Shock-to-detonation transition in nitromethane with spatially non-uniform distributions of air-filled cavities

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1 Introduction

Liquid-phase explosives can be sensitized to shock initiation by the addition of hollow micro-balloons. This sensitizing effect is attributed to the formation of localized high-temperature regions, or "hot spots", as cavities collapse over the course of the passage of an incident shock wave. The wave-interface interaction and the temperature field arising from the shock-induced collapse of a single cavity has been observed experimentally [1, 2], and finer details were revealed via numerical simulations [3, 4]. Experimental studies with a regular array of cavities indicate that the formation of a hot spot is also significantly influenced by the complex perturbation caused by the collapse of the neighboring cavities. [1, 5]

As revealed in a number of experimental studies [6, 7], the spatial distribution of mesoscale cavities in liquid explosives is highly non-uniform. For example, clusters of glass micro-balloons (GMBs) can be observed in gelled-nitromethane [7]. The question thus arises as to whether different types of spatial distributions of mesoscale heterogeneities influence the resulting hot-spot sensitizing effect on the shock initiation of heterogeneous explosives. In this study, in order to examine the collective effect of a large number of hot spots on the shock-to-detonation transition (SDT) process, meso-resolved simulations, wherein a statistically significant amount of mesoscale heterogeneities are explicitly considered, are performed.

The explosive system considered in this study is a mixture of liquid nitromethane (NM) with circular cavities filled with air. The size of the cavities is chosen to be $100\ \mu\mathrm{m}$, which is a typical size of commonly used GMBs for explosive sensitization. Via modeling the same explosive system, Mi *et al.* [8] have demonstrated that the addition of cavities results in a significantly shorter detonation overtake time than that for the case of neat NM. The current study is thus focused on examining the SDT behaviors resulting from the cases with different spatial distributions of cavities, i.e., regular, uniform, random, and clustered distributions.

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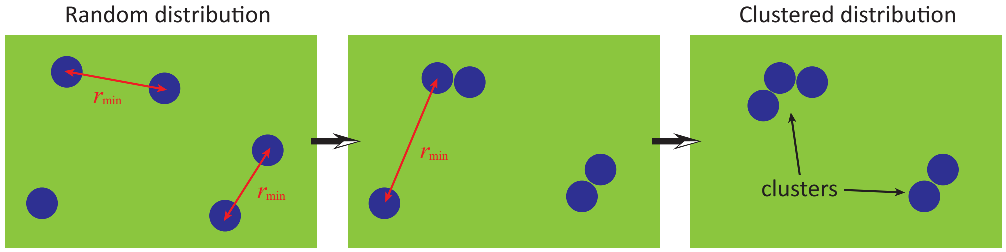

Figure 1: A schematic illustrating how a clustered distribution of cavities is created based on a random distribution.

2 Problem description

The dynamic system at hand is simulated using the hybrid formulation proposed by Michael and Nikiforakis [9] in order to treat a reactive, multi-phase flow with two immiscible materials (i.e., liquid NM and air). Liquid NM is considered to be governed by the Cochran-Chan equation of state [10]. The reaction rate of liquid NM is governed by single-step Arrhenius kinetics. The parameters used for the equations of state of air and liquid NM, and for the reaction law of liquid NM are adapted from the recent studies of Michael and Nikiforakis [4, 11] on the collapse of a single air-filled cavity in liquid NM. A complete description of the herein considered model can be found in the recent work of Mi *et al.* [8]

For each simulation, the diameter d_c of the cavities is the same. The average spacing between each two neighboring cavities is denoted by δ_c. The porosity ϕ (or the volume fraction of air-filled cavities) can be calculated as $\phi = \pi {d_\mathrm{c}}^2 / \left(4{\delta_\mathrm{c}}^2\right)$. Various types of cavity distributions are described as follows:

- Regular distribution: An array of regularly spaced cavities.
- Uniform distribution: Randomly distribute the cavities while imposing a minimum spacing of $2\delta_\mathrm{c}/3$.
- Random distribution: Randomly distribute the cavities as long as they do not overlap, i.e., with a minimum spacing of d_c.
- Clustered distribution: First generate a random distribution of cavities, and then move each cavity to its closest neighbor as illustrated in Fig. 1.

Further, a slightly perturbed regular distribution of cavities can be created, as illustrated in Fig. 2, via randomly relocating each cavity within a square region enclosing its original position within the regular array. The side length of this square region is $\sigma\delta_\mathrm{c}$. The parameter σ can thus be considered as the extent of perturbation from a regular distribution.

