

THEORETICAL AND NUMERICAL MODELLING OF MULTICOMPONENT TRANSCRITICAL DIFFUSES INTERFACES

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ABSTRACT

In this study, we present a theoretical and numerical framework for simulating transcritical flows under a variety of conditions of interest for aerospace applications. A real multi-component and multi-phase thermodynamic model, based on a cubic equation of state and vapor-liquid equilibrium assumptions, is used to describe transcritical mixtures. The versatility of this model is reported since it can represent at the same time the supercritical states and subcritical stable two-phase states at equilibrium. We emphasize the difference in the mixing behaviors conducted with and without the VLE assumptions. The well-known numerical challenges that arise with the coupling between thermodynamics and governing equations under transcritical conditions are addressed by comparing a fully conservative to a quasi-conservative scheme in the context of density-based solvers while discussing the possibility of employing a pressure-based approach given the typically low-Mach number at play for the cases of interest.

Keywords: Transcritical flow, Vapor-liquid equilibrium (VLE), Real fluids, Diffuse interfaces

1 INTRODUCTION

Liquid rocket engines combustion chambers often operate injecting cryogenic propellants at a pressure higher than the critical values of pure components. The transcritical injection and mixing at non-ideal conditions can cause an elevation of the critical point, in which the mixture locally forms the co-presence of multi-phase conditions even at a pressure higher than the reactant critical values. This generates complex mixing conditions that feature the so-called multi-component transcritical diffuse interfaces [5]. The evaluation of mixture thermochemical properties across such an interface requires real fluid thermodynamic and transport models that can take into account liquid-vapor equilibrium (VLE). From the computational fluid dynamics (CFD) standpoint, transcritical diffuse interfaces have been mainly discussed for compressible solvers in which the mixture properties non-linearity causes spurious pressure oscillations at the interface, requiring a dedicated numerical treatment [6,7,8]. In this context pressure-based and low-Mach number approaches, despite having shown promising results in a single species context [4], have found minor applications so far. The solution of a pressure-equation is a promising alternative to avoid the mentioned pressure oscillations [8], as long as a consistent thermodynamic modeling of the involved flow variables is employed. However, a complete discussion on this issue is still missing in the current literature.

In this contribution we present: (i) an extensive validation for the evaluation of multicomponent and multiphase fluid mixtures in a wide variety of extreme thermodynamic conditions, ranging from slightly below the critical pressure up to largely supercritical pressure levels. (ii) a critical assessment on the numerical issues ensuing from the multicomponent transcritical diffuse interfaces, introducing the discussion on the possible use of pressure-based approaches for this class of mixing problems.

2 MODEL FORMULATION

2.1 Governing equations

The governing equations are the multi-component, compressible Navier-Stokes equations, written in a fully conservative form as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (1)$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + p \mathbf{I}) = \nabla \cdot \boldsymbol{\tau} \quad (2)$$

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot [(\rho E + p) \mathbf{u}] = \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{u} - \mathbf{q}) \quad (3)$$

$$\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot [\rho Y_i \mathbf{u}] = \nabla \cdot (\mathbf{J}_i) \quad (4)$$

Where ρ is the density, \mathbf{u} is the velocity vector, $E = e + \frac{1}{2} \mathbf{u} \cdot \mathbf{u}$ is the specific total energy, p is the pressure and Y_i the mass fraction of species i . $\boldsymbol{\tau}$, \mathbf{q} and \mathbf{J}_i are the viscous stress tensor, the heat flux and the species diffusion flux of species i , respectively.

