A TURBULENT COMBUSTION MODEL FOR IGNITION OF RAPIDLY EXPANDING HYDROGEN JETS: VALIDATION FOR 1-D LAMINAR FLOWS

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ABSTRACT

A turbulent combustion model based on the Linear Eddy Model for Large Eddy Simulation (LEM-LES) is currently proposed to study self-ignition events of rapidly expanding hydrogen jets. The model is a one-dimensional treatment of a diffusion-reaction system within each multi-dimensional LES cell. This reduces the expense of solving a complete multi-dimensional problem while preserving micro-scale hotspots and their effects on ignition. The current approach features a Lagrangian description of fluid particles on the sub-grid for increased accuracy. Also, Adaptive Mesh Refinement (AMR) is implemented for increased computational efficiency. In this paper, the model is validated for various inviscid laminar 1-D mixing and ignition problems, shock tube problems, flames, and detonations.

1.0 INTRODUCTION

In recent years, with the emergence of new hydrogen technologies, there has been much focus on developing appropriate numerical modelling strategies in order to assess explosion and safety hazards associated with hydrogen leaks from high pressure sources. It is of fundamental importance to understand hydrogen ignition and explosion behaviour in order to develop the appropriate design codes and standards for storage facilities, fuelling stations, and other hydrogen related applications. In this paper, a novel modelling strategy is proposed for the purpose of determining spontaneous ignition limits of rapidly expanding and pressurized hydrogen jets which are suddenly released into confined oxidizer environments[1]. Furthermore, it essential to understand the physical process by which jet flames are established. Namely it is desired to isolate the roles of the diffusion-ignition mechanism[2], shock compression, and enhanced combustion due to turbulent mixing on the combustion process of such rapidly expanding turbulent hydrogen jets. Thus, it is necessary to employ a modelling strategy that captures each of these physical mechanisms in a highly compressible and reactive environment involving very rapid transients in pressure and energy. In this paper, a novel approach for modelling turbulent and rapidly expanding hydrogen jets in the framework of Large Eddy Simulation (LES) is proposed and is validated for simple 1-D laminar mixing and ignition problems where large pressure changes (i.e. shocks or expansions) are possible.

The particular problem of hydrogen jet ignition is difficult to address using either the Direct Numerical Simulation (DNS) approach of solving the Navier-Stokes equations, or the LES approach. This is primarily due to the wide range of scales that must be resolved, or modelled. While a practical problem may span several meters, it is the fast mixing and chemistry on the micro-scale that influences the overall ignition behaviour of the jet. Furthermore, for such high speed flows, the chemical reaction times and mixing times are comparable to the small scale eddy turn over times, suggesting a Damkohler number (D_a) near unity exists and must be addressed appropriately through LES. Current solutions[3-7] either involve attempts at unresolved DNS or LES strategies which are based on bold assumptions regarding the flow turn over times, mixing rates, and chemical time scales.

The LES strategy proposed in this paper is based on the Linear Eddy Model for Large Eddy Simulation (LEM-LES), which is a one-dimensional treatment of a diffusion-reaction system within each LES cell[8]. This reduces the expense of solving a complete multi-dimensional problem through DNS while preserving micro-scale hotspots and their physical effects on ignition. Furthermore, the model is appropriate for high speed flows and can treat D_a~1. This method has been successfully applied to model turbulent premixed and non-premixed flames[9,10], and also supersonic mixing layers[11]. While the method has not yet been applied to treating compressible and reactive flows, it appears to hold great promise. In this paper, the method is validated for a number of 1-D inviscid laminar problems; heat-diffusion, constant volume ignition, the shock tube problem, flames, and detonations. Results of these validation tests demonstrate the ability of the model to capture micro-scale diffusion and ignition in highly compressible flows. These preliminary results prove the model approach to be appropriate for treating ignition of rapidly expanding and pressurized jet releases, as described in [1]. Extension of the model to treat turbulent flows is currently under development and is not discussed here.

2.0 MODEL FORMULATION

2.1 Governing Equations for the Compressible and Reacting System

For the reactive and rapidly expanding hydrogen jet release described in [1], the gas dynamic evolution is governed by the compressible Navier-Stokes equations. In order to simplify the analysis, reduce computational expense, and to isolate the roles of specific physical mechanisms that influence the overall fluid flow, a number of assumptions are made. First, a calorically perfect inviscid fluid system is assumed. Also, the chemistry is simplified by considering only a single reactant species, with mass fraction *Y*, that undergoes chemical reaction that forms products according to a single-step Arrhenius reaction rate law[12]. In this study, only premixed combustion is considered, although extension of the model to non-premixed combustion is trivial. Also, for simplicity, changes in molecular weight from reactants to products are neglected. Finally, heat and mass are assumed to diffuse at the same rate, hence a Lewis number of unity is assumed. The resulting conservation equations for mass, momentum, energy, and reactant species are given below in Equations (1) through (4), respectively. It should be noted that the equations are given in non-dimensional form where the various gas properties are normalized by a reference quiescent state. Also the nomenclature for symbols found throughout the paper are given in Table 1.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \quad , \tag{1}$$

