Three-Field versus Three-Phase Flow Models

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Context

The **NEPTUNE** Project prepares a new generation of tools for multi-scale thermal-hydraulics computations in French PWR. A brief summary of NEPTUNE activities is available in the paper by Guelfi et al (NEPTUNE: a new software platform for advanced nuclear thermal-hydraulics, Nuclear Science Engineering, vol. 156, 2007). These codes will involve the system scale (real-time computation of the whole primary coolant circuit), the component scale (computation in cores and steam generators including obstacles, or equivalently CFD in porous medium) and the local CFD scale. Computations include safety analysis and thus predictions of severe accidents, such as the Loss Of Coolant Accident, and the Reflooding Phase. The latter case requires the computation of three-field models (in order to account for the dispersed liquid phase, the continuous liquid phase and the vapour phase, which is useful for instance for the reflooding phase). Up to now, the basic strategy to predict these unsteady three-field flows relies on the computation of three-phase single-pressure

models (see for instance: Jayanti and Valette, Prediction of the dryout and post dry-out heat transfer at high pressure using a one-dimensional three-field model, IJHMT, vol. 47, pp. 4895-4910, 2004). This approach is actually the straightforward counterpart of the standard two-fluid formalism, which implicitly assumes some local instantaneous pressure equilibrium between phases.

Since the lack of hyperbolicity of standard two-fluid models may lead to a blow-up of codes on fine meshes, and owing to the increasing capacities of computers, it seems necessary to anticipate this annoying trend. Thus we must propose new models -and associated numerical techniques- in order to deal with (expected well-posed) initial-value problems. We thus have a three-fold purpose, since we would like to:

- propose a class of well-posed IVP for three-phase flows;

- propose algorithms to compute unsteady approximations of the latter;

- propose a simple way to handle both standard and new three-field models.

Outline

1. The standard Three-Field Model.

2. An hyperbolic Three-Phase Flow Model.

3. A unified method to compute approximations of both models.

4. Main properties of the schemes.

5. Numerical results.

6. Conclusions and ongoing work.

7. References.

The standard Three-Fluid Model

<u>Notations</u>: Void fractions $\alpha_k > 0$ (for $k = 1, 2, 3$) comply with $\alpha_1 + \alpha_2 + \alpha_3 = 1$. Partial masses are noted $m_k = \alpha_k \rho_k$. Phase velocities U_k, mean densities ρ_k and the mean pressure P enable to define internal energies $e_k(P, \rho_k)$ and the total energy within each phase $E_k = \rho_k e_k(P, \rho_k) + \rho_k U_k^2/2$. We omit mass and energy transfer terms herein. Once interfacial momentum transfer terms I_k are given, the governing equations of the standard Three-Fluid Model are:

$$
\begin{cases}
\partial_t(m_k) + \partial_x(m_k U_k) = 0 \\
\partial_t(m_k U_k) + \partial_x(m_k U_k^2 + \alpha_k P) - P\partial_x(\alpha_k) = I_k \\
\partial_t(\alpha_k E_k) + \partial_x(\alpha_k U_k(E_k + P)) + P\partial_t(\alpha_k) = V_i I_k \\
I_1 + I_2 + I_3 = 0
\end{cases}
$$

We define $s_k(P, \rho_k)$ in agreement with: $c_k^2 \partial_P (s_k)_{|\rho_k} + \partial_{\rho_k}(s_k)_{|P} = 0$, and the entropy-entropy flux pair (η, f_η) as follows:

$$
\begin{cases}
\eta = \Sigma_k (m_k s_k) \\
f_\eta = \Sigma_k (m_k s_k U_k)
\end{cases}
$$

For regular solutions of the TFM, the governing equation for η is:

$$
\partial_t(\eta) + \partial_x(f_\eta) = \Sigma_k (a_k I_k (V_i - U_k))
$$

noting : $a_k = \left(\partial_{e_k}(s_k)_{|\rho_k} \right)$. Admissible closures for the interfacial momentum transfer terms are:

$$
\begin{cases}
I_2 = C_2^2 (a_1 (U_1 - V_i) + a_2 (V_i - U_2)) \\
I_3 = C_3^2 (a_1 (U_1 - V_i) + a_3 (V_i - U_3))
\end{cases}
$$

since in that case : $\partial_t(\eta) + \partial_x(f_\eta) > 0$.

