Modeling shocks and detonations in heterogeneous high explosives

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1 Introduction

Shock and detonations in heterogeneous materials differ widely of similar phenomena in gas mixtures as temperatures and velocities 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. Materials equations of state are obviously also very different of those of gases.

The present talk is devoted to the presentation of modern technical material in some of these areas:

- Shock relations for multiphase mixtures with stiff mechanical relaxation [1]. These relations [2] enable accurate computation of the post-shock state and energy partition among the phases.

- Generalized Chapman-Jouguet conditions [3]. In the detonation reaction zone, stiff mechanical relaxation holds but temperatures remain out of equilibrium. Heat exchanges result in non-negligible unreacted solid at the sonic surface and have similar (but weaker) effects as velocity divergence effects in non-ideal detonations.

- A flow model valid just after the shock front where mechanical relaxation is stiff to the expansion zone, where velocity disequilibrium are present [4].

- A novel equation of state, simple and accurate for condensed energetic materials and temperature computation [5].

Chemical decomposition and hot spots modelling in this theoretical frame are in progress.

The paper is organized as follows. In Section 2 the symmetric variant of the BN model [6] is presented to model non-equilibrium two-phase flow mixtures. Its mechanical equilibrium reduced version [1] is recalled in Section 3 with the associated shock relations. The CJ and ZND associated models are given in Section 4. A method to fit these shock, ZND and CJ conditions in unsteady regime, 1D and multi-D is given in Section 5.

2 Non-equilibrium flow model

A symmetric variant of the two-phase flow BN model has been derived in [4]:

$$\frac{\partial \alpha_1}{\partial t} + u_1 \frac{\partial \alpha_1}{\partial x} = \mu(\pi_1 - \pi_2)$$

$\partial(\alpha\rho)_1$	$\frac{\partial(\alpha\rho u)_1}{\partial (\alpha\rho u)_1} = 0$
∂t	$\frac{\partial x}{\partial x} = 0$
$\frac{\partial(\alpha\rho u)_1}{\partial t}$	+ $\frac{\partial(\alpha\rho u^2 + \alpha p)_1}{\partial x} = \pi_1 \frac{\partial \alpha_1}{\partial x} + \lambda(u_2 - u_1)$
$\frac{\partial(\alpha\rho E)_1}{\partial(\alpha\rho E)_1}$	$+\frac{\partial(\alpha(\rho E + p)u)_{1}}{\partial \alpha_{1}} = \pi u \frac{\partial \alpha_{1}}{\partial \alpha_{1}} + \lambda u'(u - u) - u\pi'(\pi - \pi) + O$
∂t	$\partial x \qquad \partial x \qquad \partial x$
$\partial(\alpha\rho)_2$	+ $\frac{\partial(\alpha\rho u)_2}{\partial (\alpha\rho u)_2} = 0$
∂t	$\partial \mathbf{X}$
$\frac{\partial(\alpha\rho u)_2}{\partial t}$	+ $\frac{\partial(\alpha\rho u^2 + \alpha p)_2}{\partial x} = \pi_1 \frac{\partial \alpha_2}{\partial x} - \lambda(u_2 - u_1)$
$\partial(\alpha\rho E)_2$	$\partial(\alpha(\rho E + p)u)_2 = \pi u \partial \alpha_2 - \partial u'(u - u) + u\pi'(\pi - \pi) + O$
<u>∂t</u>	$+ \frac{\partial x}{\partial x} = \pi_1 u_1 \frac{\partial x}{\partial x} - \pi u_1 (u_2 - u_1) + \mu \pi_1 (\pi_1 - \pi_2) + Q_2$

With the following definitions: $\alpha_k, \rho_k, u_k, p_k, e_k, E_k, B_k$ represent respectively the volume fractions, the densities, the velocities, the pressures, the internal energies, the total energies, the 'granular' or 'configurational' energies. The effective pressures π_k are defined as $\pi_k = p_k - \beta_k$. At mechanical equilibrium $\pi_1 = \pi_2$ and $u_1 = u_2$. The rate at which mechanical equilibrium is reached is controlled by the relaxation parameters λ and μ . The heat exchanges are represented by Q_k and mass transfer is absent for now.

The phases total energies are defined as: $E_k = e_k + B_k(\alpha_k) + \frac{1}{2}u_k^2$.

The granular pressure is defined by: $\beta_k = \alpha_k \rho_k \frac{dB_k}{d\alpha_k}$. This equation of state is determined from

pressed granular beds experiments.

