition and product formation of fuel-rich CH₄/dimethoxymethane/air mixtures

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Abstract

Flexibility between the conversion and storage of energy will be an important aspect in future energy systems. In times of high availability of renewable energy, external mechanical or electrical energy can be used in IC engines to store the energy by converting “cheap” chemicals (e.g., natural gas) into higher-value chemicals (syngas, unsaturated species). This process typically proceeds at fuel-rich conditions, far away from conventional operating regimes of ICEs. Under these conditions, chemical kinetics mechanisms need to be validated for successful implementation of such concepts. To test existing chemical kinetics mechanisms under fuel-rich conditions, we measured ignition delay times (IDTs) and the product composition of CH₄/dimethoxymethane (DMM)/air mixtures at engine-relevant conditions (30 bar, 700–1500 K) and compared the results with the predictions of literature mechanisms. For a further validation of the mechanisms ignition delay times of pure DMM were also measured. The experiments were performed in a high-pressure shock tube with driver-gas tailoring that enabled the determination of ignition delay times (IDT) up to 15 ms. Gas samples were taken from the shock tube with a fast acting valve and analyzed with GC/MS. Small amounts of DMM were used to reduce the ignition delay times of CH₄ so that engines can be used in HCCI mode without preheating the reactants. Experiments at $\phi = 2$ showed good agreement with simulations using the mechanism of Sun et al.¹ and He et al.². Syngas (CO, H₂) was observed as main product at $\phi = 2$. Beside syngas, ethane, ethylene, acetylene, propene, benzene, and toluene were observed as products at $\phi = 10$. The mechanism of He et al.² well predicted the ignition delay time measurements at $\phi = 10$ for $T < 1050$ K, whereas at higher temperatures, too long IDTs were predicted. Simulations with the mechanism of Sun et al.¹ showed a very good agreement with the measured IDTs in the whole temperature range. The measured product concentrations were not predicted well by the different mechanisms. Reactions which describe well the formation of higher hydrocarbons including benzene and PAHs must be added. These reactions are included in the mechanism of Cai and Pitsch³, which was proven to be well suited to predict products of rich CH₄ and CH₄/*n*-C₇H₁₆ oxidation⁴.

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Abstract_S5_All_05

Testing several butanol combustion mechanisms against a large set of experimental data and investigating their thermochemical data inconsistency

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Abstract

The combustion chemistry of butanol is not fully understood yet. A comprehensive set of experimental data for butanol isomers was collected and their simulation was carried out with eighteen butanol mechanisms. The performance of the mechanisms was measured and compared based on a sum-of-square error function that characterized the agreement between the experimental and the simulation data. In general, none of the reaction mechanisms could describe the combustion of all four butanol isomers in all types of experiments consistently well.

Abstract_S5_All_06

Influence of Pressure on H₂S Conversion

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Abstract

This work deals with the oxidation of H₂S under different manometric pressures (0.6-40 bar), in the temperature range of 500-1000 K and at slightly oxidizing conditions ($\lambda=2$). Experiments have been performed in a quartz tubular flow reactor. The results have shown that H₂S conversion is shifted to lower temperatures as the pressure increases. The kinetic model developed in this work is based on a previous study about H₂S oxidation at atmospheric pressure, which has been updated with a H₂/O₂ reaction subset for high pressures. Model results match fairly well the experimental ones at almost all conditions, except at 40 bar, where a shift of 50 K between experimental concentrations and model predictions is observed.

Abstract_S5_All_07

ARAS study of ethanol, butanol and DME reactions with atomic oxygen behind shock waves

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Abstract

The formation and consumption of oxygen atoms during the reaction of biofuels and oxygen at temperatures of 1600-3000 K and pressures of 200-300 kPa behind reflected shock waves using resonant absorption of O-atom line at 130.5 nm and emission of the band CH_3 ($\text{B}^2\text{A}_1 \rightarrow \text{X}^2\text{A}_2$) at 216 ± 1.6 nm have been studied. The mixtures of 10 ppm $\text{N}_2\text{O} + (20 \div 1)$ ppm $\text{C}_2\text{H}_5\text{OH}$, $\text{C}_4\text{H}_9\text{OH}$ and $(\text{CH}_3)_2\text{O} + \text{Ar}$ have been investigated. As a result, the temperatures dependences of the rate constants of reactions of biofuels with oxygen was obtained.

High temperature oxidation of 2,3-dimethyl-2-butene

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Abstract

The control and optimization of combustion in automotive engines require a perfect adequacy between the engine operation and the reactivity of the fuel. A promising way is to develop fuel formulas that are better adapted and optimized for their ignition properties. In this purpose, the search of new additives is becoming essential. Due to its branched and highly symmetrical structure, the 2,3-dimethyl-2-butene (DMB) could represent an interesting additive for gasoline. In this work, we measured the ignition delay times of DMB by means of shock tube experiments. The measurements were performed for three equivalence ratios (0.5, 1 and 2) and for a molar concentration of DMB (diluted in argon) ranging from 0.25 to 1%. Under these conditions, the temperatures (T_5) behind the reflected shock wave lies between 1250 and 1650 K, with an average pressure, P_5 , around 10 bar. In addition to this experimental study, a detailed mechanism for the combustion of 2,3-dimethyl-2-butene has been generated by means of the software EXGAS and tested to reproduce the experimental results. To improve the accuracy of the model, important pathways for the oxidation of DMB were identified from simulations and the corresponding kinetic data were computed from electronic structure calculations at the CBS-QB3 level of theory. In the same way, the combustion mechanisms of important primary products were calculated to better describe their decomposition pathways and improve the correctness of the model. Finally, the proposed model reproduce the ignition delay times and explain the main pathways involved in the combustion of 2,3-dimethyl-2-butene at high temperature. On this last point, reaction path analysis reveals that 2,3-dimethyl, buta-1,3-diene, 3-methyl,1,2-butadiene or isoprene are key primary species. Their thermal decomposition lead to strong unsaturated compounds whose combustion reaction paths remain poorly known.

Modeling of NO_x formation and consumption during oxidation of small alcohols

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Abstract

Alcohols represent an important category of biofuels and they are one of the most attractive alternatives to conventional fossil fuels and thus have been considered and used as fuel or fuel additive in internal combustion engines for a long time. They burn cleaner than gasoline and produce less emissions. However, to our best knowledge, there is no generally applicable kinetic model for alcohol combustion covering NO_x chemistry, which is validated over a wide range of experimental conditions. The focus of this study will be primarily on small alcohols/NO_x kinetics. The here derived model is an extension of our recent work Shrestha et al. [1] to include methanol and ethanol as fuel and subsequently study their interaction with nitrogen chemistry. The Model derived in this work is critically tested for speciation in plug flow reactors, in jet stirred reactors, and other burner stabilized flames, as well as for laminar flame speeds and for ignition delay times. There is only a limited number of studies on methanol and ethanol oxidation in the presence of NO_x reported in the literature. Moréac et al. [2] studied the oxidation of methanol/ oxygen/ nitrogen blends doped with NO in the jet-stirred reactor. It is found that at a lower temperature for methanol oxidation in jet-stirred reactor doping of the fuel blends with NO increase the reactivity of the system by increasing the net production of OH radicals. The increased amount of OH is formed via NO/NO₂ interconversion reaction channels NO+HO₂⇌NO₂+OH, NO₂+H⇌NO+OH, NO₂+HO₂⇌HONO+O₂, followed by the thermal decomposition of HONO producing NO and OH. At higher temperature, the formation of NO starts at the expense of NO₂ consumption mainly *via* reactions NO₂+H⇌NO+OH, CH₃OH+NO₂⇌HONO+CH₂OH, CH₃O+NO₂⇌HONO+CH₂O, and CH₂O+NO₂⇌HONO+HCO. The formed HONO is recycled back to NO *via* reaction NO+OH(+M)⇌HONO(+M). It is also found for ethanol oxidation in a flow reactor in presence of NO, the influence of oxygen concentration on ethanol conversion is not very significant at near stoichiometric and at rich conditions but influences on the onset of ethanol oxidation at the lean condition. In burner-stabilized premixed flames studied here for methanol/air and ethanol/air, NO is mainly formed via the NCN route (CH+N₂⇌NCN+H) and minor contribution comes from the NNH route (NNN⇌N₂+H). In burner-stabilized premixed methanol/air flame NO formation is less compared to ethanol/air flame.

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A novel approach for nitrogen flux accounting of NO_x formation pathways in 1D flames

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Abstract

A novel algorithm has been developed for the purpose of tracing the flux of nitrogen from the nitrogen-fixing initiating reactions, through the pool of intermediate nitrogen containing species, and ultimately to the formation of NO. As chemical kinetic mechanisms have become increasingly detailed, through the inclusion of a diverse range of NO_x formation sub-mechanisms and with continuously better measurements and estimates of reaction rates, it has become harder to distinguish the contribution to total NO formation from each sub-mechanism. This distinction of different contributions is made difficult by the flow of nitrogen through a common and finite set of intermediate species before oxidation to NO. This algorithm therefore presents a technique for tracing and allocating the contributions to the individual sub-mechanisms. Through a user-defined set of initiating reactions, which define the set of NO formation sub-mechanisms, the algorithm iteratively progresses through the flame while constantly tracing and accounting for the initial source of the fixed-nitrogen. This work will show the development and implementation of the algorithm. It will be applied to simulations of several 1D flames, using several different common chemical kinetic mechanisms of various levels of complexity. Using this algorithm, the differences in the contribution to NO formation from the different sub-mechanisms in each of the kinetic mechanisms will be highlighted. Ultimately, this algorithm is intended to be a widely available tool for analyzing pollutant formation within simulated flames.

Kinetic modeling of the destruction of organoarsenic toxics

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Abstract

Arsenical compounds have been widely used as pesticides or herbicides. A prototypical molecule is lewisite ($C_2H_2AsCl_3$), which has been manufactured as a chemical warfare agent used as vesicant and lung irritant. The destruction of stockpiles and unexploded ammunitions still found on battlefields by thermal treatments requires the development of highly safe processes. The yields of organic emissions from incinerations are mostly controlled by chemical kinetics. Lewisite is a colorless oily liquid with a geranium-like smell. It is produced through the addition of trichloroarsin $AsCl_3$ on acetylene. The product is a mixture of cis and trans isomers, the later, the most stable, accounting for around 90% in the blend. The third isomer, dichloro(1 chlorovinyl)arsine, is present with a fraction below 1%. Some theoretical works in the literature aimed to study conformers and the global rate of reaction with OH radicals, but no experimental data nor kinetic model of destruction are currently available. The development of a comprehensive detailed kinetic mechanism has been based on a theoretical investigation of decomposition reactions of lewisite, while sub-mechanisms of the combustion of light hydrocarbon and of chlorinated species were taken from previous studies of our group and from literature. The high number of electrons in arsenic ($Z=33$) makes theoretical methods usually used for combustion reactions unsuitable. It is indeed necessary to take into account the relativistic effects due to the core electrons, which are generally described by pseudo-potentials. As a result, we first performed a benchmark based on methods proposed in the literature to treat heavy atoms such as arsenic. First, the enthalpy of formation of a set of light arsenical compounds have been calculated thanks to four computational methods derived from DFT: B3LYP, Mo6-2X, mPWLYP and ω B97X-D. In a second stage, the effect of the basis set and of the pseudo potential were investigated. Eventually, an optimum between precision and calculation time has been found using the ω B97X-D method with the cc-pVTZ-PP basis set for arsenic and Def2-TZVP for other atoms. Ten core electrons of arsenic were frozen and pseudo potential were taken from EMSL Basis Set Exchange. The mechanism specific to the decomposition of lewisite includes reactions involved in combustion mechanisms, i.e. molecular eliminations, unimolecular and bimolecular initiations, H atom and Cl-atom abstractions, addition on double bond, decomposition of the radicals formed, chlorine-arsenic coupling reactions, and decomposition reactions of small species containing arsenic. Thermal decomposition and combustion of lewisite have been simulated. The main reaction paths have been derived. It appears that lewisite reacts in a radical chain reaction scheme and that the main products are carbon oxides, $AsCl_3$ and HCl.