An hyperbolic Three-Phase Flow Model

We consider the following Three-Phase Flow Model :

$$
\begin{cases}
\alpha_1 + \alpha_2 + \alpha_3 = 1 \\[4pt]
\partial_t(\alpha_k) + V_i\partial_x(\alpha_k) = \phi_k \\[4pt]
\partial_t(\alpha_k \rho_k) + \partial_x(\alpha_k \rho_k U_k) = 0 \\[4pt]
\partial_t(\alpha_k \rho_k U_k) + \partial_x(\alpha_k \rho_k U_k^2 + \alpha_k P_k) + \sum_{l=1, l\neq k}^{3} P_{kl}\partial_x(\alpha_l) = I_k \\[4pt]
\partial_t(\alpha_k E_k) + \partial_x(\alpha_k U_k(E_k + P_k)) - \sum_{l=1, l\neq k}^{3} P_{kl}\partial_t(\alpha_l) = V_i I_k
\end{cases}
$$

noting: $E_k = \rho_k e_k(P_k, \rho_k) + \rho_k \frac{U_k^2}{2}$ for $k = 1, 2, 3$. Some closure laws are required for ϕ_k and P_{kl}, which should obey :

$$
\begin{cases}
P_{12} + P_{32} = P_{13} + P_{23} = P_{21} + P_{31} \\[4pt]
\phi_1 + \phi_2 + \phi_3 = 0
\end{cases}
$$

- A first key point concerns the definition of the interface velocity V_i. For two-phase flow models, it is known that meaningful candidates are : $V_i = U_{k_0}$, or : $V_i = \frac{\Sigma_k (m_k U_k)}{\Sigma_k m_k}$. Actually, a straightforward consequence is that the field associated with the eigenvalue $\lambda = V_i$ happens to be linearly degenerated (see [CGHS02, Her03, GHS04]). Beyond this, a unique set of jump conditions holds through each isolated field. This is completely different from what occurs for the standard TFM, which involves "true" non-conservative products, which inhibits the establishment of a unique set of meaningful jump conditions. Actually , a similar result holds for the TPFM.

- The second key stone is that, given the above mentionned closure for V_i, one can exhibit a unique set of functions P_{kl} such that a meaningful entropy inequality holds, which is precisely the one discussed above:

$$\partial_t(\eta) + \partial_x(f_\eta) > 0$$

for the standard TFM, using the same notations !

Remark : When restricting to two-phase flows, we recall that the well-known Baer-Nunziato model belongs to this class.

Hence, if we choose $V_i = U_1$, the corresponding -unique- set of P_{kl} will be:

$$P_{12} = P_{23} = P_{21} = P_2$$
$$P_{13} = P_{31} = P_{32} = P_3$$

And therefore, admissible closures for momentum transfer terms are (for $k = 2, 3$):

$$\phi_k = f_{1-k} \frac{\alpha_1 \alpha_k}{P_1 + P_2 + P_3} (P_K - P_1)$$
$$I_k = \psi_k (U_1 - U_k)$$

The reader is referred to (see [Her06, Her07A]) for more details on the TPFM.

A unified method to compute

approximations of both models

1. A first evolution step computes approximations of first-order differential terms of the Three-Phase Flow Model.

2. A relaxation step computes physical source terms (drag effects here).

3. A second relaxation step either enforces the assumed instantaneous local pressure equilibrium between phases (for the TFM), or computes a true pressure relaxation (for the hyperbolic TPFM).

Each step in the above mentionned fractional step method complies with the entropy inequality. This procedure has also been applied for the computation of two-fluid models, and for the coupling of a two-fluid model with an homogeneous model through a thin interface (see AIAA paper 2007-4458 for instance).

