A Conditional Moment Closure Formulation for Large Eddy Simulation of Compressible Non-Premixed Turbulent Reactive Flows

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Abstract

This paper proposes a sub-grid closure model for Large Eddy Simulation (LES) of compressible non-premixed turbulent reactive flows. The model is an application of the Conditional Moment Closure (CMC) method to fully compressible reactive flows. In the present approach, the set of compressible reactive Navier-Stokes equations is partitioned in two sub-sets, one filtered and solved in the physical (LES) space, the other conditionally filtered and solved in the CMC space. The two sub-sets are integrated in time by means of an operator splitting technique.

1. Introduction

The Conditional Moment Closure (CMC) method [1] allows to model turbulence-chemistry interactions with large chemical kinetic mechanisms at an affordable computational cost.

The CMC model has been originally developed with reference to the low Mach number approximation, and has been used in RANS simulations to study different classes of flames, such as attached turbulent flames, lifted turbulent flames, bluff body flames, opposed jet flames, and autoignition [2, 3, 4].

Recently, the CMC equation has been formulated for LES [5], and used to study a turbulent methane/air jet flame (Sandia-D) [6], bluff-body flames [7], lifted methane flames [8], as well as autoignition problems [9].

Under the low Mach number approximation, the energy equation is coupled to the mass and momentum equations only through the equation of state, so that it can be readily conditionally filtered and solved in the CMC space, while the mass and momentum equations are solved in the physical space.

In fully compressible reactive flows, on one hand, the energy, mass, and and momentum equations are tightly coupled, and need to be integrated simultaneously in the physical space to describe the propagation of pressure waves; on the other hand, the source term in the energy equation, accounting for the heat release rate due to chemical reactions, is coupled to the species evolution equations, which are conditionally filtered and solved in the CMC space.

The CMC method has already been successfully used to solve compressible premixed reactive flows by Thornber, et al. [10]. Here we propose an application to compressible non-premixed flows, where the set of reactive Navier-Stokes equations is partitioned in two sub-sets, one filtered and solved in the physical LES space, the other conditionally filtered and solved in the CMC space. The two sub-sets are integrated in time by means of an operator splitting technique.

2. LES-CMC Formulation

The fully compressible reactive Navier-Stokes equations augmented by the transport equation of a passive scalar ξ, here referred to as ”full system”, reads:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0 \tag{1}$$

$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} + \frac{\partial p}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} = 0 \tag{2}$$

$$\frac{\partial E}{\partial t} + \frac{\partial (E+p) u_j}{\partial x_j} - \frac{\partial \tau_{ij} u_j}{\partial x_i} + \frac{\partial}{\partial x_j}\left[k \frac{\partial T}{\partial x_j}\right] + \sum_{\alpha=1}^{N} [\rho \dot{w}_\alpha \Delta h_{0_\alpha}] = 0 \tag{3}$$

$$\rho \frac{\partial Y_\alpha}{\partial t} + \frac{\partial (\rho u_j Y_\alpha)}{\partial x_j} = -\frac{\partial}{\partial x_j}\left(\rho \frac{\partial Y_\alpha}{\partial x_j}\right) + \dot{w}_\alpha \quad \alpha = 1, ..., N \tag{4}$$

$$\frac{\partial \rho \xi}{\partial t} + \frac{\partial (\rho u_j \xi)}{\partial x_j} + \frac{\partial}{\partial x_j}\left(D \frac{\partial \xi}{\partial x_j}\right) = 0 \tag{5}$$

A thermal and a caloric equation of state for mixtures of ideal gases are also provided:

$$p = \rho \overline{R}_{mix} T \qquad \overline{R}_{mix} = \sum_{\alpha=1}^{N} R_\alpha Y_{al} \tag{6}$$

$$E = \rho e = \rho \left[\frac{1}{2} u_j u_j + \sum_{\alpha=1}^{N} Y_\alpha \left(\int_{T_0}^{T} \hat{C}_{v_\alpha} T\right)\right] = \rho \left[e_{kin} + e_{sens}\right] \tag{7}$$

The state vector of this system is $\mathbf{w} = \{\rho, \mathbf{u}, E, T, p, \xi, Y_\alpha\}$, with $\alpha = 1, ..., N$, where Y_α is the mass fractions of the α-th species, ξ is the mixture fraction, a passive scalar which is a linear combination of the species mass fractions Y_α, and E is the total sensible energy. Here the subscript mix stands for the mixture value, $\overline{R}_{mix}$ is the gas constant of the gas mixture, $\hat{C}_{v_\alpha}$ is the specific heat of the α-th species. The energy release due to reactions is described by the term $\sum_{\alpha=1}^{N} [\rho \dot{w}_\alpha \Delta h_{0_\alpha}]$, where Δh_{0_α} is the formation enthalpy of the α-th species.