CaRMen: a novel software tool for the evaluation and development of reaction mechanisms

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Abstract

Given a particular chemical reaction system of interest, the literature usually contains a very large number of experimental and modeling studies, which are difficult to assess as a whole. Kinetics of heterogeneously catalyzed reactions, such as the conversion of methane over rhodium catalysts can serve as a prime example: Over the years, this system has been studied in many reactor configurations including, but not limited to, fixed beds, monoliths, and stagnation-flow setups. These experiments were carried out at different conditions (total/partial oxidation, steam/dry reforming), and have been modeled using over a dozen different reaction mechanisms, each with their own set of rate expressions. The published mechanisms tend to have a special focus on the particular application for which they were developed, and the quality and potential of that mechanism under differing conditions is either not known or hard to judge. CaRMen (catalytic reaction mechanisms network) [1] is a novel software tool that improves the current manual workflow of testing various models against real experimental data. This is achieved by automating model vs. experiment comparisons as shown in the figure below. Preparing such graphical comparisons manually is a time-consuming and error-prone process, as the problems (simulations) must be setup and run. Afterwards, the resulting data must typically be post-processed before it can be plotted. Naturally, such a tool can also be used to speed up the development of reaction mechanisms themselves. However, its applicability is more general and not restricted to heterogeneous systems. For example, the software has already been used to study ignition delay times in rapid compression machines. Furthermore, because any simulation outcome can be compared with experimental data, the software can also be used to rapidly assess the quality of physical models as well. Examples include various transport models for porous media (dusty gas vs. Thiele-modulus approach), or different flow models (laminar/plug flow). In addition, the software also serves as an archival tool for both experimental data and reaction mechanisms to enable their use by a broad audience. Hence, the tool can be a first step towards organizing the vast amounts of data available in the literature. In this contribution, the capabilities of the software are demonstrated using selected mechanisms from the literature. Experimental data from a range of reactor configurations operated under very different conditions are used in the show case to emphasize the universal applicability of the software, which is further underscored by an exemplary modeling case study. A test version can be downloaded from www.detchem.com.

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Thermochemical property estimation based on group additivity method: impact of groups on kinetic model predictions

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Abstract

The accuracy of thermochemical species properties is of large importance for predicting ignition characteristics by chemical kinetic models due to their impact on chemical equilibria of elementary reactions. They are particularly relevant in the negative temperature coefficient (NTC) regime, where the low and high temperature reaction channels compete with each other and thus, slightly shifted chemical equilibria can lead to a strong variation in predicted results [1]. Benson's group additivity method [2] is widely employed for estimating the thermochemical parameters of larger species based on contributions from the underlying chemical groups. The incorporation of revised group values [3] in recent kinetic models has considerably improved the resulting model predictions [4]. In order to shed more light on the underlying effects, the present work systematically investigates the sensitivities of ignition delay times with respect to the group values of enthalpy of formation, standard entropy, and heat capacity, employing a recent 2-methylhexane model [5]. The highest sensitivities are found at intermediate temperatures for the peroxy group OO/C/H. Other important groups include mainly those composing the intermediate species of the conventional low-temperature chain-branching pathway. Each group is typically part of different species, whose thermochemical parameters can have opposed effects on the chemical equilibria of their reactions, such as QOOH and OOQOOH species in the corresponding O₂ addition reactions. A partial compensation of the impacts of these different species' thermochemical parameters can thus be expected, lowering the net impact of the respective underlying group values on the model prediction. This compensation is evaluated for the different groups and is found to be highest for the primary and secondary alkane carbon groups. Finally, the impacts of correction groups for gauche interactions and optical isomerism on model predictions are assessed and are found to be significant. This implies that the correct application of these correction groups is as important for accurate model predictions as accurate values for the other groups. Overall, the results suggest that uncertainties in the group values would strongly propagate into the model prediction, which motivates future research towards a quantification and reduction of these uncertainties.

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Abstract_S5_All_14

On the reliability of Ab-Initio reaction rate constant estimations used for biofuel oxidation mechanisms on the example of CH₃OH + H**Heiko Minwegen*, Karl Alexander***Physico-Chemical Fundamentals of Combustion, RWTH Aachen University, Germany*

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Abstract

In a comparative study, 17 different electronic structure methods including high-level coupled cluster theories are discussed and reaction rate constants are computed. The VTST corrected for hindered rotations, and multi-dimensional tunneling rate constants, based on full core correlated CCSDT(Q)/CBS(2,3)//DSD-PBEP86/cc-pVTZ energies of H-atom abstraction for the CH₃OH+H reaction system are determined for temperatures of 300 – 2500 K to

$$k_{\text{methyl}}(T) = 2.945\text{E}+05 \text{ cm}^3\text{mol}^{-1}\text{s}^{-1}\text{T}^{2.547} \text{ EXP}(-5129.5 \text{ cal mol}^{-1} / \text{RT})$$

$$k_{\text{hydroxy}}(T) = 4.573\text{E}+07 \text{ cm}^3\text{mol}^{-1}\text{s}^{-1}\text{T}^{1.788} \text{ EXP}(-10839.4 \text{ cal mol}^{-1} / \text{RT})$$

Abstract_S5_All_15

Reduction of NO_x in combustion of solid waste fuels by the SNCR process using ammonium sulfate as alternative additive

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Abstract

The selective non-catalytic reduction (SNCR) process, with the use of ammonium sulfate as additive, was investigated experimentally in a laboratory-scale flow reactor. SNCR experiments were conducted using aqueous ammonium sulfate solutions and using NH_3 gas for comparison. The temperature range of the experiments were 950-1200 K, and the residence time was 4-6 s. A detailed chemical kinetic model for the SNCR process using ammonium sulfate was also established. The optimum temperature for NO reduction was typically located around 1125 K. It was observed that ammonium sulfate yielded lower NO reductions compared to those obtained with NH_3 . The experimental results indicated a strong inhibiting effect of SO_2 on the NO reduction, but the effect was not captured by the model. The model overestimated the NO reduction when compared to the experiments.

Experimental and modeling study of the oxidation of pentanones: 2-pentanone, 3-pentanone and 3-methyl-2-butanone

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Abstract

Industries massively use ketones as solvents and were identified as potential fuels obtained from biomass. The short carbon chain ketones are known for their high octane numbers, their knock resistance and their low soot emission. In addition, ketones are important intermediates formed during the combustion process of many hydrocarbon fuels. However, the studies on the combustion behavior of ketones, particularly in the low temperature regime, are sparse and the small ketones as acetone and butanone show a limited low temperature chemistry (LTC). Therefore, to better understand the ketones in the LTC and the effect of the functional carbonyl group, saturated five-carbon ketones (C₅) are good candidates. Experimental kinetic studies on the combustion of C₅ ketones found in the literature consist mainly of high-temperature investigation on 3-pentanone [1–4]. Fewer studies concern 2-pentanone and 3-methyl-2-butanone [5]. In this work, the reactivity of 2-pentanone, 3-pentanone and 3-methyl-2-butanone is studied in a rapid compression machine and a shock tube. The ignition delay times of stoichiometric fuel/air mixtures are measured for temperatures between 650 and 1200 K and a pressure range 20–40 bar. 2-pentanone and 3-pentanone exhibit a low temperature chemistry and a pronounced negative temperature coefficient in the range of 750 to 850 K, whereas 3-methyl-2-butanone shows a limited low temperature chemistry. A detailed kinetic model is developed to simulate these observations. A consistency has been kept during the model development concerning the reaction rate parameters for the sub-mechanisms of all three pentanones. The reaction rate parameters are adapted from the work on 2-butanone and pentane isomers [6,7].

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Formation of indene and naphthalene through $C_6 + C_3$ and $C_7 + C_3$ reaction pathways in low-pressure premixed flames

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Abstract

The objective of the present work is to develop a detailed understanding of the indene and naphthalene formation in low-pressure laminar premixed flames. To this end, detailed kinetic modeling results are compared against flame-sampling molecular-beam mass spectrometry data of fuel-rich flames fueled by mixture of benzene (or toluene) with the C_3H_4 isomers allene and propyne. The experimental data were obtained by utilizing photoionization by tunable vacuum-ultraviolet synchrotron radiation allowing the identification and separation of combustion species by their characteristic ionization energies. In these mixture flames, the phenyl + $C_3H_3 \rightleftharpoons C_9H_8$ and benzyl + $C_3H_3 \rightleftharpoons C_{10}H_8 + H + H$ should be enhanced compared to other flames because of the readily formation of these radicals from the fuel molecules. Therefore, quantitative information about the indene and naphthalene profiles in these mixture flames provides a stringent test towards understanding the importance of the proposed $C_6 + C_3$ and $C_7 + C_3$ reaction pathways. The chemical kinetic model is based on our previous work on the oxidation and aromatics formation in low pressures flames of e.g. cyclohexane [1], *n*-butanol/1,3-butadiene [2], *iso*-butanol/1,3-butadiene[3], *iso*-butanol/*n*-heptane [4], propene [5] and cyclopentene [6]. Reactions concerning the C_3H_4 network with a focus on aromatic species are revisited within the present work. Thus, the contribution of individual pathways to indene and naphthalene formation, besides to benzene formation, can be studied in detail, from fuel specific radicals, e.g. C_3H_3 . Detailed kinetic modeling results will be compared against flame-sampled molecular-beam mass spectrometry data obtained in laminar premixed flames considered. First, the predicted mole fraction profiles for important species in the mass range from $m/z=2$ (H_2) up to $m/z=128$ (naphthalene) will be compared with the experimentally observed profiles. Then, an assessment of the importance of various fuel consumption and formation pathways of indene and naphthalene, besides benzene, will be presented, by using reaction flux and sensitivity analyses.

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[3] ASTM D7655 standard.

Abstract_S5_All_18

NO emission prediction using virtual optimized chemistry

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Abstract

A reduced order kinetic model for NO (Nitric Oxide) prediction, based on the recently developed virtual chemistry methodology, is proposed in this article. Temperature and heat release are resolved through the optimization of a virtual main mechanism whereas NO emissions are reproduced through the optimization of a dedicated sub-mechanism. The proposed NO sub-mechanism is optimized over a learning database made of 1D-premixed and 1D opposed jet diffusion flames. The approach is further assessed in a direct comparison against fully detailed chemistry.

