Shock transition to detonation in channels with obstacles

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Abstract

Multidimensional numerical simulations of an unconfined, homogeneous, chemically reactive gas were used to study interactions leading to deflagration-to-detonation transition (DDT). The configuration studied was a long rectangular channel with regularly spaced obstacles containing a stoichiometric mixture of ethylene and oxygen, initially at atmospheric conditions and ignited in a corner with a small flame. The compressible reactive Navier-Stokes equations were solved by a high-order numerical algorithm on a locally adapting mesh. The initial laminar flame develops into a turbulent flame with the creation of shocks, shock-flame interactions, shock-boundary layer interactions, and a host of fluid and chemical-fluid instabilities. The final result may be eventual deflagration-to-detonation transition (DDT). Here two types of simulations are described, one with DDT occurring in a gradient of reactivity, which is common in the channels with higher obstacles, and another in which DDT arises from energy focusing as shocks converge. For the latter case, the rate of energy deposition necessary to initiate a detonation in the unburned gas is analyzed using a control volume analysis.

Keywords: DDT; Turbulent flame; Shock interactions; Direct initiation; Numerical simulations

1 Introduction

Deflagration-to-detonation transition (DDT) is a complex process involving turbulence, shock-flame interactions, shock collisions and reflections, and interactions of shocks with boundary layers. It is an important topic because DDT must be prevented in many cases [1, 2] and optimized for specific applications [3–5]. DDT may be initiated by a number of different mechanisms that have been seen in both experiments and computations [6–15]. Not all of these mechanisms, or the interplay among them, are fully understood.

Direct initiation of a detonation in a gas has been studied theoretically and experimentally [6–8]. Sufficiently large external energy addition at a timescale that is small relative to the acoustic timescale of the gas can result in a direct initiation of a detonation without first creating a deflagration [16]. Recently, the response of the gas to a localized, transient energy deposition has been studied by asymptotic analysis in an effort to quantify the gas response (deflagration or detonation) [17]. Initiation of a detonation through a gradient of chemical reactivity [18, 19] has been investigated extensively using numerical simulations, as summarized in [10]. DDT in channels with obstacles has been computed for a variety of fuel-oxidizer mixtures [11–13] and has been the subject of experimentation [20].

The effect of obstacles, often characterized by a blockage ratio (br , or the obstacle height divided by the channel height), on flame acceleration and DDT has been investigated experimentally [14, 15]

and numerically [21]. Gamezo et al. [21] noted the competing effects of high blockage ratios: larger obstacles promote non-uniform flow, which leads to fast flame acceleration and they also weaken shocks diffracting over large obstacles. These authors also observed that the location in the channel where DDT occurs does not vary significantly for $br = 0.31 - 0.56$ range, but it increases sharply outside of this interval for both higher and lower br .

As a background to this paper, a series of simulations was performed with $br = 0.05 - 0.8$ in order to identify how the mechanism of DDT changes as blockage ratio decreases. The detailed results of these simulations, and some unusual trends noted, will be presented in a subsequent paper. In several of these simulations, however, shocks and fluid instabilities evolved that caused flame acceleration and transition to detonation due to energy focusing as opposed to the more predictable detonations that occur in Mach reflections against obstacles in systems with high br . Maeda et al. [22] saw similar phenomena in their experiments in channels with $br = 0.083$ and 0.25 . The purpose of this paper is to extract results for low br and compare the mechanism of DDT with those seen for the relatively high $br = 0.5$.

2 Numerical and Physical Model

The numerical model solves the full set of Navier-Stokes equations in unsteady, fully compressible, chemically reacting gas, as described in [10]. The reaction of a stoichiometric mixture of ethylene and oxygen, with specific ethylene-oxygen parameters courtesy of Alp Ozgen, is modeled using a simplified, calibrated chemical-diffusive model of the form,

$$\frac{dY}{dt} \equiv \dot{w} = -A\rho Y \exp(-E_a/RT) \quad (1)$$

where ρ , T , Y , and $\dot{w}$ are the mass density, temperature, mass fraction of reactant, and reaction rate, respectively. A is the pre-exponential factor, and E_a is the activation energy. Thermal conductivity, κ , viscosity, ν , and mass diffusivity, D , were modeled using values of 1.0×10^{-5} g/s-cm-K^{0.7}, 7.0×10^{-6} g/s-cm-K^{0.7}, and 1.0×10^{-5} g/s-cm-K^{0.7}, respectively. A Godunov algorithm, fifth-order accurate in space and third-order accurate in time [23], is used to solve the equations on a dynamically adapting grid [24]. The simulations described below used grids with minimum size $dx_{\min} = 3.3 \mu\text{m}$ and coarsest size ranging from $dx_{\max} = 26.7$ to $53.3 \mu\text{m}$. The largest grid had 60 cells across the channel height and the smallest had 960 cells. This choice of grids was tested and shown to resolve the flames, shocks, boundary layers, and other important flow and chemical structures.

