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Jump relations across shock waves in condensed multiphase flows: a comparison between numerical and analytical solutions

Eric Daniel, Jacques Massoni

Université de Provence Polytech'Marseille,
IUSTI, UMR CNRS 6595
5 rue E. Fermi, 13453 Marseille Cedex 13
Also: INRIA SMASH Project same address.
Eric.daniel@polytech.univ-mrs.fr

Résumé

On propose de simuler la propagation d'onde de choc dans les milieux condensés en utilisant un outil de simulation directe. Ces milieux sont mécaniquement caractérisés par une pression et une vitesse unique. Dans cette étude, le mélange est constitué de grains séparés par une interface entre les matériaux : ce problème à interface est résolu par une méthode d'interface diffuse. Les solutions obtenues sont comparées à des résultats expérimentaux et à une nouvelle méthode analytique. La fraction volumique (ou la température par exemple) ne peut pas être mesurée expérimentalement et il est donc important de connaître le comportement d'une quantité phasique grâce à diverses méthodes. Une évolution non monotone de la fraction volumique en fonction de la pression derrière le choc est observé aussi bien avec les méthodes numériques que des solutions analytiques.

Mots-clefs : Shock wave, jump relations, direct numerical simulation

1 Introduction

Modelling shock wave propagation in multiphase media requires the knowledge of the Rankine-Hugoniot relations that must fit experimental results. The knowledge of the jump conditions is of prime importance to determine the complete mechanical and thermodynamical state of each phase in the mixture that is, the volume fractions, the phase densities and the temperatures together with all mixture quantities (mixture density, velocity and pressure).

In the case of mixtures governed by stiff mechanical relaxation phenomenon, and consequently evolving with a unique pressure and velocity, some analytical jump relations across a shock wave can be expressed and they fit with experimental data [5, 10]. They are consistent with conservation of mass, momentum and total energy for the mixture.

The experimental data concerning materials under strong shock wave can be found in [1, 3, 6, 7, 11]: only averaged quantities are accessible from these experiments, velocity, pressure, density and shock wave velocity. It is almost impossible to measure the volume fractions or the phase temperatures.

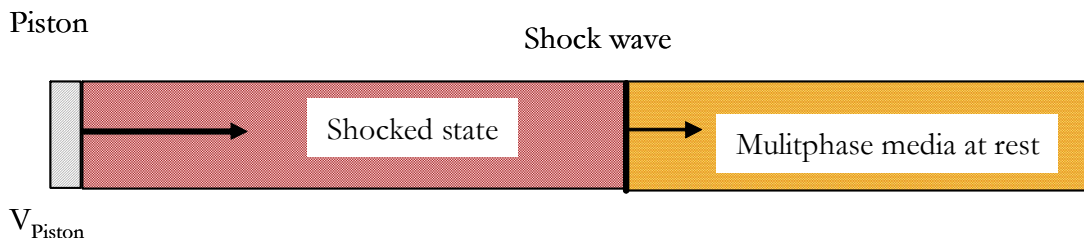


Figure 1: Schematic view of the simulation in order to determine the shock relations.

In this paper, these experiments will be numerically reproduced according to the process depicted in Figure 1. A piston moving with a high velocity hits a multiphase media and generates a shock wave that travels with constant velocity in the multiphase media. The results of the simulations lead to the knowledge of the jump of all the flow quantities across the shock wave (relations between the states of the mixture at infinity).

We propose a direct numerical simulation of shock propagation phenomena. We consider a mixture made of a collection of very small grains of single phase. Each single phase is treated as a pure phase, its dynamics is governed by Euler equations and obeys its own Equation of State (EOS). The numerical problem is then a numerical problem of interfaces. Consequently, only few assumptions can be made about the flow, which is considerably advantageous compared to other existing two-phase flows models. A diffuse interface model based on a single velocity and a single pressure is numerically solved. The numerical solution obtained is locally the solution of a one-phase flow that must be first averaged to get the characteristic states of the multiphase flow.

2 Model for the Direct Numerical Simulations

We suppose that each material obeys its own Equation of State (EOS), and that each material can be distinguished in the mixture. An ideal representation of the mixture is assumed where both phases appear as a collection of square grains at the microscopic level. It is clearly a problem of interface between each grain of each material.