In the present approach, the "full system", Eq. (1-7), is partitioned in two sub-sets: one, named "mixing system", is filtered and solved in the LES space, the other, named "reaction system", is conditionally filtered and solved in the CMC space. Mass and momentum equations are in the LES sub-set, the species evolution equations are in the CMC sub-set. The sensible energy equation is split into two contributions: (i) the heat release rate due to chemical reactions, which is conditionally filtered and solved in the CMC space, and (ii) the transport, convective and diffusive, of sensible energy in a fully compressible frozen mixture, which is filtered and solved in the LES space. This way, the LES sub-set describes a fully compressible frozen mixture mixing problem, while the CMC sub-set describes, for a given pressure field, the change in mixture composition and the energy rise owing to chemical reactions. A two-way coupling between the LES and CMC sub-sets is obtained by updating the LES temperature and composition field with the information coming from the CMC sub-set, while the conditional pressure and velocity fields, needed to solve the CMC sub-set, are known from the LES sub-set. Formally, the present formulation aims at solving the full system for the filtered variables $\mathbf{v} = \widetilde{\mathbf{w}} = \{\overline{\rho}, \widetilde{\mathbf{u}}, \widetilde{E}, \widetilde{T}, \overline{p}, \widetilde{\xi}, \widetilde{Y_\alpha}\}$:

$$\frac{\partial \mathbf{v}}{\partial t} = F(\mathbf{v}); \qquad \mathbf{v}(0) = \mathbf{v}_0 \tag{8}$$

numerically by means of an operator splitting technique as follows:

$$\mathbf{v}_m = \mathbf{v}^{(n)} + F_m(\mathbf{v}_m)\Delta t \tag{9}$$
$$\mathbf{v}_r = \mathbf{v}_m + F_r(\mathbf{v}_r)\Delta t \tag{10}$$
$$\mathbf{v}^{(n+1)} = \mathbf{v}_r \tag{11}$$

where $\mathbf{v}^{(n)} = \mathbf{v}(t_n)$ and $\mathbf{v}^{(n+1)} = \mathbf{v}(t_{n+1})$, while $\mathbf{v}_m$ and $\mathbf{v}_r$ are the state vectors of the mixing and the reaction system respectively, Eqs. (9-10]; $F(\_)$, $F_m(\_)$, and $F_r(\_)$ indicate symbolically the full, mixing, and reaction system operators, respectively; Δt is a time interval of integration which is defined on the basis of a CFL condition for the mixing system. Clearly, higher order accuracy of the operator splitting can be envisaged.

3. The Mixing System

The first sub-set, the "mixing system", has a state vector $\mathbf{w}_m = \{\rho_m, \mathbf{u}_m, E_m, T_m, p_m, \xi_m, Y_{\alpha,m}\}$ describing a chemically frozen flow, with the passive scalar $\xi = \xi(Y_\alpha)$ associated with the mixing processes:

$$\frac{\partial \rho_m}{\partial t} + \frac{\partial \rho_m u_{m,j}}{\partial x_j} = 0 \tag{12}$$

$$\frac{\partial \rho u_{m,j}}{\partial t} + \frac{\partial \rho_m u_{m,j}}{\partial x_j} + \frac{\partial p_m}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} = 0 \tag{13}$$

$$\frac{\partial E_m}{\partial t} + \frac{\partial (E_m + p) u_{m,j}}{\partial x_j} - \frac{\partial \tau_{ij} u_{m,j}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[k \frac{\partial T_m}{\partial x_j}\right] = 0 \tag{14}$$

$$\frac{\partial \rho \xi}{\partial t} + \frac{\partial (\rho u_j \xi)}{\partial x_j} + \frac{\partial}{\partial x_j}\left(D \frac{\partial \xi}{\partial x_j}\right) = 0 \tag{15}$$