Probing the low-temperature oxidation of tetrahydropyran and its effect on toluene ignition

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Abstract

In many applications, the complexity of the fuel composition requires the definition of surrogate fuels able to mimic the most significant aspects of the combustion process. Coal and biomass tar mainly comprises large molecules featuring multiple aromatic clusters as well as short aliphatic chains, oxygen, and nitrogen which reflect the initial parent coal composition (Solomon, Energy & Fuels, 1988). In this context, tetrahydropyran (THP) and toluene constitute two promising candidates for the definition of primary tar surrogates. With a structure similar to cyclohexane, differing only by the presence of the ether functional group, THP has also been proposed as a lignocellulose-derived biofuel (West, Catal. Today, 2009). The understanding of low-temperature oxidation characteristics is particularly relevant for practical application such as internal combustion engines. Besides, a recent work (Stagni, Combust. Flame, 2018) also emphasized the importance of these reactions for devices operating under partially-premixed combustion regimes, such as coal or biomass power plants and gas turbines. In this work, we analyze the oxidation chemistry of tetrahydropyran in the low-temperature regime 500-700 K. The experimental setup consists of a fused silica spherical reactor with a volume of 33.5 cm³ embedded in an electrically heated oven. Reaction products are sampled with a quartz conical probe and ionized in a Time-of-Flight mass spectrometer by tunable synchrotron-generated vacuum-ultraviolet (VUV) radiation for photoionization (PI). In a second experiment, interactive effects are investigated in THP/toluene blends at a volumetric ratio of 50/50. For better comparison, the same equivalence ratio of 0.35 and average residence time of 2.2 seconds are prescribed. The narrow width of the photon-energy distribution allows for isomer identification. In addition, thanks to the fast quenching of ongoing reactions, elusive intermediates such as keto-hydroperoxides are identified together with small hydrocarbons and oxygenated compounds. In the single-fuel case, THP reaches the maximum reactivity at 580 K, where it is converted up to 70%. In the blended case, THP conversion is hindered in favor of toluene, which benefits from the radical pool provided by THP to initiate its oxidation sequence. This results in a maximum of 57% conversion for THP and 33% for toluene. In this work, the NTC temperature range is not fully explored but its initial stage is identified around 620 K for both reactive mixtures. Concerning oxidation products of intermediate species, the addition of toluene suppresses the formation of highly oxygenated compounds directly related to the THP low-temperature reaction sequence and results in the appearance of aromatic species starting from benzene up to ethers with two aromatic rings.

Synthesized alternative kerosenes – characterization through experiments and modeling

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Abstract

In the last decade, several synthetic aviation jet fuels have been formulated, as part of the efforts to ensure sustainability in energy supplies and to mitigate effects on climate stemming from burning fossil sources [1, 2]. These synthetic kerosenes can be used as blends or even as a full substitute to kerosene; however, when it comes to global warming, a priority is given to renewable fuels. Any aviation fuel must be characterized and certified, with respect to physical and chemical properties, to ensure a safe and reliable operation for the whole flight envelope. In addition to their specification needed for their approval [3], all these advanced kerosenes must be fully compatible with today's airframe components, aero-engines, and fuel logistics to allow their use as so-called drop-in fuels in the daily operation. In the present work, we will report on fundamental combustion properties of several synthetic kerosenes, here ignition delay time from shock tube experiments and burning velocities in a laminar burner studied in a wide parameter range of temperature, pressure, and fuel-air ratio. A combined experimental and modelling effort is followed by using detailed chemical kinetic modeling exploiting the approach of a surrogate. The experimental data base will serve as validation data, for the development of the surrogate composition of the specific surrogate and their kinetic description based on an in-house reaction model. The focus is put on sustainable jet fuels; in detail, on: (i) Alcohol-to-Jet – Synthetic Paraffinic Kerosene (AtJ-SPK) from Gevo which is an iso-paraffinic jet fuel made from alcohols and can be used as 50% blend; (ii) Alcohol-to-Jet – Synthesized Kerosene with Aromatics (AtJ-SKA) from Swedish Biofuels; (iii) ReadJet – made from waste plant oils and fats by catalytic hydrothermolysis, a process developed by ARA and currently underway for certification. This synthetic jet fuel candidate consists of *n*-, *iso*- and *cyclo*-paraffins, with aromatics. Data will also be reported for Jet A-1, for comparing the results to a conventional, i.e. crude-oil based kerosene.

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[3] ASTM D7655 standard.

Ethane/nitrous oxide mixtures as a green propellant to substitute hydrazine: validation of reaction mechanism

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Abstract

Hydrazine gives the best performance and reliability as a rocket fuel, but it has a high freezing point and is too unstable to be used as a coolant. Hydrazine derivatives like monomethyl hydrazine (MMH) and unsymmetrical dimethyl hydrazine (UDMH) are used for spacecraft propulsion applications in different technological contexts. But all these fuels have the same disadvantage: They are highly toxic. Meanwhile, hydrazine consumption for European space activities is in the order of 2-5 tons per year. However, if the REACH (Registration, Evaluation, Authorisation and Restriction of Chemicals) regulation should come into full force in the upcoming years, it will severely restrict hydrazine-use in Europe, although the propellant may remain available from current sources, e.g. India and China. Nevertheless, green propellants for European space activities are an accepted challenge for research as well as technology development. Thus, within DLR's Future Fuels initiative the combustion properties of propellants like ethylene / nitrous oxide have been investigated exhibiting the potential to substitute hydrazine in chemical propulsion systems [1-3]. Measurement data from model combustors associated with investigations of fundamental combustion properties provide valuable test cases for CFD-computations, thus gaining better insights into the specific design requirements of new satellite thrusters [4]. Therefore, this contribution reports on measurements of ignition delay times of the ethane / nitrous oxide reactive system and their use for the validation of reaction mechanism capable to be applied to combustor CFD-simulations. Ignition delay times have been measured at DLR's shock tube facility at Stuttgart. Stoichiometric mixtures of C_2H_6 / N_2O diluted 1:5 with nitrogen have been shock-heated at initial pressures of p / bar = 1, 4, and 16. In addition, mixtures of C_2H_6 / ($O_2:N_2 = 1:2$) diluted 1:5 with nitrogen have been measured across the same initial range of parameters highlighting the different reaction systems' pathways. Furthermore, ethane will be compared to ethylene as a fuel. Eventually, the predictive capability of a recently published reaction mechanism [5] – adapted to the specific requirements of the C_2H_6 / C_2H_4 / N_2O reactive system – will be shown at the conditions tested. Implications to the reaction kinetics of nitrogen-containing species as well as the sensitivity of collisional partners' chaperon efficiencies on third body reactions with respect to ignition delay time will be presented completing the validation process.

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Abstract_S5_All_22

Mechanism comparison for PAH formation in pyrolysis and laminar premixed flames

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Abstract

Polycyclic aromatic hydrocarbons (PAHs) are known precursors of harmful carbonaceous particles. Accurate predictions of soot formations strongly rely on accurate predictions of PAHs chemistry. This work addresses the detailed kinetic modeling of PAH formation using two models: CRECK and ITV, aiming to compare the model predictions with experimental data in olefin pyrolysis and laminar premixed flames. The two kinetic mechanisms are validated and compared highlighting similarities and differences in PAHs formation pathways. The validation highlights the critical role of resonance-stabilized radicals leading to the PAH formation.

Ammonia oxidation in a JSFR reactor. Towards a better understanding of ammonia chemistry

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Abstract

The aim of the present work is to study the ammonia oxidation in a model reactor. Tests were performed in a Jet Stirred Flow Reactor for ammonia/oxygen/nitrogen mixtures and ammonia-hydrogen/oxygen/nitrogen mixtures, changing the mixture inlet temperature and equivalence ratio. Experimental results were compared with numerical simulations using different kinetics mechanisms available in literature. Experimental results suggested that it is possible to identify three different kinetics regimes: low, intermediate and high temperatures. The ignition temperature is independent of equivalence ratio (about 1225 K). NO_x and hydrogen concentration profiles are very similar for low and intermediate temperatures but exhibit a strong dependence on the equivalence ratio for high temperatures. None of the used kinetic models can accurately reproduce the experimental data in the considered operating conditions. The main differences among mechanisms is the description of the low-intermediate temperatures reaction rates, as suggested by flux diagrams, reaction rates and first-order temperature sensitivity analyses. Further experimental tests were realized in two different material (quartz and alumina) laminar plug flow reactors to verify the interaction between homogeneous and heterogeneous surfaces reactions.

Degree centrality of combustion reaction networks for analyzing and modelling combustion processes

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Abstract

Combustion research still needs more advanced fundamental understanding of combustion chemistry and dynamics from molecule scale to nanoparticles. The latter is also needed for soot formation and combustion system control such as Homogeneous Charge Compression Ignition (HCCI) engine and flame regimes and instability. The complex interactions between hundreds of species linked within thousands of reactions continue to be a challenge to analyze and model. The focus of this paper is to develop methods to facilitate the modelling and analysis of the detailed kinetic chemistry of fuels combustion. These methods have been validated for the combustion conditions of Rapid Compression Machine (RCM). Through the use of Combustion Reaction Networks (CRN) analysis of degree centrality, principal species were identified during a combustion process by applying an introduced definition of principal species. A principal, central or the more active species of a combustion process chemistry at a specific time step/cell is the more tied up to other species in the CRN and so have the highest value of degree centrality. The accuracy of the dynamic identification of principal species, locally adapted to the thermochemical conditions at each time step/cell of the simulated combustion process, used by the Directed Relation Graphs (DRG) method of mechanisms reduction, has been demonstrated and the fast combustion simulations were attended using an adjusted Dynamic Adaptive Chemistry (DAC) implementing approach of detailed chemistry in calculation codes. An outcome has been justified; an 'active' species in the chemistry of a combustion process isn't necessary to be considered as a part of important species set for its predictive simulations.

Abstract_S5_All_25

High temperature synthesis of TiO₂ nanoparticles using TTIP-methane flat premixed flame

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Abstract

The nanotechnologies have been extensively used in the medical fields, catalysis and energy as well as material industries. Especially, the synthesis of fine quality nanoparticles has been considered the important issue in many practical researches. And the high temperature combustion synthesis is well known to be more beneficial for the mass production of high-quality nanoparticles compared to other well known chemical process such as sol-gel. In this study, we conducted the experimental research to produce the TiO₂ nanoparticle using the TTIP (Titanium Tetra Iso-Propoxide)-methane flat premixed flame. To change the oxygen level of burnt gas, the equivalence ratio of flat premixed flame was controlled by mass flow meter and gas analyzer. To analyze the synthesis characteristics according to the TTIP concentration, the primary particle diameter and agglomeration was measured by TEM (Transmission Electron Microscopy). And XRD (X-ray diffraction) was performed to analyze the crystalline phases (rutile and anatase) of TiO₂ at different oxygen level and temperature. The temperature of the reaction region is measured by R type fine thermocouple. It is found that as the evaporated TTIP passed through a uniform high-temperature reaction zone formed from a premixed flame, an amount of the TiO₂ nanoparticles was generated effectively and the oxygen level of burnt gas is very important factor in synthesis. When the residence time was increased by changing the TTIP feed rate, the XRD result showed that the anatase phase ratio of captured nanoparticles was higher than rutile. It was also confirmed that the ratio of the rutile phase was higher when the oxygen concentration was increased by changing the equivalence ratio of the flat flame in the reaction zone.