3 Numerical methodology

The simulation code used to solve the two-dimensional reactive Euler equations is based upon a uniform Cartesian grid. The MUSCL-Hancock scheme with the van Leer non-smooth slope limiter and a Harten-Lax-van Leer-contact (HLLC) approximate solver for the Riemann problem were used [12]. The Strang splitting method was adopted to treat separately the hydrodynamic process and the reactive process. This

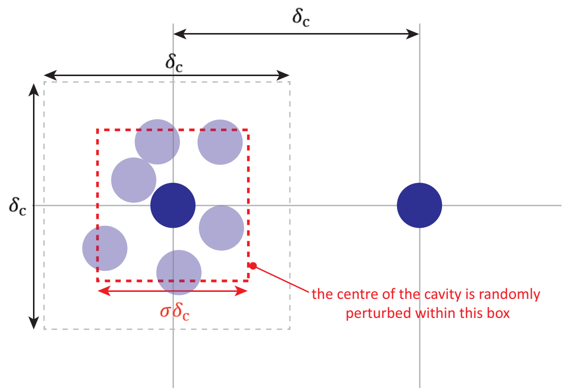

Figure 2: A schematic illustrating the introduction of slight perturbations to a regular array of cavities.

numerical scheme is thus of second-order accuracy in space and time. This code is implemented in Nvidia's CUDA programming language. The simulations were performed on Nvidia Tesla V100 16GB GPU computing processors. The use of GPU-accelerated computing platforms has been explored in several studies on gaseous detonations [13, 14]. The current work is a further development of the GPU-based code to simulate detonations in a multiphase energetic system.

4 Results and discussion

The color contour plots of NM reactant density in Fig. 3 show the initial configuration of the cases with regular, uniform, random, and clustered distributions of cavities. The cavity diameter and average spacing for these sample cases are $d_\mathrm{c} = 100\ \mu\mathrm{m}$ and $\delta_\mathrm{c} = 300\ \mu\mathrm{m}$, respectively. The corresponding porosity is thus $\phi = 8.72\%$. A rightward-going incident shock wave is realized via placing a high-pressure, inert region near the left boundary of the domain. The strength of the input shock is specified by the pressure and particle velocity in this region.

Figure 4 shows the snapshots of the flow fields at a later time ($t = 3.9\ \mu\mathrm{s}$) resulting from these four different distributions of cavities (as shown in Fig. 3). At this time, the leading shock front appears to be at increasingly advanced positions in the x-direction for the cases with regular to clustered distributions. For each case, the reaction zone behind the leading shock is the region wherein high-density NM reactant remains. While a long reaction zone continues to persist in the case with a regular distribution, as shown in Fig. 4, a very thin reaction zone attached to the leading shock occurs in the case with a clustered distribution. These results indicate that the shock-to-detonation transition progresses in an increasingly faster pace from the case with a regular distribution to the case with a clustered distribution.

The detonation overtake time for each case is measured as the time of maximum overall reaction rate as proposed by Mi *et al*. [8] The results of overtake time for the cases with different distributions are plotted as functions of input shock pressure in Fig. 5, i.e., a Pop-plot, and compared to the overtake times resulting from neat NM. The sensitizing effect (i.e., a shorter overtake time) resulting from different distributions is consistent throughout the range of input shock pressure explored in this study. The difference among the resulting overtake times from different distributions is larger for weaker input shocks.

For the lowest input shock pressure (7.04 GPa) considered in this study, additional cases with slightly perturbed regular distributions are examined to explore a more complete spectrum in sensitizing effect that

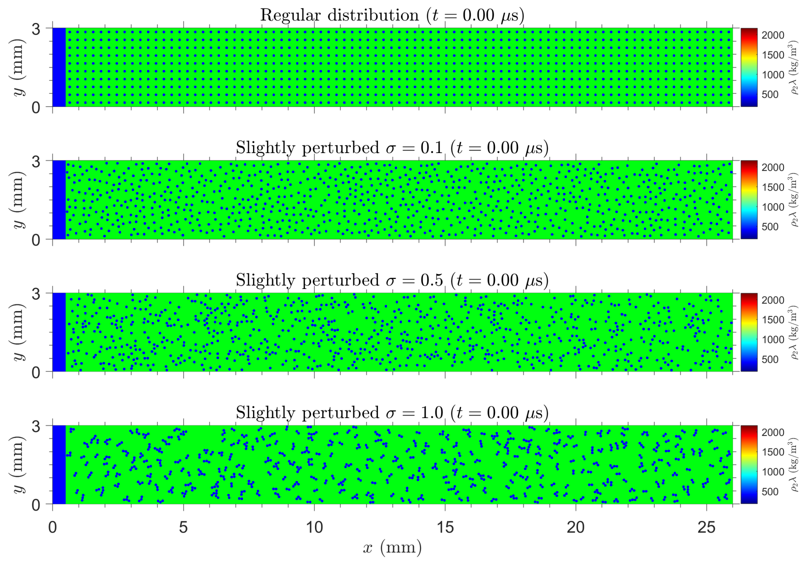

Figure 3: Contour plots of NM reactant density showing the initial configuration of the cases with regular, uniform, random, and clustered distributions of cavities. The cavity diameter is $d_\mathrm{c} = 100$ $\mu\mathrm{m}$ and average spacing is $\delta_\mathrm{c} = 300$ $\mu\mathrm{m}$.

