Simulation and Validation of a Three-Phase Flow Model

CONTEXT

The modeling and the accurate simulation of *steam explosion* is an important topic for nuclear safety analysis. This phenomenon may occur when some very hot liquid (molten metal for instance) flows down in a quiet liquid component such as water. In this case the heat transfer might lead to the rapid creation of large volumes of water vapour, so rapid that it can be *explosive* [1].

THREE-PHASE FLOW MODEL

Within each phase, $\alpha_k \in [0,1]$, ρ_k, $m_k = \alpha_k\rho_k$, $\mathbf{U}_k$, p_k, $e_k(p_k,\rho_k)$ and $E_k = 1/2\rho_k\mathbf{U}_k.\mathbf{U}_k + \rho_k e_k(p_k,\rho_k)$ represent respectively the statistical fraction, the mean density, the partial mass, the mean velocity, the mean pressure, the mean internal energy and the mean total energy of phas $k = 1 \to 3$, we note $\mathbf{W} = (\alpha_2,\alpha_3,m_1,m_2,m_3,m_1\mathbf{U}_1,m_2\mathbf{U}_2,m_3\mathbf{U}_3,\alpha_1E_1,\alpha_2E_2,\alpha_3E_3)^t$ the *state variable*. The set of PDEs that is considered is (see [6]):

$$\begin{cases} \frac{\partial\alpha_k}{\partial t} + \mathbf{V}_i(\mathbf{W}).\nabla\alpha_k = S_k^\alpha(\mathbf{W}) \\ \frac{\partial m_k}{\partial t} + \nabla.(m_k\mathbf{U}_k) = 0 \\ \frac{\partial m_k\mathbf{U}_k}{\partial t} + \nabla.(m_k\mathbf{U}_k\otimes\mathbf{U}_k + \alpha_k p_k\mathbf{Id}) + \sum_{l=1,l\neq k}^3 \Pi_{kl}(\mathbf{W})\nabla\alpha_l = \mathbf{S}_k^U(\mathbf{W}) \\ \frac{\partial\alpha_k E_k}{\partial t} + \nabla.(\alpha_k E_k\mathbf{U}_k + \alpha_k p_k\mathbf{U}_k) - \sum_{l=1,l\neq k}^3 \Pi_{kl}(\mathbf{W})\frac{\partial\alpha_l}{\partial t} = S_k^E(\mathbf{W}) \end{cases} \quad (1)$$

The statistical fraction α_1 complies with: $\alpha_1 = 1-\alpha_2-\alpha_3$, since phases are immiscible. We restrict here to the case where: $\mathcal{V}_i(\mathbf{W}) = \mathbf{U}_1$ (phase 1 denotes the liquid metal), thus following [6]:

$$\begin{cases} \Pi_{12}(\mathbf{W}) = \Pi_{21}(\mathbf{W}) = \Pi_{23}(\mathbf{W}) = p_2 \\ \Pi_{13}(\mathbf{W}) = \Pi_{31}(\mathbf{W}) = \Pi_{32}(\mathbf{W}) = p_3 \end{cases} \quad (2)$$

Closure laws for $S_k^\alpha(\mathbf{W}), \mathbf{S}_k^U(\mathbf{W}), S_k^E(\mathbf{W})$ take the form:

$$\begin{cases} S_k^\alpha(\mathbf{W}) = \sum_{l=1,l\neq k}^3 \frac{\alpha_k\alpha_l}{\tau_{kl}(\mathbf{W})}(p_k-p_l) \\ \mathbf{S}_k^U(\mathbf{W}) = \sum_{l=1,l\neq k}^3 \mathbf{D}_{kl}(\mathbf{W}) \\ S_k^E(\mathbf{W}) = \sum_{l=1,l\neq k}^3 \mathbf{V}_{kl}(\mathbf{W}).\mathbf{D}_{kl}(\mathbf{W}) + \sum_{l=1,l\neq k}^3 \psi_{kl} \end{cases} \quad (3)$$

