Effect of Thermal Nonhomogeneity on Explosion or Detonation in an Annular Cookoff

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Abstract

This computational study is motivated by recent experiments on large-scale cookoff in a confined annular geometry, where the explosive charge is heated carefully so as to produce, nominally, a uniform radial thermal gradient. In the absence of circumferential asymmetry a circular wave of explosion would traverse the charge from the hot outer boundary to the cold inner boundary. In practice, however, experimental imperfections induce weak thermal nonhomogeneities during the heating phase, leading to hot spots where ignition may occur preferentially. For a model homogeneous explosive with strongly state-dependent kinetics, this study explores the influence of the nonhomogeneities on the fate of the explosive event.

1 Introduction

Recent cookoff experiments on condensed-phase energetic materials have inspired this numerical investigation. In these experiments the nature of the explosive event is dictated, on the one hand, by the thermal field imposed upon the sample by the heating process, and on the other, by the thermally-induced damage that occurs during cookoff. Cracks, voids and pores form as the material deforms, and solid-to-solid phase transition as well as melting may occur. These changes in material morphology significantly affect mechanical behavior as well as the energy-release rate.

This study does not consider such material complexity. Rather, it limits itself to the issue of lack of simultaneity in the ignition process and addresses it in the context of a simple model of the explosive. Even though the cookoff experiment may be designed to produce a prescribed thermal field (such as a uniform radial gradient with no circumferential variation), small nonuniformities inevitably creep in. Strongly state-dependent kinetics magnifies their effect and causes the reaction to accelerate preferentially at one or more sites, or hot spots. The thermal gradients associated with the nonuniformities may then affect substantially the nature of the explosive event.

We examine two types of nonuniformities, corresponding to a linear, circumferential thermal gradient superimposed upon a uniform temperature field, and a hot spot embedded in a circumferentially uniform but radially linear temperature field. We find that in each case, the mode of evolution is strongly influenced by the presence of the nonuniformity.
2 The Model

We model the behavior of the sample using the reactive Euler equations with rate-sensitive, one-step, Arrhenius kinetics and an ideal equation of state. In dimensionless form the governing equations are

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

where

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

The variables are

- \( \rho \) = density
- \( u, v \) = \((x, y)\) velocity
- \( p \) = pressure
- \( \lambda \) = reaction progress
- \( E \) = total energy
- \( T \) = temperature

with

\[ E = \frac{p}{(\gamma - 1)\rho} + \frac{1}{2} (u^2 + v^2) - \lambda Q, \quad p = \rho T, \]

and the reaction rate

\[ R = \frac{\epsilon}{(\gamma - 1)Q} (1 - \lambda) \exp\left[\frac{1}{\epsilon} \left(1 - \frac{1}{T}\right)\right]. \]

The parameters appearing above are the scaled reciprocal activation energy \( \epsilon \) and the scaled heat release \( Q \). Pressure, density and temperature are referred to nominal values \( p_0, \rho_0 \) and \( T_0 \), velocity to \( u_0 = \sqrt{p_0/\rho_0} \), time to the constant-volume explosion time \( t_0 \) at the nominal state, length to \( u_0 t_0 \) and energy to \( u_0^2 \). For the sample explosive we take \( \gamma = 1.4, Q = 7 \) and \( \epsilon = 0.06 \). Correspondingly, the CJ speed \( D_{CJ} = 4.01 \), the constant-volume explosion pressure \( p E = 3.8 \), the CJ pressure \( p_{CJ} = 7.13 \) and the von Neumann pressure \( p_N = 13.27 \).

The bounding radii of the annulus are \( R_1 = 2R_0 \), with \( R_1 \) taken as 0.2 or 0.4 in the numerical studies. Assuming symmetry, we carry out the computations on half the annulus, \( R_0 < r < R_1, 0 < \vartheta < \pi \), for which the boundary conditions are shown in figure 1.

The initial conditions are

\[ p = 1, \quad u = v = 0, \quad \lambda = 0, \quad T = 1 - \epsilon \varphi(r, \vartheta), \]

where \( \varphi(r, \vartheta) \) is a prescribed function.

3 Numerical Results

High-resolution computations were performed using adaptive mesh refinement. Details of the numerical procedure and its implementation can be found in Kapila et al. (2002).
3.1 Evolution in a slab

In order to interpret the results of computations on the annulus, it is useful to recall existing results for the same model explosive on detonations induced by a linear temperature gradient in a slab geometry (Kapila et al., 2002). These results were computed on the domain $0 < x < 1$ with initial conditions

$$p = 1, \quad u = 0, \quad \lambda = 0, \quad T = 1 - \epsilon ax.$$  

The mode of evolution depends crucially upon the size of the gradient parameter $a$ and covers a broad spectrum. Two cases representative of the ends of the spectrum are summarized below.