Abstract_S5_All_26

Comparative mass spectrometric study of gaseous key intermediates from tetramethylsilane and hexamethyldisiloxane in silica synthesis flames

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Abstract

The synthesis of functional materials in a flame reactor is particularly attractive since it produces high-purity nanoparticles at scalable production rates in a continuous gas-phase process. In this comparative study, the reaction network of selected organosilicon precursors, e.g. Tetramethylsilane and Hexamethyldisiloxane, in laminar premixed low-pressure synthesis flames is investigated by means of Time-of-Flight Molecular-Beam Mass Spectrometry. Similarities in the precursor decomposition and cluster formation pattern will help to identify key intermediates, which can enable a chemically controlled synthesis of tailored silica nanoparticles.

Impact of the injector geometry on soot production in a model scale swirled combustor under perfectly premixed rich conditions

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Abstract

Investigations of soot formation in turbulent flames are of considerable fundamental importance and practical interest. While soot production in non-premixed flames is relatively well documented, premixed turbulent sooting flames have received less attention even if their study can bring new insights on soot production in the absence of local equivalence ratio inhomogeneities. The present investigation is carried out in a model scale swirled combustor developed at the EM2C laboratory to investigate soot production under premixed rich conditions. This device allows studies over a limited range of parameters where the production of soot is strong enough to be measurable. The effects of equivalence ratio and wall temperature on the soot yield were already characterized but it was interesting to see if a change in the injector geometry could modify the soot production pattern and level. The influence of the injector geometry on soot production is investigated in this work to assess whether a reduction of this pollutant emission can be achieved by slightly modifying the injector design. It is found that a small modification of the geometry can notably influence the flame stabilization mechanism inducing a change in the flame structure and, consequently, reducing the production of soot for the same operating point. A reference flame formed by the new injector is then characterized both in terms of soot volume fraction measured using the LII technique and of PAH presence obtained with PLIF-PAH. Finally, the evolution of soot production with equivalence ratio, flame power and wall temperature is characterized for this new injector to identify similarities and differences with respect to the behavior observed for the original injector design.

Experimental and numerical investigation of iron-oxide nanoparticles from flame assisted synthesis

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Abstract

Iron oxide nanoparticles have a wide range of advanced applications, from biomedicine and magnetic resonance imaging to heterogeneous catalysis. The synthesis route in terms of temperature, concentration and residence time history has a strong impact on the particle properties. In our current work, a modified McKenna burner is used for experimental and numerical investigation of iron oxide nanoparticles, which incorporates the ability to tune the synthesis parameters over a wide range. In the burner, the primary flame is supported on the porous sinter plate and provides the energy necessary for operation of the secondary central coaxial synthesis methane/oxygen flame to which the iron pentacarbonyl precursor is fed and where the nanoparticles are generated. The effect of varying the flow rate of the central flame on doped and un-doped flame structure and hence the nanoparticle formation are discussed and compared between measurements and detailed numerical simulations. The experiments include molecular beam sampling with particle mass spectrometer to measure the particle size and a quartz crystal microbalance for detection of condensable matter produced in the flame. Simulations of the rotationally symmetric setup are performed in a two-dimensional, rotationally symmetric domain. The flame is described with a finite rate chemistry approach and species specific diffusion, while the coupled particle dynamics are described by a monodisperse population balance model.

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Abstract_S5_All_29

Soot formation in laminar diffusion flames with population balance modelling and laser diagnostics

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Abstract

Laminar diffusion flames present an elementary configuration for investigating soot formation and validating kinetic models before these are transferred to turbulent combustors. In this work, we present a joint experimental and modelling investigation of soot formation in a laminar co-flow burner. Specifically, we combine the population balance equation (PBE), discretised with a recently developed finite volume method, with an in-house CFD code to predict the evolution of the soot particle size distribution throughout the flame. Our approach incorporates a complete set of soot kinetics for nucleation, surface growth, coagulation, oxidation and agglomeration. The diffusion flames are further analysed with the aid of laser diagnostic techniques, including elastic light scattering (ELS), OH-PLIF and light extinction measurements. The experimental dataset is supplemented by location-specific TEM images of soot particles obtained from extractive thermophoretic sampling. Additionally, the experimental light extinction signal is converted to an integrated soot volume fraction along the axial direction. Our model validation is based on a comparison of experimental laser diagnostic signals and ‘predicted signals’ computed from predictions of the gas phase scalars and the soot size distribution. The signals obtained from the PBE-based modelling approach are found to be in acceptable agreement with laser diagnostic measurements.

Absolute iron atom concentration imaging in nanoparticle flame-synthesis reactor using self-calibrating laser induced fluorescence

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Abstract

Quantitative measurements of reactive intermediates, resulting from precursor decomposition and oxidation allow to map the "genesis" of nanoparticle formation in flames and constitute a prerequisite for scaled-up predictive synthesis and model validation. Flame symmetry facilitates deduction of absolute concentrations from LIF measurement. A comparison between both LIF fluorescence patterns on both sides of axisymmetric flow configuration allows to cancel out symmetric features such as fluorescence quantum yield factors, fluorescence trapping and optical aberrations. This approach, provides a refinement of previous methods, that have used either two spectral transitions or two colinear laser beams in counter-propagating geometry. The presented method uses one laser beam and single spectral transition but nonetheless keeps up with quantitative concentration determination with reduced experimental complications. Iron distributions in IronPentacarbonyl (IPC) -doped hydrogen-oxygen-argon flame are deduced from experimental LIF patterns. Systematic off-center concentration reconstructions along with comparison to direct absorption measurements provide confidence in robustness of the deduced concentration distributions.

Newly-designed catalytic jet-stirred reactor for low-temperature oxidation of T135MB

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Abstract

The catalytic oxidation of 1,3,5-trimethylbenzene (T135MB), which is a simple model of aromatic hydrocarbons and representative component of real jet fuels, was investigated at low temperature with a newly designed catalytic jet-stirred reactor (CJSR), that ensures efficient mixing and thermal control, equipped with gas chromatography and FTIR. Thin film catalyst of pure CuO was synthesized at 325 °C using one-step pulsed-spray evaporation chemical vapor deposition. To better understand the interplay between properties and catalytic performances, the obtained catalysts were comprehensively characterized in terms of crystalline phase, morphology and surface composition. The catalytic performance based on light-off curves revealed that CuO catalyst presents a very high activity against the complete oxidation of T135MB at 330 °C. The induced catalytic effect is attributed to the open porosity, small grain size, abundance of adsorbed oxygen at the surface of CuO, and the long residence time provided by the newly designed CJSR of 1.12-7.84 seconds. Moreover, a possible mechanism is proposed for the complete oxidation of T135MB in CJSR. Accordingly, the combined diagnostic method involving the novel designed CJSR and efficient analysis devices is expected to assist in further understanding of the abatement of complex gaseous pollutants with avoiding high toxic by-products paving the way for clean combustion applications.

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Abstract_S5_AIII_32

Dehydrogenation of a chemical hydrogen carrier using a porous media burner

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Abstract

Liquid organic hydrogen carriers (LOHC) enable the permanent and safe storage of hydrogen. In existing reactors, the heat required for the release of the chemically bound hydrogen in the LOHC is usually provided by indirect heating via a heat transfer fluid or by an electric heater. The present work shows fundamental investigations to supply the heat for dehydrogenation of liquid organic hydrogen carriers by using a burner. The aim is an increase of the efficiency of the entire dehydrogenation unit. An important point is the exact regulation of the heat input to avoid decomposition of the LOHC.

Abstract_S5_AIII_33

Chemiluminescence and structure characteristics of a H_2/O_2 downward inverse diffusion flame

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Abstract

Diffusion flames are widely used in different practical combustion systems due to their safety, and wide operating range as compared to premixed combustion. Diffusion flames can be classified as normal diffusion flames (NDF), where oxidizer jet surrounds the fuel jet, and inverse diffusion flames (IDF). IDF are characterized by an oxidizer jet located in the center of the flame and surrounded by fuel jets. This configuration conserves the flame stability and adjustable flame length of a NDF, as well as its safety since the central oxidizer jet creates a negative pressure, nevertheless it affects the flame shape, OH distribution, emission, and temperature distribution. Furthermore, high temperatures with low soot emission can be obtained due the location of unburned oxidizer and fuel mixing zone. Hence, IDF is becoming more and more widespread in industrial applications such as processes of coal gasification and coke oven gas autothermal reforming technology. Several researches have studied IDF and their thermal behavior. One particular type of IDF that have been analyzed because of its high heat transfer, is the multi-fuel-jet inversion diffusion flames (MIDF), that consists in a larger central circular oxidizer jet surrounded circumferentially by a number of smaller circular fuel jets. The effect of the nozzle geometry have been studied as well as the influence of the number Reynolds and equivalence ratio on the thermal behavior. However, the comprehension of its behavior still requires more detailed research varying the fuels and design parameter of the burner (such as its geometry), and on how these features will affect the process performance. An experimental study was performed to investigate the effects of burner geometry on the thermal behavior and flame structure characteristics of a MIDF. Two different burner configurations were compared at different equivalence ratios and jet velocities. The number of fuel and oxidizer jets changes for each configuration. A downward burner was used, with H_2 and O_2 as fuel and oxidizer, respectively. Because oxyhydrogen flames have particularly high temperatures (higher than 2000°C), traditional temperature measurements are difficult to use on this research, direct visualization and the OH^* chemiluminescence are optical techniques that suit with the complex setup of this study. A post-processing of the OH^* chemiluminescence data was carried out with the Abel deconvolution. The study shows that the OH^* generated is higher when the number of O_2 jets increases, with lower O_2 jet velocities and higher H_2 jet velocities. Besides, the equivalence ratio shows to affect more the heat released than Reynolds number, nevertheless the maximum overall heat released seems not to be influenced by neither equivalence ratio nor Reynolds number. The structure of the flame is highly depending on the burner geometry as well as the number of jets (fuel and oxidizer); its dependency on H_2/O_2 ratio is also recognized.

