ON CAVITY COLLAPSE AND SUBSEQUENT IGNITION

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The collapse of a void within a reactive material has the potential to start local burning leading to partial reaction or run to detonation. There are three main features of the collapse that provide a means for ignition. The first is the formation of the high-speed jet and elevated velocities in the convergent flow around the wall of the cavity. This gives rise to heating in viscous materials. The second is the shock-heated region at the point of jet impact in an asymmetric collapse. The third is the compression of any gaseous or vapour content. These effects have been studied and experiments showing examples of each of these modes of heating giving rise to local reaction are described. Once ignited, a burning front may be quenched or may accelerate so that a transition to detonation may occur according to the confinement of the material.

INTRODUCTION

A range of modern devices may have energetic materials added in one of the following forms. The first is a pressed assemblage of explosive grains, the second is a melt-cast filling and a third is a composite, plastic-bonded explosive (PBX). These particular means of filling mean that the explosive is not a homogeneous pure material. Rather it contains different phases, included porosity and possible entrained gas. Additionally it may have been mechanically damaged during manufacture or handling. Each phase clearly has different thermal and mechanical behaviour and thus the formation of a composite may lead to increased localization such as shock focusing.

A mechanical insult results in the propagation of waves through these composite fillings. At the grain scale, the wave encounters a miscellany of phases of variable impedance and this has been illustrated in meso-scale simulations[1-3]. Sites from which propagating reaction occurs (critical hot spots) resulting from a series of mechanisms have been shown to scale with the grain size[2]. Further, the high-rate response associated with initiation occurs in a thin region consisting of only a few grains of material. The physical mechanisms by which energy is dissipated may include friction, the collapse of gas or vapour bubbles, adiabatic shear or electrical mechanisms. In a composite material, localization of energy may occur due to shock focusing and plastic work as material flows into interstitial regions[1]. Smaller crystals give rise to lower sustained stresses and temperatures since closer particle boundaries result in faster release. Since thermal conduction cools the heated zone, it is competition between energy localization and dissipation that dictates the initiation and sustaining of reaction[2].

Bowden and Yoffe[4] realised that bulk heating was insufficient to account for observed ignition or initiation. They hypothesized that application of a mechanical stimulus localized energy at some inhomogeneity in a condensed-phase explosive, which they dubbed a hot spot. Through a series of experiments they determined a range of bounding parameters upon the geometry and temperature required. In the case of the materials they studied, the hot spots were of size 0.1 - 10 μm, time duration 10 μs - 1 ms and a minimum temperature of 700 K. For the case of mechanical loading, many sites thus exist but only a few form *critical* hot spots from which propagating reaction ensues.

The collapse of cavities within a material is one of most important of the hot spot production mechanisms identified above. There has been a series of papers in which shock-induced collapse of single spherical bubbles and cavity arrays has been studied[5-10]. There are three main features of the collapse that provide a means for ignition. The first is the formation of the high-speed jet and elevated velocities in the convergent flow around the wall of the cavity. This may give rise to heating in viscous materials[11]. The second is the shock-heated region at the point of jet impact in an asymmetric collapse[12]. The third is the compression of the gaseous or vapour content of the cavity[13]. These effects have been studied[10] and experiments, showing examples of each of these modes of heating giving rise to local reaction are described below.

The morphology of voids within PBXs is generally regarded as spherical. However, given the angular nature of for instance monoclinic HMX crystals, materials that have been pressed or mechanically loaded in some manner, the void shape is likely to be more irregular. Thus although it is easiest to study spherical bubbles, in general arbitrary shapes should be considered. In most materials the effects of strength may be ignored in comparison with the strength of the shocks applied so that inert and explosive liquids and gels are used in this work.