$$\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho u u) + \nabla p = 0 \quad , \tag{2}$$

$$\frac{\partial E}{\partial t} + \nabla \cdot \left((E+p) u - u \cdot \tau \right) - \left(\frac{\gamma}{\gamma - 1} \right) \nabla \cdot (\alpha \nabla T) = -Q \dot{\omega} \quad , \tag{3}$$

$$\frac{\partial (\rho Y)}{\partial t} + \nabla \cdot (\rho u Y) - \nabla \cdot \left(\frac{\alpha}{L_e} \nabla Y \right) = \dot{\omega} \quad , \tag{4}$$

where

$$\dot{\omega} = -\rho^n A Y e^{-E_a / T} \quad , \tag{5}$$

$$E = \frac{p}{\gamma - 1} + \frac{1}{2} \rho u u \quad , \tag{6}$$

$$T = p/\rho \,, \tag{7}$$

$$L_e = 1 \,, \tag{8}$$

The various parameters and variables are given in non-dimensional form according to

$$\rho = \frac{\hat{\rho}}{\hat{\rho}_o} \,, \quad u = \frac{\hat{u}}{\hat{c}_o} \,, \quad p = \frac{\hat{p}}{\hat{\rho}_o \hat{c}_o^2} = \frac{\hat{p}}{\gamma \hat{p}_o} \,, \quad T = \frac{\hat{T}}{\gamma \hat{T}_o} \,, \quad x = \frac{\hat{x}}{\hat{L}} \,, \quad t = \frac{\hat{t}}{\hat{L}/\hat{c}_o} \,, \quad \alpha = \frac{\hat{k}/\hat{c}_p}{\hat{\rho}_o \hat{c}_o \hat{L}} \,,$$

$$L_e = \frac{S_c}{P_r} = \frac{\hat{k}/\hat{c}_p}{\hat{\rho}\hat{D}} \,, \quad E_a = \frac{\hat{E}_a}{\hat{c}_o^2} \,, \quad Q = \frac{\hat{Q}}{\hat{c}_o^2} \,, \quad A = \frac{\hat{A}}{\hat{c}_o / \left(\hat{L} \hat{\rho}_o^{(n-1)} \right)} \,, \quad \gamma = \frac{\hat{c}_p}{\hat{c}_v} \,, \tag{9}$$

where the hat represents a dimensional quantity, and the subscript '*o*' represents the reference state, usually taken as the initial quiescent fluid.

Table 1. Nomenclature.

A	Pre-exponential factor	P_r	Prandtl number
c	Speed of sound	Q	Heat release
c_p	Specific heat capacity at constant pressure	R_e	Reynolds number
c_v	Specific heat capacity at constant volume	S_c	Schmidt number
D	Mass diffusivity	T	Temperature
D_a	Damkohler number	t	Time
E	Total energy	u	Velocity
E_a	Activation energy	v	Specific volume
k	Heat conductivity	V	LES cell volume
L	Reference length scale	x	Cartesian distance coordinate
L_e	Lewis number	Y	Mass fraction of reactant
m	Mass coordinate	α	Heat diffusivity
M_D	Detonation Mach number	γ	Ratio of specific heats
N	Number of sub-grid nodes in an LES cell	ρ	Density
n	Reaction order	$\dot{\omega}$	Reaction rate
p	Pressure		

2.2 Laminar 1-D Subgrid model for Large Eddy Simulation (LES)

In order to resolve ignition problems involving hydrogen, it is proposed here to solve separately the large scale pressure evolution and the small scale mixing and reactions through appropriate coupling of the pressure and energy fields. Hence it is proposed to solve Equations (1) through (3) on the large scales without the chemical reaction terms, and then apply a model to describe the small scale molecular mixing and chemical reactions. In the proposed LES approach, the sub-grid model is a one-dimensional representation of the flow field within each LES cell whose orientation is aligned in the direction of local flow. A good general summary of the model formulation for weakly compressible flows (LEM-LES) is found in [8] and a comprehensive description of the model is found in [13]. In order to derive the sub-grid model formulation, pressure gradients are locally neglected. Thus it is assumed that pressure waves travel much faster than the flow evolution is able to expand or contract. Therefore, the pressure field evolution is solved entirely on the LES and the pressure changes are prescribed to the sub-grid in order to account for energy changes due to rapid compression or expansions. This formulation was previously applied to determine ignition limits of idealized non-turbulent and rapidly expanding hydrogen jets[14], where the large scale pressure evolution was prescribed as a source term to the 1-D sub-grid model. The previous model