The impact fragmentation tendency of limestone particles in calcium looping systems: effect of steam and sulphur dioxide

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Abstract

The Calcium Looping (CaL) process carried out in dual interconnected Fluidized Bed (FB) systems is a technique able to capture the CO₂ contained in the flue gases produced from power plants. It is based on the alternated temperature-swing CO₂ uptake by a calcium-based sorbent, with CO₂ capture taking place in a carbonator operated at around 650–700°C followed by the release of concentrated CO₂ in a calciner operated at around 900–950°C, according to the reversible carbonation reaction $\text{CaO(s)} + \text{CO}_2(\text{g}) = \text{CaCO}_3(\text{s})$. The utilization of fluidized bed reactors implies the unavoidable occurrence of attrition and fragmentation phenomena, with consequent changes in the particle size (and residence time) distribution of the sorbent, which in turn may influence its CO₂ capture capacity. Moreover, the possible presence, in the combustion flue gas entering the carbonator, of SO₂ and/or steam would have relevant effects on the sorbent reactivity. In the recent past, the effect of the presence of SO₂/H₂O in the carbonator atmosphere on the CO₂ capture capacity and on the abrasion tendency of the sorbent particles has been investigated. However, the effect of sulphur dioxide and steam on the impact fragmentation tendency of the sorbent in CaL systems has been so far neglected. Accordingly, the aim of this work was to fill this gap. Calcium looping experiments have been performed on a reference high-Ca limestone in a batch lab-scale twin fluidised bed apparatus, purposely designed for the study of chemical looping processes in conditions as close as possible to reality, in terms of cycling of temperatures and of reaction atmospheres. Six different operating conditions for carbonation were tested to study both the single effect of SO₂ and H₂O and the combined effect of them. The CO₂ capture capacity was calculated for each carbonation stage and, at the end of the test, sorbent particles were further analysed for the determination of the degree of Ca sulphation. After the CaL tests, the exhausted sorbent particles were fed to an ex situ impact test apparatus, which is based on the well-established concept of entraining particles in a gas stream at controlled velocity, and impacting them against a target. The analysis of data showed that samples obtained in the presence of SO₂ resulted to be harder than in absence of it, as higher SO₂ concentrations in the carbonator determined thicker CaSO₄-based shells around the particles. The presence of steam in the carbonator, orientating the reactivity of CaO towards CO₂ rather than SO₂ (when present), on the one hand determined particles

less resistant than those obtained in the absence of H_2O and in the presence of SO_2 . On the other hand, as steam indeed favours the carbonation reaction of CaO , we have observed particles with a larger CaCO_3 fraction and therefore more resistant than those obtained in conditions where both steam and SO_2 were absent.

Sorption-enhanced methanation in a dual fluidized bed system: evaluation of two sorbents

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Abstract

Methane is an important energetic carrier for many sectors such as industry, energy and transportation. The major share of methane comes from fossil resources, but the growing debate related to the climate change aroused a remarkable push towards the catalytic and biological production of methane. In particular, the catalytic methanation of either CO₂ or CO ($4\text{H}_2 + \text{CO}_2 = \text{CH}_4 + 2\text{H}_2\text{O}$ or $3\text{H}_2 + \text{CO} = \text{CH}_4 + \text{H}_2\text{O}$) assumes a central role when combined with the concepts of chemical storage and of CO₂ capture and utilization (CCU). Methane could be considered as the final product for the storage of solar energy, initially converted into hydrogen by electrolysis of water. Moreover, methane, contrary to hydrogen, is already extensively used in the civil and industrial sectors, as well as in the automotive industry, and consequently has a well-developed distribution and storage infrastructure in many countries, and finally benefits from a relatively large public acceptance. The commercially available methanation plants typically consist of a cascade of adiabatic fixed bed reactors with intermediate cooling, operated at high pressure, which are affected by different problems mainly related to the management of the heat of reaction. Recently, some research groups recently proposed and demonstrated, in a lab-scale fixed bed apparatus, the concept of Sorption-Enhanced Methanation (SEM), based on the Le Chatelier principle, where the steam generated by the reaction is removed from the gas phase in the catalytic bed by adding a sorbent material. In this way, the equilibrium of the methanation reaction can be shifted toward higher methane yields, allowing to lower the operating pressures. In this work, an innovative process configuration for the Sorption-Enhanced Methanation concept based on the technology of dual interconnected fluidized beds is investigated. The idea consists of a chemical looping configuration where in one reactor (the Methanator) catalytic methanation occurs simultaneously with hydration of the sorbent, to drive the equilibrium towards product formation, while in another reactor the regeneration of the sorbent (Dehydrator) takes place. Tests have been carried out at different temperatures in order to evaluate the potential of sorbents to selectively capture and release water under typical methanation conditions. Two sorbents have been selected: CaO, derived from natural limestone, and a commercial attrition-resistant Zeolite 3A. The results for CaO showed that the H₂O capture capacity (γ), expressed as the mass of captured water per mass of initial sorbent, tends to decrease with the number of cycles, reaching an asymptotic value after approximately the 5th-6th cycle. For the Zeolite 3A no decay effect of γ with the number of cycles was observed. In

general, the asymptotic values of y for CaO were in the range 0.015-0.04 g/g, while for the Zeolite fluctuated between 0.02-0.05 g/g.

Abstract_S5_AIII_36

Emissions from combustion of fuels with oleoresin-based compounds as additives

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Abstract

The search for renewable fuels or fuel additives/components which may improve/replace fossil fuels is an important step for a sustainable future. In particular, pine oleoresin, produced by conifer trees, is composed by turpentine essential oil and non-volatile rosin. In this work, oxyfunctionalized molecules from turpentine (nopol, α -terpinol, myrtenol, and borneol), and methyl ester of rosin (abietic-acid methyl-ester) were assessed as potential diesel additives/components by quantifying both the emission indices of CO, UHC and NO_x , and the flame temperature in a non-premixed co-flow burner, with n-heptane as diesel surrogate. Significant increase in flame temperature and reduction in CO and UHC emissions with respect to n-heptane were observed with nopol, terpineol and myrtenol, suggesting an improvement in combustion performance.

Abstract_S5_AIII_37

Implementation and validation of the discrete ordinates method for calculation of radiative heat transfer in the CFD software AVL FIRE™

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Abstract

It is known, that the radiative heat transfer has an impact on overall heat transfer and emissions in the engineering systems that operate at the high temperatures. The radiative heat transfer in the numerical simulations is often not considered due to its additional computational complexity and demanding of computational time. However, to precisely calculate the emissions concentrations, it is no longer enough to exclude the influence of radiative heat transfer on emission formation process. If the participation of medium in the radiative heat transfer is considered the radiative transfer equation must be solved. To solve such an integrodifferential equation, approximation with the numerical models has to be employed. In this work, the Discrete Ordinates Method (DOM) approximation featuring finite volume approach was implemented into the computational fluid dynamics software AVL FIRE™. The implemented DOM considers all radiation phenomena: absorbing, emitting, and scattering. The absorptivity and emissivity are modelled as a constant value and with the weighted-sum-of-grey-gases approach, while the scattering coefficient and scattering phase function were modelled for the homogeneous and isotropic medium. Additionally, the algorithm for spatial discretization with an arbitrary number of theta and phi angles was implemented, where to the each defined spatial angle is attributed one ordinate. After the spatial discretization is conducted, the transport equations for incident radiation in each ordinate is calculated, and its contribution is added as the radiative source term in the energy conservation equation. Furthermore, the symmetry and diffusive opaque boundary conditions are implemented for the description of incident radiation in all ordinates directions at the domain boundaries. Validation of the implemented model was conducted on simple geometry cases for which the analytical results exist, where the good agreement with analytical results is obtained. Finally, the aim of this work is to present capabilities for modelling of the radiative heat transfer in participating media with DOM and to investigate its capabilities in combination with AVL FIRE™ on a complex verification case.

Abstract_S5_AIII_38

Effects of CO₂-H₂O dilution on characteristics of CH₄-air-O₂ flames

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Abstract

This paper presents numerical and experimental results of the effects of CO₂ and H₂O dilution on CH₄-air flames enriched by oxygen. The numerical part concern the intrinsic properties of the mixture CH₄-air-O₂ diluted by CO₂-H₂O gases. The results include mainly laminar flame velocity and flame temperature. Numerical calculations are performed using the COSILAB code with the GRI-Mech 3.0 mechanism for one-dimensional premixed flames. The calculations are performed with different rates of dilution (0 to 20%) and oxygen enrichment (21% to 30%). The equivalence ratio effect is also analyzed. Calculations are compared and validated by the results from the literature. The experimental part is carried out on a coaxial swirled burner placed in a vertical combustion chamber. The flame is visualized by the chemiluminescence technique on OH* in order to locate the flame front. Measurements of combustion products such as NO_x, CO and CO₂ are done using a HORIBA PG250 multi-gas analyser. Results show that the CO₂ and H₂O dilution influences significantly the flame characteristics. Indeed, a high increase in flame velocity and pollutant emissions with the dilution is observed. The addition of H₂O/CO₂, with or without O₂ enrichment, changes significantly the form and the flame behavior such as the stability.

Abstract_S5_AIII_39

Reliability of particulate matter sensor operation during uncomfortable weather conditions

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Abstract

Particle matter (PM) concentration is one of the most important indicator of air quality due to its impact on human health, visibility and climate. European Union's Air Quality Directive 2008/50/EC (AQD), which regulates ambient concentrations of particulate matter, introduces the concept of 'indicative measurements', which have less strict data quality objectives than fixed measurements. Low-cost dust sensors may be suitable for such indicative measurements thanks to their small dimensions and high spatial resolution. The legal and procedural background is currently being developed by EU Delegated Working Groups (CEN/TC 264/WG42). Many studies related to this topic have been published in scientific journals so far; however, unanswered questions remain regarding the accuracy, reliability and reproducibility. A Honeywell particulate matter sensor was selected for investigation in this study to find out its usability at outdoors, the impact of protective casing and perform long-term (13 days) tests. Parallel tests performed with sensors of the same type have shown that the protective box formed by the lamellar exterior does not affect the accuracy of the sensors, no accumulation or loss of sensitivity occurs. The statistical relationship had been analyzed between the hourly PM_{2.5} concentrations of Honeywell sensor and OLM device by correlation coefficient (R), root mean square error (RMSE) and RMSE normalized to the OLM PM_{2.5} concentration (nRMSE). R is under 0.8 for the full period and the nRMSE is lower than 0.25. The best statistical values are under 80% RH, over 5°C and over 2 m/s windspeed. R values under 80% RH are higher with 0.37 than over 95% RH. nRMSE is almost 400 times higher over 95% RH than under 80% RH, which has the lowest nRMSE values of the investigated ranges. Ranges with R under 0.8 have not greater difference from nRMSE value of full period than 0.05.

Abstract_S5_AIII_40

Effects of inner swirl on flow and combustion patterns from non-premixed oxygen enriched flames above coaxial injectors

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Abstract

An experimental study is conducted to investigate the impact of swirl conferred to the inner stream of methane in a co-axial injector on the stabilization of non-premixed oxy-flames. The annular flow through the co-axial injector is a swirled oxygen air enriched mixture, yielding flames with a high resistance to aerodynamic strain. Increasing the axial or the tangential momentum of the inner fuel stream detaches the flame from the injector rim, whereas increasing the axial or the tangential momentum of the oxidizer annular stream reduces the flame liftoff height and provokes flame anchoring. Transitions of the flame structure are analyzed with the help of Particle Image Velocimetry (PIV) measurements. It is shown that an increase of the inner swirl level destabilizes the flow field close to the injector dump plane which impedes the diffusion flame front from stabilizing in the wake of the injector rim.