Computing the evolution step

For given values Z^n at time t^n, compute $\tilde{Z}$ as an approximation of Z solution of:

$$
\begin{cases}
\partial_t(\alpha_k) + V_i \partial_x(\alpha_k) = 0 \\[2mm]
\partial_t(\alpha_k \rho_k) + \partial_x(\alpha_k \rho_k U_k) = 0 \\[2mm]
\partial_t(\alpha_k \rho_k U_k) + \partial_x(\alpha_k \rho_k U_k^2 + \alpha_k P_k) + \sum_{l=1, l \neq k}^{3} P_{kl} \partial_x(\alpha_l) = I_k \\[2mm]
\partial_t(\alpha_k E_k) + \partial_x(\alpha_k U_k(E_k + P_k)) - \sum_{l=1, l \neq k}^{3} P_{kl} \partial_t(\alpha_l) = V_i I_k
\end{cases}
$$

This may be achieved using the non-conservative version of the Rusanov scheme, or the approximate Godunov scheme VFRoe-ncv ([BGH00]), or any Riemann solver. Owing to the well-posedness of jump conditions, <u>all mesh refinements provide the same converged solution, whatever the scheme is</u>. This is not true for the standard Three-Field Model.

Computing the pressure relaxation step -TFM-

For given values $\tilde{Z}$, compute Z^{n+1} as an approximation of the relaxation step which enforces the pressure equilibrium for the standard Three Fluid Model:

$$\begin{cases} \phi_k = 0 \\ \partial_t(\alpha_k \rho_k) = 0 \\ \partial_t(\alpha_k \rho_k U_k) = 0 \\ \partial_t(\alpha_k E_k) - \sum_{l=1, l \neq k}^{3} P_{kl} \partial_t(\alpha_l) = 0 \end{cases}$$

The last equation may be rewritten as:

$$\partial_t(m_k e_k) - \sum_{l=1, l \neq k}^{3} P_{kl} \partial_t(\alpha_l) = 0$$

An admissible discrete version to compute approximations is as follows:

For given $\tilde{Z}$:

- Compute: $(U_k)_i^{n+1} = (\tilde{U_k})_i$ and: $(m_k)_i^{n+1} = (\tilde{m_k})_i$.

- Then compute $((P)_i^{n+1}, (\alpha_k)_i^{n+1})$ solution of :

$$\begin{cases} (P_k)_i^{n+1} = (P)_i^{n+1} \\ (m_k e_k)_i^{n+1} - (\tilde{m_k})_i (\tilde{e_k})_i + (P)_i^{n+1}((\alpha_k)_i^{n+1} - (\tilde{\alpha_k})_i) = 0 \end{cases}$$

<u>Remark</u> : For perfect gas EOS, we get:

$$(P_k)_i^{n+1} = P_i^{n+1} = \frac{\gamma_2 \gamma_3 (\alpha_1 \tilde{P_1})_i + \gamma_1 \gamma_3 (\alpha_2 \tilde{P_2})_i + \gamma_1 \gamma_2 (\alpha_3 \tilde{P_3})_i}{\gamma_2 \gamma_3 (\tilde{\alpha_1})_i + \gamma_1 \gamma_3 (\tilde{\alpha_2})_i + \gamma_1 \gamma_2 (\tilde{\alpha_3})_i}$$

$$(\alpha_k)_i^{n+1} = (\tilde{\alpha_k})_i \left(\frac{\gamma_k - 1}{\gamma_k} + \frac{(\tilde{P_k})_i}{\gamma_k P_i^{n+1}} \right)$$

Computing the pressure relaxation step -TPFM-

In that case we need to compute a true pressure relaxation step. Hence, for given values $\tilde{Z}$, we compute Z^{n+1} as an approximation of the solution of:

$$
\begin{cases}
\partial_t(\alpha_k) = \phi_k \\
\partial_t(\alpha_k \rho_k) = 0 \\
\partial_t(\alpha_k \rho_k U_k) = 0 \\
\partial_t(\alpha_k E_k) - \sum_{l=1, l \neq k}^{3} P_{kl} \partial_t(\alpha_l) = 0
\end{cases}
$$

The last equation may be rewritten as:

$$
m_k \partial_t(e_k(P_k, \rho_k)) - \sum_{l=1, l \neq k}^{3} P_{kl} \phi_l = 0
$$

where $\phi_l = f_{1-l} \frac{\alpha_1 \alpha_l}{P_1 + P_2 + P_3}(P_l - P_1)$, for $l = 2, 3$.