formulation, however, contained only pressure and energy coupling in one-direction; from the large scales to the small scales. Thus, the model could only be used to determine the onset of ignition, and not the subsequent influence of ignition on the jet evolution. Therefore, this current model serves as an extension to the previous work[14] by providing two-way coupling between the large scale pressure evolution and small scale mixing and reactions. The system of equations that is solved on the sub-grid for 1-D laminar flows is the conservation of energy (10) and conservation of reactant mass (11):

$$\rho\frac{DT}{Dt}-\left(\frac{\gamma-1}{\gamma}\right)\frac{\partial p}{\partial t}-\rho\frac{\partial}{\partial m}\left(\rho\alpha\frac{\partial T}{\partial m}\right)=-\left(\frac{\gamma-1}{\gamma}\right)Q\dot{\omega} \quad , \tag{10}$$

$$\rho\frac{DY}{Dt}-\frac{\partial}{\partial m}\left(\rho\frac{\alpha}{L_e}\frac{\partial Y}{\partial m}\right)=\dot{\omega} \quad , \tag{11}$$

where *m* is a one-dimensional mass weighted coordinate whose transformation to Cartesian spatial coordinates is given by

$$m(x,t)=\int_{x_o}^{x}\rho(x,t)dx \quad , \tag{12}$$

The sub-grid model formulation in this study differs from previously published formulations, referenced in this paper[8-11,13], for several reasons. First, turbulent "stirring"[15] is normally included in equations (10) and (11) in order to treat turbulent flows (This is termed the LEM-LES approach). This treatment of turbulent terms is currently neglected since the current study only validates the model formulation for inviscid laminar test cases. Also, a pressure term is included in equation (10), which was not included in previous LEM-LES formulations. This term accounts for energy changes associated with rapid changes in pressure. It is treated as a source term where the pressure changes are obtained from the LES hydrodynamic calculations. Finally, the one-dimensional sub-grid domains are formulated with Lagrangian mass-weighted coordinates. This is done in order to account for not only expansion or contraction of the fluid along particle paths, but also changes in spatial distance between computational nodes on the subgrid ($\underline{dx}$). The transformation from Cartesian spatial coordinates to Lagrangian mass-weighted coordinates is given in equation (12). To couple the subgrid model to the large scale fluid flow, the LES simulation provides the local pressure changes at each time step to the subgrid model, while the sub-grid model provides the energy contribution due to chemical reactions to the LES. Finally it should be noted that the reactant evolution does not need to be solved on the LES scale since all of the reactant information is stored on the sub-grid. Equations (4) and (11) are completely decoupled. Numerical implementation of the model and order of operations are described in the next section.

2.3 Numerical Implementation and the LES-Subgrid Coupling

In order to solve the system of equations (1) – (4), for DNS or LES, a numerical framework developed by Mantis Numerics Ltd. is employed. The compressible flow solver features a second order accurate exact Godunov solver to treat the convection terms[16,17] and the diffusive terms are handled explicitly. Adaptive Mesh Refinement (AMR) and is also implemented for increased computational efficiency[18]. For the sub-grid model, the system of equations (10) and (11) is solved explicitly across each LES time step using operator splitting to treat the various terms. The diffusion terms are discretized using central differences and the reaction terms are solved explicitly using the Forward Euler method with variable-time stepping. For implementation of AMR for the LES approach, the sub-grid model is only solved on the finest grid level of the LES. The algorithm for implementing the LES model (for 1D laminar flows) across a single LES time step is as follows:

1. At time *t*, solve the large scale fluid motion. Solve equations (1) to (3) without chemical reactions, for a single time step, Δt, using the LES solver[16,17]. During the process store the mass flux across each LES cell face, $\rho u \Delta t$.

2. For the sub-grid simulation, at time *t*, ensure that each sub-grid node has the same initial pressure as the LES cell. If the sub-grid pressure is different (i.e. from the previous time step), account for the enthalpy change due to the constant volume adiabatic compression that occurs on the LES from the previous time step. For each sub-grid node, solve equation (13) across the time step, Δt, while holding ρ constant.

$$\frac{DT}{Dt} = \left(\frac{\gamma - 1}{\gamma \rho} \right) \frac{\partial p}{\partial t} \quad , \tag{13}$$

3. Once the sub-grid pressure is updated, update the density of each sub-grid node through equation (7).

4. Next, solve the diffusion/reaction system (10) and (11) at constant pressure for the entire LES time step, Δt. Here the initial LES cell pressure is used. For future work, turbulent stirring[15] will be implemented here. Store the amount of reactant before and after the process according to equation (14).

$$(\rho Y)_{cell} = \frac{\sum_{i=1}^{N} m_i Y_i}{V_{\text{cell}}} \quad , \tag{14}$$

5. For the LES cell, account for the pressure increase at constant volume due to the chemical reactions that occur on the sub-grid according to equation (15). This is implemented as a source term in the LES solver.

$$\Delta p_{cell} = \Delta (\rho Y)_{\text{cell}} Q \quad , \tag{15}$$

6. Implement the large scale fluid advection by transferring sub-grid mass from one LES cell to another. This is done according to how much mass flux is computed across each LES cell face (see step 1). For details on the specific splicing and re-gridding process implemented here, see [13].

