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Evolution of detonation formation initiated by a spatially distributed, transient energy source

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Detonations usually form through either direct initiation or deflagration-to-detonation transition (DDT). In this work, a detonation initiation process is introduced that shows attributes from each of these two processes. Energy is deposited into a finite volume of fluid in an amount of time that is similar to the acoustic time scale of the heated fluid volume. Two-dimensional simulations of the reactive Euler equations are used to solve for the evolving detonation initiation process. The results show behaviour similar to both direct initiation and DDT. Localized reaction transients are shown to be intimately related to the appearance of a detonation. Thermomechanical concepts are used to provide physical interpretations of the computational results in terms of the interaction between compressibility phenomena on the acoustic time scale and localized, spatially resolved, chemical energy addition on a heat-addition time scale.

Key words: combustion, compressible flows, detonation waves

1. Introduction

Detonation formation processes are usually classified as either direct initiation or deflagration-to-detonation transition (DDT). Direct initiation (Eckett, Quirk & Shepherd 2000) uses a relatively large amount of energy deposited in a short time period (classically, instantaneous energy deposition to a point) to create a significant thermomechanical response in the gas leading to a blast wave within the reactive mixture. A typical DDT process begins by igniting the gas using a comparatively small amount of energy to create a laminar flame. Surface instabilities at the flame front (Oppenheim *et al.* 1972; Roy *et al.* 2004; Oran & Gamezo 2007) transform the deflagration to a turbulent reaction front, which enhances the rate of thermal energy conversion. Compression waves are produced by a transient thermomechanical response arising from the enhanced rate of energy release from the increase in reaction front surface area. Compression waves propagate ahead of the evolving reaction zone, precondition the reactive gas ahead of the reaction front and coalesce until a detonation wave is formed. Oppenheim & Soloukhin (1973) address these concepts with the prescient remark that 'Gasdynamics of explosions is best defined as the science dealing with the interrelationship between energy transfer occurring

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at a high rate in a compressible medium and the concomitant motion set up in this medium'. In the years since their paper was published, modellers have endeavoured to quantify the cited interrelationship, including the impact of viscous/diffusive transport effects (Powers 2006; Oran & Gamezo 2007; Radulescu *et al.* 2007; Dorofeev 2011; Mazaheri, Mahmoudi & Radulescu 2012; Romick, Aslam & Powers 2012).

Direct initiation and DDT can be characterized by using concepts in the thermomechanical analyses by Kassoy (2010, 2014*a*, 2016). The first describes the consequences of localized, transient, spatially distributed thermal power deposition from a source into a volume (characteristic length-scale l) of inert gas on a time scale, t_h, that is short compared to the characteristic acoustic time, $t_a = l/a$, where a is the characteristic acoustic velocity of the heated volume. The thermomechanical response of the gas can be characterized as nearly constant volume heating when the energy addition is less than an explicitly defined maximum value. Pressure rises with temperature, leading to a pressure gradient that can accelerate fluid particles. The result is a low-Mach-number internal expansion process. Gas expelled from the original hot spot volume acts like a piston driving mechanical disturbances into the neighbouring unheated gas. The amount of energy added to the volume determines the amplitude of the mechanical disturbances (e.g, acoustic, shock, or blast waves). The maximum energy addition leads to a fully compressible expansion process characterized by an $O(1)$ Mach number and the generation of very strong shocks. In contrast, when the heating time is much longer than the characteristic acoustic time, $t_h \gg t_a$, the heat addition process occurs at a nearly spatially homogeneous pressure, with density declining inversely with temperature increase.

A detonation can be initiated by localized, transient, spatially distributed thermal power deposition on a time scale similar to the acoustic time scale of the heated fluid volume. Previous work in this area describes 1-D solutions of the reactive Euler equations (Clarke, Kassoy & Riley 1986; Clarke *et al.* 1990; Sileem, Kassoy & Hayashi 1991; Kassoy *et al.* 2008; Regele, Kassoy & Vasilyev 2012). The reactive mixture is initially at rest. Spatially resolved thermal power deposition occurs in a finite subvolume of the fluid. Shock waves are created by the initial power deposition. In the earliest work, energy is added by conduction from a planar wall located at one end of the reactive gas domain (Clarke *et al.* 1986, 1990). Alternatively, heat is added directly to a specified fluid volume (Sileem *et al.* 1991; Kassoy *et al.* 2008). Typically, an isolated high-temperature hot spot evolves spontaneously on a time scale that is short compared to the local characteristic acoustic time scale in response to exothermic reaction initiation. A detonation follows. These 1-D studies are carried out for relatively low activation energies. Recently, the work was extended to higher activation energies (Regele *et al.* 2012). Multiple isolated high-temperature hot spots characterize the combustion process in relatively high activation energy mixtures.

