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Multiscale multiphase modeling of detonations in condensed energetic materials

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ABSTRACT

Hot spots ignition and shock to detonation transition modeling in pressed explosives is addressed in the frame of multiphase flow theory. Shock propagation results in mechanical disequilibrium effects between the condensed phase and the gas trapped in pores. Resulting subscale motion creates hot spots at pore scales. Pore collapse is modeled as a pressure relaxation process, during which dissipated power by the 'configuration' pressure produces local heating. Such an approach reduces 3D micromechanics and subscale contacts effects to a 'granular' equation of state. Hot spots criticity then results of the competition between heat deposition and conductive losses. Heat losses between the hot solid-gas interface at pore's scale and the colder solid core grains are determined through a subgrid model using two energy equations for the solid phase. The conventional energy balance equation provides the volume average solid temperature and a non-conventional energy equation provides the solid core temperature that accounts for shock heating. With the help of these two temperatures and subscale reconstruction, the interface temperature is determined as well as interfacial heat loss.

The overall flow model thus combines a full disequilibrium two-phase model for the mean solid-gas flow variables with a subgrid model, aimed to compute local solid-gas interface temperature. Its evolution results of both subscale motion dissipation and conductive heat loss. The interface temperature serves as ignition criterion for the solid material deflagration. There is no subscale mesh, no system of partial differential equations solved at grain scale.

The resulting model contains less parameter than existing ones and associates physical meaning to each of them. It is validated against experiments in two very different regimes: Shock to detonation transition, that typically happens in pressure ranges of 50 kbar and shock propagation that involves pressure ranges 10 times higher.

1. Introduction

Shocks and detonations in heterogeneous materials differ widely of similar phenomena in gas mixtures as thermal and mechanical disequilibrium are present among the phases with scales much larger than molecular ones. Chemical decomposition phenomenon is different as well, the ignition being governed by local effects (hot spots) resulting of these disequilibria. Material equations of state are obviously also very different to those of gases.

Shock initiation of solid explosives is a long lasting issue. It is well known that solid temperature increase resulting of shock compression is not enough, in most situations, to achieve ignition. Part of the shock energy is focused in specific zones where local heating happens, resulting in hot spots appearance, that are considered responsible for the solid material ignition.

There are several possible causes of hot spots:

- Shear bands effects, present for example in composite explosives [6,17,45].
- Small gas pores (micrometer sizes), considered as the main ignition cause for pressed explosives [7,31,33,39].
- Big gas pores and cavities, considered responsible for the ignition of highly heterogeneous explosives [18] such as civil ones, having large amount of pores (20–30% volume).

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- Crack propagation, intergranular friction and heterogeneities are other possible sources of hot spots [9,23].

The present paper considers pressed explosives only, where small gas pores are present with typical gas volume fractions of the order of 1%.

Most existing models addressing shock to detonation transition have empirical basis. The most popular ones are the Lee and Tarver [35] model, the so-called Forest-Fire (FF) model [16] and the JTF model [29,50]. These models are widely used as they correctly predict shock to detonation transition once their parameters are calibrated. However, they have limitations:

- They usually contain many parameters: 4 and 13 parameters respectively for the FF and JTF models respectively.
- They sometimes use flow variables difficult to compute, such as the shock pressure and temperature. It means that additional equations have to be added to the flow model to transport these variables. Also, shock wave detection has to be achieved, posing non trivial issues [40].
- The various kinetic parameters mentioned previously are determined for given thermodynamics and given flow model. Most time the JWL EOS [36] is used for detonation products and the Cochran and Chan [12] EOS is used for the solid reactant. Consequently the reaction rate parameters are dependent to the EOS couple and mixture model, based in most flow models on pressure and temperature equilibrium among the phases.

In addition to these restrictions, these models are predictive only in the state variables range where the coefficients have been determined.

Attempt to build physically based models is a long lasting issue [7,31,33,39]. Khasainov et al. [33] and Kang et al. [31] are local models that consider the dynamics of isolated pores to determine the characteristic time scales of hot spots ignition. The first model addressing coupling between pore scale and wave propagation at macro-scale is due to Massoni et al. [39]. Limitations appeared however:

- Too many evolution equations were present, making the practical use difficult.
- The macro-scale model was based on solid-gas mixture Euler-type flow model where micro-scale motion was absent.

