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Effect of multi-bend geometry on deflagration to detonation transition of a hydrocarbon-air mixture in tubes☆

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ABSTRACT

We present a numerical investigation of gaseous deflagration-to-detonation transition (DDT) triggered by a shock in a multi-bend geometry. The ethylene-air mixture filled rigid tube with obstacles is considered for understanding the effects of complex confinement and initial flame size on DDT. Our calculations show generation of hot spots by flame and strong shock interactions, and flame propagation is either restrained or accelerated due to the wall obstacles of both straight and bent tubes. The effect of initial flame size on DDT in complex confinement geometry is analyzed as well as the hot spot formation on promoting shock–flame interaction, leading to a full detonation.

1. Introduction

The combustion phenomenon addressed in the present study concerns two modes of burning: deflagration and detonation. The detonation results in a rapid increase of pressure, temperature, and propagation speed of flame, leading to an extreme thermodynamic state within a very short time. When accompanied by structural failure, accidental detonation transition is a significant safety concern. Also, detonation in a fuel pipe can cause rupture or fracture that can lead to catastrophic disaster [1,2]. For this reason, deflagration-to-detonation transition (DDT) has maintained continued interest in the combustion community for experimental, theoretical, and numerical investigations [3–6].

DDT is an extremely complicated process involving deflagrations, shocks, reflected shocks, boundary layers, and their interactions. In the literature, there are known mechanisms of DDT as addressed in recent years. The Richtmyer-Meshkov (RM) instability resulting from repeated shock–flame interactions and bifurcated structure formed by reflected shock and boundary layer interaction generates turbulent flames. The turbulent flames create conditions in a nearby unreacted gas, which leads to generation of hot spots for developing a detonation through the Zel'dovich gradient mechanism [7].

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The temperature gradient triggers DDT at localized hot spots that are formed ahead of the flame front. Both modes of burning can be expressed by a single-step chemical reaction which satisfies the characteristic length and time of deflagration and detonation [4]. Another view on the DDT mechanism suggests that a temperature gradient mechanism is unnecessary, and that a multi-step chemical reaction must be considered. The pressure amplified by the positive feedback between the pressure rise and the enhanced reaction in the front edge of the flame would lead to preheat zone formation and flame acceleration, responsible for such transition to detonation [6].

These rather distinct views on the mechanism have something in common: the interaction between a strong shock wave, and the critical role of flame acceleration leading to DDT. In most laboratory experiments, the onset of DDT is believed to originate somewhere within the strange shock structure enhanced by the multiple interactions of the shock, reflected shock, and flame. This shock–flame interaction can be strengthened when encountered by complex geometries such as walls, obstacles, and curves within pipes due to multiple reflections of shocks and expanded flame surfaces.

In view of the shock–flame interaction being the main cause of DDT, researchers have looked at such phenomena in pipes in order to gain better understanding of geometrical factors responsible for DDT. In Refs. [4] and [5], comprehensive reviews on the gaseous DDT induced from the shock–flame interaction in straight tube are discussed. A consideration of the effect of obstacles is made in Refs. [5], where the enhancement of shock–flame interactions, instabilities, and flame–vortex interaction in obstacle wakes brings about the growth of the flame surface, the energy-release rate, and the intensity of the shock. Also the change in DDT triggering time and position due to the obstacle spacing and size was shown. With an emphasis on the effect of curves within pipes [8], and [9] showed how the curvature and tube diameter in a U-bend tube change the detonation propagation characteristics. Although these studies showed valuable information on a fully developed detonation in tubes, the transition study from a deflagration to a detonation subject to complex confinement geometries has not been addressed until now.

We investigate DDT in a multi-bend geometry with obstacles for comparison to a straight geometry to understand the factors responsible for triggering flame acceleration and termination. Since the initial flame size is indicative of flame surface condition [4], different flame size in two-dimensional tube geometry is also considered to provide insight into the transition dynamics of gaseous deflagrations.

