THE STRUCTURE OF DETONATION WAVES

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Résumé

Des simulations numériques multidimensionnelles dépendantes du temps ont été utilisées pour étudier l'initiation, la propagation et l'extinction des détonations en phase gazeuse et liquide. A l'aide des simulations, qui calculent le comportement détaillé de l'interaction des ondes de choc avec les zones réactives formant l'onde de détonation, on étudie l'évolution de l'instabilité qui conduit à la structure cellulaire des détonations. Les simulations portent sur les solutions à deux dimensions, dépendantes du temps, des équations de transport de convection de la densité de masse, de la densité de moment et de l'énergie couplées à des modèles de libération d'énergie chimique. Les équations de transport de convection sont résolues selon l'algorithme "Flux-Corrected Transport". Les réactions chimiques et la libération de l'énergie sont habituellement modélisées par le modèle du paramètre d'induction à deux étapes. En conclusion, le comportement de la structure multidimensionnelle d'une détonation dépend des différences entre les propriétés thermodynamiques dans les zones d'induction derrière la ligne de Mach et le choc incident. La formation de poches non réactives derrière le front de détonation dépend de l'inclinaison des ondes transversales et de la courbure des fronts de choc. Des fronts fortement incurvés peuvent entraîner de grandes poches. La dépendance en température du temps d'induction est un facteur majeur pour la régularité de la structure de détonation. La structure de détonation est affectée par les paramètres de libération d'énergie. Une libération instantanée d'énergie conduit à des structures monodimensionnelles. Une libération rapide de l'énergie donne des structures moins régulières. Une libération très lente de l'énergie entraîne de grandes poches, des fronts fortement incurvés, et la détonation peut s'éteindre.

Abstract

Multidimensional time-dependent numerical simulations have been used to study the initiation, propagation, and extinction of detonations in gases and liquids. The simulations, which calculate the detailed behavior of the interacting shock waves and reaction zones forming the detonation wave, are used to study the evolution of the instability that leads to the cellular structure of detonations. The simulations consist of two-dimensional time-dependent solutions of the convection of mass density, momentum density and energy coupled to models for chemical energy release. The convective transport equations are solved by the Flux-Corrected Transport algorithm. The chemical reactions and energy release are usually modelled by the two-step induction parameter model.

We conclude that the behavior of the multidimensional structure of a detonation depends on the differences of the thermodynamic properties in the induction zones behind the Mach stem and the incident shock. The formation of unreacted pockets behind the detonation front depends on the inclination of the transverse waves and the curvature of the shock fronts. Highly curved fronts may result in large pockets. The temperature dependence of the induction time is a major factor in the regularity of detonation structure. Detonation structure is affected by the energy release parameters. Instantaneous energy release leads to one-dimensional structures. Fast energy release results in less regular structures. Very slow energy release results in large pockets, highly curved fronts, and the detonation may die out.

1. Introduction

In this paper we summarize some of the interesting features of the structure of multidimensional propagating detonation waves in liquids and gases that we have learned from numerical simulations. A major strength of a simulation is that it is an excellent vehicle for looking at fundamental interactions in a systematic way. Thus we can isolate the major, controlling processes, and study their interactions in idealized environments. Once this is done, additional complexities may be added. In this chapter we emphasize calculations that have been done to help clarify the fundamental interactions between the fluid dynamic and chemical processes occurring in a gas-phase detonation. The research has been carried out by the authors, J. Boris, T.R. Young, J.M. Picone, and C.W. Oswald, under sponsorship from the Naval Research Laboratory through the Office of Naval Research.

This paper has four parts. First, we briefly describe the equations that must be solved, the assumptions that go into the model formulation, and some properties of the numerical solution. We then describe three important aspects of detonations waves: the development of cellular structure, the importance of transverse waves, and some potential causes of irregularity in detonation structure.