**Moderate gradient, $a = 0.38$**

After an induction period, a nearly-constant-volume thermal explosion occurs at the hot, left boundary. A supersonic, shockless, decelerating wave of reaction (a weak detonation) emerges from the explosion site, and within it there is a strong coherence among the profiles of pressure, temperature, reaction progress and reaction rate (figure 2 a). As the wave slows to the CJ velocity a weak shock appears within it at the rear of the reaction zone (figure 2 b), accelerates and strengthens rapidly, and moves towards the head of the reaction zone (figure 2 c). Within a very short time the wave transitions into a ZND detonation travelling at the CJ speed (figure 2 d).

**Large gradient, $a = 4$**

In this case the wave starts out as a low-amplitude pressure pulse (figure 3 a), generated by the explosive energy release within the initial, nearly-constant pressure explosion at the hot wall. As the pulse advances into the reacting medium it amplifies and its leading edge steepens into a shock (figure 3 b). The rising pressure within the pulse, caused by an acceleration in the reaction rate, leads to the formation of a second shock (figure 3 c). Collision of the two shocks produces an overdriven wave which relaxes in due course to the CJ speed (figure 3 d).

Very large gradients produce an essentially constant-pressure, deflagrative wave.
Figure 2: Evolution of detonation in a planar geometry, for $a = 0.38$. Profiles of pressure $p$, temperature $T$, reaction progress $\lambda$ and reaction rate $rr$ are displayed at increasing times from panel (a) to panel (d).

Figure 3: Evolution of detonation in a planar geometry, for $a = 4$. Profiles of pressure $p$, temperature $T$, reaction progress $\lambda$ and reaction rate $rr$ are displayed at increasing times from panel (a) to panel (d).
3.2 Evolution in the annulus

3.2.1 Circumferential gradient

We first consider the case of the annulus heated to a uniform temperature, upon which is superimposed a circumferential gradient. Thus the initial conditions for the post-cookoff phase are of the form

\[ p = 1, \quad u = v = 0, \quad \lambda = 0, \quad T = 1 - \frac{\epsilon \alpha \vartheta}{\pi}, \]

where \( \alpha \) now measures the strength of the circumferential gradient on the small, \( \epsilon \) scale. We consider two values of \( \alpha \).

Figure 4: Initial temperature profile for moderate gradient. The temperature decreases from \( T = 1 \) at \( \vartheta = 0 \) to \( T = 0.9772 \) at \( \vartheta = 1 \).

**Moderate gradient, \( \alpha = 0.38 \).** The evolution can be understood by examining the panels in figure 5, in which distributions of \( p \) and \( \lambda \) are displayed at increasing values of time. Following an induction period consisting of weak chemico-acoustic interaction, the evolution begins (as in the moderate-gradient planar case discussed above) as a decelerating reaction wave, or weak detonation, originating at the hot boundary \( \vartheta = 0 \) (panel a). One notices a strong coherence between the profiles of \( p \) and \( \lambda \). The larger temperature gradient at the inner boundary results in more rapid deceleration and hence higher pressure there, and as the wave proceeds, there is some acoustic release of pressure from the inner towards the outer boundary. The first appearance of a shock at the inner boundary can be seen in panel (b). The maximum pressure of 6.4 there is lower than the CJ value of 7.13 because of the radial release. As the shock strengthens and the wave transitions into the ZND structure near the inner wall, further deceleration there is halted. At the same time, the shock also travels radially outwards (panel c) into the portion of the wave that is still undergoing retardation. In panel (d) the transition of the wave into a curved, ZND front appears to be complete. Panel (e) shows the reflection of the detonation from the outer wall. The reflection appears to be regular, and the reflected shock is clearly seen in panel (f). In panel (g) the detonation has reflected from the symmetry boundary \( \vartheta = \pi \) and the evolution is nearly complete.
Figure 5: Detonation evolution in a moderate circumferential temperature gradient corresponding to $\alpha = 0.38$. Panels (a) – (g) display the distributions of pressure $p$ and progress variable $\lambda$ at increasing times. The color bars appearing on the right-hand side of each panel are static for $\lambda$, covering the interval $[0, 1]$, but dynamic for $p$, depending upon the range of pressure involved.
Large gradient, $\alpha = 3.5$. The initial profile for the large-gradient case is displayed in figure 6, and the time-evolution in the panels of figure 7. Following the induction period, we now see the appearance of a pressure pulse at the hot boundary, panel (a). The broad pulse has a larger rise in pressure at the leading edge than the drop in pressure at the trailing edge, has a higher pressure peak along the outer wall and extends considerably beyond the reaction front. In panel (b) the leading edge has stretched into a ramp near the inner wall but remains sharp along the outer wall, where the peak now appears closer to the trailing edge. The reaction zone also appears to coincide with the trailing edge. Two pressure peaks of nearly equal strengths appear along the outer wall in panel (c), one in the middle of the pulse and the other close to the trailing edge. Pressure is nearly constant in the fully-reacted region, and near the inner wall the leading ramp continues to lengthen. The rear pressure peak has become stronger in panel (d) and is followed by a reaction zone in which the pressure falls. Along the inner wall the large initial temperature gradient appears to have led to a reaction wave in which there now remains only a weak pressure drop across the reaction zone. Panel (e) shows a sharp rise in pressure (a local explosion) at the outer wall, while pressure at the inner wall remains low. A curved detonation wave emerges from the site of the local explosion, moving circumferentially forwards and radially inwards, panel (f). In panel (g) the detonation has just undergone a regular reflection at the inner wall, leading to a large pressure increase there. This regular reflection transitions into a mach reflection in panel (h), and there are signs of a similar reflection at the outer wall. The reflections flatten the wave temporarily, panel (i). In panel (j) we continue to see a mach reflection on the outer wall, but a reduction in the peak pressure at the inner wall as the wave undergoes diffraction there. In panel (k) the diffraction at the inner wall has caused the wave to fail there, as seen by an increasing gap developing between the reaction front and the leading shock. However, reflection at the symmetry boundary produces a detonation that advances into and consumes the the dead zone, panel (l).

