Simulation of flame acceleration in an obstructed tube with LES

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1 Introduction

Deflagration to detonation transition (DDT) in complex geometries is difficult to model with numerical simulation. The flame acceleration is usually dependent of several fluid mechanical phenomena. Both flame interactions with turbulent flow fields and shock waves contribute to increased heat release rates. This in turn may create more turbulence and stronger shock waves. One goal is to be able to model all possible cases with one simple model, from laminar combustion to detonation. This work explores the flame acceleration period of an explosion developing from weak ignition to a detonation. The experiments where done in a 4 long closed tube with 0.107 m diameter. One obstacle with blockage ratio of 0.92 is placed in the tube to produce transition to detonation. The experiments where performed with stoichiometric hydrogen air at atmospheric pressure and room temperature. This case is modeled by a large eddy simulation with a full set of transport equations and a reaction progress variable equation. The reaction rate is modeled by a combination of a progress variable gradient approach and a chemical kinetics Arrhenius type model.

2 Numerical Models

A transport equation for a reaction progress variable β is solved to represent the concentration of reactants and products, see equation 1.

$$\frac{\partial \overline{\rho}\tilde{\beta}}{\partial t} + \nabla \cdot \left(\overline{\rho}\tilde{\vec{u}}\tilde{\beta}\right) = \nabla \cdot \left(\frac{\mu_t}{\sigma_\beta}\nabla\tilde{\beta}\right) + \overline{\rho S_d|\nabla\beta|} \tag{1}$$

$$\overline{\rho S_d|\nabla\beta|} = max\left[\rho_u S_L \Xi|\nabla\tilde{\beta}|, r_k\right] \tag{2}$$

This model is a flame surface density model presented in [1] and [2], where Ξ is the wrinkling factor, but also include reaction kinetics, as shown in equation 2. Using the gradient formulation for the reaction term ensures physical behaviour of the flame at near laminar flow. For an extreme case the with no turbulence and no density difference across the flame the model in equation 2 propagates the flame front with the displacement speed given here as S_L. It is important for the model to behave correctly in the near laminar region for cases where the subfilter turbulence is low. In figure 1 the progress variable and normalized temperature is shown together with reaction rates. The reaction rate is highest where the progress variable gradient is highest and thus the heat release is highest. This produces pressure gradients in both directions with a peak somewhere between β=0 and β=1. These pressure gradients will create velocities in the direction of the negative pressure gradients and this leads to a significant thickening

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of the flame. As a remedy to keep flame thickness thin, an Arrhenius kinetic term is introduced. The kinetic reaction rate is controlled by temperature and the highest reaction rate is in the high temperature region.

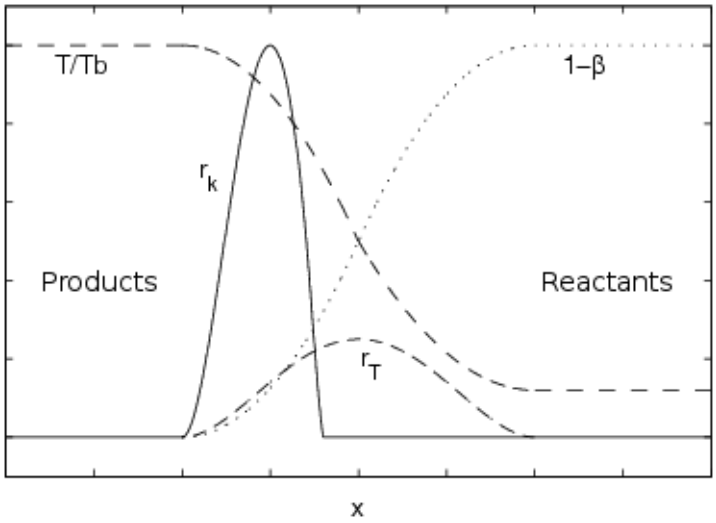

Figure 1: Schematic representation of reaction variable, temperature, and reaction rates across a filtered flame. T/Tb: temperature divided by temperature of the totally burned gas. 1-β: reaction variable. r_k: reaction rate from chemical kinetics. r_T: reaction rate from mixing rate.

An one-equation turbulence model for turbulent kinetic energy[5] is used to model the sub-filter turbulence. The transport equations are solved with the second order centered TVD scheme FLIC [3].

3 Setup

The experimental setup is shown in figure 2. It is a closed 4 m long tube with 0.107 m diameter. It is filled with stoichiometric hydrogen air at atmospheric pressure and at 293 K. The ignition is a spark set in one end wall. Placed 1 m from ignition is an obstacle, a disc with 0.03 m hole in center witch is blockage ratio 0.92. It is a pressure transducer at the ignition end. In addition it is five pressure transducers at 0.5 m intervals behind obstacle starting at 0.5 m, but these are not discussed here. The numerical