2. Problem Formulation and Numerical Solution

Numerical simulations of detonations are based on solutions of the compressible, time-dependent, conservation equations for total mass density ρ , momentum density $\rho\mathbf{v}$, and energy E ,

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \rho\mathbf{v} , \quad (1)$$

$$\frac{\partial \rho\mathbf{v}}{\partial t} = -\nabla \cdot (\rho\mathbf{v}\mathbf{v}) - \nabla P , \quad (2)$$

$$\frac{\partial E}{\partial t} = -\nabla \cdot (E\mathbf{v}) - \nabla \cdot (\mathbf{v}P) , \quad (3)$$

where $\mathbf{v}$ is the fluid velocity and P is the pressure. In a multispecies fluid, chemical reactions effect transformations among the species, we also need individual species number densities $\{n_i\}$

$$\frac{\partial n_i}{\partial t} = -\nabla \cdot n_i\mathbf{v} + Q_i - L_i n_i , \quad i = 1, \dots, N_s , \quad (4)$$

where the $\{Q_i\}$ and $\{L_i\}$ are chemical production and loss terms, respectively, for species i . The effects of molecular diffusion have been omitted from these equations because it is generally insignificant on the timescales of interest for detonations. There is a constraint which defines the total number density N ,

$$N = \sum_{i=1}^{N_s} n_i , \quad (5)$$

where N_s is the total number of different kinds of species present. The total energy is a sum of the kinetic and internal energy,

$$E = \frac{1}{2} \rho\mathbf{v} \cdot \mathbf{v} + \rho\epsilon , \quad (6)$$

where ϵ is the specific internal energy.

An ideal gas equation of state is used for the gas phase calculations,

$$P = NkT = \rho RT \quad (7)$$

Also, we assume

$$\rho\epsilon = \sum_i \rho_i h_i - P = \rho h - P \quad (8)$$

$$h_i = h_{i0} + \int_{T_0}^T c_{pi} dT, \quad (9)$$

so that the properties of the individual species are taken into account. Here k is Boltzmann's constant, $\{h_i\}$ are the enthalpies of each species i , $\{h_{i0}\}$ are the heats of formation, and $\{c_{pi}\}$ are the specific heats.

We also describe calculations of detonations in liquid nitromethane, for which we use a HOM equation of state (see Mader, 1979) for both the condensed fuel and the products. The equations of state for the condensed phase is based on the Walsh and Christian technique (1955). The equation of state of the gas products is constructed by solving the equilibrium CJ detonation problem using the BKW equation of state for the final products. The details of the equation of state are given in Guirguis and Oran (1983).

In all of the two-dimensional calculations described below, the full details of the chemical reactions are not included in the model. Instead, we use the induction parameter model that reproduces the essential feature of the chemical reaction and energy release process. In this model, three quantities must be tabulated as a function of temperature and pressure, and perhaps stoichiometry: the chemical induction time, the time of energy release, and the final amount of energy released. These may be obtained by integrating the full set of elementary chemical reactions, as we have done for hydrogen-oxygen combustion, or they may be gathered from experimental data, as we have done for liquid nitromethane. Then a quantity called the induction parameter is defined, which is convected with the fluid in a Lagrangian manner and keeps track of how long and at what temperature a fluid element is heated. When the element is heated long enough, energy release is initiated. This model for including the properties of a chemical reaction mechanism in a numerical simulation was described originally by Oran et al., (1981), and has been developed further by Kailasanath et al. (1985a,b) and Guirguis et al. (1986).

The crux of being able to simulate the multidimensional structure of detonations is solving coupled continuity equations for density, momentum, and energy with enough accuracy (Oran and Boris, 1987a,b). The numerical solution of continuity equation, which is by far the most difficult part of solving Equations (1) - (4), has been the subject of zealous arguments for the last twenty years. The problem occurs because both numerical diffusion and numerical dispersion, arising from the Eulerian finite-difference formulation, must be controlled. In addition, there are unavoidable Gibbs errors which arise simply because we are using a finite representation.