where $\tau_{kl}(\mathbf{W}) = \tau_{lk}(\mathbf{W})$, $\mathbf{D}_{kl}(\mathbf{W}) = e_{kl}(\mathbf{W})(\mathbf{U}_l-\mathbf{U}_k)$ with $e_{kl}(\mathbf{W}) = e_{lk}(\mathbf{W})$, and $\mathbf{V}_{kl} = \frac{1}{2}(\mathbf{U}_k+\mathbf{U}_l)$. τ_{kl} and e_{kl} are positive bounded functions (see [4] for pressure relaxation time scales). The heat transfer term is given by $\psi_{kl} = \frac{a_k-a_l}{\tau_{kl}^\psi}$, where $\tau_{kl}^\psi = \tau_{lk}^\psi$ is the characteristic time of heat transfer between phases k and l, and and $a_k = (s_k)^{-1}\left(\frac{\partial s_k(p_k,\rho_k)}{\partial p_k}\right)\left(\frac{\partial e_k(p_k,\rho_k)}{\partial p_k}\right)^{-1}$. We define $s_k(p_k,\rho_k)$, the specific entropy of phase k: $c_k^2\frac{\partial s_k(p_k,\rho_k)}{\partial p_k} + \frac{\partial s_k(p_k,\rho_k)}{\partial\rho_k} = 0$, and also the mixture entropy $\eta(\mathbf{W})$ and the entropy flux $\mathbf{F}_\eta(\mathbf{W})$:

$$\begin{cases} \eta(\mathbf{W}) = -\sum_{k=1}^3 m_k Log(s_k) \\ \mathbf{F}_\eta(\mathbf{W}) = -\sum_{k=1}^3 m_k Log(s_k)\mathbf{U}_k \end{cases} \quad (4)$$

Main properties:

- *The homogeneous convective subset (left hand side of* (1)*) is hyperbolic unless* $\boldsymbol{U}_1.\boldsymbol{n} - \boldsymbol{U}_k.\boldsymbol{n} = \pm c_k$*, where* $\boldsymbol{n}$ *is a normal unit vector in* $\mathbb{R}^3$*. Its eigenvalues are:*

$$\lambda_{1,2,3,4,5}(\mathbf{W}) = \boldsymbol{U}_1.\boldsymbol{n}\ ;\ \lambda_{6,7,8}(\mathbf{W}) = \boldsymbol{U}_2.\boldsymbol{n}\ ;\ \lambda_{9,10,11}(\mathbf{W}) = \boldsymbol{U}_3.\boldsymbol{n}$$
$$\lambda_{12,13}(\mathbf{W}) = \boldsymbol{U}_1.\boldsymbol{n} \pm c_1;\ \lambda_{14,15}(\mathbf{W}) = \boldsymbol{U}_2.\boldsymbol{n} \pm c_2;\ \lambda_{16,17}(\mathbf{W}) = \boldsymbol{U}_3.\boldsymbol{n} \pm c_3$$

- *The entropy inequality for smooth solutions of* (1) *reads:*

$$\frac{\partial\eta(\mathbf{W})}{\partial t} + \bigtriangledown.\mathbf{F}_\eta(\mathbf{W}) \leq 0. \quad (5)$$

- *In the* $\boldsymbol{n}$*-direction, system* (1) *admits unique jump conditions within each wave when* $\mathcal{V}_i(\boldsymbol{W}) = \boldsymbol{U}_1$*.*

NUMERICAL SCHEME

In the spirit of [2], a fractional step method is introduced to compute approximate solutions of (1) as follows:

- **Step 1 - Evolution step :** For a given initial condition $\mathbf{W}_i^n$, compute an approximate solution of $\mathbf{W}$ at time t_{n+1}, namely $\mathbf{W}^{n+1,-}$, by solving:

$$\begin{cases} \frac{\partial\alpha_k}{\partial t} + \mathbf{V}_i(\mathbf{W}).\nabla\alpha_k = 0 \\ \frac{\partial m_k}{\partial t} + \nabla.(m_k\mathbf{U}_k) = 0 \\ \frac{\partial m_k\mathbf{U}_k}{\partial t} + \nabla.(m_k\mathbf{U}_k\otimes\mathbf{U}_k + \alpha_k p_k\mathbf{Id}) + \sum_{l=1,l\neq k}^3 \Pi_{kl}(\mathbf{W})\nabla\alpha_l = \mathbf{0} \\ \frac{\partial\alpha_k E_k}{\partial t} + \nabla.(\alpha_k E_k\mathbf{U}_k + \alpha_k p_k\mathbf{U}_k) + \mathbf{V}_i(\mathbf{W}).\sum_{l=1,l\neq k}^3 \Pi_{kl}(\mathbf{W})\nabla\alpha_l = 0 \end{cases}$$

- **Step 2 - Relaxation step :** Starting with $\mathbf{W}^{n+1,-}$, compute $\mathbf{W}^{n+1}$ approximate solution of:

$$\begin{cases} \partial_t\alpha_k = S_k^\alpha(\mathbf{W}) \\ \partial_t m_k = 0 \\ \partial_t(m_k\mathbf{U}_k) = \mathbf{S}_k^U(\mathbf{W}) \\ \partial_t(\alpha_k E_k) - \sum_{l=1,l\neq k}^3 \Pi_{kl}(\mathbf{W})\frac{\partial\alpha_l}{\partial t} = S_k^E(\mathbf{W}) \end{cases}$$

This time scheme complies with the entropy inequality (5). A 3D Finite Volume scheme is built. The first evolution step - that accounts for convective effects - involves an explicit scheme (Rusanov scheme was implemented), whereas the relaxation step is implicit.