Kurtz & Regele (2014*a*,*b*) perform numerical simulations of isolated hot spots in one and two dimensions. The hot spots are modelled as a linear temperature gradient adjacent to a constant temperature plateau of some prescribed size in order to account for the finite size of localized hot spot maxima. Hot spots are shown to produce acoustic waves, compression waves and shock waves. They demonstrate that the predicted behaviour can be characterized by examining the ratio of the heating to acoustic time scale ratio t_h/t_a.

Hot spots can form inside a turbulent flame brush and initiate a rapid reaction process (explosion) to create a detonation wave (Khokhlov & Oran 1999). Obstacles inside a channel, such as a Schelkin spiral, can increase flow turbulence and reaction zone surface area/volume. The concomitant increase in rate of heat release leads to

compression waves that precondition the gas and form a detonation wave (Gamezo, Ogawa & Oran 2008). It has also been shown that boundary layers can be the sites of localized explosions that facilitate detonation formation (Ivanov, Kiverin & Liberman 2011). The Navier–Stokes (NS) equations are normally employed when performing numerical simulations of DDT (Khokhlov & Oran 1999; Khokhlov, Oran & Thomas 1999; Oran & Khokhlov 1999; Gamezo, Khokhlov & Oran 2001; Oran & Gamezo 2007; Kessler, Gamezo & Oran 2010; Ivanov *et al.* 2011). In the instances where the Euler equations are solved without the diffusive/viscous terms, the numerical diffusion implicitly present in the hyperbolic solver is used to mimic the effects of molecular viscosity/diffusion (Gamezo, Desbordes & Oran 1999). In the context of detonation evolution many investigators have assessed the impact of viscous/diffusive transport effects (Gamezo *et al.* 2001; Radulescu *et al.* 2005; Powers 2006; Radulescu *et al.* 2007; Romick *et al.* 2012; Mazaheri *et al.* 2012) and found some small-scale difference when compared to the results of fully resolved NS simulations (Powers 2006). Kassoy (2010, 2014*b*) has used non-dimensionalized inert and reactive NS equations to identify parameters that modulate viscous, conduction, diffusion and dissipation terms in order to determine when Euler equation models may be valid. The results show that all non-dimensional transport terms (differential operators) are modulated by the product of two parameters, either one of which can be asymptotically small: the inverse acoustic Reynolds number (Knudsen number) and the ratio of the heating time scale to the local acoustic time scale. Even if the latter is $O(1)$, as in the current modelling, a typical value for the Knudsen number, 10^{-7}, implies that local non-dimensional transport gradients must be enormous in order for viscous diffusion, conduction dissipation and mass diffusion to be of importance in the physics of the processes.

Sileem *et al.* (1991), Kassoy *et al.* (2008) and Regele *et al.* (2012) have modelled one-dimensional (1-D), acoustic time-scale detonation initiation using the Euler equations. The 1-D acoustic time scale detonation initiation results show that it is possible to initiate a planar detonation wave with physically plausible properties. The current objective is to extend the 1-D acoustic time scale approach ($t_h = O(t_a)$) to planar two-dimensional (2-D) Euler and NS-based models in order to describe the physics of detonation initiation. In order to maintain consistency with the previous 1-D model (Regele *et al.* 2012), a solution is pursued that is independent of diffusive/viscous transport effects. In that context, the evolution arises from the purely reactive gasdynamics envisioned by Oppenheim & Soloukhin (1973).

Consideration of multiple dimensions allows effects such as the Richtmyer–Meshkov and Kelvin–Helmholtz instabilities to exist. The Richtmyer–Meshkov instability is found to be the primary source of turbulence generation in DDT (Oran & Gamezo 2007; Gamezo *et al.* 2001). Kelvin–Helmholtz instabilities can also be found in DDT as a secondary instability and are often suppressed by diffusive effects in NS solutions (Oran & Gamezo 2007). In order to obtain a purely gasdynamic detonation initiation solution, it will be necessary to capture both the Richtmyer–Meshkov and Kelvin–Helmholtz instabilities. It will also be necessary to minimize the numerical diffusion such that any unreacted pockets will have a minimal amount of heat diffused into them so that their autoignition times can be resolved.