A diffuse interface method is used, based on a five equations model [2, 8, 9] suitable for this kind of problem. This system of equations is characterized by a single pressure and a single velocity. The interface is smeared out over a few cells.

The system of partial differential equations for a N -phases flow include five partial differential equations for scalar quantities (5 equations model):

$$\begin{aligned} \frac{\partial \rho \vec{u}}{\partial t} + \text{div}(\rho \vec{u} \vec{u} + \vec{P} \vec{I}) &= 0 \\ \frac{\partial \rho E}{\partial t} + \text{div}(\rho E + P) \vec{u} &= 0 \quad (1) \\ \frac{\partial \alpha_k \rho_k}{\partial t} + \text{div}(\alpha_k \rho_k \vec{u}) &= 0 \\ \frac{\partial \alpha_k}{\partial t} + \vec{u} \cdot \vec{\nabla}(\alpha_k) &= 0 \end{aligned}$$

The subscript k is related to the k -th phase, α_k is the volume fraction. The internal energy of phase k is related to the pressure and the phase density by the means of the Stiffened Gas EOS. The pressure is

expressed by the following analytic relation:
$$p = \frac{\rho \varepsilon - \sum_{k=1, N} \frac{\alpha_k \gamma_k P_{\infty, k}}{\gamma_k - 1}}{\sum_{k=1, N} \frac{\alpha_k}{\gamma_k - 1}}.$$

Numerical method

The conservative equations are solved by a classical Godunov scheme based on an HLLC Riemann solver. The equation of the volume fraction is non conservative. It is discretized by a simple finite volume scheme: $V_{ij} \frac{\alpha_k^{n+1} - \alpha_k^n}{\Delta t} + \sum_{M=1,4} (\alpha_{k,M}^* - \alpha_k^n) u_M^* S_M = 0$ where V_{ij} is the volume of the discrete element, S_M is the surface of M -th face defining the discrete volume. The upper-script * denotes a quantity obtained from the Riemann solver at the cell interface. The code developed on these bases is used on a cluster of 20 PCs. The parallelization of the code is done using a MPI library.

Initial condition for Direct Numerical Simulation

This paragraph concerns the initial condition for the Direct Simulation.

The solution of a field ϕ is depending on space coordinates (x, y) . This field is not suitable to achieve a quantitative comparison with the Rankine-Hugoniot solution. One must transform the 2D field, $\phi(x, y)$, into a 1D field: $\phi(X)$. In the (x, y) plane, a volume V is defined at a new abscissa X . The system of

equations (1) having no physical scale, the only real scale involved in this problem is the arbitrary size R given to the grains. Then, the flow quantity is averaged to obtain a representative values contained in $V(X)$, which must be large enough to include a sufficient number of grains in order to get a meaningful averaged quantity. The average is defined in a discrete form as follow : $f^{x,y}(X_I) = \frac{1}{V_I} \sum_{i=1, N_x} \sum_{j=1, N_y} f_{i,j} V_{i,j}$.

Several distributions of these grains in the computational domain lead to $f^{x,y}(\alpha_{1,I}) = \alpha_1$: a random distribution is suitable as well as a regular one. Because of obvious considerations about feasibility, only 2 homogeneous distributions are tested. The first one is a checkerboard distribution, the second one is made of successive vertical layers (Figure 2).

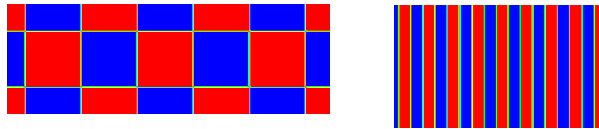


Figure 2 : Zoom on the initial condition of the volume fraction: checkerboard and vertical layers distribution. The two colours indicate the two different values of the volume fraction 0 or 1.

For the computation, a symmetry condition is used at the lower and upper boundaries of the domain. It insures a periodic reproduction of the domain in the y -direction.

3 Direct Numerical Simulation of shock wave in two-phase media

The analysis of the results is focused on the jump of quantities across a shock wave. The experiment depicted in Figure 1 is reproduced on a mixture of epoxy-spinel. The experimental values are given in [3, 7].

In the numerical simulation, the impact is modelled by a piston boundary condition, for which the velocity is imposed. When the steady state is reached, the shock velocity is also computed by the relation: $\sigma_{shock} = \frac{\rho_1 u_1}{\rho_1 - \rho_0}$. In this relation, the subscript 1 is related to the shocked state of the mixture.