7. Repeat steps 1-6 for the next time step.

A key feature of the current algorithm is that the pressures (and consequently, the internal energies) of both the sub-grid and LES cell are always returned to the same value (see step 2). This ensures that energy, along with mass, is always conserved. Although there are essentially two temperature fields (one on the LES and one on the sub-grid), as a convention the Favre-averaged temperature from the sub-grid field is the displayed quantity in the Figures shown in Section 3. The Favre-averaged sub-grid temperature is given by equation (16).

$$\tilde{T}_{\text{subgrid}} = \frac{\sum_{i=1}^{N} m_i T_i}{\rho_{\text{cell}} V_{\text{cell}}} \quad , \tag{16}$$

3.0 MODEL VALIDATION FOR LAMINAR PROBLEMS

3.1 Model Parameters

For the laminar experiments conducted in this paper, a single set of model parameters is used for simplicity and consistency, although the model has been verified to work with differing parameters. The parameters here are chosen arbitrarily, but they are to some extent representative of hydrogen ignition behaviour. The model parameters used for all of the test cases are given in Table 2. Also, for the LES simulations, each sub-grid domain is re-gridded, or initialized, with 12 nodes at each time step. This is consistent with a previously published LEM-LES approach for super-sonic flows [11].

Table 2. Summary of model parameters.

γ = 1.4	E_a = 25.0	n = 2
α = 2x10^-5	Q = 20.7	N = 12
L_e = 1.0	A = 1.5x10^5	

3.2 Diffusive Mixing

The first experiment conducted is a simple inert, and constant pressure, heat and scalar diffusion problem. The LES and sub-grid domains are initialized according to (17) and evolved up to t=1.0. A uniform flow velocity is imposed in the flow field to ensure diffusion occurs between all sub-grid nodes. This is necessary since the sub-grid diffusion of equation (10) and (11) is neglected across the LES cell faces[8,13]. The simulation is conducted for the LES model, which uses 3 levels of grid refinement, and compared against a fully resolved DNS simulation, which uses 6 grid levels of refinement. The results are also compared against an unresolved DNS simulation which has the same level of refinement as the LES model simulation. The coarse base grid resolution for all three simulations is Δx=0.01. Temperature and scalar profiles are shown in Figure 2. Results indicate that the LES model captures well the resolved trends of the DNS simulation.

$$\rho(x,0)=\begin{Bmatrix}0.5 \text{ for } x<0.1\\ 0.2 \text{ otherwise}\end{Bmatrix},\quad u(x,0)=0.2,\quad p(x,0)=0.8,\quad Y(x,0)=\begin{Bmatrix}1 \text{ for } x<0.1\\ 0 \text{ otherwise}\end{Bmatrix}, \tag{17}$$

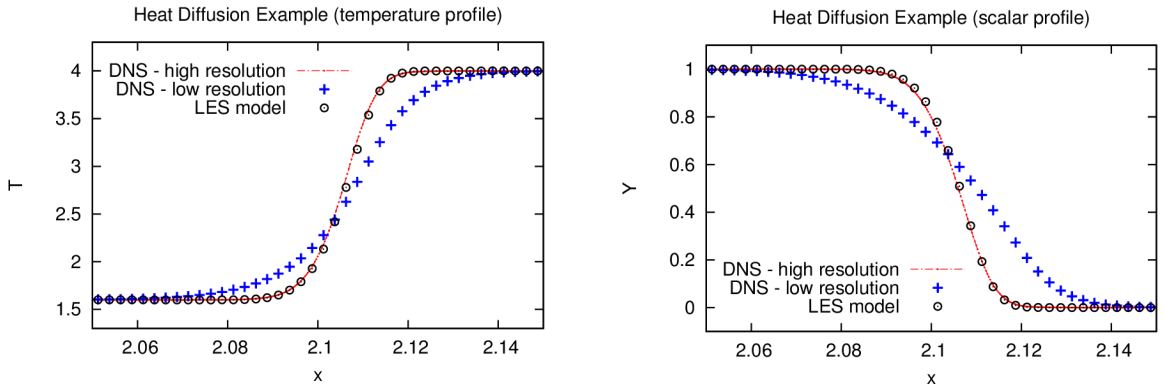

Figure 2. Heat diffusion (left) and scalar diffusion (right) at t=1.0.