Abstract_S5_AIII_41

The influence of the combustion operation parameters in the process burners on the formation of NO_x and heat fluxes

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Abstract

The paper deals with the experimental investigation of combustion operating parameters and burner's constructional parameters on the formation of nitrogen oxides and heat fluxes. The tests were carried out at BUT burners testing facility, which enables testing burners up to the capacity of 1.8 MW. Combustion tests were performed using a fuel stage burner and a fuel stage burner with integrated internal flue gas recirculation. Both prototypes have a maximum power of 1.5 MW and similar geometry. During the testing, several configurations were examined including various geometries of nozzles and numerous geometries of so-called swirl generator. The observed parameters included NO_x and CO emissions, flame stability, air temperature, turndown ratio, heat transfer from hot flue gas to the combustion chamber's shell and the distribution of in-flame temperatures measured in the horizontal symmetry plane of the chamber. The results showed that the area with the temperature peak for the fuel stage burner was not as large as for the burner with recirculation. Furthermore in close distance of a burner tile higher temperatures were observed while using the throttle with a larger diameter at burner with recirculation. The obtained shape of the heat flux curves was similar for all investigated settings. In general, the highest heat fluxes were reached in the distance 1.5 m from the burner, whereas the lowest heat fluxes were achieved in the distance 3.5 m from the burner for all three settings. In the section furthest from the burner, the heat fluxes were almost independent on combustion air temperature (ca. 25 kW·m² for all settings). With higher combustion air temperature, the heat flux is higher due to a higher amount of heat energy supplied to the combustion chamber. The abstract is prepared for inclusion in the Book of Abstracts of the ECM2019 and follows the format established in previous European Combustion Meetings. The purpose of this document is to provide rules for obtaining a high-quality proceedings volume. We urge you to submit your abstracts in the described format. The paper should begin with a four-to-six line one-column abstract as illustrated here.

Abstract_S5_AIII_42

Cold flow analysis, flame stability and emission properties of blade-based premixed swirl burners at various blade angles

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Abstract

This work presents the results of experimental investigations on the geometric design of swirl generators as used with a premixed gaseous fuel burner within a single stage combustion chamber. Three different designs of a 10-bladed swirl generator were tested, differing only by the angle α_i of the blades with respect to the axial flow of $\alpha_1=30^\circ$, $\alpha_2=45^\circ$ and $\alpha_3=60^\circ$, leading to corresponding swirl numbers of $S_1=0.42$, $S_2=0.72$ and $S_3=1.25$, respectively. Via Particle Image Velocimetry, dry-air cold flow analyses with both horizontally and vertically aligned light sheets were performed. The results demonstrate the influence of the blade angle α_i and the input flow rate on the output flow characteristics such as velocity and distribution. Notably, for a blade angle of $\alpha_2=45^\circ$, the formation of an inner recirculation zone was observed. Additionally, reference experiments with premixed methane-air flames (equivalence ratio $\phi=0.6 \dots 0.9$) reveal the limits of flame stability (blow-off and flashback) and values of exhaust gas emissions (NO_x and CO) with respect to changes to the swirl generator geometry, equivalence ratio, and input flow rate.

Abstract_S5_AIII_43

Using high-speed multispectral infrared imaging for temperature calculation of composite materials under kerosene flame

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Abstract

Over the past few years, two-color pyrometry was proven to be a fast and reliable non-invasive method to accurately determine the temperature of materials by overcoming emissivity issues usually encountered by thermal infrared cameras. However, the need for two cameras at the same time makes this method expensive. In this work, a single Telops MS M100k equipped with a fast rotating spectral filter wheel was used to accurately determine the temperature of composite materials attacked by a kerosene flame. The method was previously validated with a steel plate equipped with embedded thermocouples.

Abstract_S5_AIII_44

Natural gas replacement by syngas in Resource Energy Intensive Industries (REII) burners: numerical CFD evaluation

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Abstract

Resource Energy Intensive Industries are focused on several researches to achieve improvements in terms of energy, environmental and cost performance. One of the alternatives is the substitution of fossil fuels by alternative fuels (syngas). This paper indicates the burner modifications to achieve co-firing at 10% and 40% of energy substitution. Different bio-syngases and process-off-gases have been evaluated taken into consideration theoretical parameters such as the low heat value and the Woobe index. It has been considered a natural gas burner commonly used in ceramic sector, but relevant modifications is necessary to achieve 40% of substitution. It is essential to undertake CFD simulations to evaluate these modifications. Moreover, a combustion mechanism has been validated and several simulations have been carried out with 10% and 40% substitution.

Abstract_S5_AIII_45

Combustion-specific deep neural networks for modeling reactive flows

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Abstract

During the last years, the technique of deep learning was improved substantially and has proven to be useful in a large variety of different fields ranging from computer science to life science. As modeling of emissions and turbulence in the context of flames as well as related effects such as extinction are still challenging for current modeling approaches, the application of deep learning to reactive flows is timely and provides a data-driven approach to improve existing models. One main challenge in the context of deep learning is the generation of a task-specific neural network topology. This is addressed in the context of reactive flows in this work. As different layers, such as convolutional and recurrent layers, different solvers, such as stochastic gradient descent (SGD) or Adam, and network features, such as shortcut connections, have all shortcomings and advantages, suitable choices are not trivial and the question whether different types of combustion require different kind of networks is interesting. Therefore, two different direct numerical simulation (DNS) datasets are considered for evaluating combustion-specific networks. One dataset features a set of non-premixed, temporally evolving jet flames with Reynolds numbers ranging from 4,500 to 10,000. The other dataset represents premixed combustion in stationary gas turbines. The focus lies on the interaction of single burners with disconnected burners issuing pure air. The interaction of these jets leads to increased CO emissions similar to stationary gas turbines under part load conditions. Training is performed for several quantities such as source terms of the progress variable to predict the combustion process as well as species mass fractions and its corresponding source terms to develop models for predicting emission concentrations. Besides the focus on network effects, computing aspects are highlighted. These include the efficient use of GPUs for the training of the deep learning network on current supercomputers utilizing the state-of-the-art libraries Keras, TensorFlow, and Horovod.

Ignition and early stages of flame propagation in a non-premixed biogas planar turbulent jet

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Abstract

Localised forced ignition (spark, laser) of flammable mixture is a topic of fundamental importance in combustion science. A thorough knowledge of ignition is needed for safety standards as well as in the design of efficient and reliable Spark ignition and Direct Injection engines, in which misfire causes ineffective combustion, but also for the relight of gas turbine at altitude. The ignition of turbulent flammable mixtures is not only influenced by the minimum ignition energy or the critical flame radius, but it also is strongly dependent on the local properties of the energy deposition region (turbulence characteristics, scalar gradients, mixture composition, etc.) and of the overall flow field. The ignition of a simple canonical turbulent round methane jet in ambient air has been extensively studied by both experimental and numerical means. Furthermore, the dilution of methane by carbon dioxide is generally referred to as "biogas" and has been identified as a carbon neutral fuel when originating from anaerobic digestion of organic matter by living organisms. It is also widely accepted as a sustainable fuel that can be used either as a complement or a replacement in applications such as power generation or within the transport sector. However, to date, limited effort has been directed to the understanding of its ignition, and the uncertain combustion behaviours arising from the various amount of methane and CO₂ on the ignition process are yet to be analysed in detail. In particular, the ignition of biogas in inhomogeneous mixtures and in the presence of shear has not been studied. Building on previous numerical studies of methane/air ignition, three-dimensional compressible Direct Numerical Simulations (DNS) have been carried out to investigate the ignition of a biogas planar jet. A two-step mechanism involving incomplete oxidation of CH₄ to CO and H₂O and an equilibrium between the CO oxidation and the CO₂ dissociation has been used. This two-step mechanism captures the variation of the unstrained laminar flame speed with equivalence ratio and CO₂ dilution with sufficient accuracy when compared with detailed chemistry results. The study focuses on the three stages of flame evolution, i.e., (i) flame kernel growth, (ii) downstream flame expansion and radial propagation, and (iii) potential upstream flame propagation which relies on edge flame propagation. The flame expansion spans different combustion modes, from premixed to non-premixed in the presence of edge flames. The addition of CO₂ in the fuel stream affects significantly the flame kernel development and the subsequent flame behaviour by reducing the unstrained laminar flame speed and the heat release rate. These effects will be detailed with a focus on the edge flame speed, flame structure and reaction rate statistics with an emphasis on the differences observed with the ignition of a similar methane/air jet without CO₂ dilution.

Abstract_S5_AIII_47

Large eddy simulations of reacting spray jet with active control

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Abstract

The key features that particular combustion system must be characterized by, are low levels of instabilities, acoustic noise and vibrations, minimization of blowout probability and reliable reignition in case of extinction. These issues are related to unpredictable heat release fluctuations. Because of random nature of turbulent flames, there has been existed a constant effort into new techniques which now allows to control the flames behaviour to some extent. These techniques gave a rise to passive and active control devices. The passive control systems do not require additional energy input to the system otherwise they are active. Passive control may be realised by the use of exchangeable nozzle geometries, porous inserts into combustion chambers, swirlers or perforated liners. While the active one may be realised by introducing oscillating baffles, acoustic resonators or electrical field. The effectiveness of such devices may be different depending on details of particular combustion system, however, generally active control devices are more flexible but also more complicated. Since entrainment of fuel droplets in spray-fuelled systems significantly influences the flow field and flame and because such systems are mostly exploited in practice, detailed experimental studies have been devoted to analyse such combustion regimes. One can say that influencing the flow with spray passively or actively provides alteration of the droplets paths. Therefore, by controlling forcing the droplets can be again directed into the reaction zone. By controlling the droplet dispersion, one may also influence the efficiency of combustion process in terms of pollutants formation. The flame controlling is especially important in confined flames, e.g. in aircrafts' engines, where nozzles mutually influence each other. The strength of this effect depends on their distance and shapes. Many numerical studies have been devoted to control devices operating in single-phase combustion mode. However, facing the practical importance of the spray combustion and complexity of analysis of the flame instabilities, the only way to deal with these phenomena is by numerical simulations. In the current work, the results from experimental configuration of a two-phase jet burner are used firstly to validate the numerical code. Then it is assessed numerically to which extent the active control device (resembling the inlet oscillations), may change the flame structure in fully 3D turbulent two-phase case. The computations are carried out using a high-order compact differences in-house LES code SAILOR. The diluted ethanol polydispersed spray tracked in Lagrangian coordinates is coupled with the gas in Eulerian reference frame. The reaction rates are modelled using global chemistry with resolved scalars and implicit LES approach. The results show that the inlet flow oscillations change the angle of the jet spreading. The results may be useful for nozzle design by giving an insight into behaviour of the excited flame. Importantly

the results suggest that two-phase combustion is modified indirectly by the droplets comparing to single-phase combustion. This is due to the velocity oscillations that influence droplets dispersion.