2.2 Thermodynamic model

Dealing with transcritical mixtures requires a multi-component real fluid equation of state EoS, in this study the cubic Peng-Robinson equation (PR) [2] is used, due to its compromise between accuracy and simplicity. The PR EoS can be written as

$$p = \frac{RT}{v-b} - \frac{a}{v^2 - 2bv - b^2} \quad (5)$$

Where T is the temperature, v is the molar volume and R is the universal gas constant. The two parameters a and b , taken into account the effects of intermolecular attraction force and volume displacement [2], respectively. To extend the PR EoS to a mixture of N components, classical van der Waals mixing rules, based on pseudo-critical combination method are employed [1]. The other thermophysical properties are calculate using the departure function formalism [1]. In Figure 1 the density and the specific heat at constant pressure are compared against NIST data for pure Oxygen.

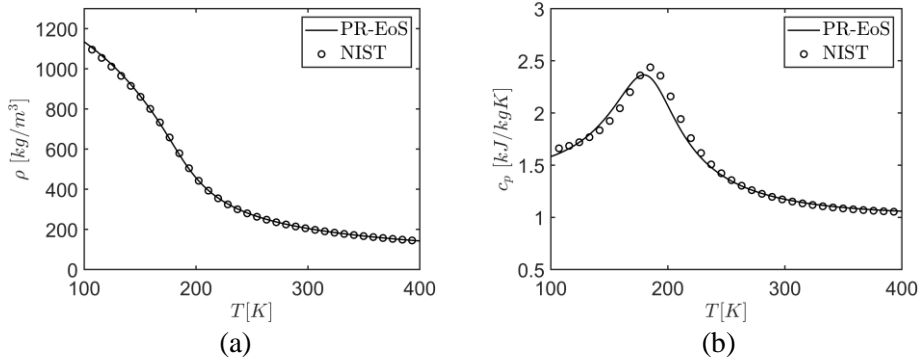


Figure 1 : Comparison of PR-EoS w.r.t NIST data results at $P=15\text{MPa}$ (a) : Density; (b) Isobaric specific heat

2.3 Vapor-liquid equilibrium solver

For a multi-component mixture, the phase equilibrium condition exists, if at the same time there is the mechanical, thermal, and chemical equilibrium of the species. So, for a two-phase system, the concept of vapor-liquid equilibrium VLE can be expressed as [3]:

$$P^V = P^L; T^V = T^L; f_i^V = f_i^L \quad (6)$$

Where f_i is the fugacity of species i , and the superscripts L and V denote the liquid and vapor phase. Figure 2 show the validation of the VLE solvers against the available experimental data of two binary mixture of Hydrogen-Nitrogen and Methane-Nitrogen.

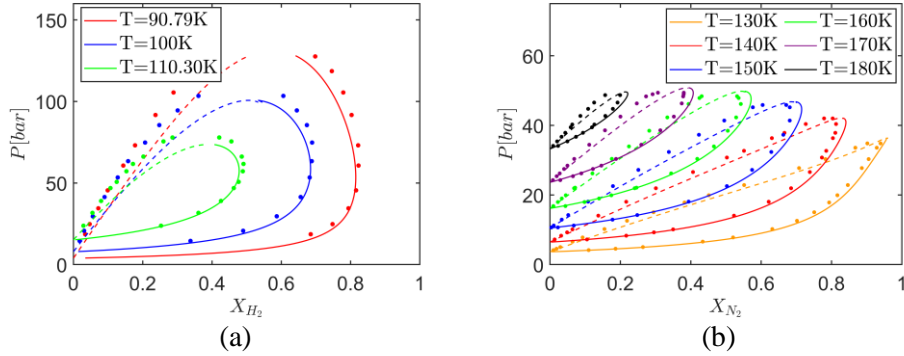


Figure 2: Pressure composition VLE diagram, the symbols denote the experimental data provided by [10],[11].
(a): $H_2 - N_2$ mixture; (b) $CH_4 - N_2$ mixture