In composite explosives, continuum analytical descriptions of response based upon measurements of state variables with present macroscopic sensors are insufficient as the measured quantity is averaged over the large sensor area[3]. Equally, measurements of the states at free-surfaces, where conditions approach uniaxial stress, or windows are not representative of bulk conditions which are uniaxial strain[3]. Thus, whilst the new generation of sensors and experiments is under development, it is necessary to probe operating mechanisms at the macroscale to validate modelling for investigation of the mesoscale. The goal of this work is to track the formation of thermo-mechanical hot spots as a result of planar shock loading of variable geometry voids and thus to further understand the processes operating in heterogeneous initiation. However, the voids studied here are large and effects such as viscosity will operate at the mesoscale.

EXPERIMENTAL

The experiments described were carried out in two and three-dimensional geometries. One of the goals of this investigation was to view temperatures generated as a result of collapse of cavities by an incident shock. For this reason, a disc-shaped cavity allowed observations of jet formation, shock and reaction within the cavities. A prepared gel slab with introduced cavity was then clamped between glass or polymethyl-methacrylate (PMMA) blocks and plane shock waves were introduced into the sheets by the impact of a flyer plate from a gas gun. In other experiments, where higher pressures were required, the shock was introduced using an explosive plane wave lens and a calibrated inert gap.

One practical problem this work aims to address is the impact-induced initiation of energetic matrices. Thus, in some experiments a 3 mm thick layer of an ammonium nitrate (AN) emulsion explosive (described elsewhere[7, 10] was contained between two, 25 mm thick PMMA blocks. High-speed framing photography at microsecond framing rates recorded the light emitted by the ignited sites. Schlieren was used to visualize the shock in some experiments whilst no external lighting was used for the ammonium nitrate (AN) experiments where reaction occurred.

NUMERICAL

Numerical studies are performed using a multi-material Eulerian hydrocode. Benson[5] loosely defines a hydrocode as a tool for solving large deformation, finite-strain transients that occur on a short timescale. This accurately defines bubble collapse problems. The equations and algorithms commonly used in hydrocodes are also introduced in Benson's review. In addition to these basic algorithms the hydrocode also has to make use of appropriate material models. The equations of state and constitutive models for the materials present in the experiment are equally important and can be a study in their own right. In this paper existing material models are used. The chemistry of the cavity gases is modelled using elements of the Chemkin II suite of programs[14]. For problems involving explosives, a model for chemical kinetics leading to explosive energy release is also needed. Again appropriate results from the literature are used.

In this study both low (*ca.* 0.3 GPa) and high pressure (*ca.* 8 GPa) shock impact on cavities of order 10 mm in diameter is considered (relatively large for explosives but allowing accurate experimental data to be acquired) thus providing good tests of the numerical models.

A schematic showing the geometry of the simulation is shown in figure 1 for the case of a circular cavity.

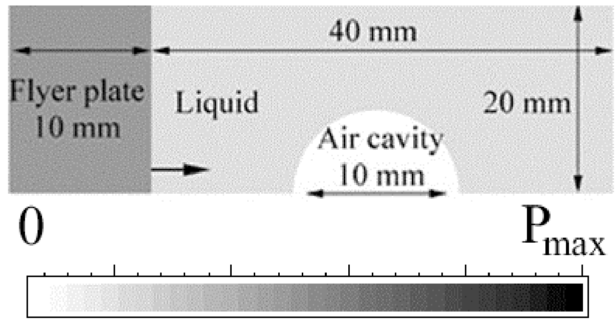

FIGURE 1. SCHEMATIC OF MODEL SYSTEM.

In all of the simulations presented below, a greyscale image of the variable considered is presented with white at ambient conditions and black at the highest value recorded, P_{max}, which is indicated in the text.