Once again, both m_k and U_k remain frozen through the relaxation step. Noting $\pi = \alpha_1 \alpha_2 \alpha_3$, we have :

$$\partial_t(\pi) = \frac{\pi}{P_1 + P_2 + P_3} \left(\sum_{l=2,3} f_{1-l}(P_l - P_1)(\alpha_1 - \alpha_l) \right)$$

Thus, we expect that void fractions remain within their bounds, and that the total energy (summed over the three phases) is conserved. We may at least propose two methods:

- The counterpart of the method introduced in [GHS04], which ensures $0 \leq \alpha_k \leq 1$, and preserves positive pressures (at least when focusing on perfect gas EOS). It enables to manage many EOS. However, in that case the discrete conservative form of total energy does not hold;

- A second method yields both requirements, by enforcing global conservation of total energy, but the existence and uniqueness of solutions may be difficult to obtain for complex EOS.

Main properties of the schemes

Property 1 (evolution step):

The Rusanov scheme enables to maintain positive values of the void fractions and partial masses, assuming a standard CFL condition. The VFRoe-ncv scheme does not.

Property 2 (relaxation step):

- The first substep in the relaxation process ensures positive values of void fractions, mass fractions and pressures P_k.

- For perfect gas EOS, the second substep (pressure relaxation step) guarantees positive values for void fractions -and mass fractions-, and positive cell values of the equilibrium presssure, when focusing on the standard TFM. The counterpart is more difficult to obtain when turning to the hyperbolic TPFM. (see [HeHprep]).

Numerical results

1. Test case 1 : An impinging jet on a wall ;

2. Test case 2 : A 1D Riemann problem with no mass transfer.
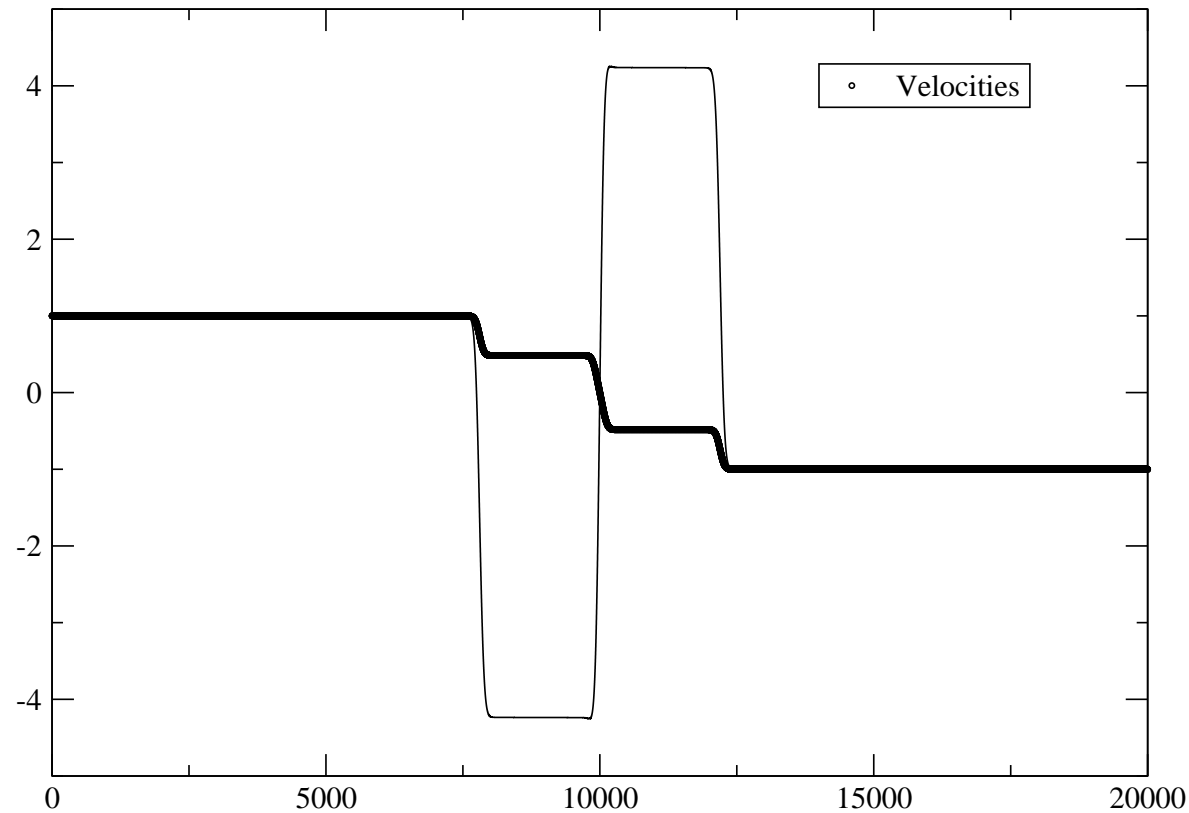
The wall is located at x=10000