3.3 Shock Tube Problem

To test the LES model's ability to capture shocks and rapid expansions, the classic shock tube problem[19] is performed. The domain is initialized according to (18) and the resulting density profiles are presented in Figure 3. The LES model captures correctly density changes arising from

rapid pressure changes. Diffusion at the density interface, near x=0.98, is also correctly captured, as can be seen at the right frame of Figure 3. Again, the high resolution DNS uses 6 levels of refinement, while the LES model and low resolution DNS only use 3. The coarse base grid resolution for these simulations is Δx=0.05.

$$\rho(x,0)=\begin{Bmatrix}1.0 \text{ for } x<0\\0.1 \text{ otherwise}\end{Bmatrix},\quad u(x,0)=0.0,\quad p(x,0)=\begin{Bmatrix}1.0 \text{ for } x<0\\0.1 \text{ otherwise}\end{Bmatrix}, \tag{18}$$

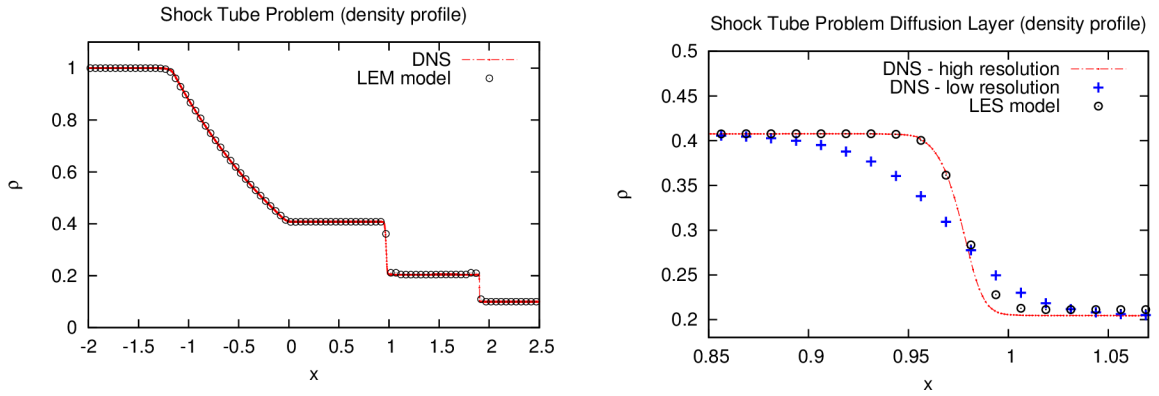

Figure 3. Shock tube problem at t=1.0. The left figure shows the entire density profile, while the right figure shows a close-up of the diffusion process at the density interface.

3.4 Constant Volume Reaction

Since the diffusion-reaction system of the LES model is formulated for constant pressure systems, it is necessary to test the model's ability to handle reactions in a simple constant volume reactor experiment. To initiate ignition, p_o=0.8, ρ_o=0.125, and Y_o=1. Comparison to DNS yields excellent agreement as can be seen by the matching temperature and reactant evolution profiles of Figure 4. Furthermore, a theoretical ignition delay time is obtained through high activation energy asymptotic expansion of the governing equations[12] and is given by equation (19). For the parameters in this study, t_{ig}=5.21E-4, which is consistent with the numerical model results shown in Figure 4.

$$t_{ig}=\frac{T_o^2\exp(E_a/T_o)}{(\gamma-1)\rho QAY_oE_a}\left(1-\exp\left(\frac{-(\gamma-1)QE_a}{T_o^2}\right)\right), \tag{19}$$

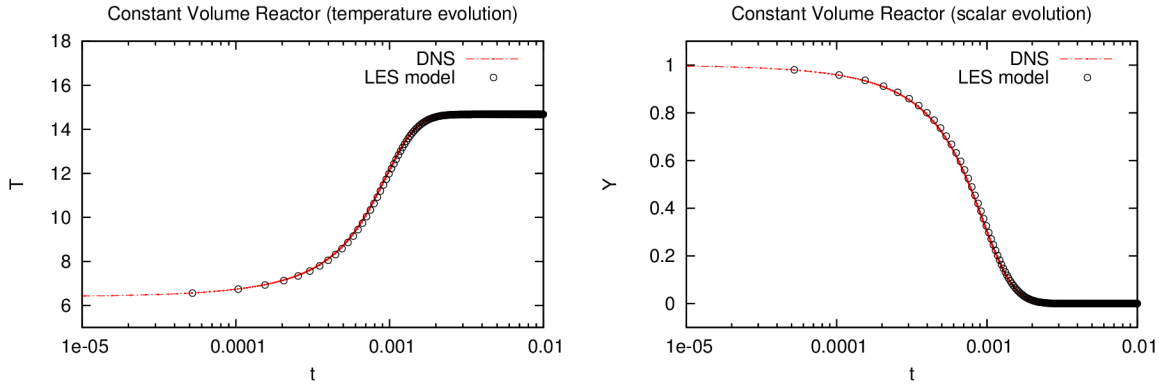

Figure 4. Constant volume reaction; temperature evolution (left) and the reactant depletion (right).