The most straightforward finite-difference approaches do not work for solving the continuity equation. The fundamental problem was stated originally by Gudonov: a linear algorithm cannot be monotone unless it is first order so that numerical diffusion damps the unphysical oscillations due to numerical dispersion. To solve shock and detonation problems, higher-order accuracy is needed, but we cannot tolerate the oscillations introduced by numerical dispersion. More complicated, nonlinear approaches are required which impose the physical requirements of positivity and monotonicity on the finite-difference algorithm itself. Flux-Corrected Transport (FCT) (see, for example, Boris, 1971; Boris and Book, 1976) was the first algorithm to do this, and since its appearance a number of algorithms have emerged based on these same principles. The Flux-Corrected Transport algorithm was used in all of the calculations presented below.

3. The Development of Cellular Structure

The front of a self-sustained propagating detonation in an energetic gas, and certainly in some energetic liquids, is not uniform. Its structure is complex and multidimensional, involving

several shocks continuously interacting with each other and the boundaries of the region through which the detonation is moving. The triple points formed at the intersection of these shocks, designated as incident shock, Mach stem, and transverse wave, trace out patterns that are called detonation cells. These structures may be degenerate for certain material conditions or if the detonation is heavily overdriven, but they can occur in all self-sustained gas-phase detonations. Extensive experimental data (see, for example, Strehow (1984) and Fickett and Davis (1979)) have shown that the size and regularity of this cell structure is characteristic of the particular combination of initial material conditions, such as composition, density and pressure.

Planar detonation fronts are unstable to perturbations in the transverse directions. One result of this is that given an initially planar front, a perturbation causes it to depart from a one-dimensional configuration. Consider Figure 1, which shows a series of pressure contours from a numerical simulation of the early effects of perturbing a planar detonation front (Kailasanath et al., 1985a). This simulation was initialized by placing an elliptical pocket of hot, unburned gas behind a planar detonation. The pocket, which was merely used as a device for initiating the perturbation, burns slowly and sends out pressure disturbances in all directions. These waves interact with the incident shock front causing the front to curve outwards. The pressure waves also reflect from the side walls of the channel and move transverse to the incident shock front, as seen in frame 2 of the figure. These pressure waves are strengthened due to collisions with each other and further increase the curvature of the incident shock front, as can be seen in frame 7. After a short time, a portion of the incident shock reflects from the side walls of the channel. Frame 8 shows a Mach reflection that has been formed between the pair of triple points. The reflected shock waves, which are the transverse waves, are initially weak but are later strengthened due to collisions with each other and the walls.

The further evolution of the pair of triple points is shown in Figure 2. The path and the direction of movement of the triple points are indicated by the lines with arrows. In the first frame, the transverse waves are moving towards each other and away from the wall. By the fourth frame they have collided with each other and are moving away from the center of the channel. In frame 7 they are again moving towards the center after colliding with the walls. Frames 7 and 8 are similar to frames 1 and 2, respectively, showing that an equilibrium configuration detonation has been established.

Calculations by Taki and Fujiwara (1981) describe a system with a number of exothermic spots, located across the path of the detonation, that perturb the planar detonation wavefront. Again, the system evolves into a group of triple points.

In the numerical simulations, the multidimensional structure can be initiated in many different ways. This includes perturbations in front and behind planar detonations, oblique shocks which transition to detonations, and explosions in corners. There have been two main approaches. The first is to set up a propagating planar detonation with some kind of a perturbation either behind or in front of it (e.g., Taki and Fujiwara, 1981; Kailasanath et al., 1985a,b). The second approach is to set off a shock or explosion in a homogeneous detonable mixture, and watch the evolution to a detonation (Oran et al., 1982). Studies for the first type of calculation have shown that the eventual detonation cell structure that forms is apparently independent of the initial perturbation, as long as the transverse perturbations are strong enough. This same result was achieved for the second method, as long as the energy deposition requirements were met well enough to detonate the material.

