Large Eddy Simulation of a Turbulent Reacting Compressible Jet

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We report results of a Large Eddy Simulation (LES) effort of turbulent compressible nonpremixed reactive jets. It is well known that there are several difficulties associated with compressible reactive flows in comparison with incompressible flows. In incompressible flows, the energy and mass conservation (for constant density flows) equations are decoupled from the velocity field. Moreover, the subgrid terms that are required in these flows need only provide with the deviatoric part of the subgrid contributions. The isotropic part can be absorbed in the pressure term. In reacting incompressible flows, one can also avoid the need to integrate the conservation equations for mass and energy by using a conserved scalar approach. In this case, both temperature and density are determined from a state relationship that is known beforehand. On the other hand, for compressible reacting flows one is not allowed to discard the energy and mass conservation equation since acoustics and in some cases shocks coexist with heat release. In the present investigation we use the totally conservative formulation in terms of total sensible energy. Other forms of the energy equation require closure for pressure velocity correlations, [1]. This is not requited in the total sensible energy form, although some other correlations are needed, notably, those between enthalpy and mass fractions of species. Furthermore, we are interested in using local subgrid models. The advantages of this kind of approach are self evident, specially in complex geometries. The results discussed in this abstract are obtained with the stretched vortex model for turbulent transport [2], scalar transport [4] and subgrid scalar variance [3]. Here, we consider a model problem of a turbulent planar nonpremixed reacting jet. The modeling assumptions are described next, followed by some preliminary results.

1 Formulation and Results

For variable density flows, the LES governing equations are formulated using Favre filtered variables, defined as $\tilde{\phi} = \overline{\rho\phi}/\bar{\rho}$, where the "conceptual" filter operator is denoted by the overbar. Conservation of mass, momentum and energy are expressed in the usual form, [5], in terms of filtered density, $\bar{\rho}$, velocity, $\tilde{u}_i$, and pressure $\bar{p}$ and the total sensible energy conservation equation is

$$\frac{\partial \bar{E}}{\partial t} + \frac{\partial}{\partial x_k}\big((\bar{E}+\bar{p})\tilde{u}_k\big) = \frac{\partial}{\partial x_k}\big(\tilde{\lambda}\frac{\partial \tilde{T}}{\partial x_j}\big) + \frac{\partial}{\partial x_k}\big(\tilde{\tau}_{kj}\tilde{u}_j\big) - \frac{\partial \sigma_k^e}{\partial x_k}. \tag{1}$$

where $\tilde{\lambda}$ is the resolved thermal conductivity. The resolved Newtonian viscous stress tensor is given as usual with $\tilde{\mu}$ as the resolved shear viscosity. The dependence on temperature of $\tilde{\mu}$ and $\tilde{\lambda}$ is typically not small for combusting flow, primarily, due to the large temperature variations in the flow. They are approximated here by $\tilde{\mu} = \mu^o(\tilde{T}/T_o)^n$ and $\tilde{\lambda} = \lambda^o(\tilde{T}/T_o)^n$, where $n = 0.7$. Finally, the total sensible energy, $\bar{E}$ is given by

$$\bar{E} = \bar{\rho}\left(\tilde{h} + \frac{1}{2}\tilde{u}_k\tilde{u}_k\right) - \bar{p} + \bar{\rho}\tilde{k}, \tag{2}$$

where $\tilde{k} = (\widetilde{u_i u_i} - \tilde{u}_i\tilde{u}_i)/2$ is the subgrid kinetic energy. The Favre filtered enthalpy is decomposed into a resolved part and a subgrid part through,

$$\tilde{h} = \sum_{i=1}^{N} h_i(\tilde{T})\tilde{Y}_i + h_s, \qquad h_s = \sum_{i=1}^{N}\big(\widetilde{h_i Y_i} - h_i(\tilde{T})\tilde{Y}_i\big), \tag{3}$$