3.5 Laminar Flames

The most important feature of the LEM-LES formulation is its ability to capture turbulent flames[9,10]. In this paper, the model's ability to capture laminar flames at various grid resolutions is assessed. To initiate a flame, a hotspot is initiated near the right boundary of the domain according to the initial conditions (20). The coarse base grid resolution, for the various flame simulations, is Δx=0.015625. The resulting flame temperature and density profiles, at t=1.0, are shown in Figure 5 for a high resolution DNS simulation using 8 levels of refinement, and also low resolution DNS and the LES model that both use 4 levels of refinement. Both boundary conditions are zero gradient type, allowing for an unsupported flame to evolve and travel in a moving fluid. Although initially there is no fluid motion initially, the pressure generated from the chemical reactions promotes fluid motion throughout the entire domain, as can be seen from the resulting velocity profiles of Figure 6. As mentioned in Section 3.2, fluid motion is required for adequate mixing of sub-grid nodes between LES cells[8,13]. Clearly, from Figures 5 and 6, the LES model captures well the temperature, density, velocity, and pressure profiles as the high resolution DNS. In comparison, the low resolution DNS flame travels much faster owing to increased numerical diffusion associated with the lower grid refinement. Finally, a comparison of steady flame speeds is made between the DNS model and the LES model for various grid level resolutions and is shown in Figure 7. In the simulations the flame speeds are calculated instantaneously by applying the conservation of mass across the flame front. Also shown in Figure 7 is the analytical solution for the flame speed based on high activation energy matched-asymptotics[12], whose formula is given below in equation (22). For the parameters here, this value was found to be $S_{L,\text{theory}}$=0.0131. Clearly, the LES model is able to capture closely the correct flame speed using less grid levels compared to the DNS model. The resolved flame speed for the LES model however, is observed slightly slower than the DNS flame speed. The resolved flame speeds for the LES model and DNS are $S_{L,\text{LES}}$=0.0123 and $S_{L,DNS}$=0.0138, respectively. This difference, however, is very minor compared to the difference in flame speeds associated with unresolved simulations.

$$\rho(x,0)=\begin{Bmatrix} 0.125 \text{ for } x>0.36 \\ 1.0 \text{ otherwise} \end{Bmatrix}, \quad u(x,0)=0.0, \quad p(x,0)=0.8, \quad Y(x,0)=1.0, \tag{20}$$

$$S_L=\frac{T_o}{E_a}\left(1+\frac{\gamma T_o}{(\gamma-1)Q}\right)\sqrt{\alpha L_e A \exp\left(\frac{-E_a}{T_o+(\gamma-1)Q/\gamma}\right)}, \tag{21}$$

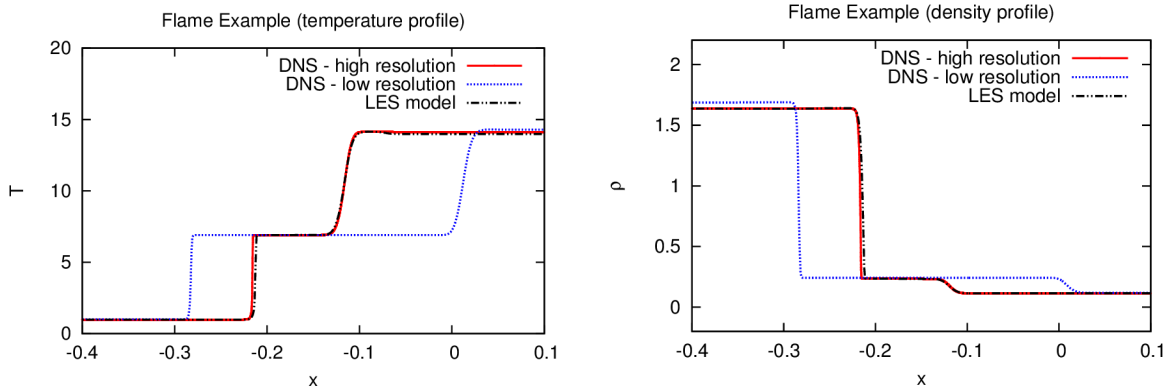

Figure 5. Flame temperature (left) and density (right) profiles at t=1.0.