SINGLE CYLINDRICAL CAVITY

The collapse of a single cavity has been studied extensively[6, 15, 16]. The upper frames of figure 2 shows four frames (each 1 μs apart) taken from a sequence in which a 12 mm cavity containing air is collapsed by a 0.3 GPa shock. Initially the incident shock has swept the cavity from the left causing the upstream wall to accelerate and a semicircular shock to be launched. The wall involutes to form a jet which may be seen in frame 1. The general form of the collapse has been investigated experimentally in previous papers[6]. This work concentrates upon the later stages where the highest temperatures occur. By the first frame, the shock in the air has crossed the cavity and rebounded twice between the stationary downstream and the involuting upstream walls. Beneath each of the experimental frames is the equivalent snapshot from a simulation showing the bubble wall and the shocks in liquid and gas. The first of these shows the entry of the air shock into the semicircular wall to the rear of the cavity. The air shock interacts with the interface and there is the development of Mach reflections at the sidewalls crossing and strengthening the air shock. The liquid shock can be seen already ahead of the downstream cavity wall.

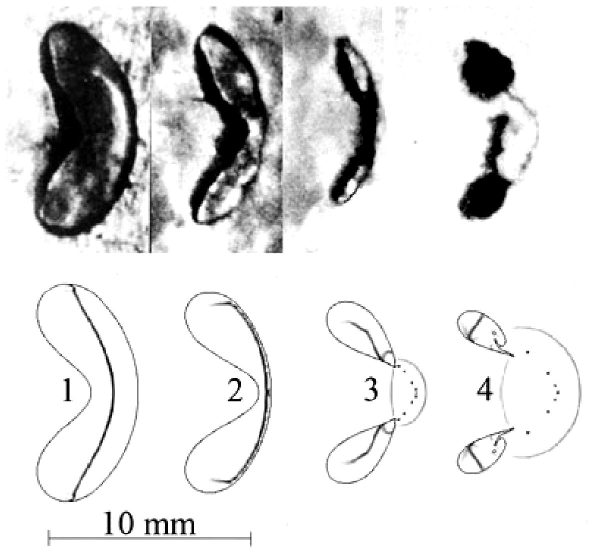

FIGURE 2. SINGLE CAVITY COLLAPSE.

As the sequence progresses, the jet and shock cross the cavity and by frame 2 they have almost reached the downstream wall. In frame 3 the jet penetrates it and shock waves travelling out from the impact point may be seen in the liquid. The pocket of gas becomes more rapidly compressed and a strong shock wave forms in the final two pockets of gas. It is at points in these lobes that the highest temperatures are reached. As can be seen, the highest temperature occurs after the jet penetration as the lobe isolated compresses. This position corresponds to that of maximum temperature.

Other experimental work has shown the presence of points of luminescence from within the enclosed interior gas soon after the jet impacts[6]. Ideal gas calculations show the gas temperature distribution to show the highest temperature achieved at the final point in the collapse of the lobe away from the symmetry axis. This corresponds to the position of the observed light emission. Calculations have also been carried out using equilibrium chemistry with a seven-species air model including electron production. This work has indicated that temperatures reach *ca.* 6000 K but only for *ca.* 100 ns[17].

