Multiscale smoothed particle hydrodynamics simulation of detonation initiation

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Abstract. Detonation initiation phenomenon in condensed explosives requires the development of multiscale simulation techniques. Contact smoothed particle hydrodynamics is applied for a mesoscopic simulation of shock initiation in a model of porous pentaerythritol tetranitrate (PETN) at low density. Our simulation of shock initiation leads to an overestimated run distance to detonation compared with Popolato curve in PETN. The consistency of the porous mesoscopic structure simulation, using a contact smoothed particle hydrodynamics and macroscopic kinetics of the pressed PETN is discussed.

1. Introduction
One of the first simulations of mesoscopic structure was used for the detonation initiation in the hydrodynamic hotspot model [1, 2]. Since 1970th mesoscopic hydrodynamics models have become widespread in numerical simulations of detonation. A run distance to detonation is one of the reference points for a calibration of shock sensitivity [3–5]. There is a discussion on the mesoscopic simulation of microstructure and the temperature of hotspots during collapsing of the pores [6–10]. Calculations of the run distance to detonation are defined by an equation of state, a macroscopic decomposition kinetic scheme and hydrodynamics. Microscopic kinetic schemes require a well-defined temperature. Mie–Grüneisen equations of state based on the reference curves for reagents and products are calibrated only for a thermal part $P–\rho–E$. There is need to take into account a heat capacity in reactants and products in different states for a correct temperature definition. An experimental measurement of the temperature during a pore collapse is developing in a group of Dlott [11,12]. As other have highlighted [13], the temperature definition is a complicated problem for reactants and products.

In this work, a three terms macroscopic kinetic scheme is used [14], which was parameterized for pressed PETN. The kinetic scheme defines energy release and transition from reactants to products. A rate of products release is depended on the local density and pressure in the material. Jones–Wilkins–Lee equation of state [15, 16] describes a pressed pentaerythritol tetranitrate (PETN) in the simulation. The equation-of-state uses temperature and pressure equilibrium of reactants and products for partially decomposed material. The simulation is done with a
2. Material model description

A porous PETN is described as a pressed substance with voids. A sequence of spherical voids is removed from the continuous sample. Such mesoscopic model with simplified geometry of pores is used in the simulation and illustrated in figure 1. The domain is a parallelepiped consisted of $L_x \times L_y \times L_z = 41000 \times 20 \times 20$ base-centered cubic (bcc) cells with SPH particles, where size of the particle conform to $L_y = L_z = 80 \, \mu m$. A periodic boundary condition is imposed in directions $y$ and $z$ which are transverse to the direction of shock propagation. First of all, SPH particles fill the whole parallelepiped domain in bcc lattice with a size corresponded to the period. After that, the sample is prepared by mixing particles as authors proposed [19]. Therefore sample has a randomly placed SPH particles distributed uniformly in the volume. The equation of state for a pressed PETN [16] at density $\rho_0 = 1.75 \, g/cm^3$ is coupled with a three-term macroscopic kinetics [14] parameterized for density $1.77 \, g/cm^3$. Pores are cut from the sample after mixing of particles. The radius of the pores is approximately $R = L_y[3(\rho_0 - \rho_p)/(8\pi \rho_0)]^{1/3} \approx 32.68 \, \mu m$, where the density of porous sample is $\rho_p = 0.75 \, g/cm^3$. The sample with pores contains 7.05 million SPH particles.

3. Shock initiation simulation

The shock wave is induced by a potential barrier of an artificial force for SPH particle. The force is growing linearly on the left of a $y$–$z$ plane at $x = 0$. This boundary condition may lead to rarefaction of the detonation products near the barrier. A thin $80 \, \mu m$ layer of non-reactive

Figure 1. The scheme of pores in mesoscopic model. The centers of pores are marked with stars. The line through the diagonal of a cube is halved twice by the centers of pores. The size of replicated periodically in $x$-direction cube is equal to the transverse direction size of $L_y = L_z = 80 \, \mu m$.

Figure 2. Maps of SPH particle density during detonation initiation simulation. The incident shock wave leads to the compactification of pores and defines the position of the shock front for three different moments of time.
Figure 3. Detonation initiation of PETN at the density $\rho_p = 0.75 \text{ g/cm}^3$ and the mass velocity $u_p = 500 \text{ m/s}$. Incident pressure amplitude is equal to $P = 0.41 \text{ GPa}$ which is the earliest profile marked at $t = 33.13 \mu s$. Calculated run distance to detonation of $l = 9.2 \text{ mm}$ is defined as moment of a shock amplitude attenuation for the first time.

PETN is placed where the potential barrier impacts on the boundary of the sample. In the beginning of simulation, the sample has a mass velocity $u_p = 500 \text{ m/s}$ in the negative direction of $x$ axis. The statement is equivalent to the barrier propagation with a positive velocity $u_p$ as shown in figure 2.

Distribution of a number density of SPH particles (in a plane $x$–$y$, the shock wave propagates along $x$ axis), shows the mesostructure of the sample before the shock arrival as shown in the scheme (see figure 1). The shock wave leads to the collapse of pores. Figure 3 shows profiles of the pressure for a sequence of moments. For the first moment $t = 33.13 \mu s$, the profile gives an amplitude of the shock $P = 0.41 \text{ GPa}$. In the same figure, three blue-coloured profiles correspond to the moments of time $t = 49.96, 50.05, 51.6 \mu s$. This is the initial stage of a detonation formation. The oscillation of pressure, near the shock front, is caused by collapsing pores. A detonation wave forms after the intensive decomposition near the piston, where the explosive was compressed at the earliest moments. A local pressure growth leads to a self-acceleration process which cause a transition of the shock wave to the detonation wave as it is shown with black-colored profiles. The detonation wave is overdriven just after the acceleration. It attenuates and propagates with oscillations near constant value correspondent to Chapman–Jouguet detonation. Experimental study of the PETN shock initiation states that the run distance is about $2 \pm 1 \text{ mm}$ at $1 \text{ g/cm}^3$ [16]. The distance is less than that we observed in our simulation.
4. Discussion
The run distance to the detonation of 9.2 mm in our simulation overestimates the comparable experimental data. Used macroscopic kinetics takes into account only a total pressure growth in the reaction rate, while a thermal part of pressure is expected to be higher inside collapsed pores. A possible way of a modification the macroscopic kinetics is accounting the thermal part of pressure inside the hot spot formed after the pore collapse. The mesoscopic simulation is able to observe a spatial non-uniformity of temperature distribution behind the shock. Analysis of the energy focusing during the shock propagation in such structures should be taken into account by the modification of the macroscopic kinetic model. The mesoscopic model should be used in a further simulation of the porous explosive to get a more universal macroscopic kinetics which is adjustable for both porous and pressed explosives.

5. Conclusions
The growth of pressure on the piston causes the detonation initiation in porous PETN. This pressure growth is caused by the acceleration of decomposition and energy release. The shock propagation leads to the compactification of explosive. The detonation initiation occurs in the part of explosive which is already compactified.

Acknowledgments
The work is supported by the Russian Science Foundation (grant No. 14-19-01599).

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