It is derived from the "full system", Eq. (1-7), under the assumption of frozen composition. Hence the chemical source term in the energy equation can be set to zero, and the species evolution equations can be replaced by a transport equation[1] of the mixture fraction ξ; here ρ_m, T_m, E_m represent the density, temperature, and total sensible energy, when they are varied by fluid-dynamics alone. The "mixing system", Eqs. (12-15), is filtered according with the LES method, to yield:

$$\frac{\partial \overline{\rho}_m}{\partial t} + \frac{\partial \overline{\rho}_r \widetilde{u_{m,j}}}{\partial x_j} = 0 \tag{16}$$

$$\frac{\partial \overline{\rho}_m \widetilde{u_{m,j}}}{\partial t} + \frac{\partial \overline{\rho_m} \widetilde{u_{m,i}} \widetilde{u_{m,j}}}{\partial x_j} + \frac{\partial \overline{p}_m}{\partial x_j} - \frac{\partial \check{\tau}_{ij}}{\partial x_j} \approx -\frac{\partial \sigma_{ij}}{\partial x_j} \tag{17}$$

$$\frac{\partial \check{E}_m}{\partial t} + \frac{\partial (\check{E}_m + \overline{p}_m) \widetilde{u_{m,j}}}{\partial x_j} - \frac{\partial \check{\tau}_{ij} \widetilde{u_{m,j}}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\widetilde{k} \frac{\partial \widetilde{T}_m}{\partial x_j}\right] \approx -\widetilde{u_{m,i}} \frac{\partial \sigma_{ij}}{\partial x_j} - \frac{\partial}{\partial x_i}[\overline{\rho} \Theta_j] \tag{18}$$

$$\frac{\partial \widetilde{\xi_m}}{\partial t} + \widetilde{u_{m,j}} \frac{\partial \widetilde{\xi}_m}{\partial x_j} - \frac{\partial}{\partial x_j}\left[D \frac{\partial \widetilde{\xi}_m}{\partial x_j}\right] = 0 \tag{19}$$

[1]For the sake of simplicity the assumption of equal diffusivities has been done. However, the formulation can be extended to the case of differential diffusivities

The "LES mixing system" has a state vector $\mathbf{v}_m = \{\overline{\rho}_m, \widetilde{\mathbf{u}}_m, \breve{E}_m, \widetilde{T_m}, \overline{p}_m, \widetilde{\xi_m}, \widetilde{Y}_{\alpha,m}\}$, where the energy $\breve{E}_m$ is the filtered total sensible energy of the frozen mixture. Closure models are required for the sub-scale stress tensor σ_{ij}, the thermal term Θ_j, as well as for the transport coefficients. So the operator F_m in Eq. (9) represents LES system of the values of the vector $\mathbf{v_m}$, Eqs. (16-19).

4. The Reactive System

The second sub-set, the "reaction system", has a state vector $\mathbf{w}_r = \{\rho_r, \mathbf{u}_r, E_r, T_r, p_r, \xi_r, Y_{\alpha,r}\}$, whose evolution is controlled by the equations of the species mass fractions, Eq. (4), and by the energy equation obtained by subtracting Eq. (14) from Eq. (3) and combining these with Eq. (7), to yield:

$$\frac{\partial \rho_r e_{sens,r}}{\partial t} + \sum_{\alpha=1}^{N} [\rho_r \dot{w}_\alpha \Delta h_{0_\alpha}] = 0 \tag{20}$$

$$\rho \frac{\partial Y_{r,\alpha}}{\partial t} + \frac{\partial (\rho_r u_{r,j} Y_{r,\alpha})}{\partial x_j} = -\frac{\partial}{\partial x_j}\left(\rho_r D \frac{\partial Y_{r,\alpha}}{\partial x_j}\right) + \dot{w}_\alpha \quad \alpha = 1, ..., N \tag{21}$$

where:

$$\rho_r e_{sens,r} = E_r - \frac{1}{2}\rho_r u_{r,j} u_{r,j} \tag{22}$$

Here the velocity field $\mathbf{u}_r$ and the pressure field p_r are assumed constant in time, while $e_{sens,r}$ and T_r are the sensible energy and temperature, whose variation is due to chemical reactions alone. A filtered reaction system, referred to as the "CMC reaction system", is still needed to describe the evolution of the filtered state vector $\mathbf{v}_r = \{\overline{\rho}_r, \widetilde{\mathbf{u}}_r, \widetilde{E}_r, \widetilde{T}_r, \overline{p}_r, \widetilde{\xi}_r, \widetilde{Y}_{\alpha,r}\}$. This is derived from the "reaction system" in Eq. (20-21), by following a CMC conditional filtering approach, to yield:

$$\frac{\partial Q_{\alpha,r}}{\partial t} + \widetilde{u_{r,i}|\eta} \frac{\partial Q_{\alpha,r}}{\partial x_i} = \widetilde{N|\eta} \frac{\partial^2 Q_{\alpha,r}}{\partial \eta^2} - \widetilde{W_\alpha|\eta} + e_Y \qquad \alpha = 1, .., N \tag{23}$$

$$\frac{\partial Q_{e_{sens,r}}}{\partial t} = \widetilde{W_{e_r}|\eta} \tag{24}$$