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The following formulation of interfacial variables render the model symmetric with respect to the phases indexes:

$$\begin{split} \mathbf{u}_{1} &= \frac{Z_{1}\mathbf{u}_{1} + Z_{2}\mathbf{u}_{2}}{Z_{1} + Z_{2}} + \operatorname{sgn}\left(\frac{\partial\alpha_{1}}{\partial\mathbf{x}}\right) \frac{\pi_{2} - \pi_{1}}{Z_{1} + Z_{2}} , \qquad \mathbf{u}_{1}^{'} &= \frac{Z_{1}\mathbf{u}_{1} + Z_{2}\mathbf{u}_{2}}{Z_{1} + Z_{2}} , \\ \pi_{1} &= \frac{Z_{2}\pi_{1} + Z_{1}\pi_{2}}{Z_{1} + Z_{2}} + \operatorname{sgn}\left(\frac{\partial\alpha_{1}}{\partial\mathbf{x}}\right) \frac{Z_{1}Z_{2}}{Z_{1} + Z_{2}}(\mathbf{u}_{2} - \mathbf{u}_{1}) , \quad \pi_{1}^{'} &= \frac{Z_{2}\pi_{1} + Z_{1}\pi_{2}}{Z_{1} + Z_{2}} . \end{split}$$

This symmetric formulation of the BN model has some advantages. As these formulas correspond to local 'granular Riemann problem' solutions, fluid-fluid interfaces, fluid-granular media interfaces as well as permeable interfaces are handled accurately by the non-conservative terms $u_1 \frac{\partial \alpha_k}{\partial x}, \pi_1 \frac{\partial \alpha_k}{\partial x}$. When dealing with the computation of material interfaces there is no need to use interface

reconstruction, Level Set, or any Front Tracking method. At interfaces, when a volume fraction discontinuity is present, interface conditions are matched automatically.

Also, this system is entropy preserving:

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$$\begin{aligned} &\frac{\partial(\alpha\rho)_{1}s_{1} + (\alpha\rho)_{2}s_{2}}{\partial t} + \frac{\partial(\alpha\rho)_{1}u_{1}s_{1} + (\alpha\rho)_{2}u_{2}s_{2}}{\partial x} = \frac{Q_{1}}{T_{1}} + \frac{Q_{2}}{T_{1}} \\ &\frac{1}{T_{1}} \left\{ \frac{Z_{1}}{\left(Z_{1} + Z_{2}\right)^{2}} \left((\pi_{2} - \pi_{1}) + \text{sgn}\left(\frac{\partial\alpha_{1}}{\partial x}\right) Z_{2}(u_{2} - u_{1}) \right)^{2} \left| \frac{\partial\alpha_{1}}{\partial x} \right| + \lambda \frac{Z_{2}}{Z_{1} + Z_{2}} (u_{2} - u_{1})^{2} + \mu \frac{Z_{1}}{Z_{1} + Z_{2}} (\pi_{2} - \pi_{1})^{2} \right\} \\ &+ \frac{1}{T_{2}} \left\{ \frac{Z_{2}}{\left(Z_{1} + Z_{2}\right)^{2}} \left((\pi_{2} - \pi_{1}) + \text{sgn}\left(\frac{\partial\alpha_{1}}{\partial x}\right) Z_{2}(u_{2} - u_{1}) \right)^{2} \left| \frac{\partial\alpha_{2}}{\partial x} \right| + \lambda \frac{Z_{1}}{Z_{1} + Z_{2}} (u_{2} - u_{1})^{2} + \mu \frac{Z_{2}}{Z_{1} + Z_{2}} (\pi_{2} - \pi_{1})^{2} \right\} \end{aligned}$$

As $Q_1 + Q_2 = 0$ and Q_1 : $(T_2 - T_1)$ all production terms are non-negative.

Last, the model is hyperbolic with 7 wave speeds instead of 6 in the BN model. This last feature is of paramount importance regarding numerical resolution [7].

