

Numerical Studies of Detonation Diffraction using the Ignition-and-Growth Model

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Introduction

The ignition-and-growth (IG) model of heterogeneous explosives originated with the work of Lee and Tarver [1], and was refined in a number of subsequent articles by Tarver and collaborators, see [2,3], for example. The model treats a heterogeneous explosive as a homogeneous mixture of two components, a reactant and a product. Each component is assigned its own equation of state, from which is constructed a mixture equation of state under certain closure assumptions such as pressure and temperature equilibrium between the two components. A single variable measures the progress of a one-step reaction. However the rate function, while remaining continuous, undergoes sudden changes in form as the progress variable crosses certain milestones. Behind this prescription of the rate law lies the nonuniform picture of the energy release process, as consisting of distinct stages in which hot spots appear, grow and merge. A number of experimentally-determined parameters appear in the equations of state. The rate law is calibrated as well, with calibrations being typically based on planar detonation-initiation experiments, and being sensitive, for example, to whether the initiating stimulus is a sustained shock or a short pulse.

A number of numerical computations have been done with IG models [1–3]. Most results are for planar geometries, but some non-planar calculations also exist [2]. While the IG model is well known, a comprehensive study of the strengths and weaknesses of the model has not been carried out. The focus of this work is to perform a detailed study of detonation diffraction in two-dimensional (and axisymmetric) expanding geometries using the IG model. The primary interest is to determine the effects of transverse disturbances introduced into the reaction zone by area changes. In expanding geometries, the detonation weakens and the reaction zone may decouple from the leading shock. This decoupling may ultimately lead to detonation failure and the appearance of dead zones. It is of interest to describe such dead zones, if they exist, and to determine, within the IG model, whether they are a short-lived feature of the solution, or whether they persist for long periods of time. It is also of interest to determine whether the weakened detonation becomes unstable and whether re-ignition occurs when the detonation passes into a converging geometry. In order to perform this study, we compute well-resolved numerical solutions of the governing equations of the IG model in various expanding geometries. The work is similar in spirit to a subset of studies reported in Arienti, Moreno and Shepherd [4], corresponding to corner-turning for a Mie-Gruneisen equation of state and a pressure-dependent reaction rate.

Governing Equations

The governing equations for the IG model have the form of the reactive Euler equations, supplemented with a mixture equation of state and a one-step reaction rate with multiple

stages. For two-dimensional flow, the model equations may be written in the form

$$\mathbf{u}_t + \mathbf{f}_x(\mathbf{u}) + \mathbf{g}_y(\mathbf{u}) = \mathbf{h}(\mathbf{u}),$$

where

$$\mathbf{u} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \\ \rho \lambda \end{bmatrix}, \quad \mathbf{f}(\mathbf{u}) = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ u(\rho E + p) \\ \rho \lambda u \end{bmatrix}, \quad \mathbf{g}(\mathbf{u}) = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ v(\rho E + p) \\ \rho \lambda v \end{bmatrix}, \quad \mathbf{h}(\mathbf{u}) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \rho \mathcal{R} \end{bmatrix}.$$

The variables are the density ρ , velocity (u, v) , pressure p , total energy E and reaction progress λ . The total energy is given by

$$E = e(\rho, p, \lambda) + \frac{1}{2}(u^2 + v^2),$$

where the internal energy $e(\rho, p, \lambda)$ is described by a mixture Jones-Wilkes-Lee (JWL) equation of state. The reaction rate \mathcal{R} involves several stages, and has the form

$$\begin{aligned} \mathcal{R} = & I(1 - \lambda)^b (\max\{\rho/\rho_0 - 1 - a, 0\})^x H(\lambda_{I,\max} - \lambda) \\ & + G_1(1 - \lambda)^c \lambda^d p^y H(\lambda_{G_1,\max} - \lambda) + G_2(1 - \lambda)^e \lambda^g p^z H(\lambda - \lambda_{G_2,\min}), \end{aligned}$$

where H is the Heaviside function. The reaction rate recognizes the role of hot spots in the reaction process and includes an ignition term that depends on the level of compression of the material and two growth terms that depend on pressure primarily. There are many parameters involved, such as I , G_1 , G_2 , ρ_0 , a , b , etc., and these are chosen to match experimental data. For example, the parameters used in the present study for both the reaction rate and the mixture equation of state are calibrated to the explosive LX-17.

Numerical Method

A numerical method has been developed to solve the reactive Euler equations in two-dimensional domains discretized using composite overlapping grids [5]. Overlapping grids are useful for complex domains including, for example, the expanding geometries considered here. The basic method is a second-order, Godonov-type, shock-capturing scheme which has been extended to handle the mixture JWL equation of state and multi-stage reaction rate for the IG model. The method incorporates a scheme of adaptive mesh refinement (AMR) in order to locally increase the grid resolution in the vicinity of detonations, shocks and contact discontinuities, and a scheme of sub-CFL time-stepping in order to accommodate the fast chemical time scale in the reaction zone.