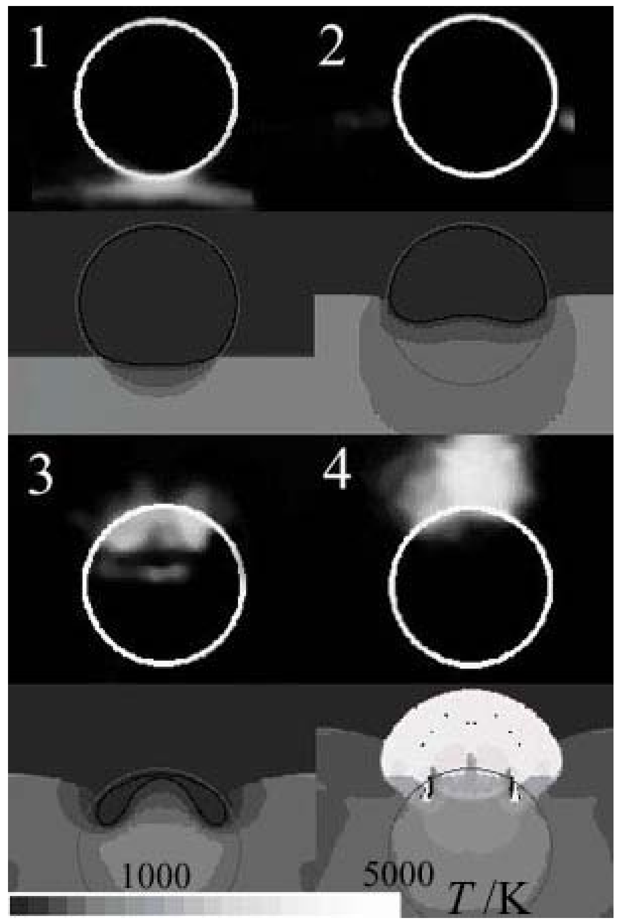

FIGURE 3. SINGLE BUBBLE COLLAPSE IN A REACTIVE MATRIX.

The highest temperatures and electron densities occur at the same positions within the collapsing lobes. Further, these are in identical regions and times as the experimentally observed flashes of light which acts as a validation for the simulation. The following experiment shows heating of an enclosed gas is not sufficient to induce propagating reaction in this case.

To illustrate qualitative features of the processes occurring, experimental data for collapse in AN emulsion is compared with simulations of collapse in nitromethane. As yet no accurate kinetic model is available for the AN emulsion. The experimental sequence of figure 3 shows 4 frames (1 µs apart) from the collapse of an air-filled cavity in AN. There is no lighting and thus in experiment and in the simulation the initial locus of the collapsing bubble is superposed as a lighter coloured circle. In frame 1, the 8 GPa shock front can be seen approaching the upstream cavity wall whilst in frame 2 it is approximately half way down it. The light here is believed to be from chemical reaction due to the rapid shock pressure jump. By frame 3, the collapse is nearing completion and the jet has crossed the cavity. There are two lobes of light which correspond to the heated gas region modelled above. The jet appears between these and is darker. In the last frame, after jet impact, there is a circular region of light centred on the impact point of the travelling jet.

The simulation records contours of temperature in the NM near to the state of minimum bubble volume (the time of peak gas temperature due to cavity collapse). The white shading corresponds to 2600 K and clearly shows the locus of ignition of the NM after jet impact in relation to the collapsed bubble. Since the ignition site is to the rear of the bubble and is moving rapidly as a result of jet impact, the growing combustion region is expected to reflect these conditions. This is confirmed both experimentally and numerically below.

OTHER GEOMETRIES

In a real assembly of crystals, whether pressed or within a PBX, entrained cavities are a series of irregular voids and occur in proximity to others of variable size. Such non-spherical geometry results in sometimes increased ability to form critical hot spots. One key requirement is the ability to form jets which travel into narrowing space. To illustrate the effects of convergence, two such geometries are illustrated to show the potential of such effects.