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Abstract_S5_AIII_48

Determination of a correlation for predicting lean blow off limits of gaseous fueled, premixed turbulent jet flame arrays enclosed in a hexagonal dump combustor

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Abstract

Combustion of natural gas with air in gas turbines is a key technology for efficient provision of electric energy and heat. More stringent regulations regarding the emission of pollutants, such as NO_x emissions, are necessitating research on technologies to reduce NO_x formation during the combustion process. One technical approach onto the reduction of NO_x -formation during combustion is fuel-lean premixed combustion. Current lean combustion concepts applied in stationary gas turbine combustors rely on flame stabilization through recirculation of hot flue gas using swirling flows. Swirl stabilized flames may be prone to combustion instabilities especially in lean premixed arrangements. Therefore, another approach is followed in the present study. In this concept, a matrix of turbulent lean premixed jet flames in a dump combustor is applied. The matrix burner consists of a nozzle with an array of circular channels in a hexagonal arrangement and a combustion chamber with a hexagonal cross section. In order to develop an appropriate burner design based on this concept, the experimental determination and theoretical evaluation of the lean blow out limit using different nozzles and operating conditions were conducted in this work in order to quantify the influence of different parameters on the flame stability. The varied geometric parameters are the diameter of the circular channels in the burner matrix as well as the ratio of the free cross section area of the nozzle to the cross section area of the combustion chamber, the combustor area dump ratio. The lean blow limit was determined at different preheating temperatures and flow velocities. The results show that the velocity at the LBO limit increases with increasing channel diameter, area combustor dump ratio and preheating temperature. The experimental results of three matrix burner are correlated in terms of a critical Damkoehler number and it is shown through experimental validation, that the Damkoehler number correlation derived is capable of predicting the LBO of a scaled matrix burner.

Large eddy simulation of a lab-scale 30 kW furnace operating in MILD combustion

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Abstract

Diluted combustion, also called Moderate or Intense Low-oxygen Dilution (MILD), is a promising type of combustion to limit pollutant emissions, especially nitrogen oxides (NO_x) emissions. Numerical simulation of MILD combustion furnaces is challenging as it involves complex interactions between turbulence, chemistry and radiation. The turbulence chemistry interaction (TCI) needs to be considered in MILD combustion as the reaction rates are lower compared to a classical combustion and the chemical time is higher, such that the Damköhler number is close to the unity. In recent literature, mainly Reynolds Averaged Navier Stokes (RANS) investigations of MILD combustion in industrial furnaces configurations can be found. However, RANS and the associated combustion models present some limitations. They do not allow to locate correctly the reaction zone and lead to over-predictions of the temperature peaks. More recently, and thanks to the computational power growth, Large-Eddy Simulations (LES) investigations become more widespread. However, most of the LES were performed on academic burners configurations, as the jets in hot and diluted coflow: the Delft-Jet-in-Hot-Coflow [Oldenhof et al., *Combust. Flame*. 158 (2011) 1553-1563] and the Adelaide burner [Dally et al., *Proc. Combust. Inst.* 29 (2002) 1147-1154]. Indeed, their dimensions and the small volume occupied by the reaction zone allows to perform LES on fairly light grids. The current study proposes to address LES simulations of furnaces close to industrial configurations. The test case considered is a lab-scale furnace with a thermal power of 30kW to limit the geometry dimensions. It has a configuration similar to industrial furnaces (burner design, high internal recirculation, load, high temperature air preheating) and in-furnace measurement were performed by Lupant et al. [*Applied Thermal Engineering* 75 (2015) 93-102]. An LES is carried out to predict the combustion phenomena in this methane/air industrial-like furnace using Finite Rate Chemistry (FRC) and radiation modelling. This simulation aims to demonstrate the possibility of obtaining accurate numerical predictions of industrial MILD combustion processes. On the other hand, experimental measurements do unfortunately not allow to access as much data as numerical simulation. In particular, the LES approach allows for true in depth analysis of the flow and flame topology, including time-averaged and root mean square (RMS) results as well as fine topological details. With fine grids, the numerical data (velocity, temperature, species mass fractions, heat release...) will constitute a detailed database for a realistic MILD combustion system.

Abstract_S5_AIII_50

Fundamental analysis of DME pilot-ignited methane-air flame

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Abstract

Dual-fuel combustion is an attractive approach for utilizing alternative fuels, such as natural gas, in compression-ignition internal combustion engines. In pilot-ignited dual-fuel engines, pilot injection of a more reactive fuel provides a source of ignition for the premixed natural gas/air. The process involves different combustion modes and transition from autoignition to premixed flame propagation in inhomogeneous mixtures. The objective of this study is to investigate dual-fuel combustion fundamentals using Direct Numerical Simulations with a realistic dual-fuel chemistry model. The configuration is based on a dimethyl ether (DME)-air mixing layer configuration previously presented in [Krisman et al. *Combustion and Flame*, 172, 326-341]. In the current study, methane is added to the oxidiser stream, as a surrogate for natural gas, at an equivalence ratio of 0.4. Methane addition affects the combustion processes both by diluting the oxidiser and through chemical involvement in the ignition process. The distinct chemical and thermal contributions of the methane addition are assessed through a numerical experiment involving an additional simulation in which methane is replaced with a chemically-inert species with thermodynamic properties identical to methane. The simulation results reveal a two-stage ignition process that develops into a poly-brachial flame structure, involving cool-flame, stoichiometric diffusion flame, rich premixed and lean premixed flame branches. Once established, the lean premixed branch proceeds to burn through the lean methane-air charge. Replacing methane with a chemically-inert substitute reduces the ignition delay time. Analysis shows that the chemical effects of methane addition retard non-premixed ignition in particular by increasing sensitivity to scalar dissipation. Ignition processes contribute a small proportion of heat release. After ignition, edge flames propagate rapidly along the stoichiometric iso-surface. The speed of the edge flames is shown to be affected by the heat release and radical species produced by first-stage ignition ahead of the edge flame. A simple model for the enhancement of flame speed due to first-stage ignition is presented.

Turbulent bluff-body flames close to stability limits revealed by coupling of high speed optical diagnostics

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Abstract

The improvement of combustion is still an important issue for the scientific community today. The requirement of the increase of efficiency and the pollutants reduction become an essential task, which imposes constraints and new physical problems for industrial burner manufacturers and furnaces users. Recent innovative combustion regimes with low pollutants emissions and high energy efficiency usually operate close to limits of stability of turbulent flames. It is then essential to have a deeper understanding of physical phenomena leading to flame stabilization and to be able to master, control and enhance it. Bluff-body burner is often used for stabilization of turbulent non-premixed flames. The internal recirculation zone generated by the wake effect of the flows downstream of the bluff-body induces then a partially mixing of the fuel with oxidant, but also a trapping of high-temperature combustion products which brings the necessary heat for the stabilization of the flame. In this configuration, the modes of stabilization of turbulent flames often take the shape of intermittent unsteady phenomena in the internal recirculation zone which are complex and still poorly understood. Their study requires the ability to make time-resolved measurements by use of high-speed optical and laser diagnostics. For this purpose, an experimental study is set up based on a bluff-body burner consisting of two coaxial jets. Methane is injected in the central jet ($D_j=7.5$ mm) while air is injected in the annular one. The 50 mm bluff-body between reactants flows induces a large blocking factor of 0.83. For a constant central methane jet velocity (i.e. thermal power), the variation of annular air velocity allows us to cover different flames modes from a fully stabilized turbulent flame to the limit of flame blow-out. The characterization of these flames is made by coupling high-speed Particle Image Velocimetry (PIV) at 5 kHz and flame imaging at 1 kHz. Time-resolved flame imaging allows to highlight the phenomenon of ejection of reactive pockets from the internal recirculation zone to the base of the main jet-like flame. Image processing of temporal series is performed to determine the characteristic frequency of this periodic ejection and its variation with the flames modes. Simultaneous PIV measurements allow to characterize the original structure of the flow downstream the Bluff-body burner, established mainly by a highly turbulent internal recirculation zone pierced by the methane central jet. Correlations determined between the periodic burning pockets ejection and the instantaneous velocity fields in this region allow to fully describe this physical phenomenon controlling the stabilization of the turbulent flame.

Abstract_S5_AIII_52

Mixing and entrainment of burned products in high Karlovitz number premixed jet flames

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Abstract

In high Karlovitz number flames, the lengthscales and timescales of the smallest and fastest turbulent structures are comparable or smaller than the corresponding characteristic scales of the flames. In this case, the inner layers of the flame structure, where preheating and chemical reactions of the fresh mixture are concentrated, can be affected significantly since the smallest turbulent eddies can penetrate these layers, modifying the reactive-diffusive imbalance. The consequences for the flame dynamics are numerous. The local reaction rate can be altered with respect to the typical behavior of an unperturbed flame, inducing local quenching and a so-called broken-reaction regime. In addition, a remarkable widening of the thickness of the flame inner layers is often observed with strong consequences on the overall flame speed and global burning rate. In addition to these phenomena, which have been studied extensively both by means of sophisticated experiments and direct numerical simulations (DNS), the intense turbulent transport that dominates high Karlovitz flames can induce mixing and entrainment of fully burned products into the low temperature regions of the premixed flame. This aspect can be very significant in jet and swirling flames, where the flames are stabilized with the heat and radical species provided by a stream of fully burned products, coming either from a pilot or from a recirculation region. Two large scale DNS of turbulent premixed combustion in jet flames are presented. The flames have the same jet Reynolds numbers of 5600 and Karlovitz number approximately equal to 40 and 400, respectively. These two high Karlovitz flames are analyzed to investigate the mixing and entrainment of fully burned products into the reaction and preheat zone of the flames. The simulations feature a 16 species, finite rate, chemical mechanism and up to 3 Billion grid points. In order to track the mixing of the coflow fluid into the flame, an equation for a tracer, i.e., a non-reactive, conserved, passive scalar with the same diffusivity of temperature, is solved in the DNS. In the higher Karlovitz number case, joint statistics of the local temperature and the tracer show that at locations where the temperature is close to that of the fresh mixture conditions, then deep in the preheat zone of the flame, up to 10% of the mixture is made of fluid coming from the coflow. This observation suggests that the flame is significantly diluted by burned products. The effects of this phenomenon on the local reactivity and dynamics of the flames are discussed. It is found that the local equivalence ratio is not affected significantly. The reaction rate of selected species is investigated. For methane, the reaction rate does not appear to be altered significantly. On the other hand, the oxidation rate of CO,

which is supposed to consume almost completely the CO formed in the inner flame zone, is strongly affected by coflow mixing. Since the final CO emission is strongly sensitive to the balance between its production and oxidation, it is likely that the coflow mixing has a significant effect on the CO emission level at high Karlovitz.

