

Simulation of FA and DDT in a channel with repeated obstacles with an under-resolved mesh

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1 Introduction

Lee et.al. [1] and Lee and Moen [2] have described different regimes of high speed flame propagation in obstructed channels. Flame acceleration may lead to three different regimes, choked regime, quasi-detonation and CJ-detonation. In quasi detonation DDT occurs but the detonation fails due to the following interactions with obstructions. Experiments with flame acceleration and DDT in obstructed channels has been presented by several authors [1, 2, 3, 4, 5]. Gamezo et.al. [6] has presented simulation results for channels with repeated obstacles with one step Arrhenius reaction rate. The flame acceleration in obstructed channels are caused by instabilities such as Rayleigh-Taylor, Richtmyer-Meshkov and Kelvin-Helmholtz, flame-shock interaction and flame-vortex interaction. Shock focusing and Mach-reflections cause transition to detonation. A comprehensive review of flame acceleration and DDT in channels is written by Ciccarelli and Dorofeev [7].

The study of simulations of flame acceleration and DDT with an under-resolved mesh is motivated by having the ability to predict DDT and fast flames in large geometries or to get simulation results within a short time. Models for sub-grid behavior of the flame-flow field interaction is important for describing the flame acceleration since the flame front is thinner than the computational mesh size. This paper describes some of the validation of a simulation codes ability to predict DDT with an under-resolved mesh.

2 Models

The numerical scheme is a flux limiter centered method (FLIC) as described by Toro [8]. This method solves the non-diffusive conservation equations of mass, momentum and energy for compressible flow. To include viscous and turbulent stresses and heat conduction the molecular transfer terms in the conservation equations are included by Godunov-splitting. The turbulence model is a one-equation model for the sub-grid turbulent kinetic energy [9]. A different combustion model used with the same numerical scheme is discussed in more detail by Vaagsaether et. al. in [10]. The combustion model is a combination of a turbulent model and a two step kinetic model and is identical to the method presented in [11].

3 Simulation set-up

Fig. 1 shows the simulation setup. This obstacle configuration is repeated along the channel length. This is the same geometry as used in the test series by Teodorczyk [5]. In this paper three different channel heights are used, 20 mm, 40 mm and 80 mm, experimental results from these geometries are presented by Teodorczyk. The blockage ratio for all experiments are 0.5. The channel is 2 m long and closed in all directions. In the experiments the channel is 110 mm wide but simulation results are performed in two dimensions thus assuming an infinitely wide channel. The ignition is in the middle of one end wall. The gas is stoichiometric hydrogen-air mixture at atmospheric pressure and 293 K. Two different mesh sizes are tested, for most of the results presented here a mesh of 1 mm is used, but results from mesh sizes of 0.5 mm is presented.

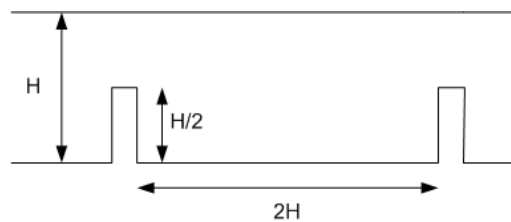


Figure 1: Experimental setup with channel height and distance between obstacles.

