

Analysis of Mobilisation and Explosion Problems in Gas and Dust Mixtures

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1 Introduction

Great effort has been done on the characterisation of multiphase problems over the years. Special attention has been paid to problems involving the mobilisation and explosion of gas and particle mixtures. This work describes the dense model implemented in DUST, a code developed by the Technical University of Cartagena, Spain and the Institute for Radioprotection and Nuclear Safety of France. It has been developed in the framework of the security of the international fusion reactor ITER. This model is based on a six-equation model which considers the effect of pressure on the solid phase by means of a compaction term. This is an Eulerian approach based on a finite volume approximation. The flux evaluation at the interfaces is carried out by means of numerical schemes extended to analyse these problems. All are approximate Riemann solvers which let us evaluate the flux accurately at each interface. The code is explicit and allows second order accuracy. This is obtained by means of variable extrapolation techniques (MUSCL approach). Some tests have been studied to analyse the behaviour of the model.

2 System of Equations

The system of equation characterising dense mixtures is given by the set of conservation of mass, momentum and energy of each phase.

$$\begin{aligned}
 & \frac{\partial}{\partial t}(\alpha \rho_g) + \vec{\nabla} \cdot (\alpha \rho_g \vec{u}_g) = \Gamma_g \\
 & \frac{\partial}{\partial t}(\alpha \rho_g \vec{u}_g) + \vec{\nabla} \cdot (\alpha \rho_g \vec{u}_g \otimes \vec{u}_g + \alpha p_g) = p_g \vec{\nabla} \cdot \alpha + \alpha \rho_g \vec{g} + \vec{F}_g^v + \vec{F}_g^{nv} + \Gamma_g \vec{u}_p + \vec{\Phi}_{gm} \\
 & \frac{\partial}{\partial t}(\alpha \rho_g E_g) + \vec{\nabla} \cdot (\alpha \rho_g \vec{u}_g H_g + \alpha p_g) \\
 & \quad = -p_g \frac{\partial \alpha}{\partial t} + \alpha \rho_g \vec{u}_g \cdot \vec{g} + \vec{F}_g^v \cdot \vec{u}_g + \vec{F}_g^{nv} \cdot \vec{u}_p + Q_g + \Gamma_g H_p + \phi_{ge} \\
 & \frac{\partial}{\partial t}((1 - \alpha) \rho_p) + \vec{\nabla} \cdot ((1 - \alpha) \rho_p \vec{u}_p) = \Gamma_p \\
 & \frac{\partial}{\partial t}((1 - \alpha) \rho_p \vec{u}_p) + \vec{\nabla} \cdot ((1 - \alpha) \rho_p \vec{u}_p \otimes \vec{u}_p + (1 - \alpha) p_p) \\
 & \quad = -p_p \vec{\nabla} \cdot \alpha + (1 - \alpha) \rho_p \vec{g} - \vec{F}_g^v + \vec{F}_p^{nv} + \Gamma_p \vec{u}_p + \vec{\Phi}_{pm}
 \end{aligned} \tag{1}$$

$$\begin{aligned} \frac{\partial}{\partial t}((1-\alpha)\rho_p E_p) + \vec{\nabla} \cdot ((1-\alpha)\rho_p \vec{u}_p H_p + (1-\alpha)p_p) \\ = p_g \frac{\partial \alpha}{\partial t} + (1-\alpha)\rho_p \vec{u}_p \cdot \vec{g} + \vec{F}_p^v \vec{u}_p - \vec{F}_g^{nv} \vec{u}_p - Q_g - \Gamma_p H_p + \phi_{pe} \end{aligned}$$

where subscripts g and p denote gas and particle phases, α stands for the void fraction, ρ is the density, u is the velocity, Γ is the generation rate ($\Gamma_p = -\Gamma_g$), p is the pressure, and g is the gravity. The left-hand side represents the advection or “Euler” part of the flow equations. The right-hand side terms include interfacial mass, momentum, and energy exchange, and viscous friction. F^{nv} is the interfacial friction and Q_g the interfacial heat transfer. The terms denoted by ϕ_i include other diffusive effects such as bulk heat conduction, the molecular and/or equivalent turbulent viscosity, and external heat sources.

The total internal energy and the total enthalpy of phase k are respectively given by $E_k = e_k + |\vec{u}_p|^2/2$ and $H_k = h_k + |\vec{u}_p|^2/2$.