Figure 1: Standard TFM - Velocity fields when the flow hits a wall boundary. U1 (plain line), U2 (dotted line), U3 (circles)
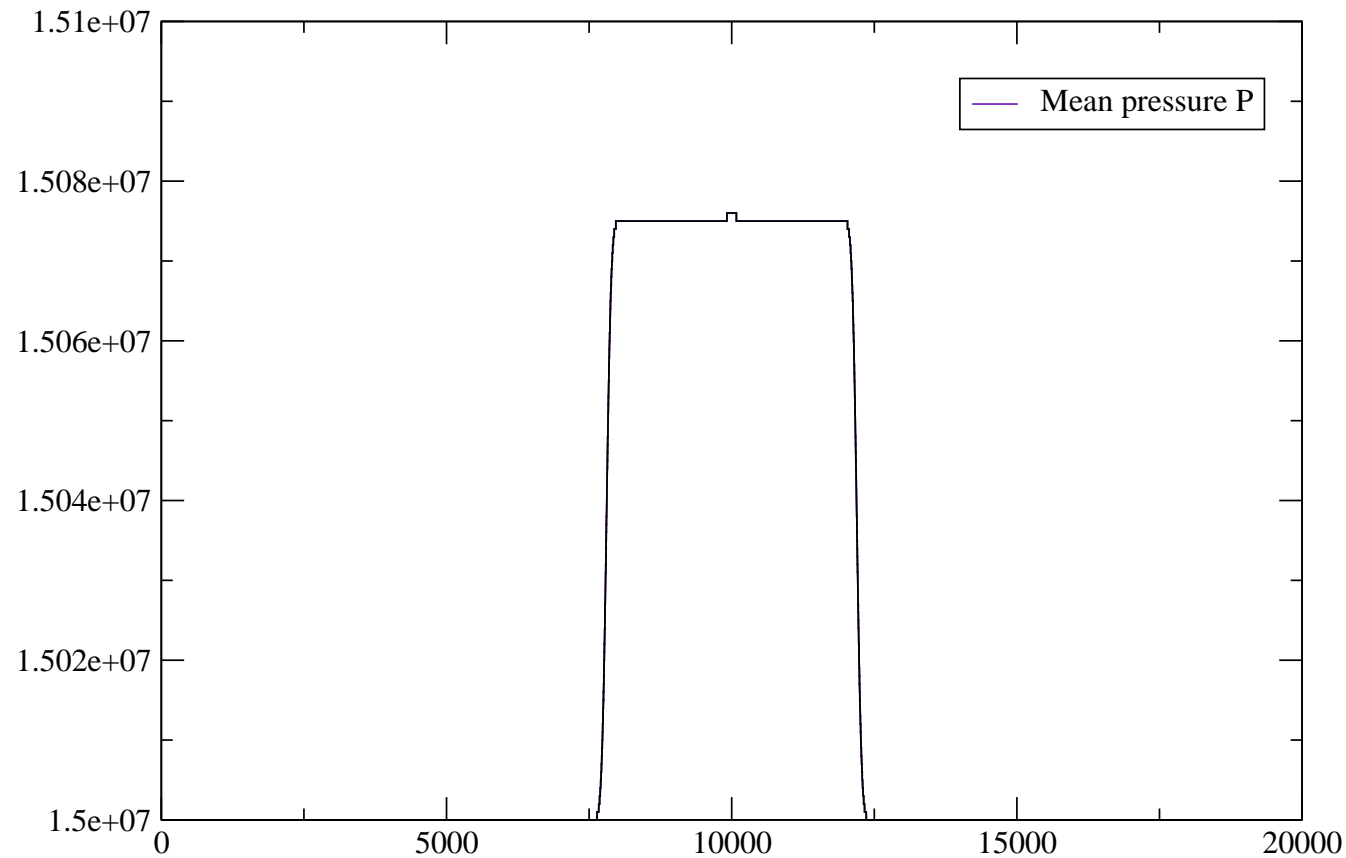
The wall is located at x=10000

