The Role of Turbulent Transport for Detonation Initiation at a Turbulent Interface

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1. Introduction

Experiments show that direct initiation of a detonation can be achieved from the rapid turbulent mixing of a jet of combustion product with an unreacted combustible mixture [1]. However, the critical conditions and the underlying mechanism for successful initiation were not established.

It has been shown theoretically and numerically that, in the absence of shock waves, a detonation may be initiated spontaneously in a reactive mixture with a gradient field of either free radicals or temperature. (See the review paper by Bartenev & Gelfand [2] for complete references). It is understood that the development of a detonation is due to a gradient mechanism leading to the proper unsteady coupling between the gasdynamics and the chemical energy release. However, in most of the previous studies the gradient field is assumed *a priori* and the analyses are for the subsequent development of the detonation. Furthermore, transport effect has mostly been neglected, though it may be of key importance for the initiation [3].

In the initiation by turbulent mixing, the diffusion process creates the gradient field. If the diffusion rate is insufficient to establish a large mixing zone, then only a flame can result. It is of interest to determine the critical mixing or diffusion rate needed to establish an adequate gradient field where the transition from flame ignition to detonation initiation can occur.

In this paper, we perform one-dimensional numerical simulations of the initiation phenomenon to investigate the mixing or diffusion process for the onset of detonation at a turbulent interface separating the combustion product from the unreacted mixture. The role of turbulence is explored by systematically varying the magnitude of the transport parameters to account for the turbulence effect. The present paper attempts to elucidate how turbulent transport may play a key role in the initiation event.

2. Mathematical model

Neglecting viscous effects, the governing equations in one-dimensional geometry that incorporate the processes of fluid flow, heat conduction, diffusion and a one-step Arrhenius chemical reaction, are given by the three conservation equations for mass, momentum and energy coupled with the transport-reaction-diffusion equation for a chemical variable, i.e.:

$$\rho_t + (\rho u)_x = 0$$

$$(\rho u)_t + (\rho u^2 + p)_x = 0$$

$$(\rho e)_t + (u(\rho e + p))_x = KT_{xx} - \rho q\dot{\omega}$$

$$(\rho \lambda)_t + (\rho u \lambda)_x = \rho \dot{\omega} + \rho D \lambda_{xx}$$

with

$$p = \frac{\rho RT}{M}, \qquad e = \frac{p}{\rho(\gamma - 1)} + \frac{u^2}{2}, \qquad \dot{\omega} = -A_k \rho \lambda \exp\left(\frac{-E_a}{RT}\right)$$

where ρ is the mass density, *u* is the particle velocity, *e* is the specific energy, *p* is the pressure, λ is the mass fraction of a reactant and $\dot{\omega}$ is the reaction rate with preexponential constant A_k and activation energy E_a . The parameters γ , *R* and *M* in the equation of state denote the specific heat ratio, universal gas constant and molecular weight. The transport coefficients, *K* and *D*, are used for the thermal conduction and mass diffusion, respectively. The chosen chemico-physical parameters of the system are presented in table 1. We used the same input parameters found in Khokhlov & Oran [4], which were selected to fit the various laminar flame and detonation properties in acetylene-air in the range of initial pressure from 0.1 to 1 atm and initial temperature of 293 K. For the transport processes, the Lewis number $Le = K/\rho c_p D$ is assumed to be unity in the present model. The coefficients for diffusion and heat conduction have similar temperature dependence of the form:

$$D = D_o \frac{T^n}{\rho}, \ \frac{K}{\rho c_p} = K_o \frac{T^n}{\rho}$$

where c_p is the specific heat at constant pressure and the index *n* is chosen to have the value of 0.7 for typical gaseous systems. D_0 , K_0 are constants and their values are also given in table 1. It should be pointed out that these constants for transport coefficients were selected to fit laminar flame and, therefore, they only account for molecular transport occurred in laminar flows.

Value	Definition
$T_{\rm o} = 293 \; {\rm K}$	Initial temperature
$P_{\rm o} = 1.33 \text{ x } 10^4 \text{ Pa}$	Initial pressure
$ ho_o = 1.58 \text{ x} 10^{-1} \text{ Kg/m}^3$	Initial density
$\gamma = 1.25$	Specific heat ratio
M = 29	Molecular weight
$A_{\rm k} = 1.0 \ {\rm x} \ 10^9 \ {\rm m^{3}/Kg/s}$	Pre-exponential constant
$E_{\rm a} = 29.3 \ RT_{\rm o}$	Activation energy
$q = 35.0 \ RT_{\rm o}/M$	Chemical energy release
$K_o = D_o = 1.3 \text{ x } 10^{-6}$	Molecular transport coefficient
$T_{\rm f}=2340~{ m K}$	Adiabatic flame temperature
$\rho_{\rm f} = 1.98 \text{ x } 10^{-2} \text{ Kg/m}^3$	Density of products

Table 1. Chemical and thermodynamic parameters for the computation

Taking into account the effect of turbulence on the transport processes, we modify the transport coefficients accordingly by defining an artificial turbulent intensity Γ . The turbulent transport coefficients $D_{\rm T}$, $K_{\rm T}$ are simply given by:

$$D_T = \Gamma \cdot D \qquad K_T = \Gamma \cdot K$$

which are used in the following computations. Turbulent flow is characterized by unsteady eddy motion. The eddies interact with each other as they move around, and they can exchange energy. Turbulence also acts as a mechanism for diffusion and heat transport. As a result of mixing between turbulent eddies of all sizes, turbulent transport is a much more effective process than molecular transport, which is a very slow process on a macroscopic scale. The turbulent transport coefficients are therefore typically several orders of magnitude larger than those for molecular transport (i.e. $\Gamma >>1$). Here, Γ is used as a control parameter to model the effect of turbulence.

