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THE ROYAL SOCIETY

The temperature of a shock-collapsed cavity

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The temperature of the gas enclosed in a cavity collapsing as the result of the passage of a shock wave has importance in considering the safety of reactive materials. This paper assesses the ability of this collapse to ignite an explosive medium in which the cavity is placed. Both jet-impact and hot-gas-ignition mechanisms are considered. A series of experiments have been conducted in which a cylindrical cavity has been collapsed under shock. This geometry has the advantage of allowing details of the gas in the bubble interior to be studied. A further series of experiments is underway to ally this disc-shaped geometry with a spherical cavity using two novel arrangements. The development of these tests has addressed the temperature increase within the cavity. For jet-impact studies, nitromethane is used as the liquid to observe ignition directly. The series of experiments has been coupled with numerical modelling of the multi-material shock interactions to indicate the mechanisms by which ignition and reaction occur.

Keywords: shock; cavity; bubble; collapse; adiabatic heating

1. Introduction

Bubbles are most often found in clouds in nature and thus flow interactions within assemblages trigger the most commonly observed phenomena. However, most work has concentrated (in the early work at least) on an isolated single cavity. If the flow direction is radially symmetric, then the motion of the bubble wall may be deduced from the equations for spherical collapse (see the review by Prosperetti & Hao (1999)), although in the majority of cases it is not. The reason for this asymmetry may be the presence of adjacent boundaries, or the acceleration of the upstream wall by a shock pulse (see, for example, Benjamin & Ellis 1966; Bourne 1989; Dear & Field 1988; Kornfeld & Suvorov 1944). In the latter situation, the impact of a resulting jet, results in a compressible problem, since a spherical shock travels outward after impact, potentially collapsing other adjacent bubbles or, if it impacts a solid surface, damaging the latter in some manner (Milne & Bourne 2002).

The complexity of the mathematics makes the description of the shock collapse of cavities both non-intuitive and nonlinear. The most complete modelling of shock interaction has considered void and matrix with the void containing different gases (see Bagabir & Drikakis 2001; Haas & Sturtevant 1987, among others). Clearly, the major effect is to accelerate the free surface under the shock so that the upstream hemisphere of the bubble travels towards the stationary downstream one (as it is shielded from the shock). Because of the geometry, there is convergence and so velocities much greater than that due to the imparted particle velocity may be achieved. In this respect, formation is equivalent to that of a shaped-charge jet. There have been several investigations that have shown that the shape and number of jets within a cavity are affected by the presence of other surfaces (Dear & Field 1988; Katz 1999), since there is an interaction due to release from free surfaces within adjacent bubbles. There has been some work to study the shock-interaction problem using a technique in which discs are used to replace drops and impacted with a metal slider (Brunton & Camus 1970; Dear & Field 1985). The advantage of studying bubble collapse two dimensionally is that details of processes occurring within the cavity can be followed without the refraction problems associated with viewing through a curved wall. Such investigations yielded a series of observations that may be summarized as follows. As the cavity diameter was reduced or the collapsing shock strengthened, the velocity of the liquid jet increased. At elevated shock pressures, the jet velocity was not constant through the collapse and, above a critical value, it exceeded the shock velocity in the surrounding liquid. By this means, information could be transmitted faster than the acoustic wave speed. After the jet hit the downstream wall, a shock wave was transmitted that travelled ahead of the shock in the liquid. Also, the area enclosed inside the cylindrical cavity (and thus its volume) was found to decrease linearly with time as the collapse proceeded (Bourne 1989; Bourne & Field 1992).

Other experiments investigated the interactions of shock waves with various cavity/particle configurations (Bourne & Field 1994). The presence of particles results in reduced collapse times and in a deviation of the jet in relation to the direction of travel of the incident shock front. The flow also contains increased vorticity, since there are variations behind the shock produced by the geometrical arrangement of the inclusions, including reflected waves propagating in the fluid (Bourne & Field 1989, 1991*a*, *b*). All of the above have application to the situation in which the liquid is reactive and the solid particles may be metal particles, which may contribute to the chemical reaction should the liquid ignite (Bourne & Field 1999*a*; Milne & Bourne 2002).

