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Flame acceleration and transition to detonation in an array of square obstacles

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ABSTRACT

We study flame acceleration and DDT in a two-dimensional staggered array of square obstacles by solving the compressible multidimensional reactive Navier–Stokes equations. The energy release rate for a stoichiometric H_2-air mixture is modeled by a one-step Arrhenius kinetics. The space between obstacles is filled with a stoichiometric H_2-air mixture at 1 atm and 298 K. Initially, the flow is at rest, and a flame is ignited at the center of the array. Computations show effects of the obstacles as a series of events leading to DDT. During the initial flame acceleration, the speed of the flame depends on the direction of flame propagation since some directions are more obstructed than others. This affects the macroscopic shape of the expanding burned region, which forms concave boundaries in more obstructed directions. As the flame accelerates, shocks form ahead of the flame, reflect from obstacles, and interact with the flame. There are more shock–flame interactions in more obstructed directions, and this leads to a greater flame acceleration and stronger leading shocks. When the shocks become strong enough, their collisions with obstacles ignite the gas mixture, and detonations form. The simulation shows four independent DDT events within a 90-degree sector, all in more obstructed directions. Resulting detonations spread in all directions. Some parts of detonation fronts are quenched by diffractions around obstacles, but they are reignited by collisions of decoupled shocks, or overtaken by other detonations. Thus detonations continue to spread and quickly burn all the material between the obstacles.

1. Introduction

Deflagration-to-detonation transition (DDT) in reactive gases usually occurs in confined or partially confined spaces. One possible configuration is an obstructed channel filled with a reactive gas. Flame acceleration and its transition to detonation in channels with obstacles have been extensively studied using experiments (Lee, Knystautas, & Chan, 1985; Teodorczyk, Lee, & Knystautas, 1988; Teodorczy, 1995) and numerical simulations (Gamezo, Ogawa & Oran, 2007; Oran & Gamezo, 2007; Gamezo et al., 2007). It has been shown that the shape and layout of obstacles have a significant effect on flame acceleration, DDT, and subsequent detonation propagation. Obstacles promote flame acceleration by creating non-uniform flows, and generating fluid dynamic instabilities. These effects stretch and wrinkle the flame surface, thus increasing the energy-release rate. The flame and flow acceleration lead to the formation of shocks that propagate ahead of the flame, reflect from channel walls and obstacles, and also propagate back to the flame. The resulting shock–flame interactions further increase the flame surface and the energy-release rate, and this process strengthens the leading shocks.

When the shocks become strong enough, the collision of the shocks with obstacles ignites detonations. This often involves Mach stems that form when shocks reflect from channels walls. The higher temperature regions behind Mach stems contribute to the formation of hot spots, where detonations can emerge spontaneously. Obstacles also affect the propagation of detonations. When a detonation passes over an obstacle, the portion of the front near the obstacle diffracts and decouples into a shock and a flame. The detonation may be reignited by decoupled shocks colliding with channel walls and obstacles.

Here, we numerically simulate flame acceleration and transition to detonation in a two-dimensional array of square obstacles. In contrast to an obstructed channel, in which both obstacles and walls restrict the flow and wave propagation, the only restrictions in the unconfined array are created by obstacles. Flame or detonation propagation through an array of obstacles, such as cylinders and beads, has been experimentally studied in (Babkin, Korzhavin, & Bunev, 1991; Chao & Lee, 2003; Hlouschko & Ciccarelli, 2007). In their studies, however, a channel is used, and the flame and the

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Table 1
Input parameters of the chemical and transport model for the stoichiometric H_2-air mixture at 1 atm.

Adiabatic index	γ	1.17
Molecular weight	W	21 g/mol
Preexponential constant	A_f	6.85×10^{12} cm^3/g·s
Activation energy	E_a	46.37 RT_0 ($T_0 = 293$ K)
Chemical energy release	q	43.28 RT_0/W
Coefficient for thermal conductivity	κ_0	2.9×10^{-5} g/s·cm·K$^{0.7}$
Lewis number	Le	1
Prandtl number	Pr	1

detonation are confined by the channel wall. In this study, a flame spreads cylindrically through an array of obstacles in an unconfined space. We study the effect of an array of obstacles on the mechanisms of flame acceleration, DDT, and detonation propagation.

2. Numerical method

The governing equations are the two-dimensional, compressible, Navier–Stokes equations including convection, chemical reactions and energy release, molecular diffusion, thermal conduction, and viscosity. The equation of state is that of the ideal gas.

The length scale of flames and detonations in hydrogen-air mixtures is $O(10^{-4}$ m), while the flow fields of our interest are O(m). Thus, we need a numerical method and the physical model that can simulate a system over this range of length scales within a reasonable amount of CPU time. We do this by using an adaptive mesh refinement method (Khokhlov, 1998) in which the mesh is dynamically refined at flames, shocks, and detonation fronts. The convective terms are discretized with a second-order Godunov method.