The other quantities of interest (pressure, density) are picked directly on computed values after averaging two-dimensional results.

Collecting this values lead to different graphs for which the abscissa is chosen to be the material velocity (the impact velocity). The mixture density, the pressure, the shock wave velocity are compared with experimental data.

In the following analysis, the experimental volume fraction is also plotted. It is contradictory with the *Introduction Section*, in which it is claimed that this quantity cannot be measured. By choosing the EOS of each material, one can extract the volume fraction from the knowledge of the experimental values of the final pressure and the mixture quantity. Combining the conservation energy across the shock and the

EOS leads to $\alpha_1 = \frac{\rho \varepsilon - \frac{P^+ P_{\infty,2}}{(\gamma_2 - 1)}}{\left(\frac{P^+ P_{\infty,1}}{(\gamma_1 - 1)} - \frac{P^+ P_{\infty,2}}{(\gamma_2 - 1)} \right)}$. This value can thus be computed from the experimental data and

may be defined as the experimental volume fraction.

The values used for the initial condition reproduce the initial state of the mixture: The pressure is set to 10^5 Pa, the volume fraction of the epoxy is 0.5965 rounded as to 0.6 (for obvious numerical considerations). The density of the epoxy is 1185 kg/m^3 and those of the spinel is 3622 kg/m^3 . The EOS parameters are $\gamma = 2.43$ and $P_{\infty} = 53.10^8 \text{ Pa}$ for the epoxy and $\gamma = 1.62$ and $P_{\infty} = 51410.10^8 \text{ Pa}$ for the spinel.

Checkerboard initial condition

The conditions of the computations are obtained from the analysis of the one-phase simulations. The numerical resolution r_{num} is imposed to be at least equal to 8 cells/grain. Increasing the resolution does not change the results. 2 grains are modelled in the y -direction.

The CFL number is equal to 0.5. The length of the sample is equal to 0.936m: this is enough to insure a steady state flow in the mixture. The total number of grain is equal to 6240. 20 processors are available for these computations, then we use a mesh of 1.248 106 cells.

Vertical layers initial condition

The same numerical experiments are reproduced with the multi-layers initial condition. The numerical resolution is set to 12 cells/grain. L_{tot} is equal to 1m. The CFL number is equal to 0.5. The results are collected the same way as for the previous case and they will be compared with the experimental results in Figure 3. The results obtained with the Direct Simulations and experimental results are in very good agreement. Whatever the initial conditions, the differences observed are quite negligible for the mixture quantities. This point must be notice, because the initial conditions are so different that one might have expected differences in the final state.