These calculations have shown that the number of triple points initially formed depends on the number and symmetry of the obstacles perturbing the planar flow. However, the calculations seem to indicate that the system relaxes toward a final state that is independent of the initial conditions. For example, the calculations by Kailasanath et al. (1985b) show that the system

Figure 1. A composite of eight "snapshots" of the pressure contours near the detonation front at intervals of $10\ \mu\text{s}$ for the early stages of the formation of a pair of triple points. The detonation is propagating in a 65 torr (8.66 kPa), 298 K stoichiometric hydrogen-oxygen mixture diluted with 60% argon (Kailasanath et al., 1985a).

Figure 2. A composite of pressure contours at later times than those shown in Figure 1. The lines with arrows show the movement of the triple points (Kailasanath et al., 1985a).

prefers to relax to a final state that is symmetric about the centerline of the tube. A typical evolution to a symmetrical solution is shown in the set of calculations by Kailasanath et al. (1985b) which modelled detonations in 5 and 10 cm tubes. The initial configurations studied are shown in Figure 3. Configurations (a) and (b) were the same, except that in case (b) the disturbance was asymmetric. The evolution of the perturbed detonation started out very different. Figure 2 shows the evolution of (a), and Figure 4 shows the evolution of (b). However, (b) goes by through a gradual change in the number and pattern of triple points and eventually becomes the symmetric cell structure seen for case (a).

The effect of changing the channel width is studied by simulating planar detonations interacting with hot spots shown in cases (b) and (c) in Figure 3. Here (b) is half of (c) and if the wall is truly a line of symmetry, the solution of (b) should be the upper half of (c). The result of (c) was a symmetrical pattern with a full cell centered in the tube and partial structures above and below it. In case (b), the triple point structure started out looking like the upper half of (c), but soon deviated and went to a structure corresponding to case (a). The conclusion is that for the dilute $H_2 - O_2 - Ar$ mixture studied, and with the restriction to two dimension and a fixed

Figure 3. Schematic of the initial conditions used to initiate the multidimensional structure of detonations (Kailasanath et al, 1985a). (a) Symmetric perturbation behind a planar front in a 5 cm tube; (b) an asymmetric initiation, (c) a symmetric initiation in a 10 cm tube.

Figure 4. Pressure contours for a detonation in a 5 cm wide channel initiated using the asymmetric pocket (Kailasanath et al., 1985b).

channel width, the wave structure tries to go to a natural mode of the system. For some other chemical systems this could take an inordinately long time, and the results might appear chaotic.

The triple point pattern in the 5 cm tube is summarized in Figure 5A. We see that the triple point structure does not appear to reflect immediately when it hits the wall, and a complete detonation cell has not been formed. A time and space gap appears at the walls as the structure reforms. (The formation of this incomplete cell is discussed further below). Increasing the width of the channel to 7 cm, as shown in Figure 5B, considerably reduces the gap in the path of the triple points near the walls. Finally, the locus of the triple points for a 9 cm wide channel, shown in Figure 5C, forms a complete detonation cell and what appears to be partial structures above

Figure 5. Calculated paths of triple points for detonation propagation in (A) 5 cm wide channel, (B) 7 cm channel, and (C) 9 cm channel.

and below it. From the figure we estimate the cell width and length to be about 8.5 cm and 19.6 cm, respectively.

4. The Importance of Transverse Waves

One surprising feature of the calculations shown in Figure 5 is the flattened shape of the cell when the channel width is less than what appears to be a natural cell size. To better understand the factors that determine the shape of the cell and thus the calculated cell size, we must look at the curvature of the transverse wave as it reflects from the wall or from another transverse wave. For the purposes of this explanation, we call that portion at and close to the triple point, the "head" of the transverse wave, and we call the "tail" that region of the transverse wave extending back towards the burned material, as shown schematically in Figure 6. This is based on the temperature, density and pressure contours from calculations for the 5 cm tube. First the transverse waves are moving towards each other (a), and the distance between the two heads is larger than the distance between the two tails. It appears the tails may collide with each other earlier than the heads. After the collision (c) the curvature of the transverse wave is reversed and the heads are closer to each other than the tails. Comparing figures (b) and (c), we see that the curvature of the transverse wave is reversed at or around the time of collision. Figure (d) shows the situation in which the tails collide with and reflect from the walls earlier than the heads. Such a reflection causes a larger pressure difference around the tail than across the unreflected front segment. This high-pressure region pushes the incident shock front forward and results in the flattened detonation cell seen in Figure 5.