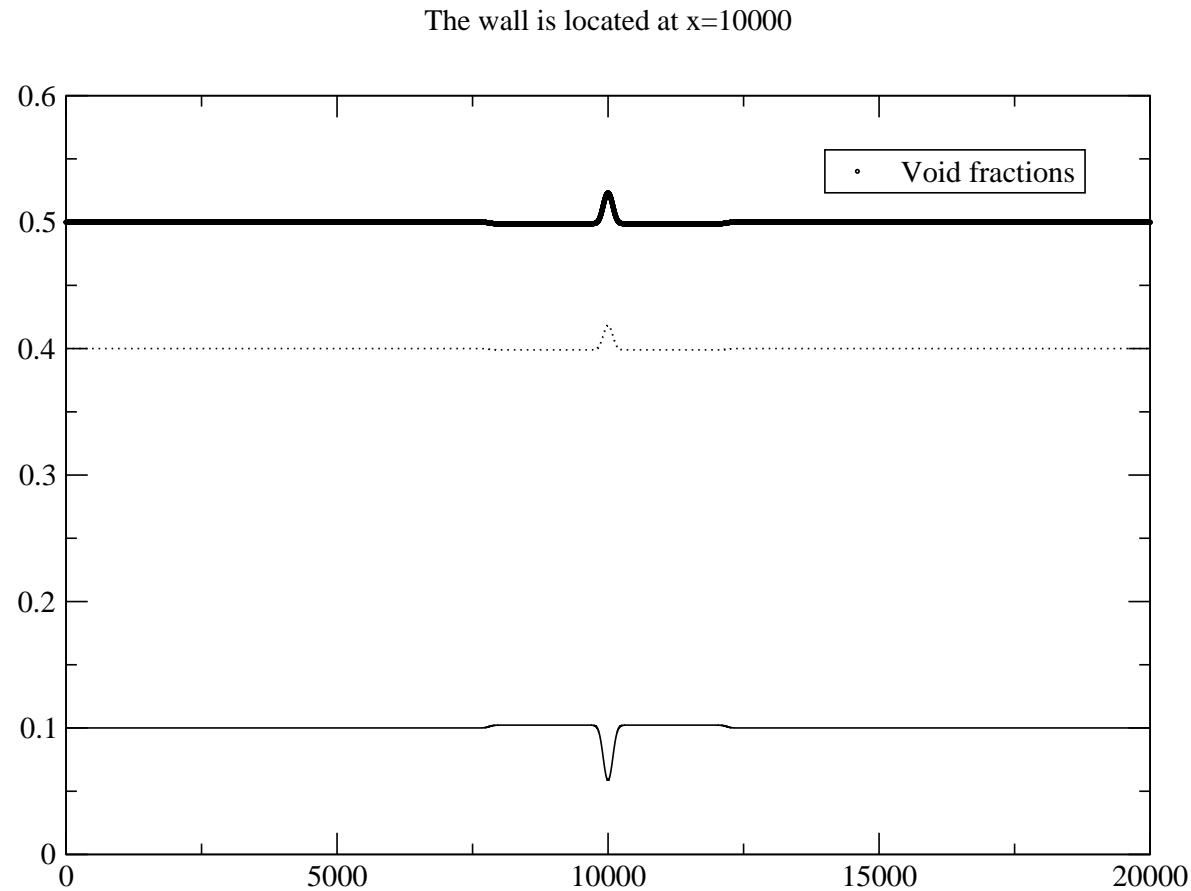Figure 2: Standard TFM - Mean pressure field P when the flow hits a wall boundary.

