Large Eddy Simulation of Deflagration to Detonation Transition using Artificial Thickening

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1 Introduction

Accurate predictions of Deflagration to Detonation Transition (DDT) in large configurations are difficult to obtain. DDT is a highly non-linear process, and very sensitive to initial fluid disturbances and chemical compositions. Direct Numerical Simulations (DNS) are not practical in large configuration and, even with strong adaptive refinement, is not possible to solve directly all scales across four or five orders of magnitude.

Large Eddy Simulation (LES) is becoming a popular tool on combustion modelling and provides a good compromise between cost and accuracy. However, LES applications on DDT are scarce in the literature. (see [1] among others). The main challenge, is that DDT occurs at sub-grid (unresolved) scales and therefore needs to be modelled.

In the present work a novel model is presented to predict DDT in the LES context. The approach follows the compressible Artificial Thickening Model (ATF) [2], where the flow features are "thickened", so they are captured by coarse mesh. The behaviour of the model is validated in one-dimensional laminar flame and in a detonation wave, testing the ability of the LES-ATF approach to work with coarse meshes. The model is then applied to a canonical three-dimensional problem of shock-induced DDT on a rectangular channel.

2 Modelling

In order to capture all relevant phenomena in a coarse mesh, the ATF model uses a geometrical transformation: $\xi_i = \mathcal{F} \cdot x_i$ and $\tau = \mathcal{F} \cdot t$ [3]. The transformation ratio, $\mathcal{F}$, is called the *thickening factor*. In the original formulation, $\mathcal{F}$ was constant, however a generalised transformation can be used if $\partial \xi_i / \partial x_i = \mathcal{F}$, where $\mathcal{F}(x_i)$ depends on the physical position x_i. The transformation factor $\mathcal{F}$ is chosen such that satisfies $\mathcal{F} \geq \Delta / \Delta_{min} \geq 1$, where Δ is the mesh size and Δ_{min} is the minimum mesh size that captures all the relevant phenomena (such as the flame thickness). If the mesh is well resolved $\Delta \approx \Delta_{min}$ and $\mathcal{F} = 1$. The original ATF formulation applied $\mathcal{F}$ to the low-speed turbulent premixed flames [4], where $\Delta_{min} = \delta_f / n$, where δ_f the laminar flame thickness, and n is the number of points desired to resolve the flame, around five in low-speed flames [5]. The ATF transformation "thickens"

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the flame by $\mathcal{F}$, but still preserves the laminar flame speed. The thickening process distorts the flame and an efficiency coefficient [4] is added to the diffusion term and chemical source. This accounts for the extra diffusion and burning due to sub-grid flame wrinkling. Unfortunately, the efficiency coefficient is not universal and depends on the fractal dimension of the flame and turbulent dynamics. In a recent paper, [2], the authors propose a novel ATF implementation, that thickness not only the flame (through the reactive scalar Y) but all the scalars; velocity, pressure and so on. The flame-fluid interactions are then preserved and an efficiency correction is not required. To be consistent with the boundary conditions, the thickening process has to be limited to a region close to the flame. A flame sensor, Ω, is then introduced as a function of the scalar Y by [6]:

$$\Omega = 16\big[Y(1-Y)\big]^2, \tag{1}$$

where $\Omega = 1$ in the flame front, and $\Omega = 0$ away from it. The flame sensor ensures that auto-ignition events are captured correctly outside the flame front. The thickening factor can be then rewritten as

$$\mathcal{F} = 1 + (\mathcal{F}_0 - 1)\Omega, \tag{2}$$

Sub-grid terms arise in LES from spatial filtering of the Navier-Stokes equations. However, these terms will be affected by the geometric transformation and will become highly anisotropic. If Δ_{min} is small enough to capture most of the small scales, then there is no need of sub-grid modelling close to the flame. The final LES-ATF equations are then:

$$\begin{aligned}
&\frac{\partial \bar{\rho}}{\partial \tau} + \frac{\partial \bar{\rho}\tilde{u}_i}{\partial \xi_i} = 0,\\
&\frac{\partial \bar{\rho}\tilde{u}_i}{\partial \tau} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{u}_j}{\partial \xi_j} + \frac{\partial \bar{p}}{\partial \xi_i} = \frac{\partial \check{\sigma}_{ij}}{\partial \xi_j} + (1-\Omega)\frac{\partial \tau_{ij}^{sgs}}{\partial \xi_j},\\
&\frac{\partial \bar{\rho}\tilde{e}}{\partial \tau} + \frac{\partial (\bar{\rho}\tilde{e} + \bar{p})\tilde{u}_j}{\partial \xi_j} = \frac{\partial \check{\sigma}_{ij}\tilde{u}_i}{\partial \xi_j} - \frac{\partial \check{q}_j}{\partial \xi_j} - (1-\Omega)\frac{\partial q_j^{sgs}}{\partial \xi_j} - \frac{\bar{\rho}q\bar{\dot{\omega}}}{\mathcal{F}},\\
&\frac{\partial \bar{\rho}\tilde{Y}}{\partial \tau} + \frac{\partial \bar{\rho}\tilde{u}_j\tilde{Y}}{\partial \xi_j} = \frac{\partial}{\partial \xi_j}\big(\bar{\rho}D\mathcal{F}\frac{\partial \tilde{Y}}{\partial \xi_j}\big) + (1-\Omega)\frac{\partial J_j^{sgs}}{\partial \xi_j} + \frac{\bar{\rho}\bar{\dot{\omega}}}{\mathcal{F}}.
\end{aligned} \tag{3}$$