As the width of the tube is increased, the transverse wave can travel faster, become weaker before collision, and the inclination of the transverse wave to the channel walls is less. If the

Figure 6. Schematic diagram corresponding to selected contours from the calculation of the 5 cm wide channel showing the structure of the transverse waves at the detonation front.

channel width is increased so that it is slightly larger than the detonation cell width, we expect new triple points to be generated in the shocked material in the direction ahead of the transverse waves. Explosion can occur only in compressed unreacted regions. This produces a new pair of transverse waves that propagates toward the two transverse waves already present in the system. The new and old waves then collide with each other, rendering the transverse wave spacing equal to the detonation cell width. Therefore in a channel slightly larger than the detonation cell width we would observe four transverse waves at certain periods in the detonation cell cycle as well as a complete detonation cell within the channel. This is what is seen in Figure 5c.

In the 9 cm channel shown in Figure 5 we also observed the presence of unburned gas pockets near the walls behind the detonation front. Such unburned gas pockets have been observed earlier both in experiments and in numerical simulations (Subbotin, 1975, Oran et al., 1982; Hiramatsu et al., 1984). The origin of these pockets in this calculation can be explained by extending the argument used above on the inclination of the transverse wave. Consider a case for which the channel width is slightly larger than the detonation cell width. In this case, a transverse wave moving towards the walls, which does not encounter another transverse wave moving in the opposite direction, continues to propagate though considerably weakened. The incident shock is also considerably weakened and hence the reaction zone ahead of the transverse wave also falls way behind. If the head of the transverse wave reflects earlier than the rear segment, the portion of the gas near the head of the transverse wave burns first, effectively cutting off a gas pocket. The formation of unburned gas pockets has been discussed in detail elsewhere (Oran et al., 1982; Kailasanath et al., 1985b) for the same gas mixture at the same initial temperature and pressure used in these calculations.

5. Irregularity in the Structure of Detonation Waves

Most of the experimental results showing detonation cells do not show the regular structure we have seen in the calculations shown above, but show irregular structure in which the size of a cell is not clearly determined. In the experiments, the regular cell patterns appear in the highly diluted argon mixtures of hydrogen and oxygen, as we have predicted in the calculations. If the mixture is less dilute, or argon is replaced by molecular nitrogen, the structure again becomes irregular.

Some insight into the mechanism causing the irregularity of the structures was provided by the recent work of Guirguis et al. (1986, 1987a) that studied detonation cell structure in liquid nitromethane. In this case, the parameters for the induction parameter model were taken from ex-

Figure 7. Pressure contours of a detonation wave propagating in a channel filled with liquid nitromethane. Solid traces are loci of main triple points, dashed traces are loci of secondary triple points. Induction time and energy release parameters derived from experimental data. (Guirguis et al., 1986, 1987.)

perimental data, as opposed to being derived from a detailed chemical reaction mechanism. Guirguis defined two quantities, the induction parameter, defined in the form, $\tau_i = A^i \exp(E^i/RT)$, and an energy release time, which also had an Arrhenius form, $\tau_r = A^r \exp(E^r/RT)$. The initial calculations were performed with the experimentally derived values of the τ_r and τ_i , and typical results are shown in Figure 7. The outstanding feature of this figure is that the structure appears very irregular. The solid lines drawn through the pressure contours outline the movement of the stronger triple points, and the dashed lines indicate weak triple points.