4 Results and Discussion

The results are presented as contour plots of gradients of density and flame speeds along the channel length. The flame speeds presented are just below the top wall. The present simulations are 2D simulations. Gamezo et.al. [6] argued that there are minor differences in 2D and 3D simulations of a case similar to the case presented here. For all channel heights the flame accelerates and a shock wave is formed ahead of the flame. When this shock passes an obstacle a diffracted shock front reflects of the bottom wall and creates a Mach-stem. Both the leading shock and Mach-stem reflects on the obstacles and is focused in the corner between the bottom wall and obstacle. This effect can ignite the gas behind the focused shock and sends a strong shock wave into the products that diffracts over the obstacles and reflects of the top wall. This shock interacts with the flame from the product side and accelerates the flame and may even heat the reactants in front of the flame and cause DDT. This effect is seen and discussed by several authors [1, 2, 3]. Figure 2 (left) shows the simulated DDT process in the 40 mm channel. The simulated flame speed shown in figure 2 (right) indicates that the flame experiences DDT at one point and failure at the next obstacle. This process repeats itself and can be interpreted as a quasi detonation as discussed by Lee and Moen [2] and Lee et. al. [1]. In the experiments by Teodorczyk [5] the flame experience DDT between 0.9 m and 1.0 m from the ignition end for 40 mm channel. The simulation shows DDT at 1.2 m for the 1 mm mesh and at 1.0 m for the 0.5 mm mesh size. Figure 3 shows the simulated flame speed of the 20 mm channel (left) and 80 mm channel (right) along the channel length. Experiments show a possible DDT in the 20 mm channel at 0.7 m, but the experiments scatter. The simulated flame speed reach a quasi steady propagation at about 0.6 m and might be interpreted as choking regime. The simulated flame speed for the 80 mm channel show an increase in flame speed at about 1.4 m but the DDT is achieved at 1.6 m. The experiments indicate DDT for this case at about 1.6 m.

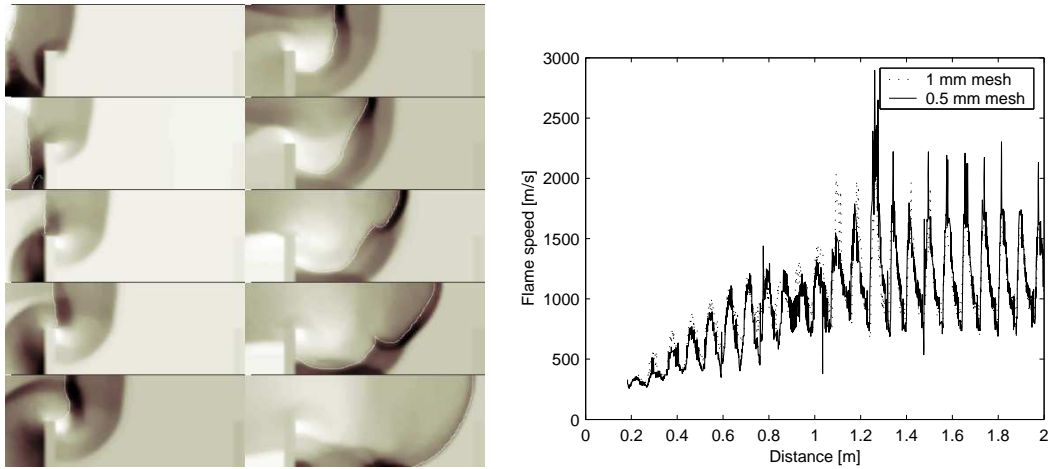


Figure 2: Left: Simulated density gradient contours of the DDT process with 1 mm mesh for the 40 mm channel. Right: Flame speed along the channel length for both 1 mm and 0.5 mm mesh size for the 40 mm channel.