A moderately low activation energy will be used that is similar to that of the mildly unstable detonation case in Radulescu *et al.* (2007) and Radulescu & Maxwell (2011). The approach taken in this work is to quantitatively justify the use of the Euler equation model and solve them with increasing levels of resolution until the detonation formation time and the spatially integrated chemical heat release transient

are no longer affected by the unresolved local flow structures. In this paper a series of numerical experiments with progressively increasing resolution is conducted in order to quantitatively demonstrate that acoustic time-scale detonation initiation is dominated by purely gasdynamic effects and is independent of diffusive/viscous transport effects. These Euler simulations are cross-referenced against solutions of the NS equations with sufficiently large Reynolds numbers to demonstrate the validity of the approach.

2. Mathematical model

The mathematical model for quantifying the thermomechanical response of a compressible, reactive gas to localized, spatially distributed power deposition from an external source and ultimately from a one-step Arrhenius-type chemical reaction is based on the vector form of the non-dimensional reactive NS equations

$$\rho_t + \boldsymbol{\nabla} \cdot \rho \boldsymbol{u} = 0, \tag{2.1a}$$

$$(\rho \boldsymbol{u})_t + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\boldsymbol{\nabla} P + \frac{1}{Re_a} \boldsymbol{\nabla} \cdot \boldsymbol{\tau} \tag{2.1b}$$

$$(\rho e_T)_t + \boldsymbol{\nabla} \cdot (\boldsymbol{u}(\rho e_T + P)) = \dot{Q}(\boldsymbol{x}, t) + \dot{W} q + \frac{1}{Re_a Pr} \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} T) + \frac{1}{Re_a} \boldsymbol{\nabla} \cdot (\boldsymbol{u} \cdot \boldsymbol{\tau}) \tag{2.1c}$$

$$(\rho Y)_t + \boldsymbol{\nabla} \cdot \rho Y \boldsymbol{u} = -\dot{W} + \frac{1}{Re_a Sc} \boldsymbol{\nabla} \cdot (\rho \boldsymbol{\nabla} Y). \tag{2.1d}$$

Here the stress tensor is $\boldsymbol{\tau} = -(2/3)(\boldsymbol{\nabla} \cdot \boldsymbol{u})\boldsymbol{I} + \boldsymbol{\nabla}\boldsymbol{u} + \boldsymbol{\nabla}\boldsymbol{u}^{\mathrm{T}}$, where $\boldsymbol{I}$ is the identity matrix. These equations are complimented by an equation of state written in terms of e_T and $\boldsymbol{u}$

$$P = (\gamma - 1)\rho \left(e_T - \frac{\boldsymbol{u} \cdot \boldsymbol{u}}{2} \right). \tag{2.1e}$$

Finally the reaction rate is defined by

$$\dot{W} = B \rho Y e^{-E/T}, \tag{2.1f}$$

where the temperature is expressed as $T = \gamma P/\rho$ and $\dot{Q}(\boldsymbol{x}, t)$ is the non-dimensional thermal power deposition term.

The non-dimensional thermodynamic variables are defined by

$$(\rho, P, T) = \left(\frac{\rho'}{\rho_0'}, \frac{p'}{\gamma p_0'}, \frac{T'}{T_0'} \right), \tag{2.2}$$

where primes denote dimensional variables and (ρ_0', p_0', T_0') are the reference (initial) values of the density, pressure and temperature. The non-dimensional velocity is defined by

$$\boldsymbol{u} = \frac{\boldsymbol{u}'}{a_0'}, \tag{2.3}$$

where a_0' is the acoustic speed in the reference state. The space and time variables are defined by

$$\boldsymbol{x} = \frac{\boldsymbol{x}'}{l'}, \quad t = \frac{t'}{t_a'}, \tag{2.4a,b}$$

where l' is the characteristic length-scale of the volume affected initially by the external non-dimensional power source $\dot{Q} = \dot{Q}'/a_0'^2$, defined with respect to the dimensional power source $\dot{Q}'$ and the square of the sound speed in the reference state.