3 Mechanical equilibrium model and shock relations

When shock and detonation waves propagate in condensed energetic materials mechanical relaxation is so stiff (see [1,2] for relaxation time estimates) that a single pressure-single velocity model is enough accurate to describe the dynamics of such flows. The reduced model that results of asymptotic analysis at leading order reads [1],

$$\begin{aligned} \frac{\partial \alpha_1}{\partial t} + u \frac{\partial \alpha_1}{\partial x} &= \frac{\left((\rho_2 c_2^2 - \beta_2) - (\rho_1 c_1^2 - \beta_1)\right)}{\frac{\rho_1 C_1^2}{\alpha_1} + \frac{\rho_2 C_2^2}{\alpha_2}} \frac{\partial u}{\partial x} + Q_1 \frac{\alpha_2 \Gamma_1 + \alpha_1 \Gamma_2}{\alpha_2 \rho_1 C_1^2 + \alpha_1 \rho_2 C_2^2} \\ \frac{\partial (\alpha \rho)_1}{\partial t} + \frac{\partial (\alpha \rho)_1 u}{\partial x} &= 0, \qquad \qquad \frac{\partial (\alpha \rho)_2}{\partial t} + \frac{\partial (\alpha \rho)_2 u}{\partial x} = 0, \\ \frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2 + p}{\partial x} &= 0, \\ \frac{\partial \rho E}{\partial t} + \frac{\partial (\rho E + p) u}{\partial x} &= 0, \end{aligned}$$

where, Γ_k is the Gruneisen coefficient of phase k and $C_k^2 = c_k^2 + \alpha_k^2 \frac{d^2 B_k}{d\alpha_k^2}$ represents the 'effective'

sound speed. The total mixture energy is defined as,

$$E = Y_1(e_1(\rho_1, p_1) + B_1(\alpha_1)) + Y_2(e_2(\rho_2, p_2) + B_2(\alpha_2)) + \frac{1}{2}u^2.$$

The mixture pressure is given by a mixture equation of state $p = p(\rho, e, \alpha_1)$ derived from:

 $\pi_1 = \pi_2$, the mechanical equilibrium condition and,

 $e = Y_1(e_1(\rho_1, p_1) + B_1(\alpha_1)) + Y_2(e_2(\rho_2, p_2) + B_2(\alpha_2)), \text{ the mixture internal energy definition.}$

This flow model is valid to describe mixtures of materials in mechanical equilibrium but is also very well suited to the computation of mixture cells (artificial smearing zones) in multi-material codes [8,9]. The volume fraction equation of this flow model being non-conservative it is not possible to derive conventional shock relations. The following Hugoniot system was proposed in [2] and was demonstrated valid in the weak shock wave limit. For strong shocks is at been compared in the same reference to most published data and has shown excellent agreement as well. It reads,

$$Y_{k} = Y_{k}^{0},$$

$$\rho(u - \sigma) = \rho^{0}(u^{0} - \sigma) = m$$

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$$\begin{split} p - p^0 + m^2 (v - v^0) &= 0, \\ e_k - e_k^0 + \frac{p + p^0}{2} (v_k - v_k^0) &= 0. \end{split}$$

The key point relies in the last relations, that means that each phase evolves along its own Hugoniot curve, in pressure equilibrium with the other phases.

4. Generalized CJ and ZND

From the Neumann spike to the CJ point mechanical relaxation effects are stiff and the flow evolves in pressure and velocity equilibrium but in thermal and Gibbs free energy disequilibrium. Chemical decomposition effects result in mass transfer terms that must be added to the former flow model [10]. They result in the following volume fraction and mass equations, the remaining mixture momentum and energy equations being unchanged:

$$\frac{\partial \alpha_{1}}{\partial t} + u \frac{\partial \alpha_{1}}{\partial x} = \frac{(\rho_{2}c_{2}^{2} - \beta_{2}) - (\rho_{1}c_{1}^{2} - \beta_{1})}{\rho_{1}C_{1}^{2}} \frac{\partial u}{\partial x} + \dot{m} \frac{\frac{c_{1}^{2}}{\alpha_{1}} + \frac{c_{2}^{2}}{\alpha_{2}}}{\rho_{1}C_{1}^{2}} + H(T_{2} - T_{1}) \frac{\frac{\Gamma_{1}}{\alpha_{1}} + \frac{\Gamma_{2}}{\alpha_{2}}}{\rho_{1}C_{1}^{2}} + \frac{\rho_{2}C_{2}^{2}}{\alpha_{2}}},$$
$$\frac{\partial \alpha_{1}\rho_{1}}{\partial t} + \frac{\partial \alpha_{1}\rho_{1}u}{\partial x} = \dot{m},$$
$$\frac{\partial \alpha_{2}\rho_{2}}{\partial t} + \frac{\partial \alpha_{2}\rho_{2}u}{\partial x} = -\dot{m}.$$