The input parameters in Table 1 were chosen to reproduce the flame and detonation properties of the

Table 1. Input model parameters and output combustion wave properties for stoichiometric ethylene and oxygen initially at 1 atm and 298 K.

Input		
P_o	1 atm	Initial Pressure
T_o	298 K	Initial Temperature
ρ_o	1.27×10^{-3} g/cm ³	Initial Density
γ	1.2195	Adiabatic Index
M	31 g/mol	Molecular Weight
A	1.05×10^{12} cm ³ /(g s)	Pre-Exponential Factor
E_a	$39.2RT_o$	Activation Energy
q	$59.7RT_o/M$	Chemical Energy Release
ν_o	7.0×10^{-6} g/s-cm-K ^{0.7}	Viscosity
$\kappa_o = D_o$	1.0×10^{-5} g/s-cm-K ^{0.7}	Transport Constants
Output		
S_L	413 cm/s	Laminar Flame Speed
T_b	$11.7T_o$	Post-Flame Temperature
ρ_b	$0.085\rho_o$	Post-Flame Density
x_l	8.88×10^{-3} cm	Laminar Flame Thickness
D_{CJ}	2.20×10^5 cm/s	CJ Detonation Velocity
P_{ZND}	$54.5P_o$	Post-Shock Pressure
P_{CJ}	$27.8P_o$	Pressure at CJ Point
T_{ZND}	$6T_o$	Post-Shock Temperature
T_{CJ}	$15.5T_o$	Temperature at CJ Point
ρ_{ZND}	$9.8\rho_o$	Post-Shock Density
ρ_{CJ}	$2\rho_o$	Density at CJ Point
x_d	3.2×10^{-4} cm	Half-Reaction Thickness
λ	~ 0.02 cm	Detonation Cell Size

ethylene-oxygen mixture initially at 298 K and 1 atm. Using the input parameters in one-dimensional (1D) and two-dimensional (2D) solutions of the Navier-Stokes equations produces the output flame and detonation properties listed. To estimate the detonation cell height, λ , for this model, a 2D detonation was computed and an average was taken of cell sizes after an initially overdriven detonation had decayed to the Chapman-Jouguet velocity. The value $\lambda = 0.2$ mm agrees surprisingly well with reported experimental results, which range from 0.1 mm to 2 mm [25].

The geometrical setup is shown in Fig. 1. Obstacles are uniformly spaced along the wall. The obstacle width and height are constant through the channel. The br for the simulations discussed here are 0.5 and 0.1. The channel is open at the right, with symmetry planes at the left and top boundaries. The bottom wall and all obstacle surfaces are no-slip adiabatic boundaries. To ignite the mixture, a circular region of hot, burned product at 3500 K and 1 atm is placed at the left wall. A channel height of 0.32 cm was chosen for several reasons. Experimental data for DDT in small channels with stoichiometric ethylene-oxygen, such as the work by Wu et al. [25], is available for comparison. The small scale detonation properties of this fuel-oxidizer mixture, such as small detonation cell sizes, fast reactions, and energy release, make ethylene-oxygen an ideal fuel-oxidizer mixture for studying DDT

in small channels.

Fig. 1. Computational setup in units of cm. Obstacles evenly spaced along channel length L . Radius of the initial burned region is 0.08 cm. Blockage ratio is 0.1 in this case.

3 Flame Acceleration and DDT

Fig. 2. Accelerating flame and detonation in 2D quarter-channel with $br = 0.5$. Time in milliseconds is shown in the frame corners. Obstacles are numbered.

Previous work [11, 12] has shown that flame acceleration is rapid in channels with $br = 0.5$ for stoichiometric mixtures of hydrogen and air. Figure 2 shows flame acceleration and transition to detonation for the stoichiometric ethylene and oxygen mixture for $br = 0.5$. As the flame passes over obstacles, its surface area increases due to expansion and fluid instabilities (Rayleigh-Taylor, Richtmyer-Meshkov, and Kelvin-Helmholtz), shocks and all of their interactions. Strong leading shocks propagate into the unburned gas. The leading shock diffracts over obstacles and reflects from the channel floor, eventually forming a Mach stem (0.1126 ms). At 0.1355 ms, detonation occurs in hot, unburned gas as a Mach stem reflects from an obstacle and leaves a hot spot in a gradient of reactivity. In Fig. 2, the unburned material detonates behind a Mach stem reflection from obstacle 7 at 0.1355 ms.