It has been shown that when a gas void sits within a reactive material there is additional potential to start local burning, which leads to partial reaction or runs to full detonation (Bowden & Yoffe 1952). 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 (Frey 1985). The second is the shock-heated region at the point of jet impact in an asymmetric collapse (Mader & Kershner 1985). The third is the compression of the gaseous or vapour content of the cavity (Chaudhri & Field 1974). These effects have been studied (Bourne & Field 1991*b*) and an experiment, showing examples of each of these modes of heating giving rise to local reaction, is described below. 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. These features may be accentuated if the void is non-spherical (Bourne & Milne 2003).

The first two mechanisms identified for heat generation are connected, in that asymmetric collapse and the formation of a jet cause the highest local flow velocities. Typically, a jet may cross a cavity at *ca.* 1 km s^{-1}, and at this velocity a stress of *ca.* 1 GPa is induced in the surrounding fluid. It is only required that a hot spot is formed in the explosive, which requires the heated zone to exist for a minimum temperature and time. Bowden & Yoffe identified several mechanical and electrical mechanisms that might lead to thermal hot spots (Bowden *et al.* 1947; Bowden & Yoffe 1949, 1952). They realized that bulk heating was insufficient to reach the necessary ignition temperatures for observed reaction, identifying friction, pore collapse and adiabatic shear as some of the mechanical processes that might localize heating (see the review by Field *et al.* (1992)). They suggested a minimum dimension of *ca.* 0.1 μm for a hot spot from which ignition might occur. Additionally, they specified that the temperature should be *ca.* 700 K or greater and that the source should be maintained for a minimum of *ca.* 10 μs. In any event, many such points may exist, but only a few form *critical* hot spots from which an event may originate (Bowden & Yoffe 1952).

There is evidence of sensitization of material and also of associated shock heating of the impacted explosive. Mader has modelled shock-induced hot spots (Mader 1989; Mader & Kershner 1985). His model predicts jets impacting in a local high-pressure area, followed by compression of this material with attendant heating. His models do not require a gas-filled bubble to achieve the necessary ignition temperatures. This mode was considered by Kang *et al.* (1992). However, there are other potential heating mechanisms that may occur in materials with viscosity and/or strength where friction between, and shear within, explosives may be present. In a visco-plastic material, work is done at internal interfaces, leading to heating and the formation of a melted layer at the edge of a pore at which surface burning may start (Carroll & Holt 1972). These effects may be summarized by stating that low viscosity and small bubbles decrease sensitivity.

In each mode of loading and particular geometry, the size of the cavity will determine which mechanism gives rise to heating that may ignite the matrix with flow favoured at the smallest scale, and gas compression and jet impact at the largest. Clearly, the viscosity of a liquid, or strength of a solid matrix, increases the potential range of heating mechanisms by adding shear. Indeed, shear dominates the impact region for a material with strength (Frey 1985). However, account must be taken of the size of the void under consideration. Bubbles with diameter ranging from microns to hundreds of microns may be added to commercial explosives to render them more sensitive. Equally, voids between crystals in a pressed crystalline compact and inhomogeneities in a polymer-bonded formulation are of equivalent size. On the other hand, the space left by contraction on cooling at the base of shells may be hundreds of microns to millimetres. At the largest scale, detonating an explosive charge underwater produces explosion bubbles of diameter metres or tens of metres. The medium in this case is inert, so that no further reaction occurs. However, the collapse of such large bubbles is such that the force due to buoyancy is significant, interacting with the external flow (Blake & Gibson 1987).

It will be seen that the potential for reaction about a collapsing void depends on the type of the loading and the geometry of the void. In cast or plastic-bonded explosives, this size is most likely to be in the micron range. In the following work, however, larger cavity diameters in the millimetre range are considered, as they are experimentally easier to visualize. Nevertheless, accurately capturing the various mechanisms operating leads to an appreciation of effects at a smaller scale.

In this work we aim to couple numerical studies of bubble collapse with experiment. The main goal is to specifically address the temperature state achieved at the final stages of collapse of a shocked bubble. It should be emphasized that the shock-induced collapse is not generally considered, so that there are few other works considering this geometry. The numerical work makes use of a two-dimensional multi-material Eulerian hydrocode with a range of models for material equations of state. Coupling of numerical predictions with experimental data provides an important cross-check on assumptions. We consider here a wide range of initial conditions and develop numerical models aimed at enhancing our understanding of which physical mechanisms dominate at any given time.

