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Simulation of shock–turbulence interaction in non-reactive flow and in turbulent deflagration and detonation regimes using one-dimensional turbulence

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ABSTRACT

The one-dimensional turbulence (ODT) methodology is extended to include an efficient compressible implementation and a model for capturing shock-induced turbulence is presented. Lignell et al. recently introduced a Lagrangian ODT implementation using an adaptive mesh. As the code operates in the incompressible regime (apart from constant-pressure dilatation) it cannot handle compressibility effects and their interactions with turbulence and chemistry. The necessary algorithmic changes to include compressibility effects are highlighted and our model for capturing shock–turbulence interaction is presented. To validate our compressible solver, we compare results for the Sod shock tube problem against a finite volume Riemann solver. To validate our model for shock–turbulence interaction, we present comparisons for a non-reactive and a reactive case. First, results of a shock traveling from light (air) to heavy (SF_6) with reshock have been simulated to match mixing width growth data of experiments and turbulent kinetic energy results from LES. Then, for one-step chemistry calibrated to represent an acetylene/air mixture we simulate the interaction of a shock wave with an expanding flame front, and compare results with 2D simulation (2D-sim) data for flame brush formation and ensuing deflagration-to-detonation transitions (DDT). Results for the Sod shock tube comparison show that the shock speed and profile are captured accurately. Results for the non-reactive shock–reshock problem show that interface growth at all simulated Mach numbers is captured accurately and that the turbulent kinetic energy agrees in order of magnitude with LES data. The reactive shock tube results show that the flame brush thickness compares well to 2D-sim data and that the approximate location and timing of the DDT can be captured. The known sensitivity of DDT characteristics to details of individual flow realizations, seen also in ODT, implies that model agreement can be quantified only by comparing flow ensembles, which are presently unavailable other than in an ODT run-to-run sensitivity study that is reported herein.

1. Introduction

Due to its huge complexity, progress in understanding and prediction of turbulent combustion is extremely challenging. The picture is complicated even further when compressibility effects and their interaction with turbulence and chemistry are included. In principle, progress is possible through direct numerical solution (DNS) of the exact governing equations, but the wide range of spatial and temporal scales often renders it unaffordable, so coarse-grained 3D numerical simulations with subgrid parameterization of the unresolved scales are often used. This is especially problematic for multi-physics regimes such as reacting flows because much of the complexity is thus relegated to the unresolved small scales.

One-dimensional turbulence (ODT) is a stochastic model for turbulent flow simulation. ODT has two key features. First, the properties of the flow reside on a one-dimensional domain. This 1D formulation allows full resolution of the interaction between large scales and molecular transport scales within computationally affordable simulations. The lack of spatial and temporal filtering on this 1D domain enables a physically sound multiscale treatment that is especially useful for combustion applications where, e.g., sharp interfaces or small chemical time scales have to be resolved. ODT resolves flame structure in 1D without compromising chemical-state accessibility, and achieves major cost reduction relative to DNS through reduced spatial dimensionality. Second, because vortical overturns cannot occur on a 1D domain, turbulent advection is represented using mapping events whose occurrences are governed by a random process. Unlike the Reynolds-averaged Navier–Stokes (RANS) model and large-eddy simulation (LES), which model the small scale

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phenomena and retain the 3D representation of the flow, ODT resolves all the scales of motion but models 3D turbulence. Hence ODT cannot capture geometrical effects and coherent flow structures, other than the so-called eddy events of ODT. In ODT, velocity components are transported and are used to determine the eddy frequency and eddy-size distribution, thereby providing a phenomenologically sound basis for driving turbulence.

As a stand-alone model, ODT has been successfully used to simulate homogeneous turbulent non-reacting [1–6] and reacting flows [7–12]. However, for stand-alone modeling of turbulent flows using ODT, one must define the dominant direction of mean property variation. For complex flows that do not have a single dominant direction, ODT has been used as a sub-grid scale model in both RANS [8,13] and LES [14] to provide closure for reacting scalars in combustion. An alternative multi-dimensional approach called ODTLES is discussed in [15,16].

Lignell et al. [17] recently introduced an efficient ODT Lagrangian implementation using an adaptive mesh. Like most ODT formulations, this also is formulated for zero Mach number, with constant pressure assumed, except when hydrostatic equilibrium is invoked in some applications to buoyant stratified flow. In this manuscript we extend the scope of the Lagrangian formulation of ODT, especially for reacting flows, by introducing a compressible formulation. A variant of the existing ODT model in an Eulerian reference frame with a compressible formulation was developed by Punati et al. [18,19] and applied to non-reacting and reacting jets. One-dimensional compressible hydrodynamic turbulence has also been developed by Ni et al. [20]. In their formulation, fluctuations of thermodynamic variables and velocity are generated by stochastic forcing rather than by the physical mechanism of advective stirring. The inclusion of the physically based turbulent enhancement of the mixing process is what is unique to the ODT formulation and makes it suitable for reactive flows with finite-rate kinetics.