When br is much smaller, 0.1 shown in Fig. 3, the flame accelerates more slowly and stays laminar

Fig. 3. Full simulation for blockage ratio of 0.10. Time in milliseconds is shown in the frame corners. Obstacles are numbered.

longer as it propagates into the channel. For $br = 0.5$, detonation occurs at 0.136 ms at 3.5 cm from the left edge, having passed six obstacles. When the $br = 0.1$, detonation occurs against the lower wall at 0.271 ms at 7.25 cm, having passed 11 obstacles. Despite the major differences in time and distance to DDT, the flame development is similar in both cases. Unburned gas is driven downstream over obstacles causing vortex shedding from the obstacle's leading edges (seen starting at 0.1804 ms in Fig. 3). Vortices coalesce behind obstacles to form regions of recirculation. The flame surface area increases as it is pulled into the recirculation region and becomes turbulent as the acoustic waves shed by the vortices propagate through the flame. Shocks form as the flame accelerates, increasing in strength as they reflect off the obstacles, and these shocks collide with one another. Rather than seeing the rapid development of a strong leading shock that is closely coupled with the flame, as seen in Fig. 2, a relatively large unburned, turbulent region filled with shocks and strong vortices now forms between the flame and the leading shock. Figure 4 shows the complexity and dynamic structure in this shock-flame complex.

Figure 5 is an enlargement of the detonation that occurs in Fig. 3 for $br = 0.1$. Two shocks, labeled

Fig. 4. Numerical schlieren showing the turbulent region.

Fig. 5. Multiple shock collision and detonation. Time is shown in ms.

S1 and S2 at 0.2689 ms, collide at 0.2696 ms. Shock S1 is immediately ahead of the flame, traveling to the right, and shock S2 is reflected from the downstream obstacle (shown in white in the lower right corner of Fig. 5) and is traveling to the left. The shock collision ignites two hot spots in the boundary layer, labeled H1 and H2. By 0.2707 ms, H1 evolves into a flame and shock, and H2 evolves into a detonation. The analysis below shows that the confluence of shocks causes transition to detonation in hot unburned gas. This detonation mechanism has elements of both gradient ignition and direct initiation of detonation.

To quantify the change in state of unburned material compressed during the multiple-shock collision, a control volume analysis was performed on a small $33.3 \mu\text{m} \times 33.3 \mu\text{m}$ region at the location where H2 forms and becomes a detonation. The analysis tracked the change in pressure, temperature, density, and energy release rate over a $0.2 \mu\text{s}$ period from $270.5 \mu\text{s}$ to $270.7 \mu\text{s}$. This corresponds to a time before the region is compressed by the shock collision to a time after the detonation formed and propagated through the region. Figure 6 shows the trends of the state variables. Shock compression begins at $270.55 \mu\text{s}$, and the material begins to react chemically at $270.65 \mu\text{s}$. The pressure and density increase dramatically, first from shock compression and then after the detonation. As the detonation propagates out of the region, the pressure and density decrease. The average temperature in the control volume

prior to combustion is ~ 850 K.

Fig. 6. State variables in the control volume from 270.5 μ s to 270.7 μ s (a) Shock compression (b) Detonation. The gas begins to react chemically at 270.65 μ s.

Fig. 7. Rate of energy deposition in control volume during (a) Shock compression (b) Detonation.

Figure 7 shows the rate of energy deposition into the control volume. Chemical energy is defined as heat release per kg of reactant, q , internal energy is $P/(\gamma - 1)$, and kinetic energy is $0.5\rho u^2$, where u is the magnitude of velocity. As the material in the region is compressed, rates of internal and kinetic energy increase, followed by a second peak as the material detonates. The detonation carries energy out of the region as it propagates into the surrounding gas, resulting in the negative energy rates seen after 270.66 μ s. The total energy content in the region, defined as the sum of chemical, internal, and kinetic energies, increases by a factor of 15 during shock compression.

Prior work [11] has shown that for hydrogen and air mixtures in channels of different sizes, there were different regimes of DDT. The authors found that in some of these regimes, the detonation mechanism was more sensitive to the turbulence in the flow. The variations in br described in this paper reflect the same phenomenon, that there are different regimes of DDT with varying sensitivity of the detonation mechanism to turbulence. In the $br = 0.1$ regime, the sensitivity of the solution to the turbulence causes the detonation to occur at slightly different times and locations for cases with modified initial conditions.