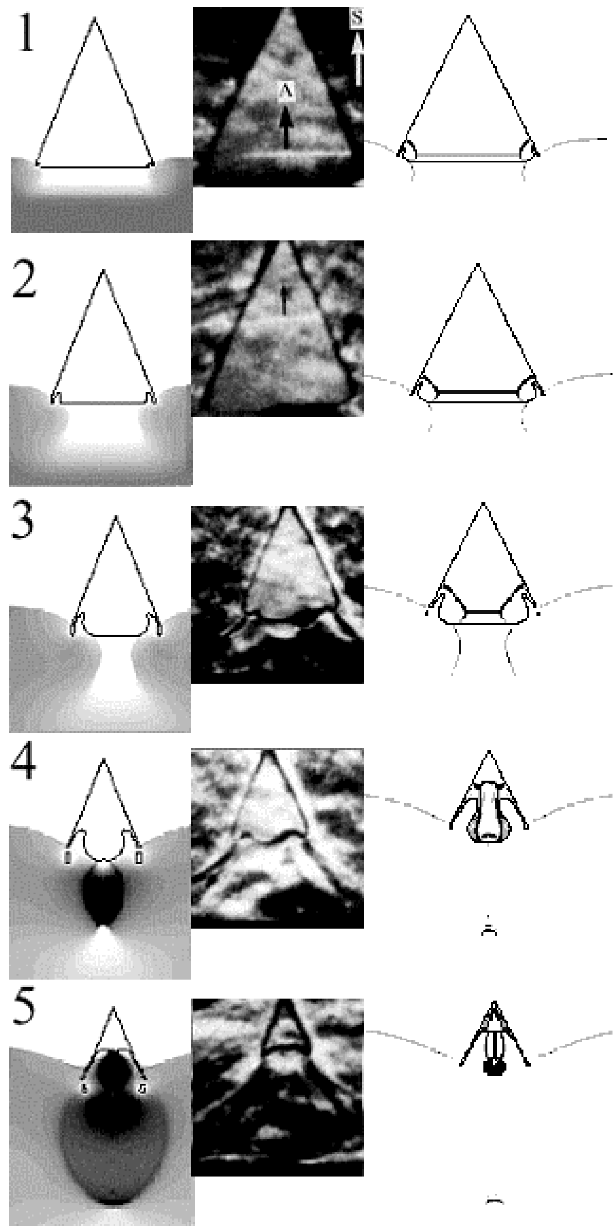

FIGURE 4. COLLAPSE OF A TRIANGULAR CAVITY SHOCKED FROM BELOW. BLACK 10 GPa.

In the first, a triangular cavity is shocked from the flat base. The shaped-charge configuration[9], where the apex of the triangle is swept first, has been much studied and will produce the high-speed jets expected. In this geometry narrow jets impinge upon flat planes and lateral release quickly damps high pressures. However, in the former situation (figure 4), the impact is such that the time for which high pressure and temperature lasts is greater. To the left are contours of pressure from a simulation, in the centre are experimental frames, and to the right, the shock locus is shown. The simulations shows pressures with white indicating ambient conditions and black the maximum pressure achieved which is 10 GPa. The interaction of the shock starts disturbances travelling from the corners of the triangle towards the centre that converge towards the final frames (4 and 5) to give the highest pressures. In the final frame of the simulation the void is finally closed and the maximum temperatures and pressures are reached.

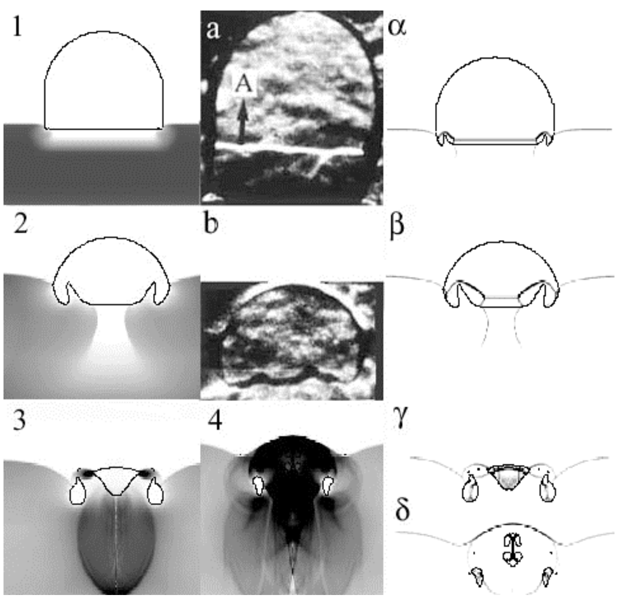

FIGURE 5. COLLAPSE OF A SEMI-CIRCULAR CAVITY. BLACK; 30 GPa.

It will be noticed that the convergent geometry gives rise to high values of both the above variables but also leads to the prolonging of the time over which they are achieved. It is important to consider this factor when one considers hot-spot formation since there is a minimum value required for ignition.