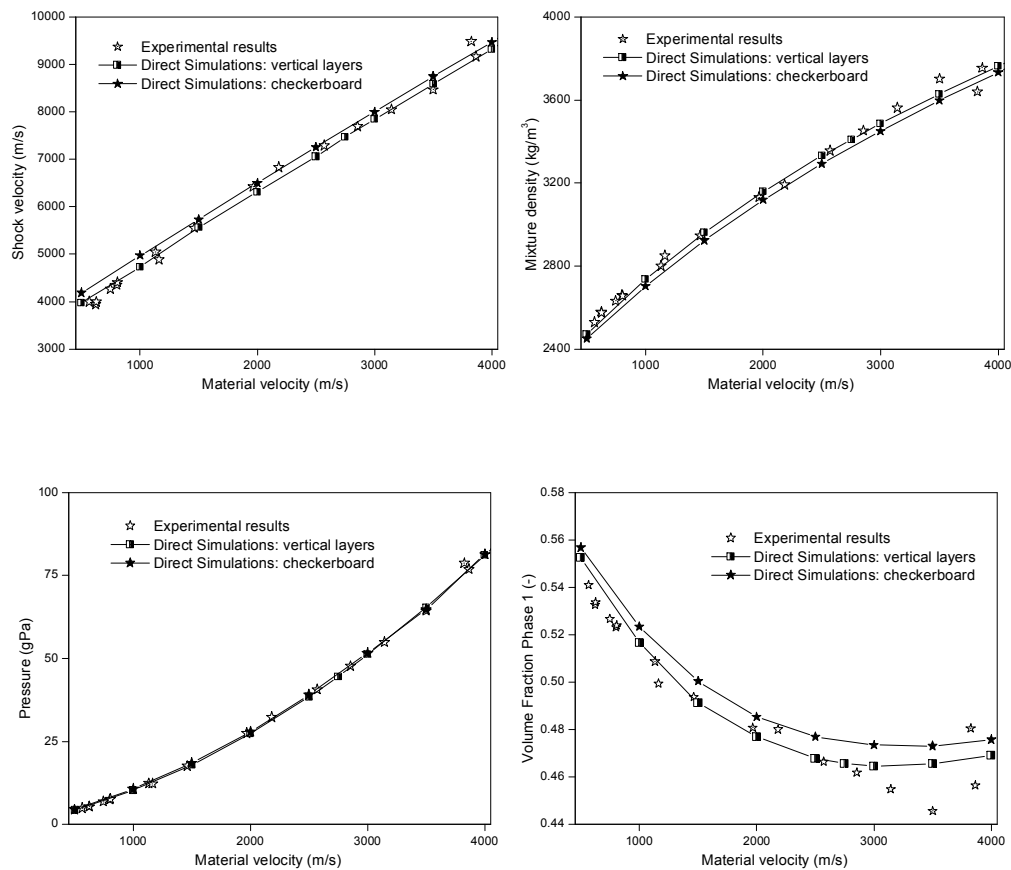


Figure 3: Direct numerical simulation results for the shock wave propagation in epoxy-spinel compared with experimental data.

The differences between both initial conditions are more visible on the volume fraction. They both fit well the experimental results but the checkerboard initial condition gives slightly larger values than the vertical layers initial condition. The differences may be explained by a difference of “turbulent energy” associated to the two-dimensional motion of the flow: The checkerboard initial condition might generate more turbulent energy that will insure an homogeneous flow. This point has been underlined in [4]. Nevertheless, the scale of the graph magnifies this difference.

The non monotonous behaviour of the volume fraction according to the material velocity is noticeable. Experimental results also show this tendency. Actually, one can think this behaviour is mainly driven by the evolution of the EOS with the pressure. Indeed, it is possible to find out a limit value of the volume

fraction when the pressure tends to infinity: $\alpha_1^{\text{lim}} = \frac{\delta_{\infty,2}}{\alpha_2^0 + \frac{\delta_{\infty,1}}{\alpha_1^0}}$. With the value related to each material

(Table 1), $\delta_{\infty,1} = 2.40$ and $\delta_{\infty,2} = 4.22$, then $\alpha_1^{\text{lim}} \approx 0.725$. This result is coherent with an increase of the volume fraction versus the flow velocity, or equivalently versus the pressure, like observed in Figure 3.

The direct simulations provide very interesting results because they are free of any constraint: the solution is mainly driven by the EOS of each material. These EOS are the same in all models used in this paper. We get excellent agreement with the experimental results.

It is now interesting to compare these results with results provided by analytical solutions or multiphase flow numerical model. These comparisons will be based only on the checkerboard initial conditions.

4 Direct numerical simulation vs analytical solution

As said in the *Introduction Section*, it is important to obtain the Rankine-Hugoniot relations of such mechanical system. A nice solution is proposed in Ref.[10] and it does appear interesting to compare the solution of this problem with this numerical method. We first recall the basic of the Rankine-Hugoniot solution.