Figure 8 shows the detonation in another simulation with $br = 0.1$ with slightly different initial conditions. A smaller coarse mesh size of 26.7 μ m was used, as compared to 53.3 μ m in the previously

Fig. 8. Shock reflections and collisions result in initiation of two detonations. Time is shown in ms.

described $br = 0.1$ case shown in Fig. 3. The location of the detonation is ~ 1.2 cm further along the channel boundary than the detonation that occurred in Fig. 5, however, it again appears where shock collisions and reflections are focused. The shock immediately ahead of the flame, labeled S3, reflects off the channel boundary and ignites a hot spot H3 in the boundary layer. The hot spot becomes a detonation while another shock ahead of the flame, labeled S4, reflects off the obstacle shown in the lower right corner of the figure. The reflection of S4 ignites another hot spot, labeled H4, that also becomes a detonation. The two detonations combine and propagate down the channel. Although the time and location of detonation is stochastic due to turbulence in the flow, which is heavily dependent on initial conditions such as grid size, the detonation mechanism in the low br regime is robust. This is consistent with previous work investigating the stochasticity of DDT in flow regimes that are sensitive to turbulence in the flow [11].

Fig. 9. Forward position of the reaction front within the channel as a function of time for 0.1 and 0.5 blockage ratio cases. Detonations occur at inflection points on the curves.

A comparison of the simulations with $br = 0.5$ and 0.1 shows that obstacle size plays a major role in the flame acceleration, turbulence in the flame and unburned gas, shock formation, time or distance

to detonation, and detonation mechanism. Figure 9 shows the position of the tip of the reaction front as a function of time for both blockage ratios. Higher values of br result in a more predictable flow as strong leading shocks form very close to the flame. These obstacles consistently produce Mach-stems and detonations that form behind Mach-stem reflections. For this stoichiometric ethylene and oxygen mixture, the flame never falls more than ~ 0.2 cm behind the leading shock. When br decreases, the leading shocks form as far as 1.5 cm ahead of the flame tip, creating a large, unburned turbulent region ahead of the flame. Rather than the detonation always occurring in a Mach reflection against an obstacle, they may occur anywhere that energy is focused sufficiently to initiate the detonation. The actual detonation location is stochastic because the turbulent region is filled with shock collisions and reflections that may focus sufficient energy to detonate the unburned gas anywhere within the turbulent region ahead of the flame.

Turbulence, an essentially stochastic process, dominates this region of shock collisions, shock-boundary layer interactions, and fluid instabilities. This is complicated even further by the nonequilibrium nature of the turbulence itself in these scenarios.

4 Conclusions

Multidimensional, unsteady numerical simulations of an initially homogeneous mixture of ethylene and oxygen in partially blocked channels were performed to determine how the mechanism of DDT changes as the blockage ratio (br) is decreased. This paper compared two cases, $br = 0.5$ and 0.1 .

For $br = 0.5$, detonation occurs due to the creation of a hot spot in a gradient of reactivity that forms behind a Mach reflection [11–13]. This was shown for a different fuel-oxidizer mixture than used in previous work. In the case with $br = 0.1$, shock collisions increase the temperature, pressure, and density of the unburned material. These effects and interactions occur frequently due to the complexity of the shock structures and interactions in the unburned turbulent region between the flame and the leading shock. As the flame propagates down the channel, the strength of the shock collisions and reflections increases in this region. Multiple shocks collide and reflect against the channel boundary, focusing energy in a localized region of unburned material and detonating the mixture. These results are consistent with direct initiation theory [16] and with detonations seen in experiments using similar blockage ratios ($br < 0.3$) [22]. Sufficient energy is deposited into a localized region on a timescale that is small relative to the acoustic timescale of the gas, initiating a detonation.

An additional simulation, with $br = 0.1$, investigated the sensitivity of the solution to initial conditions. Modifying the coarse mesh size resulted in a difference in detonation time and location of 0.02 ms and 1.2 cm, respectively, but the detonation mechanism was the same. This phenomenon was also

seen in previous work with a different fuel-oxidizer mixture [11], where it was determined that some regimes of DDT are especially sensitive to turbulence in the flow, which is heavily dependent on initial conditions.

It is important to understand the similarities and differences in flame acceleration and DDT with different fuel-oxidizer mixtures. The small detonation cell size, fast reactions, and rapid energy release in the combustion of ethylene-oxygen result in a smaller length scale than in previous work with other mixtures [11–13], however, the detonation mechanism for the $br = 0.5$ case in previous work with other mixtures is the same as what is observed for the $br = 0.5$ case for ethylene-oxygen. Future work to directly compare results from different mixtures, such as where and when DDT occur, the flow structures that form ahead of the turbulent flame, and whether the flame is galloping or fast, will be a useful contribution to the study of DDT in channels.

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