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A coupled LES-ODT model for spatially-developing turbulent reacting shear layers

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ABSTRACT

Large-eddy simulation (LES) for momentum transport combined with the one-dimensional turbulence (ODT) model for momentum and reactive scalars' transport is designed to capture subgrid scale (SGS) turbulence-chemistry interactions. An extension of the original LES-ODT formulation is developed to capture these interactions in turbulent spatially-developing reacting shear layers. The LES-ODT results are compared to results from direct numerical simulations (DNS). Lewis number parametric variations for the variable-density simulations are carried out. The validation with DNS shows that the LES-ODT approach can qualitatively and quantitatively capture important salient features of turbulent shear layers statistics, including large-scale flow patterns, shear layer growth and mean and RMS statistics of velocity and reactive scalars.

1. Introduction

A principal challenge in turbulent combustion modeling is the capture of subgrid scale effects associated with the coupling of chemistry and molecular transport. A common strategy in turbulent combustion models is to exploit the separation of scales (e.g. the eddy-dissipation concept (EDC), the eddy break-up (EBU) model and the flamelet model [1–3]) or the behavior of thermo-chemical scalars in terms of a subset of scalars in composition space (e.g. the conditional moment closure (CMC) model, [4,5]). Other modeling approaches adopt a fundamentally different strategy by directly evaluating closure terms, which renders them more regime-independent [6]. Such modeling approaches include the PDF-transport methods [7] and the models based on coupling the linear eddy model (LEM) [8] and its extension to LES, the LEMLES approach [9,10] and the one-dimensional turbulence model (ODT) [11,12] and its extension to LES [13–18].

The LES-ODT framework attempts to combine two solutions: a 3D LES solution on a coarse grid with embedded 1D ODT solutions in the computational domain. the fine-grained ODT solutions are designed to capture unresolved subgrid scale (SGS) effects and address the problem of closure for turbulence-chemistry interactions.

The objective of the present study is to extend the LESODT framework originally developed for combustion by Cao and Echekki [13] to turbulent shear layers where velocity and scalar gradients are dominated by one principal direction. Some of the key contributions related to this study pertain to the different treatments implemented in the different directions of the flow. This includes a variable mesh implementation along the transverse direction and the implementation of different boundary conditions in the 3 directions, including inflow and outflow boundary conditions in the streamwise direction, vanishing gradients in the transverse direction and periodic boundary conditions in the spanwise direction. More importantly, a new treatmet at the so-called "nodes" is implemented to establish a robust coupling between the 3 directions of the flow. Such a treatment is important to reproduce the spatial structures associated with turbulent shear layers. The model is validated against direct numerical simulations (DNS) for turbulent spatially-developing shear layers. The paper is organized as follows. The model formulation is presented in Section 2 and its numerical implementation is discussed in Section 3. Results are presented in Section 4 for both constant density and variable density simulations based on comparison with DNS statistics.

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2. Model formulation

Different variants of the LES-ODT method have been studied. Balasubramanian [19] and Sedhai [20] implemented a formulation, which advects the ODT domains along the flame brush in a Lagrangian fashion. In the Cao and Echekki [13] formulation, which is used as a starting point for the work, the ODT domains are fixed in space. This conforms to an Eulerian description of the flow field. More recent work by Park and Echekki [14], Ben Rejeb and Echekki [15] and Fu and Echekki [16] are based on this Eulerian formulation.

The ODT formulation simulates the time evolution of velocities and scalars along a one-dimensional domain. This domain represents a notional line of sight through turbulent flow. In Cartesian coordinates and in the Eulerian context, such a one-dimensional domain can be thought to be aligned with the (x_1)-coordinate for example. Contribution along this line can be spatially and temporally resolved; whereas contributions from the second (x_2) and third (x_3) orthogonal directions need to be modeled. The same principle applies for notional lines parallel to the other two coordinate directions.

Fig. 1 shows the embedded 1D ODT domains as a three-dimensional lattice in the LES computational domain, illustrated here with one LES cell. The ODT domains are aligned with the LES cell edges and can span the extent of the computational domain. An ODT node is defined as the intersection point of three orthogonal ODT domains. In the present work, the ODT grid is aligned in such a way that the ODT node coincides with the LES node, which in the general case is not necessary. It is important to note that at the ODT node, all three orthogonal directions represented by the 2 ODT domains are resolved, such that no modeling is necessary. Outside these nodes, the ODT governing equations, as discussed below, exhibit both resolved and unresolved contributions with the latter requiring additional modeling.

2.1. LES governing equations

In LES-ODT, the LES governing equations cover only the large-scale motion using mass and momentum conservations (or momentum and the Poisson equation under the low-Mach number assumption). By performing a density-weighted (Favre) filtering operation on the Navier-Stokes equations the filtered LES governing equations are obtained, which are given as.