Figure 6: Initial temperature profile for large gradient. The temperature decreases from $T = 1$ at $\vartheta = 0$ to $T = 0.790$ at $\vartheta = 1$. 
Figure 7: Detonation evolution in a strong circumferential temperature gradient corresponding to $\alpha = 3.50$. 
3.2.2 A hot spot

![Figure 8: A hot spot superimposed upon a radial temperature distribution.](image)

We now turn to an exploration of the manner in which the insertion of a hot spot into an otherwise radial thermal field affects the evolution. The initial temperature distribution is shown in figure 8. It corresponds to a radial variation from 0.930 on the inner boundary to 0.950 on the outer boundary, on which is superimposed a hot spot with a temperature maximum of unity, situated at mid radius on $\vartheta = 0$. On the $\epsilon$ scale the imposed circumferential gradient has the value 1.1 compared to the radial value of 5.5 between the hot spot and the outer boundary.

The results of the computation are shown in panels (a) – (j) of figure 9. Following an induction delay a finger-shaped reaction front, circumferentially long and radially slender, emerges from the hot spot, panel (a). The associated pressure disturbance is wider in the radial direction, in keeping with the stronger radial temperature gradient applied initially. Panel (b) shows the pressure disturbance reflecting from the radial boundaries, and surging ahead of the reaction front in the circumferential direction. Collision of the two laterally reflected disturbances causes the pressure behind the leading front to rise. Panel (c) shows that the outer wall, acting as a converging channel, produces a stronger reflection than the inner wall. Panel (d) shows a continuing strengthening of the pressure peak behind the lead wave, and in panel (e) one sees the beginning of a local explosion at the tip of the reaction front. The explosion has transitioned into a detonation in panel (f). Observe that the very large initial radial gradient in temperature results in only a very slow radial spreading of the reaction front. In panel (g) the detonation is about to reflect from the outer boundary. The reflection generates a backward-propagating detonation as well, which consumes the thin ribbon of explosive adjacent to the outer boundary. Reflection of the forward wave from the inner boundary is imminent in panel (h), and following reflection, a second backward-propagating detonation along the inner wall can be seen in panel (i). The three-front system is now well-established to consume the remaining explosive, panel (j).
Figure 9: Detonation evolution due to a hot spot embedded in a radial temperature gradient.
4 Closing Comments

By means of well-resolved numerical computations, it has been shown that even weak temperature nonuniformities generated during cookoff can have a substantial impact on the manner in which an explosive event unfolds in an annular configuration. Results have been presented for three representative situations, two corresponding to purely circumferential initial temperature gradients of different sizes, and the third corresponding to a hot spot embedded in a radial temperature field. In each case the lack of simultaneity in ignition leads to the generation of a reaction wave that ultimately transits into a detonation, although the precise transition scenarios are quite different. Preliminary results for a slab configuration ease interpretation of results for the annulus. The explosive has been modelled as a homogeneous, polytropic fluid with a one-step, Arrhenius rate law, and attention is restricted to temperature inhomogeneities. It is recognized that a mechanically complex explosive, capable of suffering thermal damage during cookoff, may well behave differently.

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Reference