3. Computational setup

To initialize the computation, the initial conditions are described by two thermodynamic states separated by an interface. For x < 2.5 cm, the state corresponds to the computed properties T_f and ρ_f of the laminar flame given in table 1. The state on the other side of the interface is simply the uniform initial properties. The detailed evolution process from the initial condition is then simulated numerically, taking into account the chemical reaction, "turbulent" transport effects and compressible effects for a one-dimensional geometry. The governing equations are solved numerically using the method of Strang's operator splitting, separating the hyperbolic part of system from the additional chemical and parabolic terms in the model. The hyperbolic Euler equations without the transport effects are approximated using a second-order centered scheme, namely the slope-limiter centered (SLIC) integration scheme [5]. The additional parabolic terms in the model are treated using explicit second-order finite-difference approximations. In the present work, adaptive mesh refinement (AMR) is also adopted as a technique for manipulating the local resolution of numerical simulations based on a hierarchical series of Cartesian grids [6].

4. Numerical results

4.1 Small turbulent intensity $\Gamma \sim 10$

For small turbulent intensity $\Gamma \sim 10$, the laminar flame continues to propagate and no abrupt explosion occurs near the interface. The evolution process is essentially controlled by slow molecular transport effects and chemical reactions. Figure 1 shows the temperature profiles for the laminar flame at equal time intervals. In this case, the transport processes has no time to establish a gradient field prior to ignition. Hence, no explosion occurs. A laminar flame is ignited, and the compressibility effect is negligible in its subsequent propagation.



Figure 1. Temperature profiles for the case of $\Gamma = 10$ at t = 0.1, 0.2, 0.3 and 0.4 ms

4.2 Moderate turbulent intensity $\Gamma \sim 80$

For the case of moderate turbulent intensity $\Gamma \sim 80$, a mild explosion takes place at the interface due to the mixing between reactants and products and to the heat exchange between the two zones. In figure 2, we can see an overpressure at the interface, however the corresponding pressure increase resulting from the explosion is essentially too weak to provoke direct initiation of detonation in the unreacted mixture. The steady solution is similar to a fast deflagration wave.

4.3 Large turbulent intensity $\Gamma > 250$

In contrast, direct initiation of detonation at the interface may be possible when the transport processes become significant by increasing the turbulent intensity $\Gamma > 250$. During the early stage, the chemical reaction undergoes induction process at the interface while temperature and species concentration gradients are established by rapid turbulent diffusion. Subsequently, the interface is surrounded by a layer of reactive mixture with a large non-uniform concentration and temperature distribution established by diffusive mixing. This causes an explosion at the interface and eventually leads to the formation of the detonation, as shown in figure 3.



Figure 2. Pressure and temperature profiles for the case of $\Gamma = 80$ at t = 10, 20, 30, 40, 50 and 60 µs



Figure 3. Pressure and temperature profiles for the case of $\Gamma = 280$ at t = 20, 24, 28, 32 and 36 µs

5. Discussion

The mechanism for successful detonation initiation observed in the latter case of large turbulent intensity is very similar to that of detonation formation in a temperature gradient field [2]. The initiation process is related to a gradient mechanism due to the unsteady coupling between the gasdynamics and the chemical reaction. However, instead of imposing explicitly a linear temperature or concentration gradient into the problem and analyzing the subsequent evolution due to such a gradient field, the gradient field itself is generated implicitly by turbulent transport from the given initial conditions of an interface in the present investigation. In our results, we have illustrated through a simple model how the turbulent mixing rate may be of key importance in such spontaneous initiation phenomenon.

For successful initiation, the formation of detonation takes places only when the local temperature gradient is smaller than a critical value or the length of mixing zone has to be larger than a minimum value [2]. In this study, we found that an adequate temperature gradient to initiate a detonation can only be established if the turbulent intensity at the interface is sufficiently high. The magnitude of the turbulent transports must be of the order of 250 greater than that of laminar molecular transport.

6. Concluding remarks

The present study demonstrates how turbulent transport plays a key role in the process of initiation by turbulent mixing. When the turbulent intensity in the mixing zone at the interface becomes dominant, it can create a smooth gradient field which is responsible for the onset of detonation. Nevertheless, the key element still relies on the ability to generate a proper gradient field for the coupling between gasdynamics and chemical reaction leading to the formation of detonations.

References

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