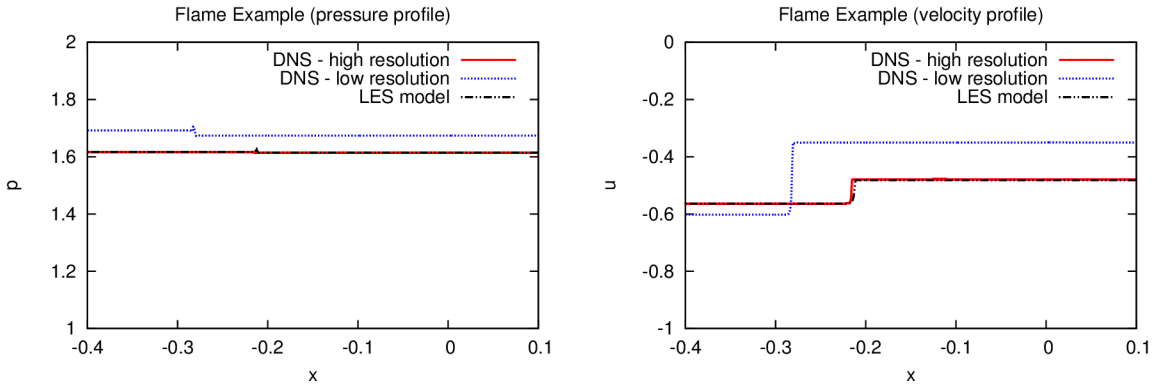

Figure 6. Flame pressure (left) and velocity (right) profiles at t=1.0.

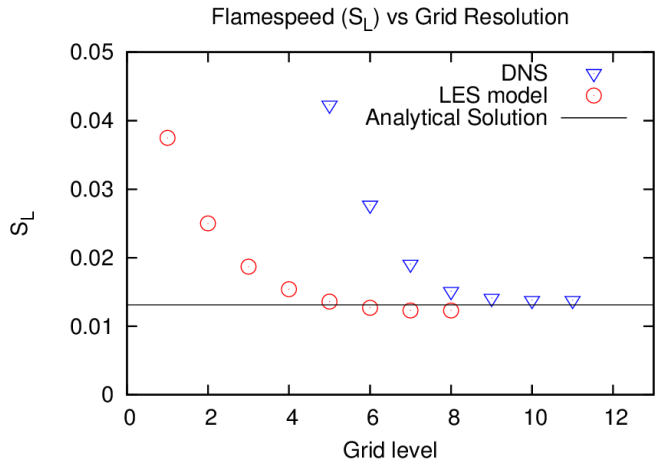

Figure 7. Steady flame speed vs. grid resolution.

3.6 Piston Driven Detonation

The final experiment conducted in this study is to test the LES model's ability to capture steady detonations. To initiate a detonation wave for the parameters given in Section 3.1, a piston traveling at the required velocity to drive a Chapman-Jouguet (CJ) detonation[12] in a reactive mixture is simulated in the frame of reference of the piston itself. The computational domain is initialized according to (22) where the left boundary is a wall type boundary, representing the piston, and the right boundary is fixed with the unburned mixture properties flowing into the domain. In order to determine the piston velocity, the CJ detonation Mach number for the reactive mixture is first determined by equation (23) and has a value of $M_{D,CJ}$ = 6.46. The piston velocity is then given by equation (24). The resulting steady state pressure, density, and velocity profiles of two DNS simulations and the LES simulation at t=0.1 are shown below in Figure 8. The base grid resolution used for the simulations is Δx=0.0005. The high resolution DNS simulation used 7 levels of refinement and the low resolution DNS and the LES model both used 3 levels or refinement. The principle observation made from Figure 8 is that the LES model gives the correct values for the detonation products. Furthermore, the LES model is able to capture well the Von-Nuemann properties[12] observed at the detonation front compared to the low-resolution DNS. Despite this, the LES detonation structure remains stretched spatially, compared to the high-resolution DNS as the pressure evolution remains unresolved. The detonation velocities of all three simulations are estimated instantaneously by applying the conservation of mass across the structure. All three simulations were found to give the exact CJ detonation Mach number of M_D = 6.46. Finally, it should be noted that although the LES model gives the correct CJ detonation velocity, the front is observed to follow only a few grid points behind the DNS simulations. The reason for this is currently under investigation.

$$\rho(x,0)=1.0\ ,\quad u(x,0)=-u_p\ ,\quad p(x,0)=0.714\ ,\quad Y(x,0)=1.0\ , \tag{22}$$

$$M_{D,CJ}=\sqrt{1+(\gamma^2-1)Q\left(1+\sqrt{1+\frac{2}{(\gamma^2-1)Q}}\right)}=6.46\ , \tag{23}$$

$$u_p=-(\gamma-1)QM_{D,CJ}\left(1-\sqrt{1+\frac{2}{(\gamma^2-1)Q}}\right)=2.63\ , \tag{24}$$