Mass transfer (m) modelling is not addressed herein. As chemical decomposition is absent in the shock front, the Rankine-Hugoniot set given in the former paragraph is unchanged. Between the shock front and the CJ state, the ZND model corresponds to the former two-phase flow model in steady regime and expressed in the shock front moving frame:

$$\begin{split} \frac{\partial u}{\partial x} &= \frac{1}{\rho(C_w^2 - \overline{u}^2)} \times \\ \left\{ \frac{\left(\Gamma_1 \rho_2 c_2^2 - \Gamma_2 \rho_1 c_1^2\right)}{\left(\alpha_2 \rho_1 C_1^2 + \alpha_1 \rho_2 C_2^2\right)} H(T_2 - T_1) + \left(\frac{\left(\alpha_2 c_1^2 + \alpha_1 c_2^2\right)}{\alpha_1 \Gamma_2 + \Gamma_1 \alpha_2} \left(\frac{\Gamma_1 \rho_2 c_2^2 - \Gamma_2 \rho_1 c_1^2}{\alpha_2 \rho_1 C_1^2 + \alpha_1 \rho_2 C_2^2} \right) + \left(\frac{\Gamma_1 \Gamma_2}{\alpha_1 \Gamma_2 + \Gamma_1 \alpha_2} \right) \left((h_2 - \frac{c_2^2}{\Gamma_2}) - (h_1 - \frac{c_1^2}{\Gamma_1}) \right) \right) \dot{m} \right\} \\ \frac{\partial \rho}{\partial x} &= -\frac{\rho}{\overline{u}} \frac{\partial \overline{u}}{\partial x} ; \frac{\partial p}{\partial x} = -\rho \overline{u} \frac{\partial \overline{u}}{\partial x} ; \frac{\partial Y_1}{\partial x} = \frac{\dot{m}}{\rho \overline{u}} ; \\ \frac{\partial \alpha_1}{\partial x} &= \frac{\left(\rho_2 c_2^2 - \rho_1 c_1^2\right) \frac{\partial \overline{u}}{\partial x} + H(T_2 - T_1) \left(\frac{\Gamma_1}{\alpha_1} + \frac{\Gamma_2}{\alpha_2} \right) + \dot{m} \left(\frac{c_1^2}{\alpha_1} + \frac{c_2^2}{\alpha_2} \right)}{\overline{u} \left(\frac{\rho_1 C_1^2}{\alpha_1} + \frac{\rho_2 C_2^2}{\alpha_2} \right)} \cdot \end{split}$$

The velocity in the detonation frame of reference is denoted by $\overline{u} = u - D$, with D the detonation velocity. The first equation of this system provides the generalized temperature non-equilibrium CJ condition [3, 11]:

$$\frac{\left(\Gamma_{1}\rho_{2}c_{2}^{2}-\Gamma_{2}\rho_{1}c_{1}^{2}\right)}{\left(\alpha_{2}\rho_{1}c_{1}^{2}+\alpha_{1}\rho_{2}c_{2}^{2}\right)}H(T_{2}-T_{1})+\left(\frac{\left(\alpha_{2}c_{1}^{2}+\alpha_{1}c_{2}^{2}\right)}{\alpha_{1}\Gamma_{2}+\Gamma_{1}\alpha_{2}}\left(\frac{\Gamma_{1}\rho_{2}c_{2}^{2}-\Gamma_{2}\rho_{1}c_{1}^{2}}{\alpha_{2}\rho_{1}c_{1}^{2}+\alpha_{1}\rho_{2}c_{2}^{2}}\right)+\left(\frac{\Gamma_{1}\Gamma_{2}}{\alpha_{1}\Gamma_{2}+\Gamma_{1}\alpha_{2}}\right)\left(\left(h_{2}-\frac{c_{2}^{2}}{\Gamma_{2}}\right)-\left(h_{1}-\frac{c_{1}^{2}}{\Gamma_{1}}\right)\right)\right)\dot{m}=0$$

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at sonic point defined by $\overline{u} = C_w$.

The mixture sound speed is given by $\frac{1}{\rho C_W^2} = \frac{\alpha_1}{\rho_1 C_1^2} + \frac{\alpha_2}{\rho_2 C_2^2}$.

This algebraic system contains the conventional CJ conditions in the single phase limit and in the absence of heat transfer (or in the temperature equilibrium limit). Conventional CJ conditions are $\dot{m} = 0$ at sonic point defined by $\bar{u} = c$.

Generalized CJ conditions allow incomplete reactions at the sonic surface. More precisely, exothermicity of the chemical reaction is balanced by the internal heat exchange between the phases.

The detonation wave structure can be computed with conventional ZND algorithms. For a given detonation speed:

- The Hugoniot system is used to compute the Neumann spike.
- The ODE system is solved from the Neumann spike to the CJ point.
- Generalized CJ conditions have to be fulfilled at the sonic surface, otherwise the presumed detonation velocity has to be changed.