Micro-macro scale motion coupling has been addressed by van Wijngaarden [51] in the context of bubbly liquids with a model involving a single velocity. Extension to two-phase mixtures in velocity disequilibrium was addressed in Drumheller et al. [13], Bedford and Drumheller [3] and Gavrilyuk and Saurel [21]. In the present work micro inertia is neglected, as assumed in Baer and Nunziato [1] type models. Here the symmetric variant of Saurel et al. [48] is considered and the pressure relaxation process is used to model pore collapse. The visco-plastic heat deposited at pore surfaces is determined through a simple approach based on 'configuration' pressure [1,42] and radial pore collapse velocity, determined through a pressure relaxation process. This method considerably simplifies the approach of Khasainov et al. [33], Kang et al. [31] and Massoni et al. [39] as no radial integration normal to the pore interface is needed. Relaxation terms combined with the 'granular equation of state' summarize 3D subscale motion and associated dissipation. Efforts in the same direction of simplification were done formerly by Gonthier [24], Hamate and Horie [26] and possibly other researchers.

From pore collapse, heat is deposited at pore surface and hot spots are created. These hot spots may be subcritical or supercritical depending on heat losses. Dominant heat loss occurs in the solid phase, between the (hot) pore interface and the (cold) solid core. Its determination usually needs resolution of the heat equation and this is problematic as the solid temperature varies as a consequence of shock propagation and compressibility effects as well as subscale heat diffusion.

A method is developed herein to compute heat losses without subscale resolution. It uses on one hand the time varying volume average solid temperature, determined from the solid phase balance energy equation, and the solid core temperature that varies as a consequence of compressibility and shocks. Its precise evolution is determined through a non-conventional energy equation, or more precisely through two-phase shock jump relations.

Having in hand the mean solid temperature and the solid core temperature, the interfacial heat flux (heat loss) is determined from an approximate profile expressing correctly the physics of heat transfer.

At this point, both subscale heat production and heat loss are computed without subscale resolution. These heat sources enter in the definition of the interface temperature that now involves all relevant contributions reported in shock ignition sensitivity studies: pore size, shock pressure, thermal conductivity, subscale plastic stress, pressure relaxation rate (related to pore collapse velocity). Transient evolution of these variables directly enters in the interface temperature formulation.

This temperature is used as criterion to initiate solid deflagration, modeled by Vieille's law. Collective effects of subscale deflagrations are summarized at global scale, in the two-phase model, through the specific interfacial burning surface. At short times, total pore surface is used in the global mass transfer rate to compute the burning surface. After some time, the fluidization limit of the granular bed is reached and burning continues through the outer grains surface.

Last the model is extended to deal with quasi-steady detonation propagation in explosive cylinders of variable diameters. To this end, modification of the decomposition kinetics with burning area increase is addressed. With this modification good agreement with experimental measurements of detonation velocity as a function of charge diameter is obtained. The full model is thus able to deal with both shock to detonation transition, occurring in pressure ranges of 50–100 kbar, and detonation propagation regime, occurring in pressure ranges of 300–1000 kbar.

The paper is organized as follows. The macro-scale flow model is presented in Section 2, as an extension of the Saurel et al. [48] model, this one being itself a modification of the Baer and Nunziato [1] model. The various closure relations are provided in the same section. Section 3 analyses pore collapse dynamics and hot spot creation through relaxation effects of the former model. Section 4 analyses the extra evolution equations used to determine the solid core temperature. This temperature is used to compute the solid-gas interface temperature as well as the interfacial heat flux. Section 5 addresses validations of shock to detonation transition in 1D for PBX9501 explosive. A sensitivity analysis of the flow model to the various parameters is done in the same section. Validations against experimental data of velocity of detonation as a function of charge diameter are addressed as well. Conclusions are given in Section 6.

2. Multiscale multiphase model

The flow model of Saurel et al. [48] is considered as symmetric variant of the Baer and Nunziato [1] two-phase flow model. It is complemented by extra equations used to compute pore and grain radii, important for interfacial area determination. Extra equations are also added to determine solid core temperature, important for the computation of conductive heat loss at pore scale. For the sake of simplicity the equations are given in 1D.