Where $\bar{\cdot}$ indicates conventional filtering (with filter width Δ) and $\tilde{\cdot}$ indicates density-weighted filtering. The filtered tensor is $\check{\sigma}_{ij} = 2\mu\mathcal{F}\Big(\tilde{S}_{ij} - \frac{1}{3}\delta_{ij}\nabla\cdot\tilde{\mathbf{u}}\Big)$ where $\tilde{S}_{ij}$ is the filtered strain tensor. The filtered heat flux is calculated from Fourier's Law as $\check{q}_j = -\lambda\mathcal{F}\vec{\nabla}\tilde{T}$. The term $(1-\Omega)$ in front of the sub-grid terms, cancels the sub-grid contribution in the region close to the flame, and no "turbulence" model exists within the thickened region. The filtered reaction rate can then by directly approached by $\bar{\dot{\omega}} = -A\bar{\rho}\tilde{Y}e^{-Q/R\tilde{T}}$. To simplify the complexity of the problem, one step kinetics is maintained; where the pre-exponential factor A, the activation energy Q and the energy released by combustion q are selected to reproduce the laminar flame speed [7]. The ideal equation of state is used $p = \rho RT/M$ and a perfect gas is assumed. The coefficients of dynamic viscosity, μ, heat conduction, λ, and mass diffusion, D, are assumed to depend only on temperature and followed a Sutherland-type empirical law.

The sub-grid terms are closed using a gradient approach, where $\tau_{ij}^{sgs} = \mu_{sgs}\tilde{S}_{ij}$ (similarly for the sub-grid scale transport of energy and mass, q_j^{sgs} and J_j^{sgs}). The sub-grid viscosity is modelled using a conventional Smagorinsky model where $\mu_{sgs} = (C_s\Delta^2)||\tilde{S}_{ij}||$. The sub-grid model is independent on the ATF approach, and other approaches (such as a dynamic Smagorinsky model, or WALE) could be used. The Smagorinsky model has been retained in this work for simplicity. The model was implemented in an in-house three-dimensional LES solver. The code is fully compressible, using the HLLC Riemann Solver [8], with fifth-order WENO reconstruction [9] . The code has been used to model shock waves and shock/boundary layer interactions.

3 Results and Conclusions

Although, the thickening effects on the laminar flame speed have been extensively investigated [3], its effects on detonation wave propagation have not yet been studied. The performance of the model was tested on both a one-dimensional laminar flame and a detonation wave. Several mesh spacings were employed to test the convergence of major parameters and grid sensitivity. The coarsest meshes employed, completely under-resolve the flame: For the laminar flame test, $\Delta_1 = 10\delta_f$ and for the detonation wave $\Delta_1 = 100\delta_f$. Subsequent grid-spacings are defined as $\Delta_{n+1} = \Delta_1 2^{-n}$. In one-dimensional calculation, doubling the mesh spacing (increasing n by 1), quadruples the computational effort (to maintain a constant CFL).

Figure 1 shows the results of laminar flame and detonation speed versus Δ. Three conditions are tested: No model (shown as Δ), ATF only on the reactive scalar, denoted as (Δ, F) and ATF on all scalars (Δ, F, H). The results showed that without ATF model, the laminar flame speed converges with $\Delta < \Delta_5$ (finer meshes not shown). The predicted laminar flame speed increases linearly with mesh spacing, from 0.57 m/s to the steady-state value of 2.57 m/s. The ATF model, as expected, reproduces the laminar flame speed even in the coarsest mesh Δ_2. Is interesting to show that, if the energy equation is not thickened (mostly through $\check{q}_j$), the flame speed is not predicted accurately for the coarse meshes Δ_1 and Δ_2 .