Compared to the conventional ZND model based on the Euler equations knowledge of the heat exchange coefficient is needed. Computations have been done in [12] assuming zero heat exchange in various liquid explosive mixtures loaded by aluminium particles. In the absence of heat exchanges the CJ conditions reduce to $\dot{m} = 0$ when $\bar{u} = C_w$. As the sound speed C_w has non-monotonic behavior versus the volume fraction, important difference appear in the flow behavior and detonation speed compared to the conventional CJ condition $\bar{u} = c$. Non-negligible improvement in the detonation speed computation have been reported with this temperature disequilibrium approach [12, 13].

5 Multi-D computations

From the above theory and space and time relaxation scale analysis important facts appear:

- At the shock front the jump conditions given in Section 3 are appropriate. But a difficulty appears at the discrete level. How to impose them in practical computations?

- In the reaction zone, from the shock to the CJ surface the flow evolves in temperature disequilibrium but in pressure and velocity equilibrium. How to impose such behavior in the computations?

- At the sonic surface some amount of solid is unreacted as a consequence of heat exchanges competition with exothermic reaction as well as front curvature. Consequently reacting material will possibly react in the expansion zone. But in this zone, as the detonation products density decreases mechanical relaxation is no longer stiff and the flow evolves in velocity disequilibrium. How to model and reproduce these effects?

These various layers are schematized in Figure 1.



Figure 1. Schematic representation of a detonation wave and various specific zones.

For the sake of conciseness, these specific treatments will be presented at the ICDERS 2015 oral session and in a forthcoming full length paper.

References

[1] Kapila, A. K., Menikoff, R., Bdzil, J. B., Son, S. F., & Stewart, D. S. (2001). Two-phase modeling of deflagration-to-detonation transition in granular materials: Reduced equations. Physics of Fluids (1994-present), 13(10), 3002-3024

[2] Saurel, R., Le Metayer, O., Massoni, J., & Gavrilyuk, S. (2007). Shock jump relations for multiphase mixtures with stiff mechanical relaxation. Shock Waves, 16(3), 209-232

[3] Petitpas, F., Saurel, R., Franquet, E., & Chinnayya, A. (2009). Modelling detonation waves in condensed energetic materials: Multiphase CJ conditions and multidimensional computations. Shock waves, 19(5), 377-401

[4] Saurel, R., Le Martelot, S., Tosello, R., & Lapébie, E. (2014). Symmetric model of compressible granular mixtures with permeable interfaces. Physics of Fluids (1994-present), 26(12), 123304

[5] Le Metayer, O. and Saurel, R. (2015) The Noble-Abel-Stiffened-Gas equation of state. Int. J. Thermal Sciences, submitted

[6] Baer, M. R., & Nunziato, J. W. (1986). A two-phase mixture theory for the deflagration-todetonation transition (DDT) in reactive granular materials. International journal of multiphase flow, 12(6), 861-889

[7] Furfaro, D., & Saurel, R. (2015). A simple HLLC-type Riemann solver for compressible non-equilibrium two-phase flows. Computers & Fluids, 111, 159-178.

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[8] Murrone, A., & Guillard, H. (2005). A five equation reduced model for compressible two phase flow problems. Journal of Computational Physics, 202(2), 664-698

[9] Saurel, R., Petitpas, F., & Berry, R. A. (2009). Simple and efficient relaxation methods for interfaces separating compressible fluids, cavitating flows and shocks in multiphase mixtures. Journal of Computational Physics, 228(5), 1678-1712

[10] Saurel, R., Petitpas, F., & Abgrall, R. (2008). Modelling phase transition in metastable liquids: application to cavitating and flashing flows. Journal of Fluid Mechanics, 607, 313-350

[11] Schoch, S., Nikiforakis, N., Lee, B. J., & Saurel, R. (2013). Multi-phase simulation of ammonium nitrate emulsion detonations. Combustion and Flame, 160(9), 1883-1899

[12] Baudin, G., Lefrancois, A., Saurel, R., Petitpas, F., Metayer, O. L., Massoni, J., ... & Zotov, E. (2010). Toward a thermal disequilibrium multiphase model for high explosives containing metallic particles. Journal of Energetic Materials,28(S1), 154-179

[13] Pei, H., Nie, J., & Jiao, Q. (2014). Study on the Detonation Parameters of Aluminized Explosives Based on a Disequilibrium Multiphase Model. Central European Journal of Energetic Materials, 11(4)