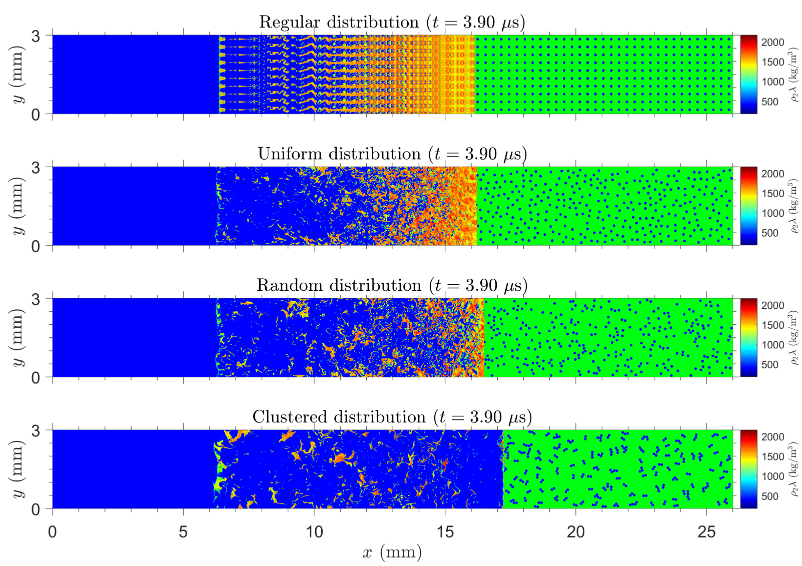

Figure 4: Contour plots of NM reactant density at $t = 3.9$ μs for the cases with regular, uniform, random, and clustered distributions of cavities. The cavity diameter is $d_\mathrm{c} = 100$ $\mu\mathrm{m}$ and average spacing is $\delta_\mathrm{c} = 300$ $\mu\mathrm{m}$. The input shock pressure is 7.04 GPa.

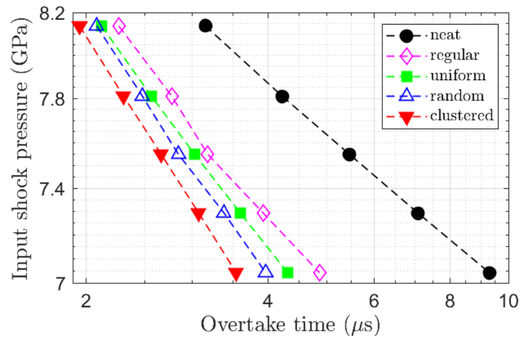

Figure 5: The results of detonation overtake times plotted as a function of input shock pressure for the cases with neat NM and various distributions of cavities. The cavity diameter is $d_\mathrm{c} = 100\ \mu\mathrm{m}$ and average spacing is $\delta_\mathrm{c} = 300\ \mu\mathrm{m}$

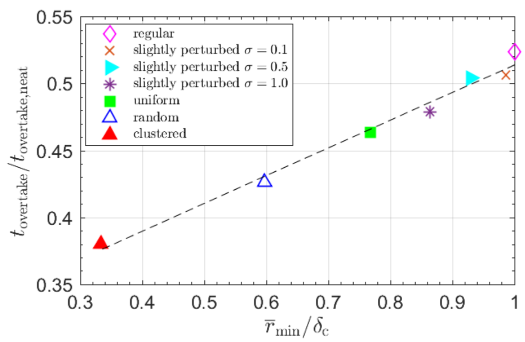

Figure 6: Detonation overtake times resulting from various distributions of cavities normalized by the overtake time for the case of neat NM plotted as a function of mean minimum spacing $\overline{r}_\mathrm{min}$ normalized by the average spacing δ_c of the initial distribution. The cavity diameter is $d_\mathrm{c} = 100\ \mu\mathrm{m}$ and average spacing is $\delta_\mathrm{c} = 300\ \mu\mathrm{m}$. The input shock pressure is 7.04 GPa.

varies from clustered to regular distributions. The overtake times resulting from seven different distributions (including three slightly perturbed regular distributions with $\sigma = 0.1$, 0.5, and 1.0) normalized by the overtake time for neat NM are plotted as a function of mean minimum spacing $\overline{r}_\mathrm{min}$[1] normalized by the average spacing $\delta_\mathrm{c} = 300\ \mu\mathrm{m}$. The scatter of data points exhibits a linear correlation between the resulting overtake time and mean minimum spacing.

5 Concluding remarks

Two-dimensional, meso-resolved simulations of liquid NM mixed with air-filled cavities reveal that the spatial distribution of mesoscale heterogeneities may significantly influence a hot-spot-driven SDT process in heterogeneous explosives. In an order of increasingly pronounced sensitizing effect (i.e., shorter detonation overtake times), the distributions examined in this study can be ranked as follows: $\mathrm{Regular} \to \mathrm{uniform} \to$

[1]For each cavity, the minimum spacing is the distance to its closest neighbor; $\overline{r}_\mathrm{min}$ is the minimum spacing averaged over the entire distribution of cavities in the domain

$\mathrm{random} \rightarrow \mathrm{clustered}$. The mean minimum spacing, which describes the nature of the initial distribution of heterogeneities, seemingly characterizes the sensitizing effect on the overall SDT process of heterogeneous explosives.

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