3 VLE EFFECT ON MIXING PROCESS

To have a direct interpretation of the effect of the VLE model on the mixing process, we employed the single and the two-phase thermodynamic in a 0-dimensional mixing model. Two thermodynamic mixing processes were analyzed, the adiabatic and the isochoric model, calculated according to [7,9] respectively. As shown in figure 3(b), for the adiabatic mixing, the almost isothermal behavior in the single-phase case does not occur with the VLE assumptions, the VLE mixing line exhibits a linear function within the two-phase regime and a higher estimate of the mixing temperature. On the contrary, for the isochoric case, the temperature estimated with the VLE is lower than in the single-phase case. It is also interesting to note that on the outside of the two-phase dome, the two thermodynamic models collapse. In addition to the difference in mixing temperature, it is important to underline how the intrinsic difference between the mixing trajectories, induce, when the VLE is taken into account, profoundly different behavior in the phase equilibrium composition. This can be seen in

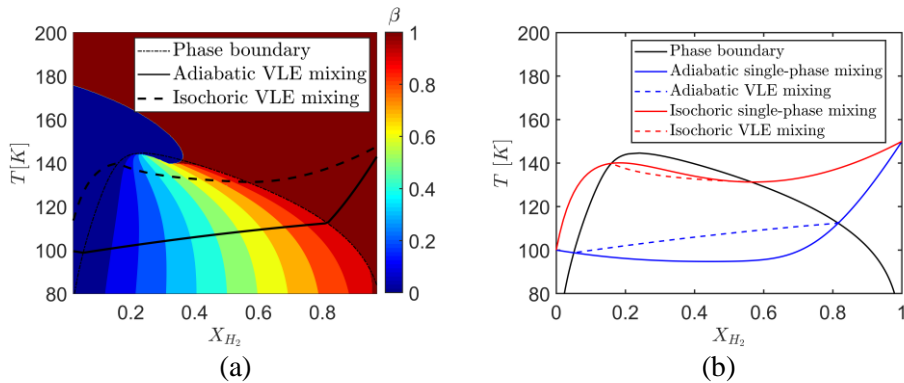


Figure 3: (a): Vapor phase fraction for $H_2 - O_2$ mixing at 100bar in composition-temperature plane; (b) Adiabatic and isochoric mixing lines for the same case with and without the VLE

Figure 3 (a) where the mixing lines are superimposed on the phase fraction β field. The relatively higher temperature of the isochoric mixing results in a higher vapor fraction in the vapor phase, and therefore, as a direct consequence a lighter homogeneous mixture is obtained, this has a huge impact on the flow variable.

4 NUMERICAL METHODS

Reducing the system of equations in section 2.1 to the Euler form (no molecular diffusion and viscosity), is discretized using a finite-difference method. Two approaches are used in the context of a density based solver, namely the standard Fully-Conservative FC scheme and the Quasi-Conservative QC scheme featuring the double-flux method DF developed in [6]. A first-order spatial integration is employed for both the approaches while the temporal integration is performed using the high-stability third-order Runge-Kutta scheme. Two cases of one-dimensional advection problems are simulated, which are a common benchmark problem used in the literature to validate the performance of the numerical schemes against the exact solution. For all simulations, the CFL number is set to 0.8.

4.1 LN2-GH2 interface advection problem results

The interface consists of a contact discontinuity of liquid and gas-like nitrogen. The operating pressure is $p = 5$ MPa, and the advection velocity is $u = 50$ m/s. The computation domain has a length $L = 1$ m. The initial conditions in terms of temperature (and so the density) are the same as [8]. Figure 4 shows results for both FC and QC schemes, the computation is conducted for three different uniform grids, with $N = 100, 300,$ and 500 points, respectively. The simulation is run for 0.02 s.