Figure 1 shows that the ATF model performs also well in a planar detonation wave. Without the model, the detonation wave speed is larger at coarse meshes. With ATF, the detonation wave speed in Δ_1 is the same as in the fine mesh. Heat transfer is not an important mechanism across the detonation wave and detonation flame speeds with (Δ, F) and $(\Delta, \mathrm{F}, \mathrm{H})$ are nearly identical.
Figure 2 shows the normalised thermal properties close to detonation front for a coarse and fine mesh. Although, the detonation speed is maintained by the ATF model, the coarse mesh smears the Von-Neumann spike over several cells. Nevertheless, the results converge to the fine mesh after a few cells (without ATF density is 20 % lower) and the results can be consider acceptable.

The full LES-ATF methodology was then investigated in the DDT set-up investigated by Gamezo *et al.* [10]. It consists of a rectangular shock tube filled by a stoichiometric mixture of ethylene/air at 13 kPa and 293 K. The mixture is ignited by a spark ahead of an incident shock wave at $M_s = 1.8$ travelling into the mixture. Non-slip, adiabatic walls were considered, and no wall-functions were therefore used to modify the sub-grid terms.

Figure 3, shows the evolution of the scalar iso-surface LES simulation on DDT, mesh size is $\Delta \sim \delta_f/2$. Initially, the shock waves travels toward the right, interacts with the flame and distorts it. The shock wave and flame interacts with each other, increasing turbulence. When the shock reflects back from the wall, hot spots are generated within the flame at approximately 280 μs and DDT occurs at 296 μs, where detonation propagation speed is measured at around 1900 m/s. A detonation wave is generated, its front swallow unburned fuel rapidly at it overtakes the reflected shock shortly afterwards.

The results showed good performance of the ATF model and three-dimensional LES simulation can be obtained relatively quickly. Comparing to the DNS results of [10], LES does not cature the smallest flow features (as the grid is much coarser) but the predicted detonation times are very similar and an acceptable solution could be obtained in a much shorter time scale than the DNS.

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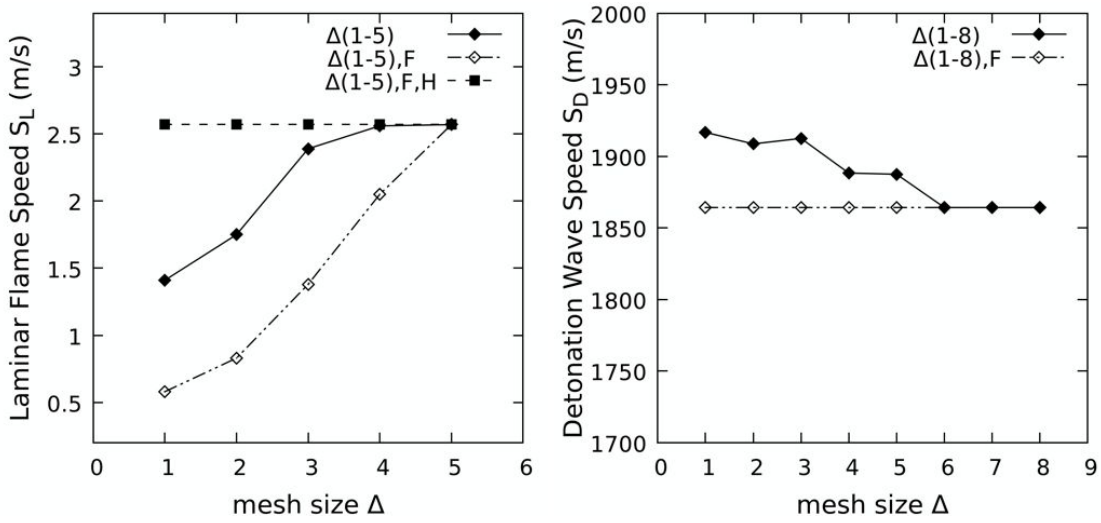

Figure 1: Left: Laminar flame speed in the 1D laminar flame Right: Detonation wave speed in a 1D detonation wave. (Δ) indicates results without model; (Δ, F) indicates results using ATF only on the reactive scalar; and $(\Delta, \mathrm{F}, \mathrm{H})$ indicates results using ATF on all scalars.