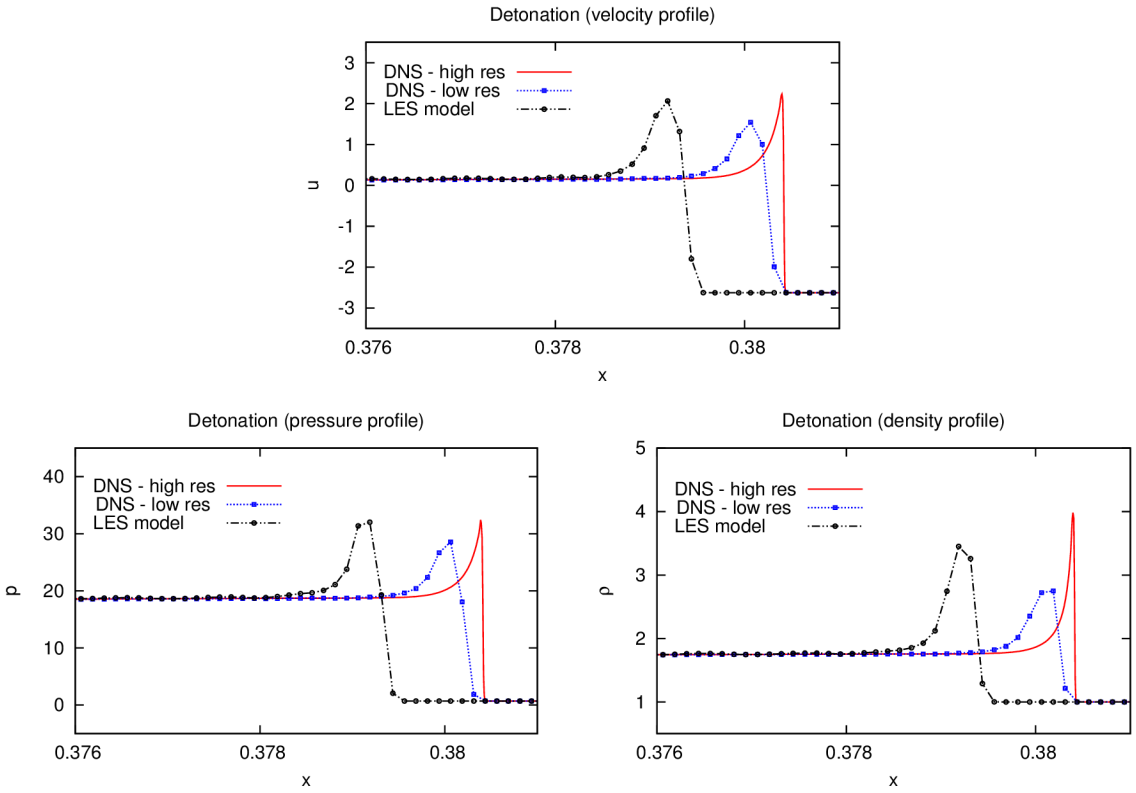

Figure 8: Steady detonation velocity (top), pressure (left), and density (right) profiles at t=0.1.

4.0 DISCUSSION, CONCLUSIONS, AND FUTURE WORK

In this paper an LES model (based on LEM-LES) is proposed for investigating the ignition limits of pressurized and turbulent hydrogen jets which are released into turbulent oxidizer environments. The model has been demonstrated to combine well with Adaptive Mesh Refinement (AMR) for increased computational efficiency and is also threaded for parallel computations. The fundamental assumption of the model is that the scales of pressure evolution are separated from the scales of molecular diffusion and chemical reaction. In general, the LES model performs well at modeling the laminar experiments presented in Section 3. Simple heat diffusion, shock tube, and constant volume ignition problems are captured exactly when compared to high resolution DNS simulations. Furthermore, the model is able to correctly capture detonation wave speeds, and also laminar flame speeds in moving fluids. A fundamental limitation of the model is that fluid motion is required in order to achieve diffusion between neighboring LES cells, and thus correct flame speeds and diffusion rates. For the jet release problem[1], ignition occurs in a very fast moving fluid medium. Therefore the model is expected to perform well for predicting the ignition limits and also the transition to jet flame in a turbulent environment. Future work on the project involves investigating Deflagration to Detonation Transition (DDT) limits in the context of 1-D shock-flame interaction simulations[20]. Inclusion of turbulent stirring terms and extension to 3-D is also planned for the near future model development.

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