NUMERICAL RESULTS

Verification test case : Riemann problem

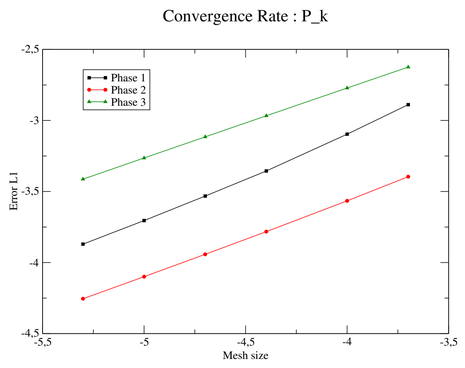

Figure 1: L^1 norm of the error wrt the mesh size h

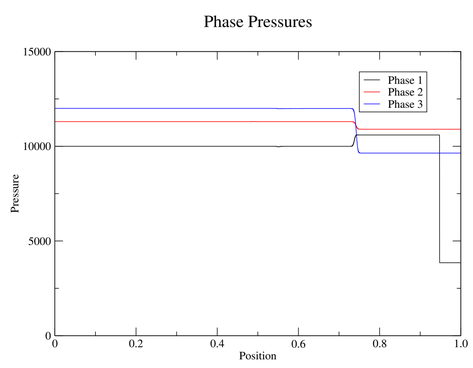

Figure 2: Pressure profiles at the final time $T = 8ms$.

Validation test case :
See [3] for the experimental setup, and [2] for a barotropic approach:

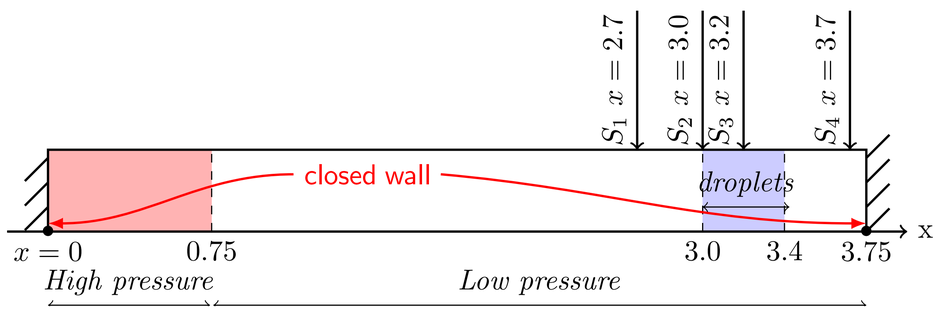

Figure 3: Sketch of the experimental shock tube apparatus.

Simulation results for solid droplet test case:

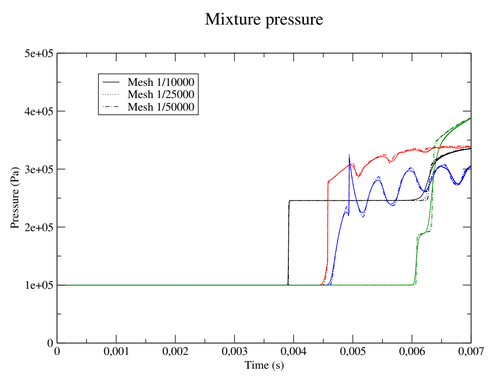

Figure 4: Mixture pressure on S1 (black) S2 (red) S3 (blue) S4 (green).

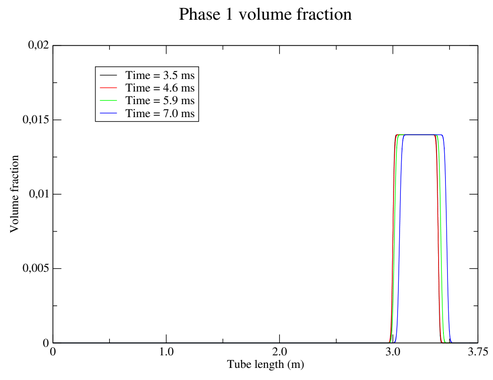

Figure 5: Phase 1 volume fraction in 4 time instants.

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