The reaction model is based on one-step Arrhenius kinetics,

$$\frac{dY}{dt} = -\rho Y A_f \exp\left(-\frac{E_a}{RT}\right),$$

where Y is the mass fraction of the unburned material, A_f is the preexponential constant, and E_a is the activation energy. The transport properties are also simplified. The thermal conductivity κ (cm^2/s) is approximated as,

$$\frac{\kappa}{C_p} = \kappa_0 T^n,$$

where κ_0 and $n = 0.7$ are model constants, and $C_p = \gamma R/W(\gamma - 1)$ is the specific heat. The Lewis number and the Prandtl number are assumed to be constant. This model has been extensively tested and used for DDT problems (Gamezo, Khokhlov, & Oran, 2001; Khokhlov & Oran, 1999; Khokhlov, Oran, & Thomas, 1999).

The input parameters are calibrated to reproduce the laminar flame speed, the flame thickness, the detonation velocity, and the detonation cell size for the stoichiometric H_2-air mixture at 1 atm and 293 K. Input parameters are summarized in Table 1, and the computed properties are compared with the experimental and theoretical values in Table 2.

Table 2
The computed properties of the stoichiometric H_2-air mixture using the present model.

	Present model	Experiment
Laminar flame velocity [m/s]	2.98	2.15
Laminar flame thickness [m]	3.3×10^{-4}	3.5×10^{-4}
CJ Detonation velocity [m/s]	1.993×10^3	2.028×10^3
Detonation cell width [cm]	1–2	1–2

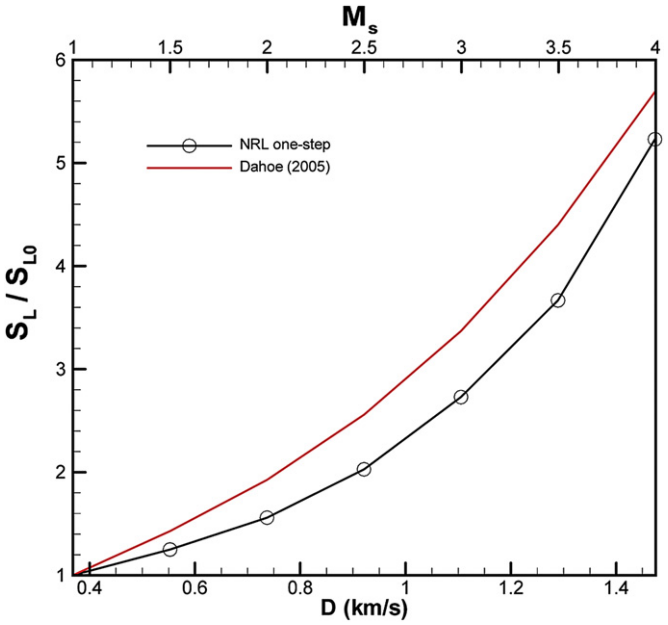

Fig. 1. The normalized laminar flame speed S_L/S_{L_0} at the conditions behind a shock, where S_{L_0} is the laminar speed of the referenced state, 293 K and 1 atm. The shock speed is D, and its Mach number is m_s. The result of the NRL one-step model is compared with the formula based on the experimental data by Dahoe (Dahoe, 2005).

To simulate flame acceleration and DDT in this study, we first place a flame in a quiescent unburned material at the standard condition, 293 K and 1 atm. As the flame accelerates, a shock is formed ahead and is strengthened until it ignites a detonation. Thus, combustion takes place in an unburned mixture compressed by the leading shock of a wide range of strength. Here, we study the properties of the one-step reaction model for post-shock conditions. First, we calculate laminar flame speeds by

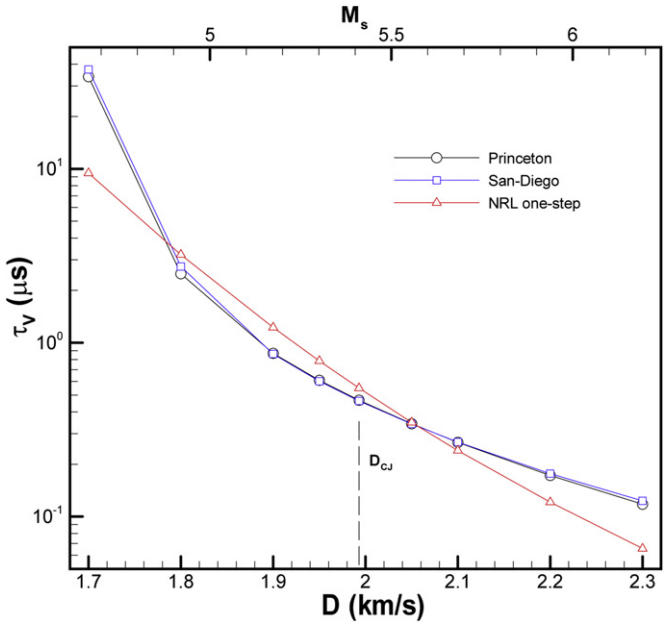

Fig. 2. The ignition delay time τ_v at the conditions behind a shock with speed D and Mach number m_s. The CJ detonation speed is denoted as D_{CJ}. The plot compares the result of the detailed reaction models, the Princeton (Burke) (Burke et al., in press) and the San Diego 12-step H2-O2-N2 mechanisms (Boivin et al., 2011) along with the result of the NRL one-step model.