A second geometry considered is one in which a flat-walled semicircular cavity is collapsed by a similar planar shock. The sequence and simulation are shown in figure 5. The shading and organisation of the results are the same as figure 5. The maximum pressure achieved is 30 GPa for this geometry. In the first frame the shock has just encountered the flat, upstream wall which is accelerated downstream. Frame a shows the experimental situation at the same time in which the conditions in the contained gas may be seen.

An air shock (white in the sequence; see ‘a’ and ‘α’) is accelerated by the flat wall. Corner waves can be seen, most clearly coming from the right hand side and strengthening the shock as they spread. Development of the two jets proceeds as seen for the triangular cavity above by perturbations starting from the corners and propagating across.

By frame 2 and ‘b’ they have developed sufficiently to be easily resolved. As the collapse progresses they proceed across the cavity until they have again isolated three regions of entrapped gas. Pressures and temperatures in the region down the central axis and close to the cavity become elevated in the later stages of the process. During the final frames the jet impact and penetration gives a long lasting and large region in which conditions for hot spot creation are favoured even over the triangular geometry considered above. This is seen in frame 4 of the simulation that shows the large, dark high region which exhibits *ca.* 3 times the pressure and 5 times the area as that of the triangular geometry of figure 4. Further, the time for which it exists is *ca.* 5 times longer.

ARRAYS OF VOIDS

Having observed the collapses of isolated cavities in semi-infinite fields it seems prudent to consider the effects of other voids nearby within a distance close enough to affect each others collapses. It has been found that this region of influence extends to *ca*. two diameters for modest shock pressures (0.3 GPa). In the following example an array of cavities is collapsed within the same reactive material discussed earlier.

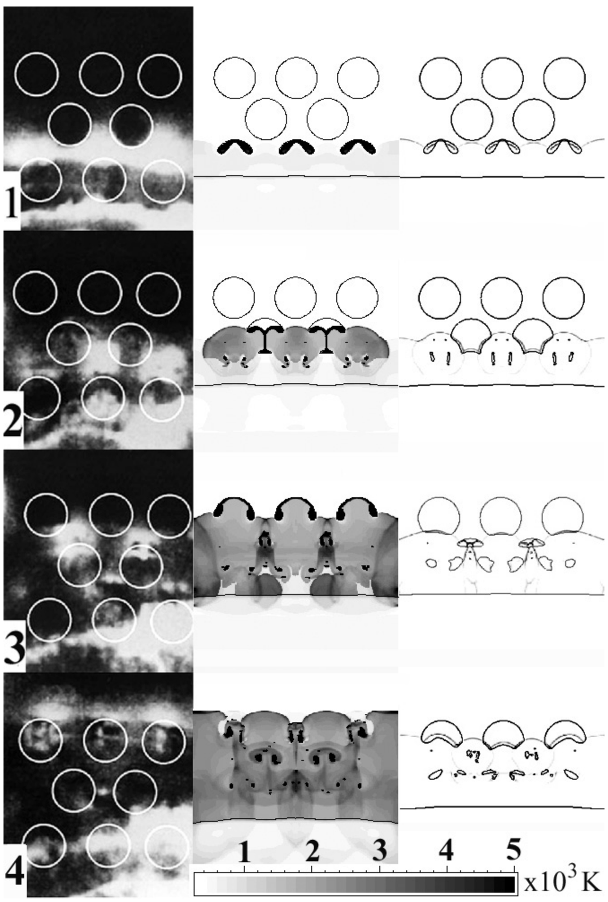

FIGURE 6. COLLAPSE OF A HEXAGONAL ARRAY IN AN EMULSION EXPLOSIVE BY SHOCK AMPLITUDE 8 GPa. CENTRE FRAMES; CONTOURS OF TEMPERATURE FOR COLLAPSE IN NITRO-METHANE. RIGHT FRAMES; SHOCK FOR ARRAY IN WATER.