Numerical Results

Numerical results have been obtained for planar detonation diffraction at corners of varying angles, and for axisymmetric detonation diffraction at a 90° corner. Most of the results are for rigid confinement, but some cases of compliant confinement have been considered. Only a brief discussion is given here, and we will focus on planar detonation diffraction. For example, Figure 1 shows the behavior of the pressure and reaction progress for detonation diffraction at a 90° corner. In this calculation, a steady Chapman-Jouguet detonation propagates from

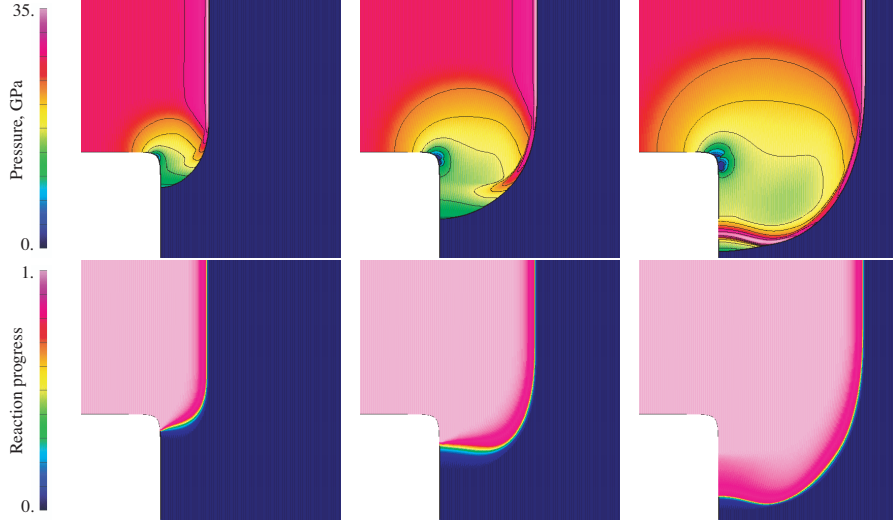


Figure 1: Detonation diffraction at a 90° corner. Pressure and reaction progress at $t = 0.3$, 0.6 and $0.9\mu\text{s}$. (The detonation reaches corner at $t = 0$.)

the left to the right in the portion of the domain to the left of the corner. The curved lower boundary is taken to be a rigid wall in this calculation and the upper straight boundary is a line of symmetry. The detonation weakens upon diffraction by the corner and the reaction zone separates from the lead shock (left frames at $t = 0.3\mu\text{s}$ in the figure). The unreacted ‘dead zone’ behind the lead shock is only temporary as the detonation re-ignites and strengthens near the vertical wall at later times. Two basic mechanisms for this re-ignition are observed. The first is a strengthening of the detonation away from the vertical wall due to a pressure gradient transverse to the diffracted wave (middle frames at $t = 0.6\mu\text{s}$) and the second, which develops slightly later in time but becomes the dominant re-ignition mechanism, is a strengthening along the vertical wall due to the growth terms in the IG reaction rate (right frames at $t = 0.9\mu\text{s}$). The latter effect dominates when the pressure behind the weakened diffracted shock is high enough so that the detonation re-ignites along the vertical wall before the transverse wave reaches the wall.

Planar detonation diffraction at a 140° corner is shown in Figure 2. As before, the weakened leading shock separates from the reaction zone at early times (left frames at $t = 0.5\mu\text{s}$), but now the unreacted region behind the shock is larger due to the larger turning angle which results in a weaker leading shock. The pressure behind the shock is correspondingly lower so that a re-ignition along the oblique wall does not occur in contrast with the previous calculation. Here, the dominant re-ignition mechanism is a strong transverse detonation that develops away from the oblique wall and propagates through the unreacted region behind the separated shock to the wall (middle and right frames). In both of these calculations, and for other calculations not shown, no permanent dead zones have been observed for the IG model and there is no indication of instability along the diffracted detonation wave.

Conclusions

Computational studies of detonation diffraction at a sharp corner and in a variety of configurations have been carried out with the IG model. We conclude that there is a local

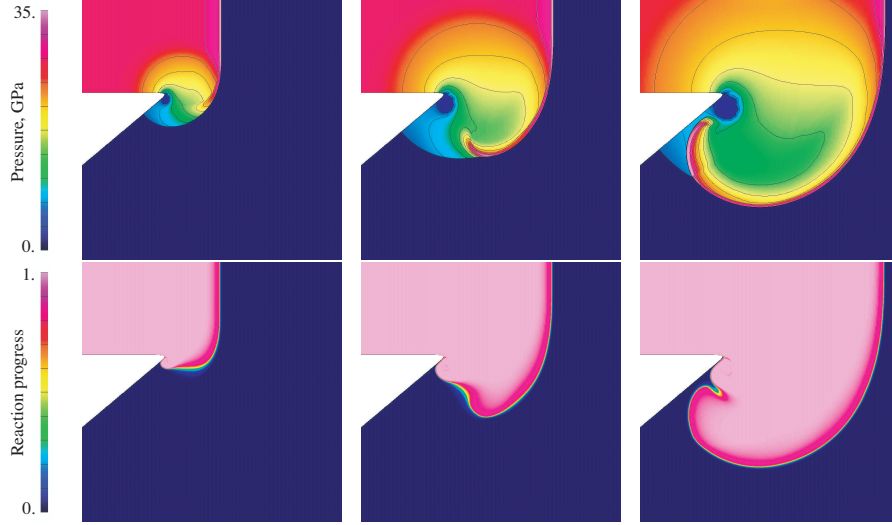


Figure 2: Detonation diffraction at a 140° corner. Pressure and reaction progress at $t = 0.5, 1.0$ and $1.5\mu\text{s}$. (The detonation reaches corner at $t = 0$.)

failure of the detonation at the corner, manifested in the weakening of the lead shock and its decoupling from the reaction zone. These results are similar to those presented in [4] for the Mie-Gruneisen equation of state and a pressure-dependent reaction rate. However, for the IG model, the weakly-shocked explosive reignites in due course, either by a local strengthening of the growth stage of the IG reaction rate or by being swept over by a transverse detonation that developed elsewhere. A fully fledged detonation reappears, and there remain no sustained dead zones. It appears, therefore, that if experimentally observed dead zones are to be captured, the IG model must be suitably modified, possibly by accounting for the observed desensitization of heterogeneous explosives by the passage of a weak shock.

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