Numerical tests in which the timestep and computational mesh spacing were varied proved that these results are a physically correct property of the calculation, and not numerically induced. The next question is what is the origin and what controls this structure. Figure 8 shows the results of increasing the value of E^i in the expression for the induction time. This has the effect of increasing the difference of the size of the induction zones behind the Mach stems and reflected shocks. The structure is now quite regular and qualitatively similar to the dilute hydrogen-oxygen calculations described above. An interesting feature of this calculation is the formation of large unreacted pockets behind the propagating detonation front, which was not really seen in the calculations represented in Figure 7. The formation of such a pocket is shown in Figure 9, which shows how they form as two triple points collide.

Similar studies were carried out which varied the energy release parameters. From these,

Figure 8. Pressure contours of a detonation wave propagating in a channel filled with liquid nitromethane with modification to the temperature dependence of the experimentally derived induction time. (Guirguis et al., 1986, 1987.)

Figure 9. Pressure and temperature contours behind the detonation wave, showing the collision

we found that detonation structure is also affected by the energy release parameters, A_r and τ_r . Instantaneous energy release leads to a one-dimensional structure. Very fast energy release results in less regular structures, and very slow energy release results in large pockets and highly curved fronts. In this last case, the detonation may die out.

The obvious question now is what can we say about irregularity in the gas phase. To answer these questions, we have been doing calculations of detonations in hydrogen-oxygen diluted with argon, as above, and compared these to calculations of hydrogen-oxygen diluted with nitrogen, which we know gives irregular structures (Guirguis et al., 1987b). The calculations indicate that the nitrogen dilution has a tendency to give irregular structures. This result indicates that the multidimensional structure of a detonation depends on the differences of the thermodynamic properties in the induction zones behind the Mach stem and the incident shock. Whereas the chemical induction times for equivalent nitrogen and argon dilutions are the same, the rate and the amount of energy release are different, and so are the relative sizes of the induction zones behind the Mach stem and incident shock and different for argon and nitrogen dilution.

6. Summary

From our two-dimensional calculations of the structure of propagating detonations in liquids and gases, we have been able to conclude:

- The multidimensional structure of a detonation depends on the differences of the thermodynamic properties in the induction zones behind the Mach stem and the incident shock.
- The formation of unreacted pockets behind the detonation front depends on the inclination of the transverse waves and the curvature of the shock fronts. Highly curved fronts may result in large pockets.
- The temperature dependence of the induction time is a major factor in the regularity of detonation structure.
- Detonation structure is affected by the energy release parameters. Instantaneous energy release leads to one-dimensional structures. Fast energy release results in less regular structures. Very slow energy release results in large pockets, highly curved fronts, and the detonation may die out.

Future work will continue the gas-phase studies, and we also hope to extend the work to three-dimensions.

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Commentaire - G. DUPRE

You talked about the difference in regularity of detonation structure between $H_2/O_2/Ar$ and $H_2/O_2/N_2$ systems, saying that comes from the size in induction zone.

Experimentally it has been seen that $H_2/O_2/Ar$ systems give much more regular structure than $H_2/O_2/He$ systems. How can it be explained? Can you predict that from your computations?

An interesting experiment would be to look at the influence on structure regularity by changing the nature of the monoatomic diluent, that is He, Ne, Ar, Kr.

Conclusion : Synthèse de la discussion - C. FAUQUIGNON

- Gaz* : Importance dominante de la structure cellulaire plus ou moins régulière.
Effort actuel pour lier la dimension de la cellule aux conditions aux limites, aux propriétés thermodynamiques, à la cinétique réactionnelle du milieu.
- Liquide* : Mécanisme réactionnel complexe du nitrométhane qui pourrait expliquer l'impossibilité d'utiliser l'énergie d'activation unimoléculaire classique dans le calcul du temps d'induction.
- Solide* : Mécanisme séquentiel à points chauds (hétérogénéité) ignition (ou explosion thermique) combustion, équilibre (plan sonique de Chapman Jouguet).
Question d'actualité : non idéalité par suite de la différence entre les cinétiques de condensation du carbone et, chimique, de formation des produits de réactions (cinétique lente dans le premier cas et cinétique ultra-rapide dans le second).