Time derivatives of void fraction are considered in the energy equations following Gidaspow recommendations [1]. According to him these terms Clausius-Duhem inequality is satisfied when they are included.

Particle-particle interaction is negligible in dilute or high dilute gas-particle flows. Only when the particle concentration becomes important, particles collide with each other and they lose kinetic energy. In dense flows, the force on the particle due to shear stress is often neglected and, instead, a term is added to the particle momentum equation [2,3,4]. This approach has been adopted in this model so p_p is substituted by

$$p_p = p + T$$

where

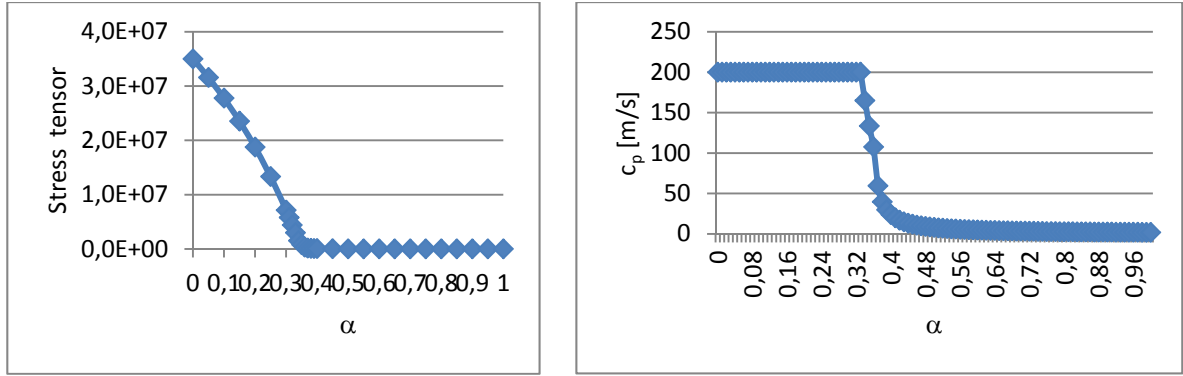
$p = p_g$ and T is the stress tensor given by

$$T(\alpha) = \begin{cases} \rho_p c_{p0}^2 \left(1 - \frac{\alpha_{p0}}{1-\alpha}\right) & \text{if } \alpha \leq \alpha_1 \\ T_1 + \frac{(T_2 - T_1)}{(\alpha_2 - \alpha_1)}(\alpha - \alpha_1) & \text{if } \alpha_1 < \alpha < \alpha_2 \\ \rho_p \beta (q_p^2)_0 \frac{1}{1 - \frac{(1-\alpha)}{\alpha_{pmax}}} & \text{if } \alpha \geq \alpha_2 \end{cases} \quad (2)$$

where c_{p0} is a reference speed of sound ($c_{p0} = 200 \text{ m}\cdot\text{s}^{-1}$ and $\alpha_{p0} = 0.35$ in [3]), $\beta = \frac{2}{3}$, $(q_p^2)_0 = 7.5 \text{ m}\cdot\text{s}^{-2}$ and $\alpha_{pmax} = 0.64$ according to [4], T_1 and T_2 have been evaluated at two arbitrary values α_1 , α_2 and. This has been represented in Fig. 1. The speed of sound of the solid phase, c_p is evaluated by

$$c_p = \begin{cases} \left[c_{p0}^2 - \frac{p}{\rho_p} \right]^{\frac{1}{2}} & \text{if } \alpha \leq \alpha_1 \\ c_{p1} + \frac{(c_{p2} - c_{p1})}{(\alpha_2 - \alpha_1)}(\alpha - \alpha_1) & \text{if } \alpha_1 < \alpha < \alpha_2 \\ \left[\frac{\alpha_{pmax}^2 \beta (q_p^2)_0}{(\alpha_{pmax}^2 - \alpha_p^2)} \right]^{\frac{1}{2}} & \text{if } \alpha \geq \alpha_2 \end{cases} \quad (3)$$

where c_{p1} and c_{p2} have been evaluated at two arbitrary values α_1 , α_2 . It has been defined in a way that it converges to zero when α goes to zero which is typical in high dilute mixtures. This has been represented in Fig. 1 as well. Equations 2 and 3 are the combination of the expressions used by Rogue et al. in [3] when $\alpha \leq \alpha_1$ and that suggested by Combe and Herard in [4] when $\alpha \leq \alpha_2$. Between α_1 and α_2 , a linear interpolation may be used.