2. Numerical model

2.1. Formulation of the problem

To simulate the DDT process, we solved multidimensional, time-dependent, and reactive compressible Navier–Stokes equations, which include models for viscosity, thermal conduction, molecular diffusion, and chemical reaction. Equations (1)–(6) are the conservation equations of mass, x-axis momentum, y-axis momentum, energy, and species, and the equation of state of ideal gas in a two-dimensional rectangular coordinate:

$$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x}(\rho u)+\frac{\partial}{\partial y}(\rho v)=0 \tag{1}$$

$$\frac{\partial}{\partial t}(\rho u)+\frac{\partial}{\partial x}\left(\rho u^2+P\right)+\frac{\partial}{\partial x}(\rho uv)=\frac{\partial \tau_{xx}}{\partial x}+\frac{\partial \tau_{yx}}{\partial y} \tag{2}$$

$$\frac{\partial}{\partial t}(\rho v)+\frac{\partial}{\partial x}(\rho uv)+\frac{\partial}{\partial y}\left(\rho v^2+P\right)=\frac{\partial \tau_{xy}}{\partial x}+\frac{\partial \tau_{yy}}{\partial y} \tag{3}$$

$$\begin{aligned}\frac{\partial}{\partial t}(\rho e)+\frac{\partial}{\partial x}[u(\rho e+P)]+\frac{\partial}{\partial y}[v(\rho e+P)]&=\frac{\partial\left(u\tau_{xx}+u_y\tau_{xy}-q_x\right)}{\partial x}\\&+\frac{\partial\left(u_x\tau_{yx}+u_y\tau_{yy}-q_y\right)}{\partial y}+\rho Q_i\dot{w}_i\end{aligned} \tag{4}$$

$$\frac{\partial}{\partial t}(\rho Y_i)+\frac{\partial}{\partial x}(\rho Y_i u)+\frac{\partial}{\partial y}(\rho Y_i v)=-\frac{\partial d_x}{\partial x}-\frac{\partial d_y}{\partial y}+\rho\dot{w}_i \tag{5}$$

$$P=\frac{\rho RT}{M} \tag{6}$$

where ρ, u, v, P, e, Y_i, R, and M are density, x-axis velocity, y-axis velocity, pressure, total energy density, mass fraction of a reactant, the universal gas constant, and molecular weight, respectively. In the source term, $\vec{q}=k\nabla T$ is the thermal conduction, $\dot{w}_i\equiv\partial Y_i/\partial t|_{Chem}=A\rho Y\exp(-E_a/(RT))$ is the reaction rate described by the first-order Arrhenius kinetics, $\vec{d}=\rho D\nabla Y_i$ is the mass diffusion, and τ_{xx}, $\tau_{xy}=\tau_{yx}$, and τ_{yy} are the viscous stresses that are calculated by constitutive relation. Here, k is the thermal conduction coefficient, A is the pre-exponential factor, E_a is the activation energy, and D is the mass diffusion coefficient. We assume that kinematic viscosity, diffusion, and heat conduction coefficients are dependent on temperature. Also, non-dimensional Lewis, Prandtl, and Schmidt numbers are assumed to be unity, as these assumptions do not affect the physical changes in the flame structures, partial flame extinguishing, and outbreak of distributed flames [4]. For description of an incident shock wave, we use uniform shocked flow condition with parameters (P_s, ρ_s, and T_s) determined from the Rankine-Hugoniot conditions for a given Mach number as shown in equation (7).

$$\begin{aligned}P_s&=P_0\left(\frac{2\gamma M_s^2}{\gamma+1}-\frac{\gamma-1}{\gamma+1}\right)\quad \rho_s=\rho_0\left(\frac{\left(\frac{\gamma+1}{\gamma-1}\right)\frac{P_2}{P_1}+1}{\left(\frac{\gamma+1}{\gamma-1}\right)+\frac{P_2}{P_1}}\right)\quad T_s\\&=T_0\left(\frac{\left(1+\frac{\gamma-1}{2}M_s^2\right)\left(\frac{2\gamma}{\gamma-1}M_s^2-1\right)}{\frac{(\gamma+1)^2}{2(\gamma-1)}M_s^2}\right)\end{aligned} \tag{7}$$

Convection is handled by the convex Essentially Non-Oscillatory (CENO) method rather than the weighted ENO (WENO) method due to its efficiency and robustness in simulating strong shock dominant phenomena for spatial discretization, and a third-order Runge-Kutta (RK) integration is used for temporal discretization [10]. Viscous, heat conduction, and mass diffusion fluxes are evaluated using the second-order finite difference method. The subgrid models are not considered for small turbulent eddies. Instead, the