2. Experimental

The experiments described were carried out in two- and three-dimensional geometries. The goal 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 clamped between glass or polymethylmethacrylate (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, 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 in Bourne (1989)) 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, while no external lighting was used for the AN experiments where reaction occurred. Other, specifically experimental, work using these geometries and methods of introducing the shock has more detail concerning the development and use of these respective geometries and techniques (Bourne & Field 1999*a*, *b*).

3. Numerical

Numerical studies are performed using a multi-material Eulerian hydrocode. Benson (1992) loosely defines a hydrocode as a tool for solving large-deformation finite-strain transients that occur on a short time-scale. 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 (Kee *et al*. 1992). 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) and high-pressure (*ca.* 3 GPa) shock impact on cavities of order 10 mm in diameter is considered (relatively large for explosives,

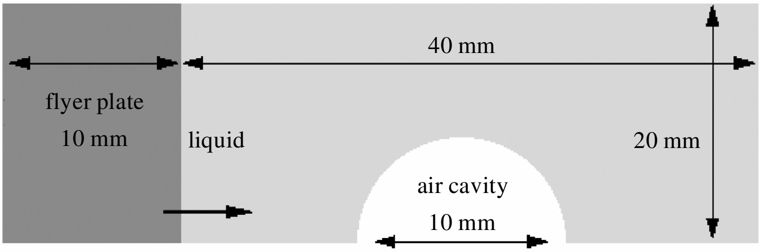

Figure 1. Schematic of the model system.

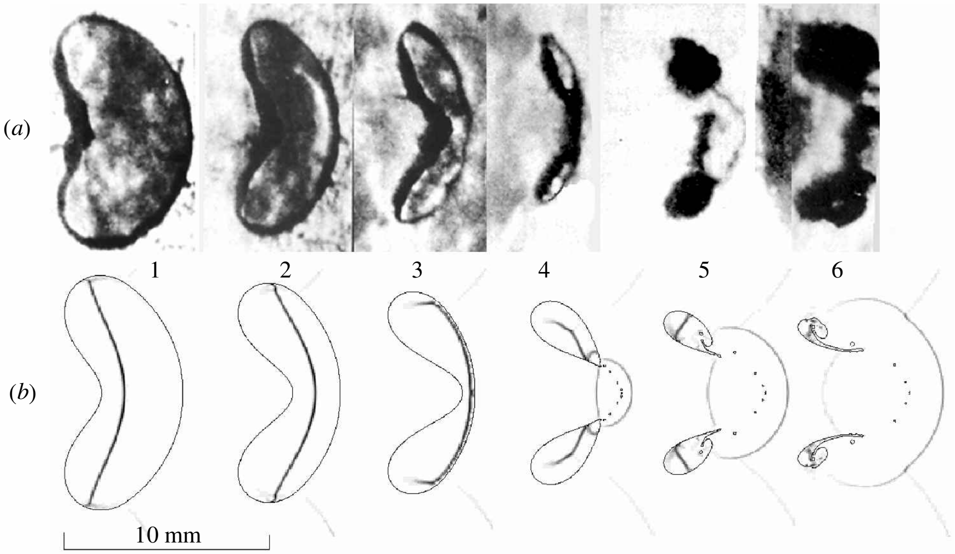

Figure 2. (*a*) Closure and jet penetration for the low-pressure collapse of a 12 mm diameter cavity shocked to 0.3 GPa. (*b*) Simulation tracks both shocks and the cavity walls.

but allowing accurate experimental data to be acquired), thus providing good tests of the numerical models. In the lower-pressure regime, the temperature of the gas in the collapsed cavity is deemed to be the major concern, while in the higher-pressure regime, jet impact is seen as the more important feature when considering the likelihood of explosive ignition. The geometry of the problem is shown in figure 1.