Figure 1. Variation of the $T(\alpha)$ and c_p as a function of α .

3 Numerical methods

As mentioned above a finite volume approximation is followed as in [5]. System of equations 1, may be written in vector form as

$$\frac{\partial U}{\partial t} + \vec{\nabla} \cdot H = S$$

where the conserved variables U , the flux vector/tensor $[F, G, H]$ and the source term S are

$$\begin{aligned}
 U &= \begin{bmatrix} \alpha_g \rho_g \\ \alpha_g \rho_g u_{gx} \\ \alpha_g \rho_g u_{gy} \\ \alpha_g \rho_g u_{gz} \\ \alpha_g \rho_g E_g \\ (1-\alpha) \rho_p \\ (1-\alpha) \rho_p u_{px} \\ (1-\alpha) \rho_p u_{py} \\ (1-\alpha) \rho_p u_{pz} \\ (1-\alpha) \rho_p E_p \end{bmatrix}, F = \begin{bmatrix} \alpha_g \rho_g u_{gx} \\ \alpha_g \rho_g u_{gx}^2 + \alpha_g p_g \\ \alpha_g \rho_g u_{gx} u_{gy} \\ \alpha_g \rho_g u_{gx} u_{gz} \\ \alpha_g \rho_g H_g u_{gx} \\ (1-\alpha) \rho_p u_{px} \\ (1-\alpha) \rho_p u_{px}^2 + (1-\alpha) p_p \\ (1-\alpha) \rho_p u_{px} u_{py} \\ (1-\alpha) \rho_p u_{px} u_{pz} \\ (1-\alpha) \rho_p (E_p + \frac{p_p}{\rho_p}) u_{px} \end{bmatrix}, G = \begin{bmatrix} \alpha_g \rho_g u_{gy} \\ \alpha_g \rho_g u_{gx} u_{gy} \\ \alpha_g \rho_g u_{gy}^2 + \alpha_g p_g \\ \alpha_g \rho_g u_{gy} u_{gz} \\ \alpha_g \rho_g H_g u_{gy} \\ (1-\alpha) \rho_p u_{py} \\ (1-\alpha) \rho_p u_{px} u_{py} \\ (1-\alpha) \rho_p u_{py}^2 + (1-\alpha) p_p \\ (1-\alpha) \rho_p u_{py} u_{pz} \\ (1-\alpha) \rho_p (E_p + \frac{p_p}{\rho_p}) u_{py} \end{bmatrix}, \\
 H &= \begin{bmatrix} \alpha_g \rho_g u_{gz} \\ \alpha_g \rho_g u_{gx} u_{gz} \\ \alpha_g \rho_g u_{gy} u_{gz} \\ \alpha_g \rho_g u_{gz}^2 + \alpha_g p_g \\ \alpha_g \rho_g H_g u_{gz} \\ (1-\alpha) \rho_p u_{pz} \\ (1-\alpha) \rho_p u_{px} u_{pz} \\ (1-\alpha) \rho_p u_{py} u_{pz} \\ (1-\alpha) \rho_p u_{pz}^2 + (1-\alpha) p_p \\ (1-\alpha) \rho_p (E_p + \frac{p_p}{\rho_p}) u_{pz} \end{bmatrix}, S = \begin{bmatrix} \Gamma_g \\ p_g \frac{\partial \alpha}{\partial x} + \alpha \rho_g g_x + \vec{F}_{gx}^v + \vec{F}_{gx}^{nv} + \phi_{gmx} \\ p_g \frac{\partial \alpha}{\partial y} + \alpha \rho_g g_y + \vec{F}_{gy}^v + \vec{F}_{gy}^{nv} + \phi_{gmy} \\ p_g \frac{\partial \alpha}{\partial z} + \alpha \rho_g g_z + \vec{F}_{gz}^v + \vec{F}_{gz}^{nv} + \phi_{gmz} \\ -p_g \frac{\partial \alpha}{\partial t} + \alpha \rho_g \vec{u}_g \cdot \vec{g} + \vec{F}_g^v \vec{u}_g + \vec{F}_g^{nv} \vec{u}_p + Q_g + \phi_{ge} \\ \Gamma_p \\ -p_p \frac{\partial \alpha}{\partial x} + (1-\alpha) \rho_p g_x - \vec{F}_{gx}^v + \vec{F}_{px}^{nv} + \phi_{pmx} \\ -p_p \frac{\partial \alpha}{\partial y} + (1-\alpha) \rho_p g_y - \vec{F}_{gy}^v + \vec{F}_{py}^{nv} + \phi_{pmy} \\ -p_p \frac{\partial \alpha}{\partial z} + (1-\alpha) \rho_p g_z - \vec{F}_{gz}^v + \vec{F}_{pz}^{nv} + \phi_{pmz} \\ p_g \frac{\partial \alpha}{\partial t} + (1-\alpha) \rho_p \vec{u}_p \cdot \vec{g} + \vec{F}_p^v \vec{u}_p - \vec{F}_p^{nv} \vec{u}_p - Q_g + \phi_{pe} \end{bmatrix} \quad (4)
 \end{aligned}$$