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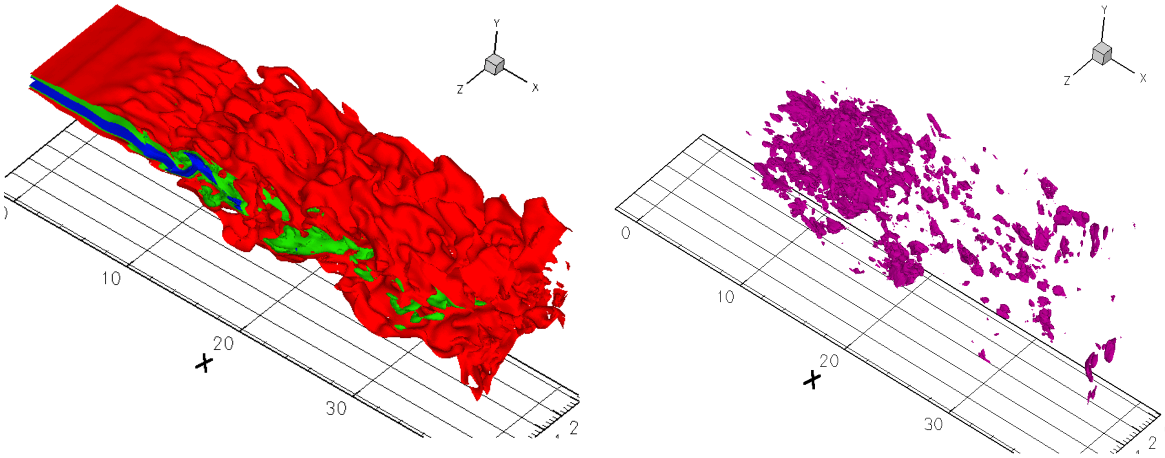

Figure 1: Mixture fraction and subgrid kinetic energy distribution.

where N is the number of species, h_i is the enthalpy of component i, given by

$$h_i(\tilde{T}) = h_i^o + \int_{T_o}^{\tilde{T}} c_{pi}(T^*)dT^*, \tag{4}$$

and the system of equations is closed by the equation of state,

$$\bar{p} = \bar{\rho}R^o\tilde{T}\sum_{i=1}^{N}\frac{\tilde{Y}_i}{W_i} + p_s, \qquad p_s = \bar{\rho}R^o\sum_{i=1}^{N}\frac{\widetilde{TY}_i - \tilde{T}\tilde{Y}_i}{W_i} \tag{5}$$

c_{pi} is the specific heat of component i, h_i^o is the enthalpy of formation of the corresponding species, R^o is the gas constant and W_i is the molecular weight of species i.

Combustion is handled through the conserved scalar approach, where a a mixture fraction field, Z, is used to obtain the mass fraction of the different species. The quantities that need to be modeled are the subgrid momentum stresses, scalar transport and subgrid total energy transport, defined as

$$\sigma_{ij} = \bar{\rho}\big(\widetilde{u_i u_j} - \tilde{u}_i\tilde{u}_j\big), \qquad \sigma_j^z = \bar{\rho}\big(\widetilde{Zu_j} - \tilde{Z}\tilde{u}_j\big), \qquad \sigma_j^e = \bar{\rho}\big(\widetilde{hu_j} - \tilde{h}\tilde{u}_j\big) + \frac{\bar{\rho}}{2}\big(\widetilde{u_k u_k u_j} - \widetilde{u_k u_k}\tilde{u}_j\big). \tag{6}$$

The triple correlations in σ_j^e of Eq. (6) are neglected and the other terms are modeled using the stretched vortex model. The combustion related terms, h_s and p_s, are closed through an assumed beta pdf model, where the subgrid scalar variance needed in the assumed pdf model is obtained from the approximate reconstruction model of [3]. The governing equations are integrated using a compact Padé scheme in space of sixth order and a third-order low-storage Runge-Kutta scheme in time. The chemistry is modeled as an infinitely fast one step methane-air reaction. This determines a state relation of the form $Y_i = Y_i(Z)$. The stoichiometric mixture fraction was set to 0.2. The cold Reynolds number was set equal to 20000 and the jet Mach number was equal to 0.6. Figure 1 shows mixture fraction isosurfaces (a) and subgrid kinetic energy (b) at one instant in time. Further details will be provided in the presentation.

References

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