4. Results and discussion

The first sequences presented address the lower-pressure regime discussed above. The upper frames of figure 2 shows six 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. The beginning of the sequence shows the incident shock sweeping the cavity wall. The upstream wall starts to accelerate behind it and a semicircular shock is launched across the cavity. The wall involutes to form a jet, which has already formed at the start of the above sequence. The general form of the collapse has been investigated experimentally in previous papers (Bourne & Field 1992, 1994). This work concentrates on the later stages, where there is development of the highest temperatures. In frame 1, the collapsing surface has crossed the cavity. The shock in the air within the cavity

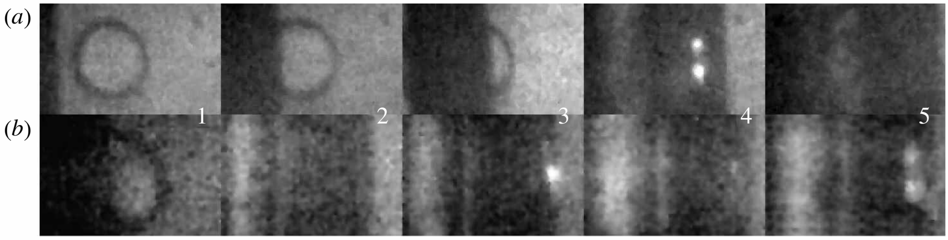

Figure 3. Collapse of 6 mm cavities under 2 GPa shock waves. The first frames show initial cavity positions. (*a*) Inter-frame time 1 μs. (*b*) Inter-frame time 0.2 μs.

is launched by the accelerating upstream wall and, by the stage shown above, 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 (Lesser & Finnstrom 1987). The liquid shock can be seen already ahead of the downstream cavity wall.

As the sequence progresses, the jet and shock cross the cavity and, by frame 3, they have almost reached the downstream wall. In frame 4, the jet penetrates the wall 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 shown in frame 6. It is at points in these lobes that the highest temperatures are reached.

Other experimental work has shown the presence of luminescence from the enclosed interior gas soon after the jet impacts (Bourne & Field 1999*b*). It was thus considered important to investigate such phenomena numerically. Figure 3 shows the collapse of a 6 mm cavity by a 2 GPa shock photographed at two different framing rates (inter-frame times of 1 and 0.2 μs for (*a*) and (*b*), respectively). Frame 1 of each sequence shows the initial cavity position. The sequence (*a*) is taken at equal frame intervals to show the collapse process. Sequence (*b*) shows an initial frame and then 2–5 are at high rate to show the processes occurring. There are two bright flashes of light in frame 4 of the slower sequence, which are shown in greater temporal detail in (*b*). First, a single flash occurs in frame 3, which appears to be at the shock front, given that there are minimal refraction effects. In the next frame 4, little is seen, except perhaps some faint remnants of the bright flash in frame 3. However, in frame 5, two regions of luminescence are seen, which correspond in position to the two flashes seen in frame 3 of sequence (*a*). The durations of the flashes are bounded by the framing rate and exposure time of the camera. One may estimate 200 ns for the first, then a delay of 200 ns, but then it can only be hypothesized that the duration of the pair is less than 1 μs, since this was the end of the sequence. The position of the flashes shows that the single flash occurs symmetrically between the pair. Since there is no indication of it in the slower sequence that is averaging the output, one might assume that its brightness is very much lower than that of the later pair. It is interesting to note the similarity with sonoluminescence, where the source of light is believed to be weak bremsstrahlung radiation (Hilgenfeldt *et al.* 1999). Recent work

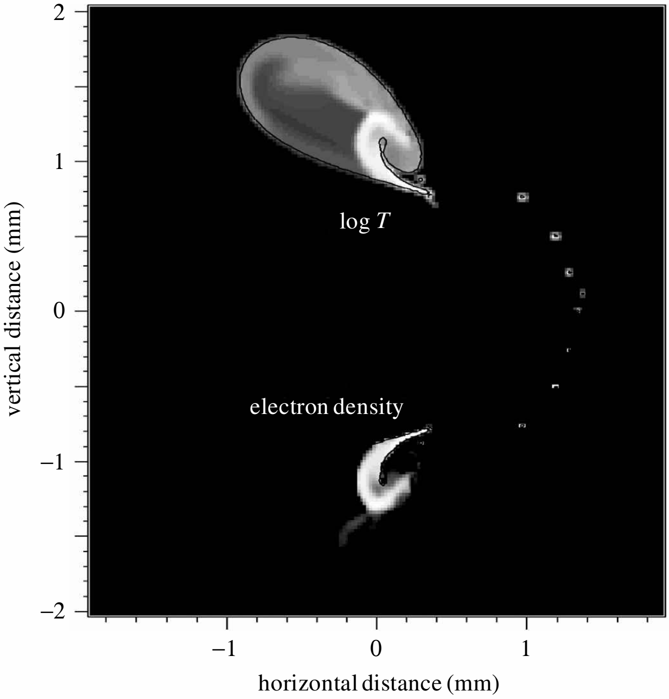

Figure 4. Collapsed bubble shape showing logarithm of temperature at the top, with electron concentration below.