It is important to observe that the non-conservative terms have been included in the source term.

As far as the numerical schemes are concerned, several approximate Riemann solvers may be found in the existing literature [3]. In this case, several versions of the AUSM family of schemes have been implemented. The details of these approaches can be found in [5]. Non-conservative terms are evaluated by means of a centred approximation, so the void fraction gradient is calculated by

$$\vec{\nabla}\alpha \approx \frac{1}{\Omega} \sum_{stencil} \frac{\alpha_i + \alpha_{i+1}}{2} \vec{n}_{i+\frac{1}{2}} |N_i, N_{i+1}|.$$

where $\alpha_i = \alpha(N_i)$ and $|N_i, N_{i+1}|$ is the length of the segment joining the centres of the elements i and $i+1$.

Time derivatives of void fraction are approximated by means of

$$p \frac{\partial \alpha}{\partial t} \approx p_j \frac{\alpha_j^n - \alpha_j^{n-1}}{\Delta t^{n-1}}$$

leaving the scheme explicit in time.

4 Numerical results

In this section, the fluidisation effect of a shock induced on a particle bed is numerically studied and compared to the experimental results obtained by Rogue et al. in [3]. They studied the fluidisation of different particle beds by means of experimental and analytical methods. The model considered in their work is a one-pressure model which is in fact the result of considering only a weak compaction in System 1. They tested several types of particles (nylon and glass) under the action of distinct shocks (Mach numbers from 1.3 to 1.5). The geometry specifications can be found in [3,5]. In the present case, aimed at validating this development, a test with glass is carried out numerically, the shock considered is given by a Mach number of 1.3 and the initial conditions are:

- *Driven part*: a density and a pressure of $\rho_g = 1.2 \text{ kg/m}^3$ and $p = 10^5 \text{ Pa}$ are respectively considered. The particle bed is characterised by a gas volume fraction of 0.35.
- *Driver part*: By taking into account the above values and by solving Rankin–Hugoniot jump conditions for a shock of Mach number 1.3.

Besides, for the glass a density of $\rho_p = 2500 \text{ kg/m}^3$ and a particle diameter of $d_p = 1.5 \text{ mm}$ is set.

The interfacial friction has been characterised by the following drag force expression:

$$\vec{F}_{dg} = -\frac{3}{4} C_d \frac{\rho_g}{d_p} (1 - \alpha_g) |\vec{u}_g - \vec{u}_p| (\vec{u}_g - \vec{u}_p)$$

In addition to the constant value suggested in [3] for the drag coefficient $C_d = 0.6$, in this work the expression proposed in [4] has been studied. As is shown in Fig. 4, the results registered for pressure at two different positions of the tube match quite well to the experiments. These are better in the second case.

The interfacial heat transfer has been evaluated by

$$\dot{Q} = \pi d_p (1 - \alpha) \lambda_g \text{Re}^{0.7} \text{Pr}^{0.33} (T_p - T_g)$$

where Pr is the Prandtl number of the gas phase and the Reynolds number is given by $\text{Re} = \rho_g |\vec{u}_g - \vec{u}_p| d_p / \mu_g$.

An example of the mesh used in 3D for the study of this test and the results obtained for the pressure at different times are those gathered in Fig. 5.