The goal of this study is to extend the adaptive ODT methodology to handle compressibility effects and their interactions with turbulence and chemistry and to study shock–turbulence interaction and the deflagration-to-detonation transition (DDT). The shock–turbulence interaction, which is related to the Richtmyer–Meshkov instability, plays a fundamental role in the context of many physical settings, both natural and man-made. To list a few, it finds applications in natural phenomena like supernova collapse [21], pressure wave interaction with flame fronts [22], and supersonic and hypersonic combustion [23,24]. In the interaction of shock waves with flames it plays an important role in the DDT [25–27], and in inertial confinement fusion [28].

This paper is organized as follows. Section 2 gives an overview of the modeling approach. Section 3 gives a short overview of ODT. For further depth on ODT, the reader is referred to [1,29,30]. Section 3.3 discusses the strategy of incorporating instabilities caused by acceleration of a variable density flow into ODT. Section 3.3.1 presents the model representation of the Darrieus–Landau instability caused by unsteady dilatational flow and Section 3.3.2 introduces the ODT representation of shock–turbulence interaction. Section 4 presents results for (1) Sod's shock tube problem with comparison to a Riemann solver, (2) non-reacting shock-tube results with comparison to experimental and LES data, and (3) reacting shock-tube results with comparison to 2D simulation data. The details of the numerical implementation and the shock–turbulence interaction model are provided in Appendix A and Appendix B respectively.

2. Modeling approach

2.1. Overview

In this section we give a general overview of our modeling approach. To the authors' knowledge, the current state of the art for modeling compressible turbulence in 1D is by Ni et al. [20]. In their formulation, the flow is entirely confined to a 1D line and turbulent fluctuations are generated by stochastic forcing. Our intention is to improve on this formulation by introducing a physically based turbulence model, namely ODT, that is also capable of mixing scalars which is ideal for combustion. We therefore have a hydrodynamic model that is based on the truncated 1D Navier–Stokes equations and a turbulence model that emulates 3D turbulence.

The physics of the turbulence model are described in detail in [17] and briefly in Sections 3.1 and 3.2 and have been validated generally in many ways. A submodel of ODT, intended to represent unsteady dilatation, termed the Darrieus–Landau (DL) instability, is described in Section 3.3.1 and has been validated in a turbulent counterflow configuration [12] and a turbulent wall flame fire [31]. For flows involving shocks, in Section 3.3.2 a model for representing shock–turbulence interaction (STI) is introduced, which is based on the validated concept of the DL instability model. To validate the STI model, in Section 4.2 we compare ODT results with experimental data for a non-reactive shock tube with reshock. As this is a non-reactive case, dilatational effects are minimal in comparison to the instability generated by a shock traveling over a density interface and therefore is an ideal test case for the STI model.

The formulation for the hydrodynamic model and its implementation is described in Appendix A. It is an extension of the code described in [17] to include finite Mach number effects. In Section 4.1 we compare the hydrodynamic model to a 1D gas dynamics solver for Sod's shock tube problem. This and the laminar simulations carried out for the non-reactive and reactive shock tubes in Section 4.2 and 4.3 respectively are verifications of the 1D hydrodynamic solver, as in these cases the turbulence model is turned off.

In general, the ODT methodology views the 1D line as a closed system. In the example of the counterflow configuration [12], the 1D line is taken to be the center line connecting two nozzles facing each other. For such a configuration, mass conservation dictates a mean off-line flow. In [12] the necessary additional modeling needed to take into account off-line flow was developed. For the applications discussed in the current paper, although expansion and compression can occur in off-line directions, they are statistically 1D flows and we neglect off-line effects to maintain simplicity in the formulation. Results shown in Section 4 validate the hypothesis that a treatment of off-line effects is not needed.

2.2. Governing equations

We time advance the truncated 1D equations and interrupt time advancement to implement eddy events EE as discussed in Section 3.1. Further explanation of the formulation and numerical solution of the governing equations is provided in Appendix A. The truncated differential equations for continuity, momentum, species and enthalpy are written as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_1)}{\partial x} + \mathrm{EE}(\rho) = 0, \tag{1}$$

$$\frac{\partial u_i}{\partial t} + u_1 \frac{\partial u_i}{\partial x} + \mathrm{EE}(u_i) = \frac{1}{\rho}\left(-\frac{\partial p}{\partial x}\delta_{i1} + \frac{\partial \sigma_{i1}}{\partial x}\right), \tag{2}$$

$$\frac{\partial Y_\alpha}{\partial t} + u_1 \frac{\partial Y_\alpha}{\partial x} + \mathrm{EE}(Y_\alpha) = \frac{1}{\rho}\left(-\frac{\partial j_\alpha}{\partial x} + \dot{\omega}_\alpha\right), \tag{3}$$

$$\frac{\partial h}{\partial t} + u_1 \frac{\partial h}{\partial x} + \mathrm{EE}(h) = \frac{1}{\rho}\left(\frac{\partial p}{\partial t} + u_1 \frac{\partial p}{\partial x} - \frac{\partial q}{\partial x} + \sigma_{i1}\frac{\partial u_i}{\partial x}\right), \tag{4}$$

with $\alpha = 1, \ldots, n_\alpha$ and n_α is the number of different species in the gas mixture. Subscripts $i \in \{1, 2, 3\}$ denote the $\{x, y, z\}$ spatial directions where x is the spatial direction along the ODT line and summation over repeated indices i is implied. u_i denotes the three ODT velocity components, ρ is the density, Y_α is the mass fraction of species