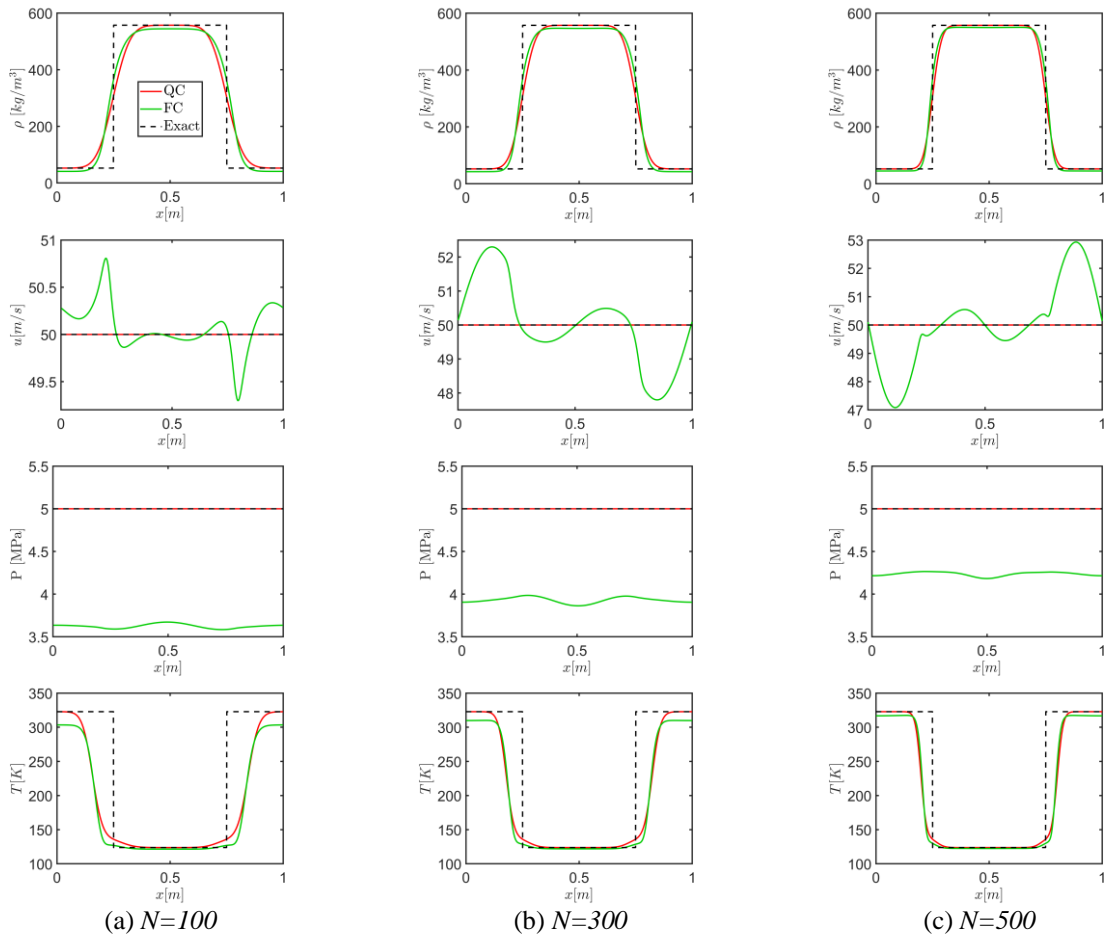


Figure 4: Simulation results for one-dimensional advection of LN2-GN2 contact discontinuity at $t=0.02$ s. TLN2 = 122.8 K, TGN2 = 332.8 K

The results show that for the QC scheme, density and temperature are captured very well despite the harsh cryogenic conditions, the velocity and pressure equilibriums are maintained without the generation of spurious oscillation for each grid resolution. The FC scheme does not maintain the equilibrium of pressure and velocity, the lower estimate of the pressure along with the entire domain, influences temperature and density, the same behavior was highlighted in the previous study by Terashima and Koshi [8].

4.2 LOX-GH2 interface advection problem

The second test case considered is in the context of a multi-component flow, we consider the advection of a contact discontinuity between liquid oxygen LOX and gaseous hydrogen GH2. The pressure is set to 22MPa, the advection velocity, the computational domain, and the grid points are the same as the previous case study.