The wall is located at x=10000

Figure 3: Standard TFM - Void fraction distribution when the flow hits a wall boundary. α_1 (plain line), α_2 (dotted line), α_3 (circles)
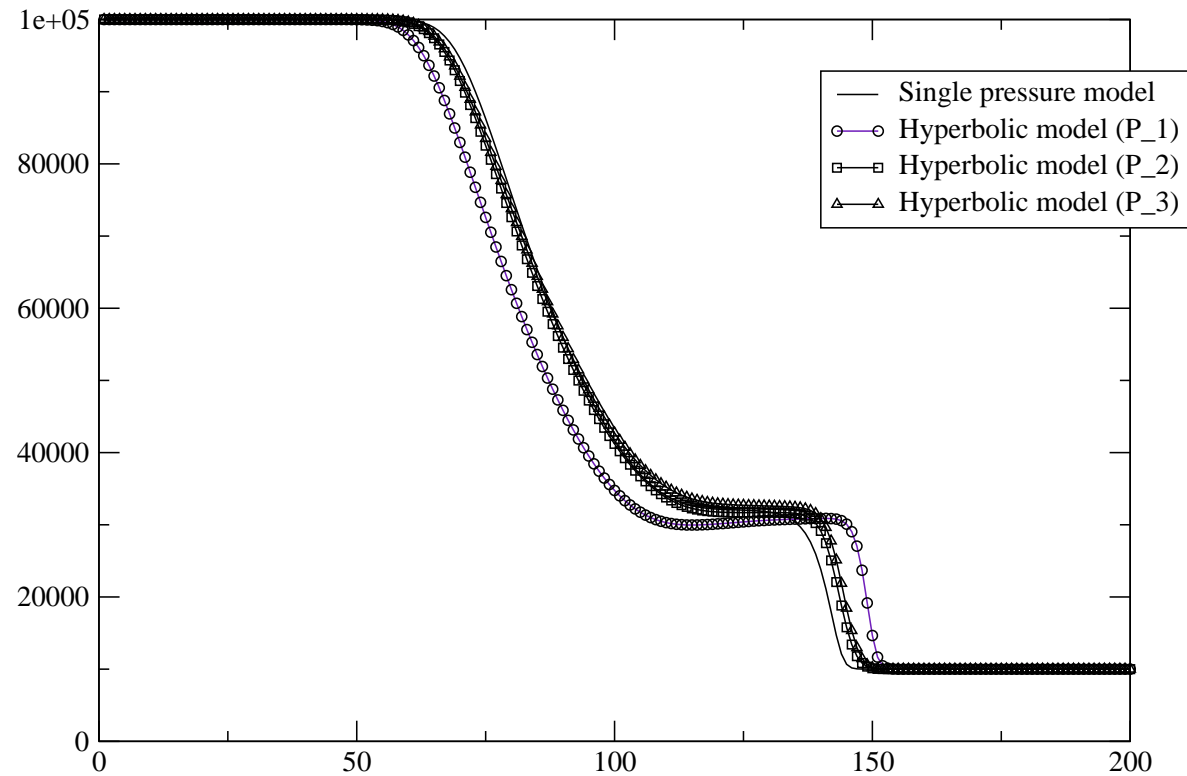
Figure 4: Shock tube experiment. Both approaches are compared using large pressure and velocity relaxation time scales.

Conclusions and further work:

- The present algorithm, which combines a new formulation for three-phase flows and the relaxation procedure, handles both the Three-Phase Flow Model and the standard Three-Field Model (see [Her07a, Her07b]);

- The algorithm is stable: when the initial-value problem is well-posed, a mesh refinement provides a - unique - converged approximation ; moreover it does not hide deficiencies of the TFM when h tends to 0 (see [HeH05]);

- We need to extend these results for flows in a porous medium (following [Hersub], [AGGHsub] for instance) ;

- We also work on some accurate and stable enough algorithms based on approximate Riemann solvers.

References

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