To check if the model converges to the high dilute one, another test has been studied. This is a shock tube test proposed by Miura and Glass in [6]. It is a 2 m long tube with two parts characterised by:

- *Driven part*: a concentration of $\sigma = \rho(10^5 \text{ Pa}, 300 \text{ K}) \text{ kg/m}^3$ is assumed. Pressure and temperature are respectively $p = 10^5 \text{ Pa}$ and $T_g = T_p = 300 \text{ K}$. Phases are considered at rest.
- *Driver part*: in this case a concentration of 0 kg/m^3 is assumed. Pressure is $p = 10^6 \text{ Pa}$. The same temperatures and velocities as in the driven part are considered.

The results obtained in this case are depicted in the Fig. 6 which are very similar to those provide by the referred authors in their paper.

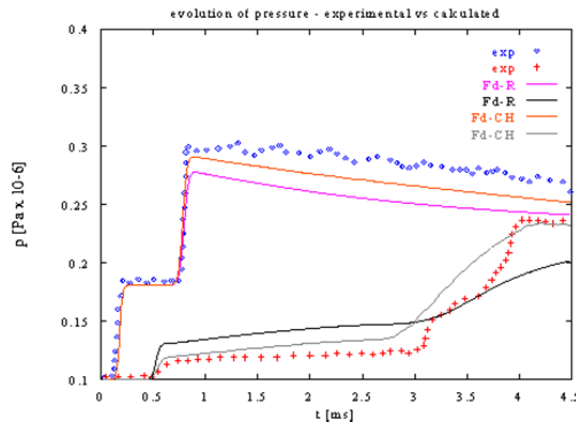


Figure 4. Pressure registered at two different positions in the tube calculated vs experimental.

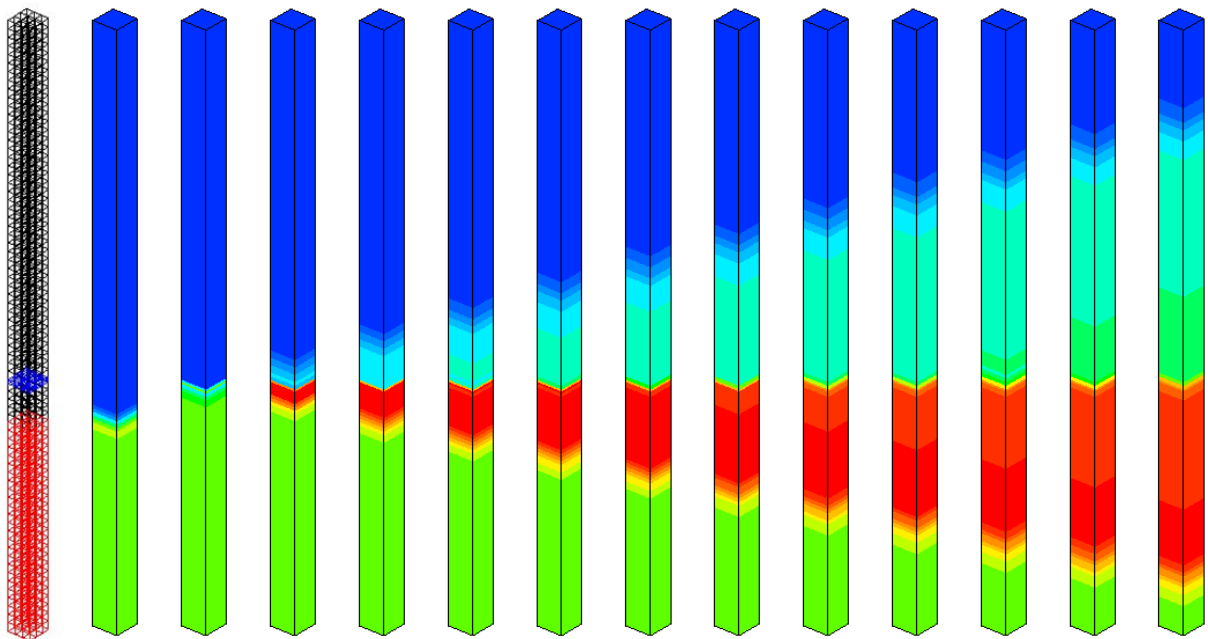


Figure 5. Mesh used in the 3D analysis of Rogue et al. test (left) and distribution of pressure at different times.