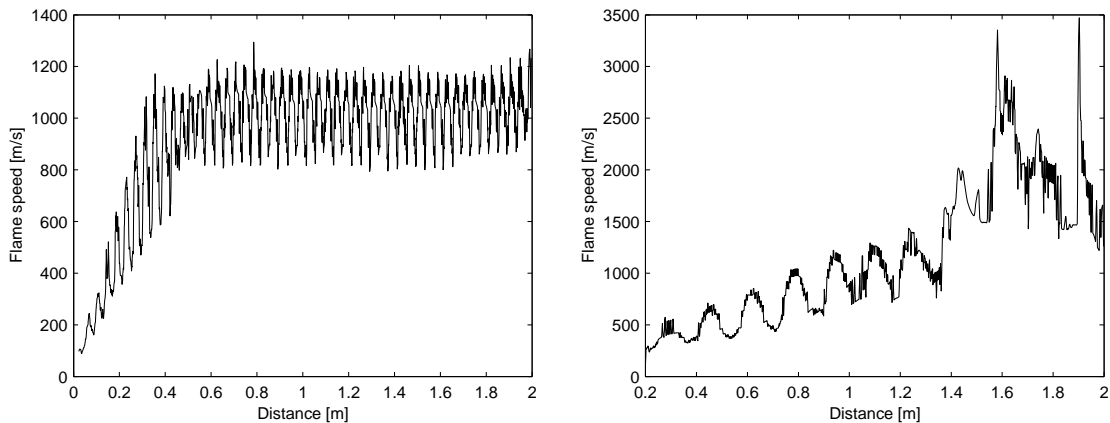


Figure 3: Left: Simulated flame speed along the channel with 1 mm mesh for the 20 mm channel. Right: Simulated flame speed along the channel with 1 mm mesh for the 80 mm channel.

5 Conclusion

The simulation of experiments by Teodorczyk [5] show that the choking regimes, quasi detonation regime and detonation all are controlled by the interaction of a shock wave interacting with the flame from the product side. This effect can be handled on an under-resolved mesh as shown here. For the 20 mm channel the shock interacts with the flame and increase the flame speed and compresses the reactants but is not strong enough to sufficiently heat the reactants. This can be interpreted as the choking regime with average flame speed of 900-1000 m/s. For the 40 mm channel the shock is strong enough, but the detonation fail when it passes an obstacle, this process of DDT and failure to propagate is repeated until the end of the channel. This may be seen as the quasi detonation regime with average flame speed of 1400 m/s. For the 80 mm channel the flame experiences DDT and propagate as a detonation. The simulation of these cases on an under-resolved mesh show that it was possible to reproduce the different phenomena as is seen in the experiments [1, 2, 3, 4, 5]. This might suggest that the process of DDT in a channel with repeated obstacles are controlled by large scale effects, like the ignition of reactants in the

corners between the obstacles and bottom channel wall. The grid test did not show too large deviance between two different mesh sizes for the 40 mm case but the position of the DDT is predicted differently.

References

- [1] Lee JHS, Knystautas R, Chan CK. (1985). Turbulent flame propagation in obstacle-filled tubes. *Proc. Combust. Inst.* 20: 1663.
- [2] Lee JHS, Moen IO. (1980). The mechanisms of transition from deflagration to detonation in vapor cloud explosions. *Prog. Energy Combustion Sci.* 6 359–389.
- [3] Teodorczyk A, Lee JHS, Knystautas R. (1988) Propagation Mechanism of Quasi-Detonations. 22nd Symp. (Intl.) on Combustion. The Combustion Institute. 1723.
- [4] Dorofeev SB, Sidorov VP, Kuznetsov MS, Matsukov ID, Alekseev VI. (2000) Effect of scale on the onset of detonations. *Shock Waves* 10: 137.
- [5] Teodorczyk A. (2008) Scale effects on hydrogen-air fast deflagrations and detonations in small obstructed channels. *Journal of Loss Prevention in the Process Industries* 21: 147.
- [6] Gamezo VN, Ogawa T, Oran ES. (2007) Numerical simulations of flame propagation and DDT in obstructed channels filled with hydrogen-air mixtures. *Proceedings of the Combustion Institute* 31: 2463.
- [7] Ciccarelli G, Dorofeev S. (2008) Flame acceleration and transition to detonation in ducts. *Prog. Energy and Comb. Sci.* 34: 499.
- [8] Toro EF. (1999) *Riemann solvers and Numerical methods for fluid dynamics*. Springer-Verlag Berlin Heidelberg, (ISBN 3-540-65966-8).
- [9] Menon S, Vaidyanathan S, Stone C. (2003) Subgrid combustion modeling for the next generation national combustion code. NASA/CR-2003-212202.
- [10] Vaagsaether K, Knudsen V, Bjerketvedt D. (2007) Simulation of flame acceleration and DDT in H₂-air mixture with a flux limiter centered method. *International Journal of Hydrogen Energy* 32: 2186.
- [11] Vaagsaether K, Bjerketvedt D. (2007) Simulation of flame acceleration in an obstructed tube with LES. ICDERS 21. Poitiers France.