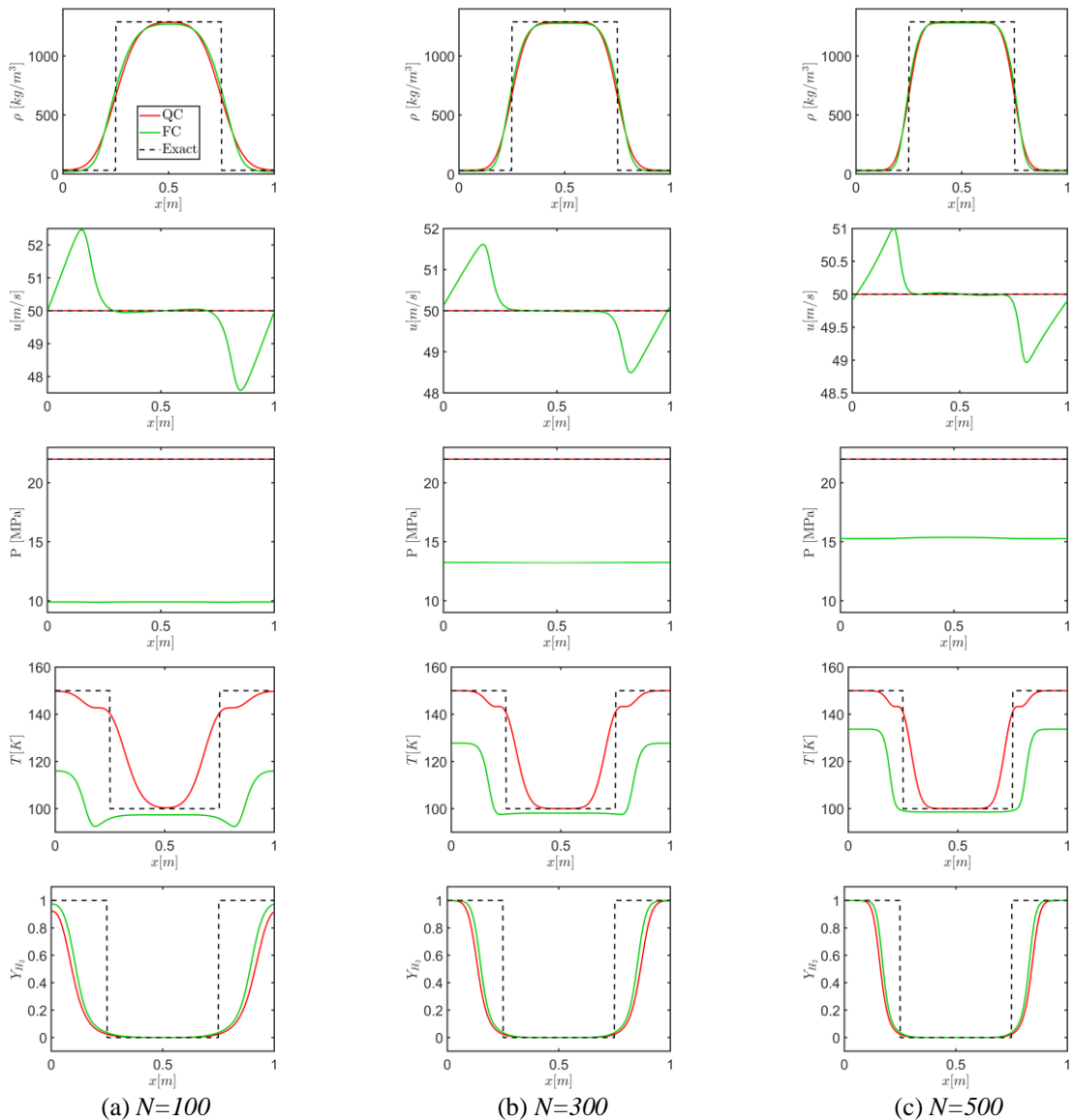


Figure 5: Simulation results for one-dimensional advection of LOX-GH2 contact discontinuity at $t=0.02s$.
TLOX = 100 K, TGN2 = 150 K

