Deflagration-to-Detonation Transition in Obstructed Spaces

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1 Introduction

Deflagration-to-detonation transition (DDT) in reactive gaseous mixtures usually occurs in confined or partially confined spaces that can be filled with obstructions. Mechanisms of flame acceleration and DDT in these conditions are often studied experimentally in channels with obstacles [1]. Recent numerical simulations [2, 3, 4] reproduced main results of these experiments and identified key mechanisms responsible for the detonation initiation in simple obstructed channel configurations. The same mechanisms are likely to remain relevant for more complex geometries, though additional phenomena may also play important roles in DDT. In this work, we consider two-dimensional (2D) unconfined arrays of obstacles as shown in Fig. 1, and model the flame propagation through these obstructed 2D spaces. For these configurations, the gas flow and wave propagation are only restricted by obstacles, but not by any external confinement.

2 Numerical and Physical Model

The numerical model is based on reactive Navier-Stokes equations coupled with the ideal-gas equation of state and a one-step Arrhenuis kinetics of energy release

$$dY/dt = -A\,\rho\,Y\,\exp(-E_a/RT), \tag{1}$$

where Y is the unburned mass fraction, A is the pre-exponential factor, and E_a is the activation energy. The equations are solved using the explicit, second-order, Godunov-type numerical scheme incorporating a Riemann solver, and the FTT-based structured adaptive mesh [5]. The mesh refinement is dynamically controlled by gradients of density, pressure, velocity, and composition. This model has been extensively tested and used to solve combustion and detonation problems including shock-flame interactions and DDT [6, 7, 8, 9] and cellular detonations [10, 11, 12].

Parameters of the reactive system described in detail in [3] approximate a stoichiometric hydrogen-air mixture at 1 atm and 293 K. The one-step Arrhenius kinetics used in this model cannot exactly reproduce all properties of the stoichiometric hydrogen-air mixture for different combustion regimes, including laminar flames, detonations, and DDT. The model does, however, give a reasonable approximation of the length and time scales for the problem considered. This allows us to use this model for a qualitative analysis of the behavior of the stoichiometric hydrogen-air mixture.

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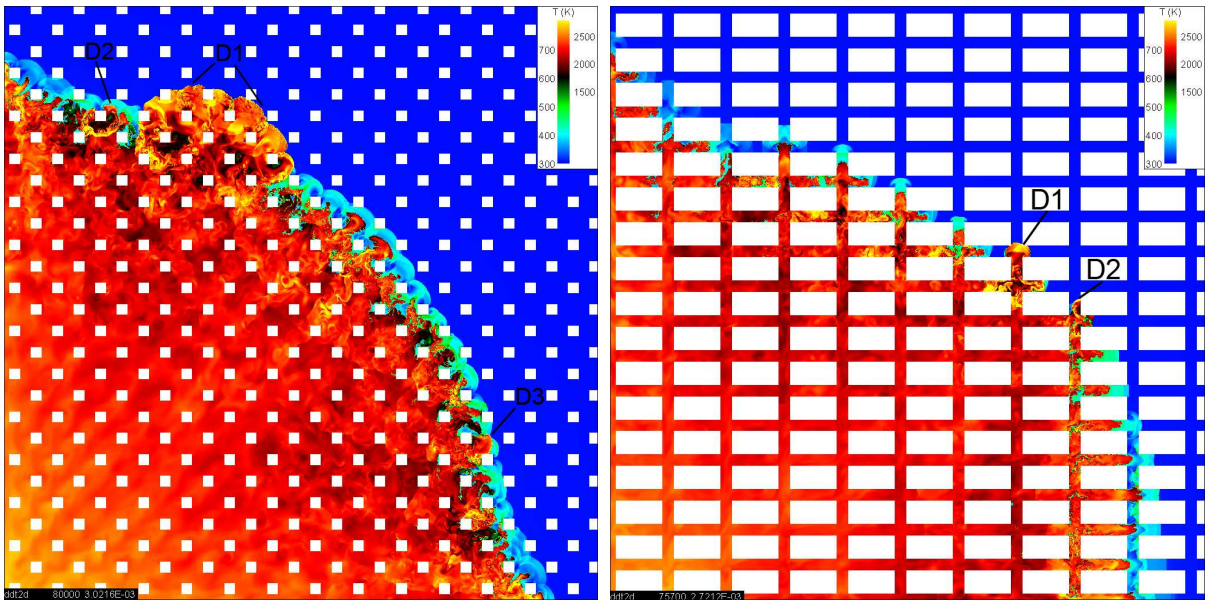
Computations were performed for the minimum computational cell size $dx_{min} = 1/128$ cm, which corresponds to 4.5 computational cells per laminar flame thickness. Resolution tests performed for obstructed channels [2, 3] have shown that this resolution is adequate for the numerical analysis of flame acceleration and DDT.

3 Results of Simulations

Figure 1 shows the results from simulations of flame propagation through two different 2D arrays of obstacles. For such multidimensional arrays, the area blockage ratio (BR) is often replaced by the volume blockage ratio (VBR) defined as the fraction of volume occupied by obstacles. The two configurations shown in Fig. 1, corresponding to (a) VBR=0.125 and (b) VBR=0.533, differ by obstacle sizes, shapes, and location patterns. For both configurations, the flame was ignited at the left bottom corner of the computational domain in a soft mode. It spread in all directions, first without shocks, mostly with the flow created by expanding combustion products. At initial stages, the flame surface area, and therefore the energy generation rate, increased due to the interaction of the flame with large-scale vortices created by flow-obstacle interactions. Then the flame became turbulent, accelerated to supersonic velocities, and generated strong shocks. Shock-flame interactions, shear layers, and RT instabilities contributed to the increase in energy-release rate in the same way as we observed in channels with obstacles [2, 3, 4].



(a) **(b)**

Figure 1: Premixed hydrogen-air flame propagating through 2D array of obstacles for two different obstacle configurations. Obstacle size 1×1 cm (a) and 4×2 cm (b). Times shown correspond to 3.0 ms (a) and 2.7 ms (b) after soft ignition in the left bottom corner. Distance between neighboring rows of obstacles 1 cm. dx_{min}=1/128 cm. D1, D2, D3 indicate detonations.

The configuration (b), which can be considered as a network of channels, shows the importance of interactions between shocks and flames approaching channel intersections from different directions. These shocks are equally strong (comparable to the leading shock in a single channel with obstacles), but they often approach the channel intersection at different times. As a result, a strong shock, which approaches an intersection a little later, often interacts with a turbulent flame that propagates in a hot material compressed by another shock, which already crossed this intersection. This results in

a rapid shock acceleration and a formation of hot spots when strong shocks propagating in a shock-compressed material interact with obstacles. Some of these hot spots generate detonations that appeared independently in three different locations.

The configuration (a) shows similar phenomena involving interactions of strong shocks with flames and obstacles in a shock-compressed material, and a detonation initiation behind the leading shock. In total, four detonations independently appeared in the system, resulting from multiple shock-obstacle, shock-shock, and shock flame interactions. None of these involved Mach stems or was ignited by a direct collision of the leading shock with an obstacle, as we often observed in single channels [2, 3, 4].

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