Species Mixing under Supercritical Pressure Conditions

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1 Introduction
Mixing of species under supercritical pressure conditions occurs in gas-turbine engines, liquid-rocket combustion chambers, diesel engines and Homogeneous Charge Compression Ignition engines. The multiple application of this phenomenon to automotive, aeronautics and astronautics areas makes this subject of high interest and explains why there has been substantial activity over the years on this topic. During approximately the last decade, there are several examples of experimental studies [1-5] and of modeling and numerical studies [6-12] that have changed the understanding we have of supercritical species mixing. Unlike in atmospheric flows, mixing in supercritical flows occurs in filamentary structures which populate the entire flow. These filamentary structures have been experimentally observed in fully turbulent situations [1,2,4] and have been predicted numerically through Direct Numerical Simulation (DNS) that reached transitional states. These states are characterized by a smaller Reynolds number value than in the fully turbulent cases, however, the flow exhibits the characteristic smooth velocity-fluctuation spectrum of full turbulence [7, 8]. Since DNS is not a practical methodology for computing the fully turbulent flows in the aforementioned applications, another methodology, Large Eddy Simulation (LES), has been considered instead. In LES, the computational grid is coarser than in DNS, which means that the small-scale effects which are not computed must be filtered out, but since they cannot be neglected they are replaced by models called, for obvious reasons, subgrid-scale (SGS) models. The success of LES depends to a great extent on how faithfully the SGS models reproduce the small-scale behavior. For supercritical flow, the existence of the filamentary structures introduces a level of SGS modeling complexity not encountered in atmospheric-pressure flows where LES originated. Because filtering may remove a substantial part of the filaments' structure, which is crucial to mixing, models must be devised to reintroduce in the equations the filtered-out structure. The mathematical equivalent to this description is presented next and some examples of SGS modeling for terms particular to supercritical mixing are further presented.

2 LES governing equations
According to Selle at al. 2007, the LES governing equations for supercritical flow are:
\[
\frac{\partial \tilde{p}}{\partial t} + \frac{\partial \tilde{p}u_j}{\partial x_j} = 0
\]

\[
\frac{\partial \tilde{p}Y_a}{\partial t} + \frac{\partial \tilde{p}Y_a u_j}{\partial x_j} = -\frac{\partial j_{aj} \langle \phi \rangle}{\partial x_j} - \frac{\partial}{\partial x_j}(\tilde{p} \eta_{aj})
\]

\[
\frac{\partial \tilde{p}e_t}{\partial t} + \frac{\partial \tilde{p}e_t u_j}{\partial x_j} = -\frac{\partial}{\partial x_j}(\tilde{p}\zeta_j) - \frac{\partial}{\partial x_j}(q_{IKj} - q_{IKj} \langle \phi \rangle)
\]

where \( \rho \) is the mass density, \( x_j \) is the jth spatial coordinate, \( t \) is time, \( u_j \) is the velocity in the jth direction, \( p \) is the pressure, \( \sigma_{ij} \) is the \((i,j)\) component of the stress tensor, \( \tau_{ij} \) is the \((i,j)\) component of the SGS stress tensor, \( Y_a \) is the mass fraction of species \( \alpha \), \( j_{aj} \) is the mass flux of species \( \alpha \) in the jth direction, \( \eta_{aj} \) is the SGS species mss flux, \( e_t \) is the total energy, \( q_{IKj} \) is the jth coordinate of the heat flux and \( \zeta_j \) is the jth coordinate of the SGS enthalpy flux. Variable \( \phi \) represents the vector of conservative variables. The overbar denotes regular filtering and the tilde labels Favre filtering. The above equations result from an assessment of all terms obtained from filtering, with some terms being negligible and thus not appearing in the equations above. These differential equations are coupled to the Peng Robinson equation of state for which detailed information has been presented elsewhere [8, 13].

Under atmospheric-pressure, or more generally subcritical-pressure conditions, the SGS modeling is restricted to \( \tau_{ij}, \eta_{aj} \) and \( \zeta_j \). For supercritical-pressure conditions one must additionally model the last terms in brackets in the momentum and energy equations. The fact that these terms cannot be neglected is a direct manifestation of the subgrid-scale activity which prevents replacing the filtered quantity (i.e. \( p \) or \( q_{IKj} \)) with the same quantity computed as a function of the filtered flow field. In particular, it should be noted that the filtered \( p \) or \( q_{IKj} \) may be very close to the respective quantity computed using the filtered flow field, but that the corresponding difference between gradients represented by the terms in the governing equations may be large. According to the chemical species, one of these terms may be important, or both may be important. To isolate the effect of each of these terms, we present results for heptane/nitrogen mixing for which only the new SGS term in the momentum equation is important (based on an assessment of the DNS database), and for oxygen/hydrogen mixing for which only the term in the energy equation is important (also based on an assessment of the DNS database).

### 3 Results: A posteriori study

The focus is here only on the new SGS terms as we use conventional models for the SGS fluxes \( \tau_{ij}, \eta_{aj} \) and \( \zeta_j \).