LES continuity

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i}{\partial x_i} = 0 \tag{1}$$

LES momentum

$$\bar{\rho}\frac{\partial \tilde{u}_i}{\partial t} = -\bar{\rho}\tilde{u}_j\frac{\partial \tilde{u}_i}{\partial x_j} - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\tau}_{ij}}{\partial x_j} + \frac{\partial \tau_{ij}^{SGS}}{\partial x_j}, \tag{2}$$

assuming negligible external body forces. The symbol "-" corresponds to spatial filtering by a filter function G with a characteristic

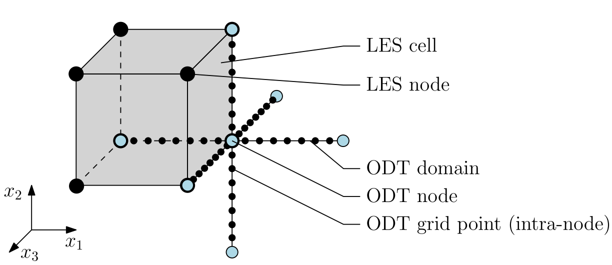

Fig. 1. Three-dimensional alignment of LES cell and ODT domains.

filter size Δ, such that a generic filtered quantity $\bar{\varphi}$, defined at a spacial position, x, and time, t is expressed as

$$\bar{\varphi}(x_j, t) = \int_{\Delta} \varphi(x_j', t) \cdot G(x_j - x_j', \Delta) dx_j'. \tag{3}$$

The symbol "$\sim$" corresponds to Favre filtering

$$\tilde{\varphi}(x, t) = \frac{\overline{\rho\varphi}}{\bar{\rho}}. \tag{4}$$

The subgrid scale (SGS) stress tensor, τ_{ij}^{SGS}, given as

$$\tau_{ij}^{SGS} = \bar{\rho}(\tilde{u}_i\tilde{u}_j - \widetilde{u_i u_j}). \tag{5}$$

The viscous stress tensor $\bar{\tau}_{ij}$ is expressed in terms of the dynamic viscosity μ and the strain rate tensor, S_{ij}

$$\bar{\tau}_{ij} = 2\mu S_{ij}, \tag{6}$$

where

$$S_{ij} = \frac{1}{2}\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}\frac{\partial \tilde{u}_k}{\partial x_k}. \tag{7}$$

where μ is the dynamic viscosity. In the present validation studies, τ_{ij}^{SGS} given in Eq. (5) is modeled using the Smagorinsky model:

$$\tau_{ij}^{SGS} = 2\bar{\rho}\nu_T S_{ij}, \text{ where } \nu_T = (C_S\Delta)^2\left(2\bar{S}_{ij}\bar{S}_{ij}\right)^{1/2}. \tag{8}$$

In this expression, C_S is the Smagorinsky constant. Within the context of the present LES-ODT formulation, the filtered density is computed by spatially filtering the ODT density, which is evaluated on the subgrid based on an equation of state, such as the ideal gas equation. The density filtering is a substitute for the solution of the continuity equation in LES. Instead, the Poisson equation is solved to enforce continuity and resolve the pressure field. In a recent study by Fu and Echekki [16] both the continuity equation and density filtering from ODT are solved together to yield a "smooth" solution for the density field using Kalman filtering. However, this approach is not adopted here.

2.2. ODT governing equations

The ODT governing equations include transport for the momentum components and the thermo-chemical scalars, expressed here in terms of the temperature and the species equations:

1D momentum

$$\frac{\partial u_i}{\partial t} = \underbrace{\left[-\tilde{u}_1\frac{\partial u_i}{\partial x_1} + \frac{1}{\rho}\frac{\partial \tau_{i1}}{\partial x_1} + \Omega_{u_i}\right]}_{\text{resolved}} + \underbrace{\left\{-\left(\tilde{u}_2\frac{\partial u_i}{\partial x_2} + \tilde{u}_3\frac{\partial u_i}{\partial x_3}\right) + \frac{1}{\rho}\left(\frac{\partial \tau_{i2}}{\partial x_2} + \frac{\partial \tau_{i3}}{\partial x_3}\right)\right\}}_{\text{modeled}}, \tag{9}$$

1D energy

$$\frac{\partial T}{\partial t} = \underbrace{\left[-\tilde{u}_1\frac{\partial T}{\partial x_1} + \frac{1}{\rho c_p}\left(\frac{\partial \dot{q}_1''}{\partial x_1} - \sum_{k=1}^{N} h_k\dot{\omega}_k\right) + \Omega_T\right]}_{\text{resolved}} + \underbrace{\left\{-\left(\tilde{u}_2\frac{\partial T}{\partial x_2} + \tilde{u}_3\frac{\partial T}{\partial x_3}\right) + \frac{1}{\rho c_p}\left(\frac{\partial \dot{q}_2''}{\partial x_2} + \frac{\partial \dot{q}_3''}{\partial x_3}\right)\right\}}_{\text{modeled}}, \tag{10}$$

1D species

$$\frac{\partial Y_k}{\partial t} = \underbrace{\left[-\tilde{u}_1\frac{\partial Y_k}{\partial x_1} + \frac{1}{\rho}\frac{\partial J_{k,1}}{\partial x_1} + \frac{\dot{\omega}_k}{\rho} + \Omega_{Y_k}\right]}_{\text{resolved}} + \underbrace{\left\{-\left(\tilde{u}_2\frac{\partial Y_k}{\partial x_2} + \tilde{u}_3\frac{\partial Y_k}{\partial x_3}\right) + \frac{1}{\rho}\left(\frac{\partial J_{k,2}}{\partial x_2} + \frac{\partial J_{k,3}}{\partial x_3}\right)\right\}}_{\text{modeled}}. \tag{11}$$