on the chemical effects present in cavitation bubbles by Suslick (Didenko & Suslick 2002) has demonstrated that the presence of chemical species will limit the maximum attainable temperature. However, he notes that considerable light emission is still possible under the conditions he infers from states in single-bubble sonoluminescence.

To attempt to explain these effects, different approximations for the equation of state of air have been investigated. Ideal gas calculations show the gas-temperature distribution to mimic the experimental results, with the highest temperature achieved at the final point in the collapse of the lobe away from the symmetry axis. This corresponds qualitatively with the position of the observed flashes of light in the sequences of (*a*) and (*b*), but to fully explain the latter feature requires more complex modelling for the gas. The exact nature of the observed luminescence is unknown; however, it may be assumed that the mechanism will involve some dissociation mechanism in the air. Calculations have thus been carried out using equilibrium chemistry with a seven-species air model including electron production. The aim here is to predict this degree of dissociation. This performs two purposes. In the first instance, it provides an improved model for the air equation of state and thus a more accurate prediction of temperature. In the second, it allows indication of the distribution of dissociated air products (here principally electrons) and treats this as a more accurate estimate of luminescence.

Strong shocks exist within the bubble and (as Ball *et al.* (2000) have recently shown) adiabatic collapse models will significantly underestimate the peak temperatures.

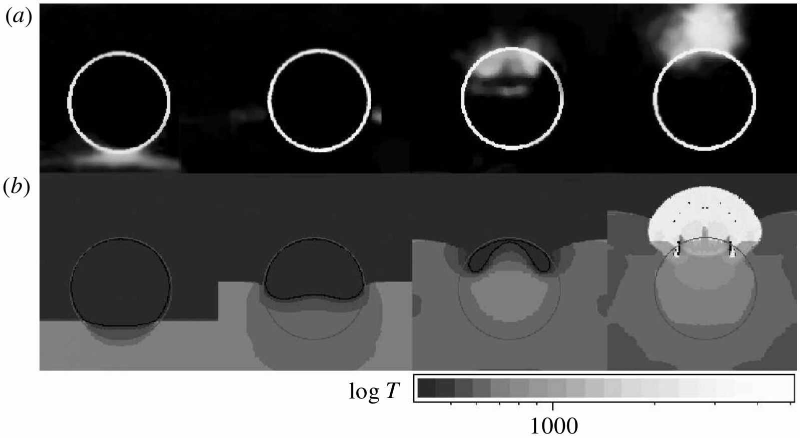

Figure 5. Experiment and simulation of bubble collapse in a reactive matrix. (*a*) Experiment in which a large (6 mm) cavity collapsing in an AN matrix. Light is due to reaction. Inter-frame time 1 µs. (*b*) Temperature field around a cavity collapsing in NM showing similar reaction sites.

The distribution of temperature and electron density is plotted at a selected time in the collapse process in figure 4. The time chosen is that at which the peak temperature is reached in the cavity. The upper region (where vertical distance is positive) shows a grey-scale representation of the logarithm of the temperature in the cavity lobes that ranges from 300 to 6000 K. The lower (where vertical distance is negative) part of the figure shows the predicted electron-density distribution at the same time. The two are plotted in this manner to emphasize the correlation between the highest temperatures and electron densities. It is beyond the scope of this paper to determine the detailed physical mechanism of luminescence. It is simply indicated here that the location of the luminosity is related to temperature. If luminosity is considered proportional to temperature or if luminosity is proportional to electron density (i.e. a complicated nonlinear function of temperature), the peak value is at the leading edge of a shock within the cavity. The key observation is that the light emission recorded from the collapse lies at identical time and position both in the predictions of figure 4 and in the frames of the sequences presented in figure 3.