#### 3a. Heptane/Nitrogen

To model the last term in the momentum equation, the following model has been proposed [12]

\[
\rho(\phi) = \rho(\overline{\phi}) + \frac{\partial p}{\partial \phi_m} \bigg|_{\phi=\overline{\phi}} (\phi_m - \overline{\phi_m})
\]
where $\phi_m$ represents the conservative variables and the derivatives of the pressure with respect to them are computed from the equation of state. The model has been implemented in the code as

$$\nabla (p(\phi)) + \nabla (p(\langle \theta \rangle)) = \nabla (p(\langle \phi \rangle)) = \nabla \left( p(\langle \phi \rangle) + \left. \frac{\partial p}{\partial \phi_m} \right|_{\phi=\langle \phi \rangle} (\phi_m - \langle \phi_m \rangle) \right)$$

and for obvious reasons it is called a pressure correction.

This model has been tested in LES and comparisons were made between LES devoid of it and LES including it. The template for comparison for both of these LES has been the filtered-and-coarsened (FC) DNS database. This database has been obtained in the context of a temporal mixing layer of coordinates $(x_1, x_2, x_3)$. The mixing layer progressed from its initial conditions to a transitional state exhibiting turbulent characteristics. It is this transitional state which was considered representative for the LES capabilities. Illustrated in Fig. 1 is the FCDNS on the top row, a LES using the constant-coefficient scale-similarity model for the SGS fluxes but not using the pressure correction on the middle row, and a LES utilizing the constant-coefficient scale-similarity model for the SGS fluxes and utilizing the pressure correction on the bottom row. In both cases the LES grid spacing was four times that of the DNS and the grid filter width was twice the DNS grid spacing; the test filter width was twice that of the grid filter width, as usually recommended. The constant coefficient value was found from calibrating the scale-similarity model with the DNS database. The comparisons show that using the pressure correction introduces more realism in the pressure and the mass fraction fields, although the density gradient magnitude does not benefit from this model. Figure 2 depicts a comparison between the FCDNS and the LES conducted the dynamic-coefficient mixed scale-similarity model (i.e. combination of the Smagorinsky and scale-similarity models, where the coefficient of the Smagorinsky model is computed dynamically and that of the scale-similarity model assumes the theoretical value of unity). It is clear that compared to the constant coefficient scale-similarity model using the pressure correction, we have now improved the quality of the simulation by better recovering not only the pressure and mass fraction fields but also the density gradient magnitude field. The latter is important, as experimental observations showed that it governs the distribution of turbulence in the flow [14].

3b. Oxygen/Hydrogen

To model the last term in the energy equation, we recall that $q_{IK}$ is the sum of three terms, each being the product of the gradient of a thermodynamic variable and a coefficient which is a complex function of the thermodynamic variables. Examination of the heat flux revealed that its behavior is dominated by the gradients of the thermodynamic variables rather than the coefficients, which put the modeling burden on reproducing the filtered gradients from the gradients of the filtered solution. To this end, we adopted the Approximate Deconvolution Model (ADM) where

$$\phi^* = 3\phi - 3\phi + \bar{\phi} + \ldots$$

is the reconstructed DNS flow field from the known LES flow field. Thus, without heat-flux correction

$$\left( \nabla \cdot q(\phi_{LES}) + \left( \nabla \cdot q(\phi) - \nabla \cdot q(\phi_{LES}) \right) \right)$$

is computed as $\nabla \cdot q(\phi_{LES})$

whereas with the heat flux correction

$$\left( \nabla \cdot q(\phi_{LES}) + \left( \nabla \cdot q(\phi) - \nabla \cdot q(\phi_{LES}) \right) \right)$$

is computed as $\nabla \cdot q(\phi^*)$.

The reconstruction has been performed on the conservative variables rather than the primitive variables, to enhance its accuracy since the LES solution is obtained for the conservative variables. Computations performed with LES excluding the heat-flux correction or including it showed that when compared to the FCDNS, the results of the latter are more accurate, including the higher order quantities [15]. Particularly, success in reproducing the heat flux may have substantial implications for liquid-rocket simulations which focus on the ability to predict the heat flux to the wall [16]. Since
ADM depends on the LES solution which is SGS-flux model dependent, the success of the endeavor was variable according to the SGS-flux model used.

4 Conclusions

It has been shown that for supercritical-pressure conditions, the LES equations contain additional subgrid terms which have magnitude comparable to other terms traditionally retained in the equations. Modeling of these new terms has been proposed, and LES computations including these terms have been shown to be more accurate than those excluding them. The next challenge is to use these models in a practical LES computation.

Figure 1. Comparison of $|\nabla \rho|$ in kg/m$^3$ (first column), $p/p_0$ (second column) and the heptane mass fraction $Y_h$ (third column) at the transitional state of the DNS in the between-the-braid plane ($x_3/L_3=0.06$) for: First row represents the filtered and coarsened DNS. Second row represents LES using the constant-coefficient scale-similarity model for the SGS fluxes and not including the pressure correction. Third row represents LES using the constant-coefficient scale-similarity model for the SGS fluxes and including the pressure correction.
Figure 2. Comparison of $|\nabla \rho|$ in kg/m$^3$ (first column), $p/p_0$ (second column) and the heptane mass fraction $Y_h$ (third column) at the transitional state of the DNS in the between-the-braid plane ($x_3/L_3=0.06$) for: First row represents the filtered and coarsened DNS. Second row represents LES using the dynamic-coefficient mixed scale-similarity model for the SGS fluxes and including the pressure correction.

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References


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Supercritical-pressure mixing