Its state vector is $\mathbf{q}(\mathbf{x}, t, \eta) = \{\widetilde{Y_{r,\alpha}|\eta}, \widetilde{e_{sens,r}|\eta} = \{Q_{e_{sens,r}}, Q_\alpha\}$; where $\widetilde{Y_{r,\alpha}}$ and $e_{sens,r}$ are related to $\mathbf{v}_r$ by means of the thermal and caloric equations of state. The CMC space involves the physical space $\mathbf{x}$ as well as the mixture fraction η as additional dimension. Eq. (23) is derived from Eq. (4), while Eq. (24) is obtained by conditionally filtering the source term $\overline{\sum_{\alpha=1}^{N} [\rho w_\alpha \Delta h_{0_\alpha}]}$ of the energy equation, Eq. (3).

The CMC variables $\mathbf{q}$ and the LES physical filtered variables are linked by convolution operations; for the generic function f these are:

$$LES \rightarrow CMC : \quad \widetilde{f|\eta}(\eta; x, t) := \frac{\int_{V_{CMC}} \overline{\rho} \widetilde{f|\eta} \widetilde{P}(\eta) dV'}{\int_{V_{CMC}} \overline{\rho} \widetilde{P}(\eta) dV'} \tag{25}$$

$$CMC \rightarrow LES : \quad \widetilde{f}(x, t) := \int_0^1 \widetilde{f|\eta} \widetilde{P}(\eta; \xi(x, t)) d\eta \tag{26}$$

where $P(\eta)$ if a presumed-shape, filtered density function. Hence the operator F_r in Eq. (10) is composed of the following phases:

1 Conditional filtering of $\mathbf{v}_r$ according with Eq. (25), to set the initial condition of the state vector $\mathbf{q}$ in the CMC system;

2 Time evolution of the state vector $\mathbf{q}$ as described by the CMC system, Eqs. (24-23);

3 Convolution of the state vector $\mathbf{q}$ according with Eq. (26), to find the updated state vector $\mathbf{v}_r$.

Note that the global time interval of integration, defined on the basis of a CFL condition for the LES mixing system, is usually larger than the time interval required to integrate the CMC reaction system. Hence, multiple CMC time-steps are required per each LES time-step.

5. Numerical Issues

The numerical implementation of the LES-CMC formulation here presented has been accomplished on the basis of a fully compressible turbulent LES flow solver developed by S. Pirozzoli [11] for non reactive single species flows. Pirozzoli's flow solver is 4-th order accurate in time and 6-th order accurate in space. Time integration is explicit to achieve a highly scalable parallel performance. The energy conserving space discretization prevents erroneous drifts of invariant properties of the fluid dynamics.

The CMC system, Eq. (23-24), is solved by means of an operator splitting technique; the convective and diffusive operators are solved explicitly in time with 3-rd order time accuracy and with 2-nd order space accuracy, while the source term are integrated in time by means of a point implicit technique (DVODE).

6. Discussion

The proposed approach allows to generate a suite of off-the-shelf CMC libraries which can be interfaced with different RANS and LES legacy flow solver platforms. Clearly, this implies an additional computational work associated to the the transfer of information to and from the CMC space (conditional filtering and convolution).

The weak space sensitivity of the conditionally filtered values allows to adopt a CMC mesh with a resolution coarser than the one usually required by the LES system, this implying a lower computational cost. On the other hand, the LES-CMC introduces the mixture fraction η as additional dimension, and thus, the CMC system has to be solved in general in a four-dimensional space.

However, according to the degree of symmetry of the problem of interest, the CMC space can be reduced from three to two, or even one physical dimensions.

It should be noted that the pressure field is not strongly dependent on the mixture fraction, this means that this formulation works efficiently with weakly compressible flows.

Finally, it is worth observing that a CMC code can be operated as if it were a classical flamelet model, simply by setting the conditional velocity $\widetilde{\mathbf{u}|\eta}$ to zero. It can also be used for diagnostic purposes under the equilibrium assumption, if the scalar dissipation $\widetilde{N|\eta}$ is also set to zero.

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