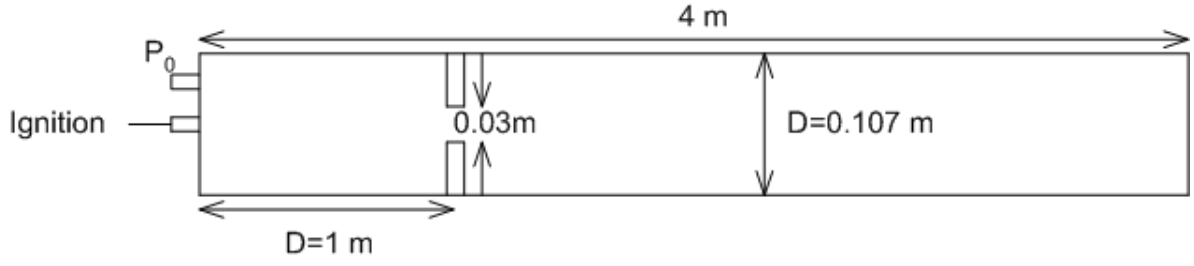

Figure 2: Experimental setup of a 4 m long tube.

experiments are done in axisymmetric cylindrical coordinates and with two homogeneous meshes with 1 and 2 mm sizes.

4 Results

Figure 3 shows the pressure records from transducer P_0 for the experiments and two simulations with two different mesh sizes, 1 mm and 2 mm. This simulation time is up to the time the flame passes the obstruction. Figure 4 shows the simulated flame front at different times from ignition time.

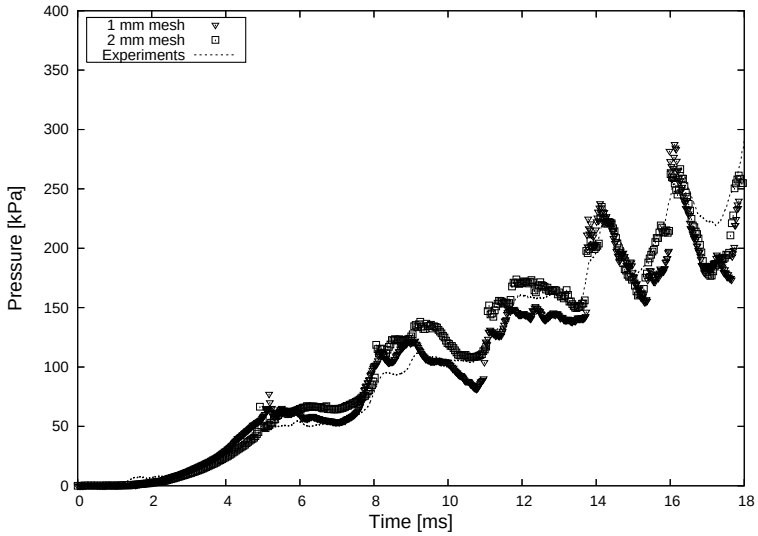

Figure 3: Pressure history for simulations with 1 mm mesh and 2 mm mesh, and for experiments.

5 Discussion

Both simulated pressures and shock wave arrival times from both the 1 mm mesh and 2 mm mesh are similar to the experimental values as can be seen in figure 3. The assumption of axisymmetric geometry should not be too rough, the Reynolds stresses in the axial-tangential plane and the radial-tangential plane is possibly small in this case. The most rapid strain rates are in the axial-radial plane due to the hemispherical development of the flame from central ignition and the cylindrical geometry. The flame is highly distorted by shock waves, as seen in figure 4. These large scale distortions are probably the most important effects that contribute to flame acceleration before the flame reaches the obstacle. By comparing simulated and experimental pressure histories it is possible to see that the simulated flame speed is reasonable. Propagating shock waves are reflected from the flame front and these waves are captured by the transducer. The combustion model keeps the flame thin and propagation is controlled by the flame surface density model for the most part. The Arrhenius rate expression is only active in areas of high temperature and low values of β and only help to keep the flame thin in this part of the explosion.

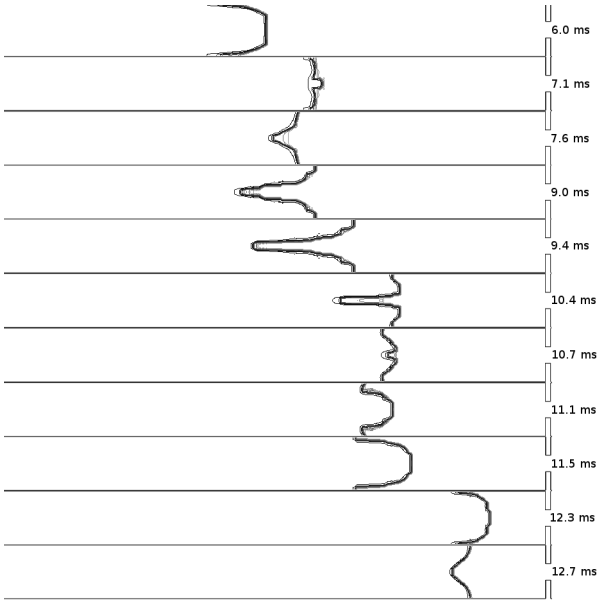

Figure 4: Flame front development at time intervals from ignition.

6 Conclusion

The combustion model behaves reasonable and simulations with this model shows promising results for cases with large flame deformation due to propagating shock waves. Simulated pressures and shock wave time of arrival are similar to experimental results. Simulations with two different mesh sizes showed small differences in pressures. This model should be able to simulate DDT and detonations as it is, but more experiments must be done to verify this.

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