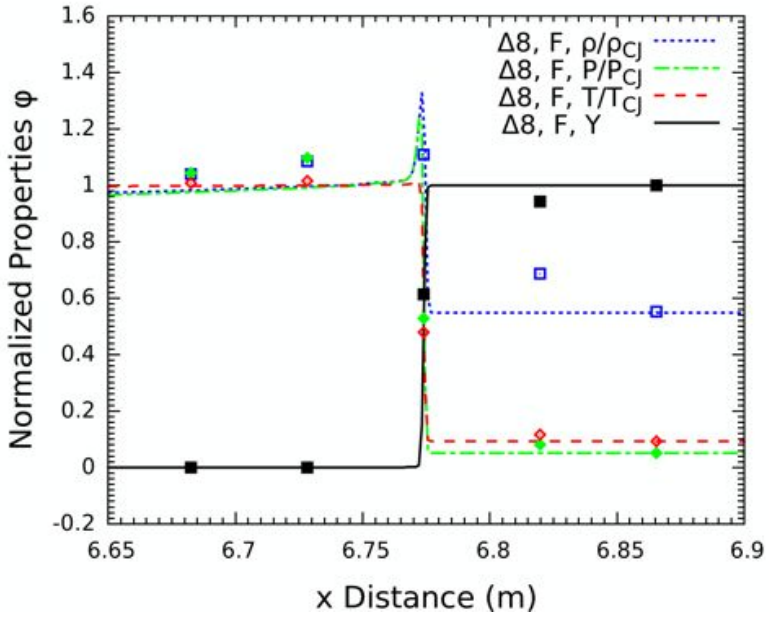

Figure 2: Normalized scalars of 1D detonation wave in a coarse Δ_2 (dot) and fine mesh Δ_8 (line) using the ATF model. The scalars are normalized to their CJ values.

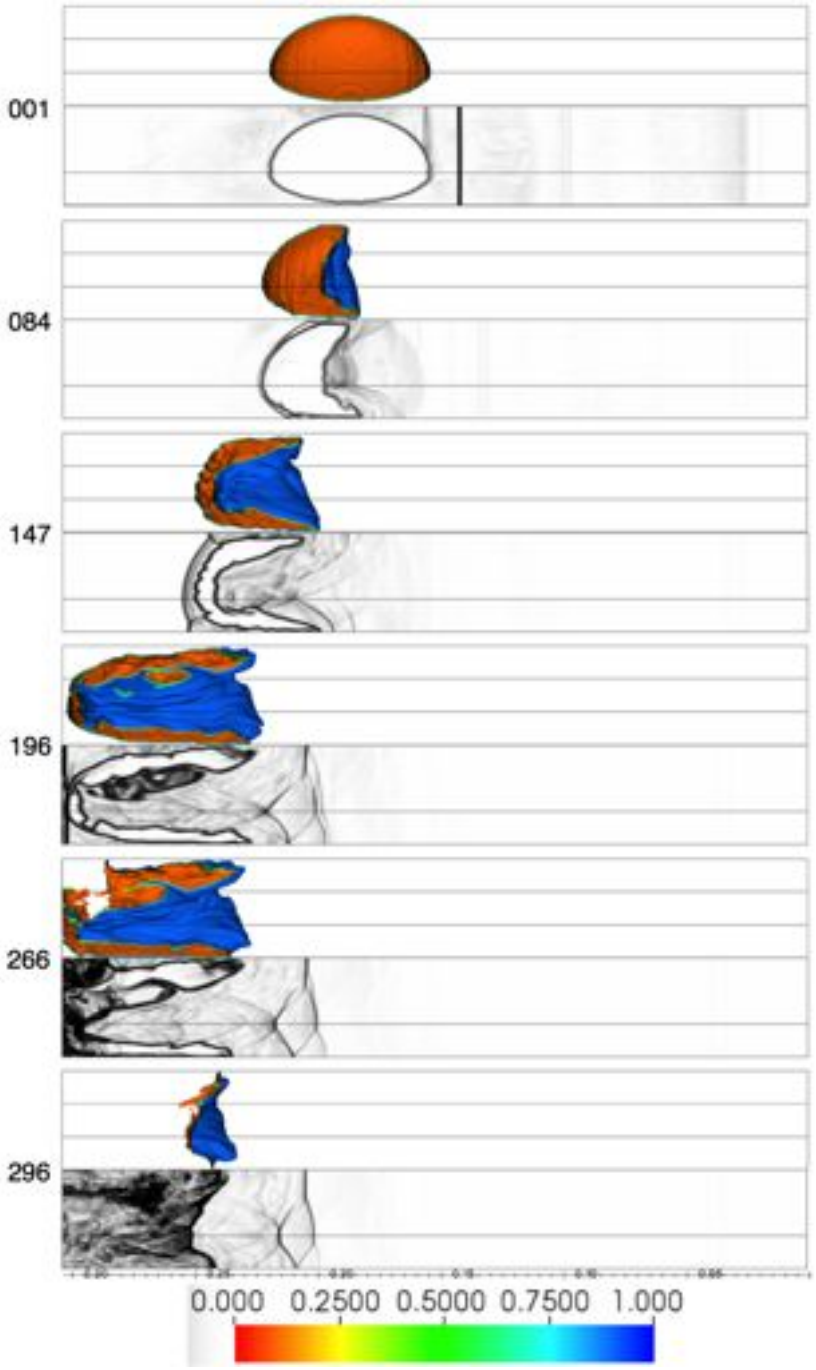

Figure 3: LES-ATF of Ethylene/Air. The colour plots are iso-surfaces of fuel mass ratio Y. The black and white plots are numerical Schileren. Time step is counted by μs.