The results above have addressed the temperature in the gas cavity. This is an important diagnostic of the cavity collapse but is not necessarily the cause of ignition in a reactive medium. Shock-driven cavity collapse naturally leads to high gas temperatures, but these only exist in the collapsed cavities for short periods of the order of 200 ns. The jet-impact ignition source occurs well before peak gas temperature is achieved. For a spherical bubble, a 1000 $\mathrm{m\,s^{-1}}$ plate impact results in a 4000 $\mathrm{m\,s^{-1}}$ jet speed. For a cylindrical bubble, this speed reduces to 3200 $\mathrm{m\,s^{-1}}$. Thus, in asymmetric cavity collapse, the main mode of ignition of a reactive medium is the shock heating at the point of jet impact in the surrounding fluid. The following illustrates this mode drawing on both experimental and numerical results.

To accurately model jet ignition requires an accurate numerical model, so simulation of the collapse of a bubble in nitromethane (NM) was undertaken using an Arrhenius kinetics model for the reactive liquid within the hydrocode. This was chosen since a calibrated NM kinetics scheme has been fitted by Cook *et al*. (1998) from bullet-impact studies and thus is well suited to jet impact.

To illustrate qualitative features of the processes occurring, experimental data for collapse in AN emulsion is compared with simulations of collapse in NM. As yet, no accurate kinetic model is available for the AN emulsion and further work is underway to repeat experiments in NM. The jet-ignition mode is illustrated in figure 5, which shows experimental results of a 6 mm cavity collapsing under an 8 GPa shock in an AN emulsion explosive and a simulation of a cavity collapsing in NM under similar geometry and conditions (parts (*a*) and (*b*), respectively).

The experimental sequence of figure 5*a* shows four frames, 1 μs apart, from the collapse of an air-filled cavity in AN. There is no lighting, so that bright features correspond to luminescence or chemical reaction. In frame 1, the shock front can be seen approaching the upstream cavity wall, while in frame 2 it is approximately halfway down it. The light here is believed to be from chemical reaction, which does not propagate after the rapid shock jump passes. 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. There is some luminosity progressing from the lobes of the collapsing bubble into a roughly circular region behind the jet-impact site. This may be due to partial reaction due to heat conduction from the heated region. In the last frame, after jet impact, there is a circular region of light centred on the impact point of the travelling jet, which is hypothesized to result from the jet impact. The heat conduction seen earlier has affected a different region which does not react with the same intensity as observed here.

The calculation in figure 5*b* mimics the stages of the collapse shown in part (*a*). The simulation only 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 in figure 5*b* 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.

Thus the early luminosity in the lobes is due to high temperatures in the gas cavity. Imaging the light emission provides a useful diagnostic of the collapse mechanism. However, the temperature in the cavity reaches high values towards the end of the collapse, and although there is reaction in the vapour within the cavity as the jet is close to impact, the calculations show that it is the temperature and pressures generated at the impact site itself that causes ignition of the surrounding fluid. Thus, while there is luminosity in the circular region of figure 5*a* due to combustion adjacent to the high temperatures (of thousands of kelvins) generated, it is the jet impact that gives rise to the main ignition.

5. Conclusions

A range of experiments and simulations has illustrated an approach to understand gas luminescence and the formation of hot spots in reactive media by the collapse of cavities. Experiments have illustrated features of the shock collapse of large (millimetre-sized) cavities in spherical and cylindrical form to observe details occurring within the cavity. In a typical pressed explosive, these cavities are usually of the order of microns. A numerical scheme with suitable representation of liquid and included gas has been developed and has been shown to reproduce the wall geometry, the included gas behaviour (including the electron density consistent with observed luminescence) and the temperature field within the bubble.

The experiments show the development of a jet that impacts the rear of the gas cavity. Two lobes of gas are present after this impact and have been observed by several workers as the source of luminescence. Experimental examples have been compared with numerical predictions and these simulations clearly show detailed shock structures within the cavity and associate luminosity with the gas temperature or electron-density distributions that follow these shock structures.

When a reactive liquid is present, late-time luminosity occurs downstream of the jet-impact point. Comparing calculations with experiment relates this to reaction in the energetic material as a result of jet-impact ignition, not heat transfer from the gas cavity. Further work is in progress to further elucidate the mechanical and chemical mechanisms by which the processes operate.

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