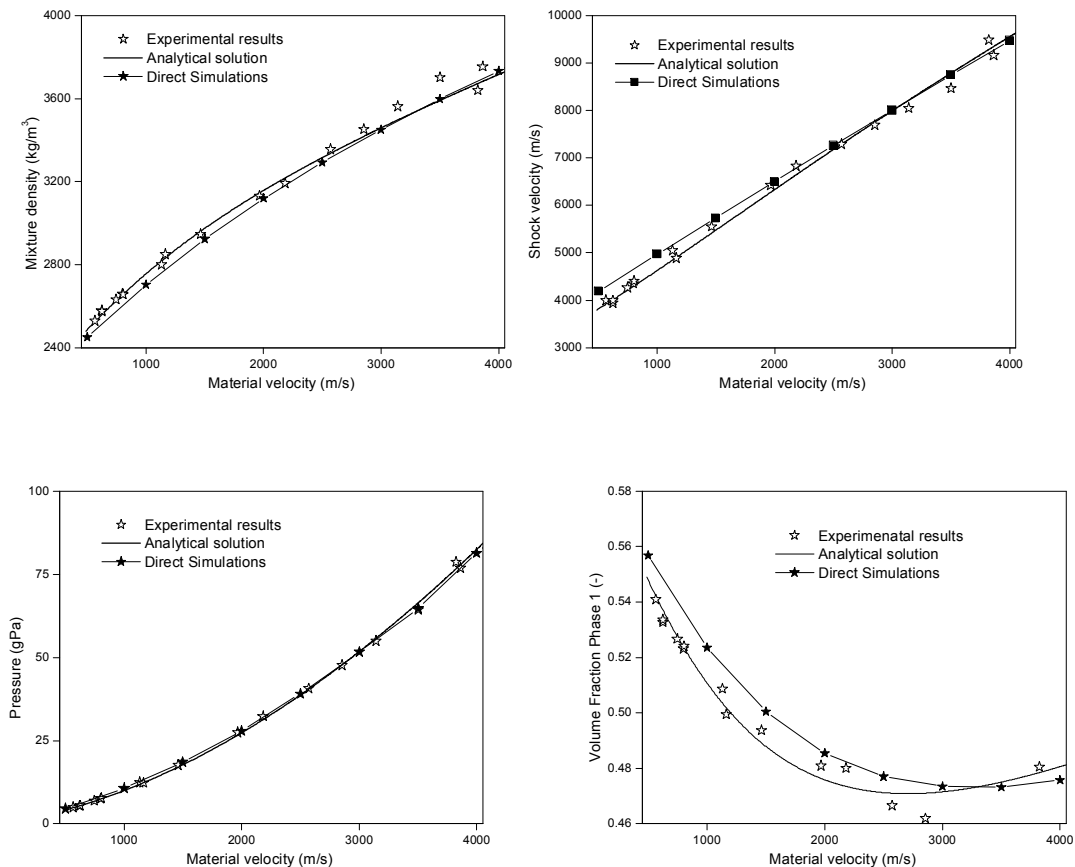


Figure 4: Direct numerical simulation and analytical results for the shock wave propagation in epoxy-spinel compared with experimental data.

The difficulty to obtain this solution lies in the non-conservative equation evolution of the volume fraction that cannot be directly integrated. In [10], this operation is possible by assuming each phase obeys its own Hugoniot curve across the shock. This closure relation is proved to be in excellent agreement with experimental results and works much better than other closure relations. The complete solution is obtained by solving the following non-linear algebraic system:

$$P_1 - P_0 + m^2 \left(\frac{1}{\rho_1} - \frac{1}{\rho_0} \right) = 0; \quad \rho_{k,1} (u_1 - \sigma) = m; \quad e_{k,1} - e_{k,0} + \frac{P_1 + P_0}{2} \left(\frac{1}{\rho_1} - \frac{1}{\rho_0} \right) = 0 \quad (6)$$

In Figure 4, the results of the direct numerical simulation are compared with analytical solution results. Both results are in very good agreement with the experiments.

The noticeable point is that both methods lead to very close results for the volume fraction evolution. It is important, because there is no experimental data for the jump of the volume fraction across a shock, and the fact that such different methods lead to very close results indicate that the assumptions involved in the analytical solution lead to really good results: one can be very confident in using these relations for a numerical purpose.

5 Conclusions

In this study we use a solver for interfaces problem based on a 5 equations model in a particular context: This model, used for Direct Numerical Simulations, is proven to be efficient to solve the propagation of a shock wave in condensed multiphase material. The agreement is very good with experimental results for jump quantities across the shock.

The advantage of the direct simulations lies in the fact there is a minimum number of assumptions: the only one concerns the Equation of State for each material

A major point also was the determination of a phase quantity, the volume fraction. Indeed, there is no measurement of this quantity and only numerical or theoretical results leads to this quantity.

The analytical Rankine-Hugoniot solution clearly shows a non-monotonous behaviour of the volume fraction versus the pressure. We find out the same evolution of the volume fraction with the direct simulations and the results are quantitatively very close. We can then be very confident in using analytical Rankine-Hugoniot relations in Riemann solvers for finite volume methods.

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