Abstract_S5_AIII_53

Multi-scalar and velocity measurements in a turbulent bluff-body flame using spectral fitting of spontaneous Raman scattering and PIV

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Abstract

Depletion of fossil fuels and environmental issues make necessary an in-depth study of combustion processes to improve the energy efficiency and adaptability of industrial burners. Bluff-body burners are widely used to ensure stabilization of large turbulent non-premixed flames. The presence of a bluff-body generates a recirculation zone of high temperature combustion products that partially mix the central jet of fuel with the co-flow of oxidant and provide the required heat to ignite reactants and stabilize the flame. However, operating conditions leading to an increase of energy performance and reduction of pollutants emission are quite close to the limits of stability of turbulent flames. The objective of this study is to experimentally investigate the complex shear and mixing layers of the recirculation zone at the exit of a canonical bluff-body burner by spontaneous Raman scattering and PIV, in order to have a deeper understanding of combustion mechanisms that lead to the stabilization of the flame. Simultaneous temperature and multi-species density numbers from Spontaneous Raman Scattering (SRS) measurements provide valuable information to describe such turbulent flames. However, in the case of highly turbulent and locally rich hydrocarbon flames, single-shot SRS measurements require powerful excitation system and sensitive detection system with short exposure time because of the low cross-section of SRS and the strong radiation from the flame. In this study, the excitation source consists in a high energy Nd:YAG laser system (1.8 J per pulse at 532 nm with a pulse duration of 1 μ s) and the detection system is a Bi-CCD Camera, combined with an ultra-fast electro-optical shutter that offers an exposure time of 1.05 μ s. 1D single-shot SRS measurements with 330 μ m spatial resolution are collected in the core of the recirculation zone, for several radial positions to get a complete profile of about 3 cm, from the methane central jet to the ambient air. Quantitative number densities for all major species (N_2 , O_2 , CO, CO_2 , H_2O and CH_4) are extracted simultaneously from single-shot spectra using a spectral fitting method. Temperature of the probe volume is obtained from the minimization of synthetic spectra of N_2 with the experimental ones. In the fuel jet where nitrogen is absent or in too low concentration, temperature is extracted up to 1500 K from spectral fitting of methane SRS. In rich and luminous regions of the flame, strong interferences from C_2 emission on N_2 and CO Raman scattering spectra are rigorously removed by spectral fitting of the Swan bands. Temperature and multi-species number densities profiles across the recirculation zone of the bluff-body burner are compared with velocity measured by PIV and flame imaging results to identify and characterize precisely all the specific features of the flame in the recirculation zone consisting in eddies of partially burnt gas and a diffusion flame of CO close to the annular air flow.

Data-driven model development for CO emissions in stationary gas turbines

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Abstract

The assessment of pollutant formation plays a pivotal role in the development of next-generation gas turbine combustors. Especially for stationary gas turbines under part load conditions, CO emissions can increase drastically, which limits the load range. In this work, a comprehensive direct numerical simulation (DNS) dataset, featuring some essential characteristics of stationary gas turbines under full load as well as part load, is analyzed using the optimal estimator concept with the long-term goal of improving current LES of stationary gas turbines. The optimal estimator concept is a data-driven approach to investigate the modeling error and to assess its parts individually. The DNS configuration consists of three parallel slot jets separated by laminar pilots. All three jets are loaded with a premixed, lean methane/air mixture for the full load case. For the part load case, only the central jet is charged with the reactive mixture, while pure air is issued from the two outer jets. The perturbation of the combustion process by the unloaded jet burners leads to a significant increase of CO emissions for the part load case. A series of artificial neural networks (ANN) is trained with the DNS dataset using state-of-the-art libraries. These ANNs are trained to predict the target quantity, the CO source term ω_{CO} . The irreducible error, which is only related to input parameters of the model, is used to identify the optimal sets of input parameters for each simulation case. The ANNs are well suited for such a regression task, and they are able to achieve an optimal prediction as they minimize the prediction error for the corresponding data with respect to the set of input parameters. All quantities accessible from the DNS are taken as potential input parameters, with the progress variable C being fixed as one input parameter for each data set. It is found that mainly that species mass fractions, and especially some radicals, dominate the optimal sets of input parameters. Furthermore, it is evaluated how well ANNs trained for one simulation case predict the source term ω_{CO} of another simulation case.

The influence of the reactor model on EDC's mean reaction rate - a study on the relevance of choice

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Abstract

In their paper from 1996, Gran and Magnussen implemented chemical kinetics into the Eddy Dissipation Concept by treating the smallest scale eddies as transient, isobaric, homogeneous reactors. The stiff, time-dependent set of ordinary differential equations that describes the reactor was integrated to steady state. The choice of integration time is crucial as numerical stability and reliability of results strongly depend on it. The integration operation constitutes a major portion of the computational effort related to the EDC combustion simulation. Because mathematically easier to handle, in some CFD-codes the ODE of the PSR is replaced by the ODE of a plug flow ($u=const.$, batch) reactor. Few studies have examined possible differences between the two approaches. Investigations that exist so far found very good agreement for main species and temperature and small deviations for minor species such as CO and OH. Most of the studies focused on testing the influence of the reactor model choice on individual simulations and did not provide sufficient reasoning for the observed behavior. For this study, a combined approach of CFD simulations and separate reactor analysis was chosen. The aim was to connect phenomena observed in the simulations to features inherent to the reactor models. Therefore, the focus of the reactor study was placed on actual parameter combinations determined from simulations to improve its explanatory value. Both the PFR ($u=const.$, batch) and the PSR model were used within EDC to simulate Sandia Flames D and E. The idea behind simulating Sandia Flames D and E was that E is operated with higher Reynolds number for both jet and pilot and, hence, shows increased turbulence. The EDC parameters fine structure mass fraction γ^* and residence time τ^* define the turbulence input variables for the chemical reactor and are both influenced by changing the turbulence conditions. For Flame E, the difference between the two reactor models increased in regions where the PFR predicted higher species mass fractions while better compliance was reached for regions where the PSR predicted higher values. One aspect that needs to be considered is that the reaction path in the PFR is independent from the EDC parameters while they control the continuous flow through the PSR and, thereby, have an important influence on the reaction path. No qualitative impact of the reactor model on the global flame structure could be observed within this study. Quantitative differences existed but were not the relevant source of error in a RANS context. Contrary to previous studies, no differences between the minor and main species groups could be found concerning orders of magnitudes for mass fraction discrepancies. The reactor model analysis was used to connect the deviations between the reactor models with a time scale ratio between the transport and chemical processes of the PSR. This idea was

based on the assumption that the PSR is controlled by the interaction of transport and chemical processes and varies between residence time and chemical time scale controlled conditions. Both reactors share the residence time but differ in the reaction rate, which would indicate that differences between the reactor models are likely to increase where the reaction speed becomes more important.

Abstract_S5_AIII_56

Flame stabilization in a cavity based scramjet

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Abstract

Large eddy simulations (LES) of non reactive and reactive flows in a cavity-based scramjet combustor configuration from the U.S Air Force Research Laboratory (AFRL) are reported in this paper. The present LES are performed for a medium-high fuel-loading case for which the combustion is stable. A good agreement is found between experimental data (velocities measured by PIV) and results from the LES. The reactive simulation shows the persistence of the two recirculation zones already present in the non reactive flow. The globally high temperature into the cavity helps to sustain a reactive zone located in the mixing layer above the cavity. Combustion first occurs in a diffusion dominated regime followed by the efficient burning of a well stirred mixture (rich then lean). A significant diffusion dominated burning is also found inside the cavity. A priori test of a tabulated approach of the chemistry is performed based on premixed flamelet library.

Modelling and simulation of high-pressure flows

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Abstract

The modeling and simulation of supercritical mixing and combustion requires attention to the problems usually encountered at low pressure, but also to the problems posed by the introduction of non-ideal phenomena related to high pressure. It is now established that studying supercritical flows requires a dedicated framework that includes a real-gas equation of state (EoS) and non-ideal transport fluxes. It is also a scientific challenge to process with detailed high pressure chemistry since it has been shown that supercritical laminar diffusion or premixed flames can be less thick than one micron if the stretching of the flame becomes significant [1]. Dealing with supercritical flows also poses numerical challenges linked to the presence of strong density gradients that can lead to spurious numerical oscillations. Hence, introducing detailed chemistry in the context of realistic high pressure configurations requires lowering the numerical cost of simulations but preserving the physical modeling of non-ideal phenomena. The numerical benchmark proposed by Ruiz et al. [2] for high-Reynolds-number supercritical non-reactive flow tends to satisfy this compromise. A splitter-plate configuration is studied with a two-dimensional DNS allowing a good description of the mixing of liquid oxygen (LOx) with hydrogen under high pressure. In the present study, different modeling levels are evaluated for the combustion of hydrogen with LOx under supercritical conditions. In particular, the focus is on the modeling of the diffusion velocity of species, and the evaluation of binary diffusion coefficients at high pressure. A two-dimensional splitter-plate configuration, inspired from [2] for computational cost considerations, serves as numerical reference for this reacting flow. The impact of non-ideal transport modeling is addressed on the configuration of the 2D splitter-plate with and without combustion. With this modeling the diffusion velocity of species is described from the gradient of chemical potential coupled to the Peng-Robinson equation of state. A comparison with the classical low-pressure approach, which only uses the gradient of species molar fraction, is also performed. The results show that the non-ideal transport has a non-negligible impact on the flame structure and consequently on the flame temperature. This observation means that such an approach must be taken into account in the case of realistic simulations at high pressure. Also, the multi-component approach with Soret effects are found non-negligible for the combustion of H_2/O_2 . Finally, the development of high-pressure models for large-scale simulations can now be achieved through the analysis of this database.

[1] G. Ribert et al., *Combust. Flame*, 154 (2008) 319-330.

[2] A. Ruiz et al., *AIAA J.*, 54 (2016) 1445-1460.

Abstract_S5_AIII_58

Mesh partitioning of reactive flow simulations – speed-up and other side effects

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Abstract

Despite continuously increasing computational power, an efficient use of the available resources remains important. Reactive flow simulations differ from other simulations due to their high complexity. For efficient use of computational resources for reactive flow simulations we conducted a case study in OpenFOAM®, an open-source code for computational fluid dynamics. For coupling turbulence and chemistry the well-known Eddy Dissipation Concept was chosen. Guidelines on how to choose optimal partition size depending on reaction mechanism size were derived and interesting speed-up behavior for small meshes was observed. The influence of common speed-up techniques, such as tabulation are presented as well.

Auto-ignition characteristics of transient methane, biogas and syngas jets at elevated pressure and temperature conditions: an axisymmetric DNS study

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Abstract

The auto-ignition characteristics of spatially and temporally evolving methane, biogas and syngas jets at elevated pressure and temperature conditions are investigated by axisymmetric direct numerical simulations using a 20-species reduced reaction mechanism for methane/air. The composition of the biogas (CH_4/CO_2) and the syngas (H_2/CO) are defined based on a literature review of biogas and syngas production and application in internal combustion engines. In a first step, the most reactive mixture fraction is evaluated using homogeneous reactor, and one dimensional flamelet calculations, in order to identify the pre-ignition and thermal runaway marker species, for each fuel type. In the axisymmetric setup, a jet is injected at constant velocity through a nozzle into a chamber filled with quiescent air at elevated temperature and pressure. The ignition characteristics, and the ignition delay time and location are mapped for the different fuels. Global phenomenological observations based on the temporal and spatial development of relevant fields show the dynamics leading to the onset of ignition. Finally, the distribution of relevant fields in mixture fraction space is presented to highlight the role of the addition of CO_2 , H_2 and CO on the auto-ignition characteristics.



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