As in the previous case, the QC schemes maintain the pressure and velocity at the same values as the initial conditions. The density and mass fraction are in good agreement w.r.t the analytic solution, while the temperature exhibits at low-resolution a little fluctuation in the proximity of the discontinuity, which can be mitigated by increasing the number of grid points. On the other hand, the

FC scheme does not maintain equilibrium. The density and mass fraction are captured well, while the temperature highlights numerical errors due to the coupling between the EoS and the scheme, which need a high resolution to be mitigated. The solution obtained with the QC scheme can be considered a good starting point for the development of a low-Mach number pressure-based numerical framework.

5 CONCLUSIONS

A brief description of a comprehensive theoretical and numerical framework for simulating multi-species transcritical flows has been presented. A real multi-component and multi-phase thermodynamic model, based on a cubic equation of state and vapor-liquid equilibrium assumptions that can effectively describe transcritical mixtures has been validated. This modelling framework has allowed the discussion on the impact of VLE assumptions on the mixing behaviors of a conducted with and without the VLE assumptions. In the context of transcritical multi-species interfaces also the well-known numerical issue caused by the coupling between thermodynamics and governing equations have been briefly discussed. A fully conservative and a quasi-conservative scheme have been compared showing the superior performance of the second approach which is expected to be used as a reference for the development of pressure-based numerical framework.

REFERENCES

- [1] Poling, B., Prausnitz, J., O'Connell, J.; "The properties of Gases and Liquids", Fifth-Edition McGraw-Hill, 2001.
- [2] Peng, Ding-Yu & Robinson, Donald. (1976). New Two-Constant Equation of State. *Industrial & Engineering Chemistry Fundamentals*. 15. 10.1021/i160057a011.
- [3] Elliot, J. R., and Lira, C. T., *Introductory Chemical Engineering Thermodynamics*, Prentice-Hall, Upper Saddle River, NJ, 2012.
- [4] Lapenna, P. E., and F. Creta. "Direct numerical simulation of transcritical jets at moderate reynolds number." *AIAA Journal* 57.6 (2019): 2254-2263.
- [5] Urzay, Javier. (2021). Transcritical diffuse-interface hydrodynamics of propellants in high-pressure combustors of chemical propulsion systems. *Progress in Energy and Combustion Science*. 82. 100877. 10.1016/j.pecs.2020.100877.
- [6] Ma, Peter & Lv, Yu & Ihme, Matthias. (2017). An entropy-stable hybrid scheme for simulations of transcritical real-fluid flows. *Journal of Computational Physics*. 340. 10.1016/j.jcp.2017.03.022.
- [7] Ma, P. C., Wu, H., Banuti, D. T., Ihme, M., "On the numerical behavior of diffuse-interface methods for transcritical real-fluid simulations." *International Journal of Multiphase Flow*. 113:231-249, 2019.
- [8] Terashima, H., Koshi, M., 2012. Approach for simulating gas-liquid-like flows under supercritical pressures using a high-order central differencing scheme. *J. Comput. Phys.* 231 (20), 6907-6923.
- [9] Qiu, L., Reitz, R., 2015. An investigation of thermodynamic states during high-pressure fuel injection using equilibrium thermodynamics. *Int. J. Multiphase Flow* 72, 24-38.
- [10] Streett, W. B., and Calado, J. C. G., "Liquid-Vapour Equilibrium for Hydrogen+Nitrogen at Temperatures from 63 to 110 K and Pressures to 57 MPa," *Journal of Chemical Thermodynamics*, Vol. 10, No. 11, 1978, pp. 1089-1100.
- [11] Kidnay, A. J., Miller, R. C., Parrish, W. R., and Hiza, M. J., "Liquid-Vapour Phase Equilibria in the N₂ CH₄ System from 130 to 180 K," *Cryogenics*, Vol. 15, No. 9, 1975, pp. 531-540.