5 Conclusions

In this paper, the development of a dense model for the analysis of dense mixtures of dust and gases has been presented. This is a combination of two different models, one applied by Rogue et al. to analyse the fluidisation of a particle bed and another used by Combe and Herard to study some numerical tests: a shock tube and a dusty flow compression. This second one is a particular case of Gidaspow model. In the proposed model, the effect of solid compaction is taken into account by means of a stress tensor and a speed of sound. They have been defined to ensure the convergence to the high dilute model when void fraction goes to 1mm or what is equivalent that the stress tensor and the speed of sound go to zero when the flow get more dilute. This model has been implemented in DUST for the analysis of 2D and 3D problems involving dense mixtures. The proposed numerical method for studying these types of problem is based on a finite volume approximation.

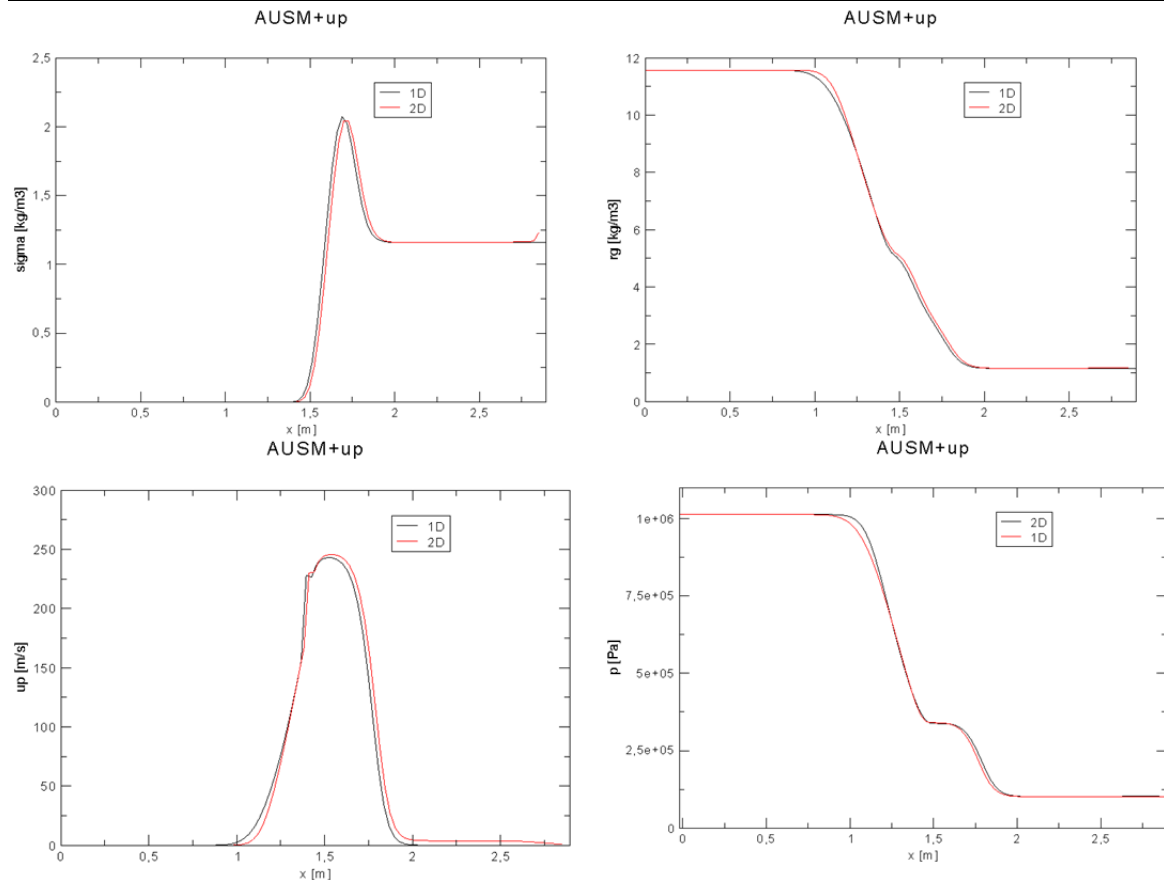


Figure 6. Numerical results obtained for the Miura and Glass test. From top to bottom, left to right: particle concentration, density, particle velocity and pressure.

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