Figure 6 shows the interaction of a hexagonal array of 5 mm cavities with an 8 GPa incident shock. The interframe time is 2 µs. The first row of sites has just formed in frame 1. The simulation in the centre shows temperatures in a nitromethane fluid. The simulation to the right has water as the fluid and is intended to show the position of shock fronts. Shock diffraction around the cavities is clearly visible. These sites are producing less light in frame 2 and the characteristic kidney shape is apparent. There are two heated regions apparent in the simulation where the collapsed lobes of the first row were. The second row is nearing collapse with highest temperature within the collapsing cavity and where there is interaction between the flow fields from the first collapse. The flow simulation in the inert fluid shows that the shock is behind that for the case of the reactive medium. The chemical energy has accelerated the wave-front in the energetic matrix.

By frame 3 there are two more reaction sites at the points of jet impact as the second row has entirely collapsed. The central simulation shows that the reaction has occurred faster in the NM than the emulsion in the experiment as by this stage the third row has almost collapsed. Nevertheless, two high-temperature reaction regions may be seen behind the shock. Again the shock simulation with an inert fluid shows the shock lagging further behind. By the fourth frame the collapse of the final row of cavities is finishing. The sites start around the point of jet impact and take a characteristic kidney-shaped form. Flame fronts enter each frame from below but do not interfere with the reacting sites. The simulation shows high temperature sites persisting at the positions of the shock-induced collapses. The highest calculated temperature points are 4000-5000 K whilst the bulk is at a value in the range 2000-3000 K.

In all experimental frames, ignition was first seen at the point of jet impact at the downstream cavity wall. The main areas of light emission were then seen to be within explosive downstream of this region. The initial site was always *ahead* of the collapsing shock. This indicates that the reaction was supersonic which emphasises the importance of the jet in this ignition process. There are never any ignitions observed in the jet material itself. In fact there is often an area along the central axis that is darker than the rest of the cavity. The sites remain after the shock and then travel downstream in the following flow. Their shape and position suggests that reaction may be occurring in the highly mixed regions left after the collapse. Simulations confirm these observations. The shock is accelerated relative to the inert simulation but the high temperature sites correlate well with the light emission observed in experiment.

CONCLUSIONS

This paper has examined a series of mechanisms and geometries important in the collapse of cavities in reactive matrices. The geometry was macroscopic so that effects due to viscosity have been rendered relatively unimportant.

An incident shock wave in the surrounding fluid induces convergent flow at the upstream cavity wall. This leads to the formation of a high-speed jet. At a later stage in this process the compression of lobes of gas will cause sufficient heating that material to either side of this initial site may ignite by thermal conduction. However, there is insufficient time for this to occur in the geometries considered here. In situations where bubble size is an order of magnitude smaller, there is even less time for heat conduction, so this mechanism is not of great importance. Emulsion contained in small quantities within the cavity may react at the elevated collapse pressures but again this is not generally the case. Also, reaction may be occurring in the emulsion/gas boundary before the final closure of the cavity. After final collapse, the mixing within the vortex site favours the continuation of the reaction. The highest temperatures are observed to persist at the Lagrangian position of the inhomogeneity. The primary ignition event is caused by the high-speed jet and ignition of material will occur at its point of impact if pressures and temperatures are maintained for long enough.

When an array of cavities is considered, it is quickly clear that the effects of the incident shock are rapidly mediated by the multiple rows of cavities and that a concerted collapse mechanism quickly takes over. Nevertheless, collapses still leave an inhomogeneous temperature field in the reactants after the wave has passed that does not rapidly diffuse.

The spatial extent of the high temperature site is favoured by considering other geometries, particularly involving flat back faces and convergent downstream walls. Further pressures are greater. Finally the time for which the high pressure and temperature are achieved is also elevated.

The formation of a critical hot spot is a function of its volume, duration and temperature achieved. Thus critical hot spots are favoured by non-spherical voids. The suppression of porosity, and its formation (by cracking for example during ageing or by non-routine impulsive mechanical loading) is thus a pressing need.

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