Numerical Simulation of Two-Phase Flows using a Pressure-based Solver

Lei Zhang [1]   Anela Kumbaro [2]   Jean-Michel Ghidaglia [1]

[1]CMLA, ENS Paris-Saclay, France

[2]CEA Saclay, France

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1 Introduction
- Introduction
- Mathematical model

2 Numerical method
- Semi-implicit method
- Conservative semi-implicit method

3 Numerical results
- Application to benchmark test cases
- Application to test cases with experimental data

4 Conclusions et perspectives

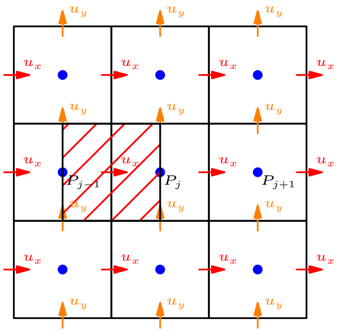
Introduction

Motivation

- Industrial need for calculation of thermohydraulic components in nuclear reactors by sophisticated models such as the bi-fluid 6-equation model.

Context of numerical simulation

- Density-based solvers : upwind scheme for all the waves (material and pressure) (e.g. OVAP, component code) on unstructured grids with colocated variables, accurate but present inconsistency problems at low Mach number.
- Pressure-based solvers : on structured grids with staggered variables (e.g. CATHARE, system code), perform well at low Mach number, but not extended over unstructured grids.



1 : A structured grid with staggered variables.

Mathematical model

Bi-fluid 6-equation model

Mass, momentum and energy equations ($k = v, l$):

$$\frac{\partial}{\partial t}(\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) = \Gamma_k, \tag{1}$$

$$\alpha_k \rho_k \frac{\partial}{\partial t}\mathbf{u}_k + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k \otimes \mathbf{u}_k) - \mathbf{u}_k \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) + \alpha_k \nabla P + (P - P^{int}) \nabla \alpha_k = \alpha_k \rho_k \mathbf{g} + \mathbf{M}_{ik} + \Gamma_k \mathbf{u}^i - \Gamma_k \mathbf{u}_k, \tag{2}$$

$$\frac{\partial}{\partial t}(\alpha_k \rho_k h_k) + \nabla \cdot (\alpha_k \rho_k e_k \mathbf{u}_k) = \alpha_k \frac{\partial}{\partial t} P - P \nabla \cdot (\alpha_k \mathbf{u}_k) + Q_{ik} + \Gamma_k h_{ik}. \tag{3}$$

- Interfacial terms: Γ_k, Q_{ik}, $\mathbf{M}_{ik}$, h_{ik}, $\mathbf{u}^i$.
- Basic model ($P^{int} = P$) is not hyperbolic.
- Intermediary model[1] for the interfacial pressure default:

$$P - P^{\text{int}} = \delta \frac{\alpha_v \alpha_l \rho_v \rho_l}{\alpha_v \rho_l + \alpha_l \rho_v} |\mathbf{u}_v - \mathbf{u}_l|^2 + \frac{1}{c_v^2} \left(\rho_v - \delta \frac{\alpha_v \alpha_l \rho_v \rho_l}{\alpha_v \rho_l + \alpha_l \rho_v} \right) |\mathbf{u}_v - \mathbf{u}_l|^4.$$

[1] M. Ndjinga. Quelques aspects de modélisation et d'analyse des systèmes issus des écoulements diphasiques. PhD thesis, École Centrale de Paris, 2007.

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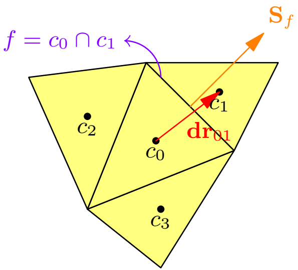
Semi-implicit method[2]



[2] D. R. Liles and Wm. H. Reed. A semi-implicit method for two-phase fluid dynamics. Journal of Computational Physics, 1978.

Semi-implicit method[2]

- The discretized momentum equation for phase k:

$$(\alpha_k\rho_k)^n_{c_0}\frac{(\mathbf{u}_k)^{n+1}_{c_0}-(\mathbf{u}_k)^n_{c_0}}{\Delta t}+\frac{1}{V_{c_0}}\sum_f(\alpha_k\rho_k\mathbf{u}_k)^n_f(\Phi_k)^n_f-\frac{(\mathbf{u}_k)^n_{c_0}}{V_{c_0}}\sum_f(\alpha_k\rho_k)^n_f(\Phi_k)^n_f$$
$$=(\alpha_k\rho_k)^n_{c_0}\mathbf{g}-(\mathbf{u}_k\Gamma_k)^n_{c_0}+(\Gamma_k\mathbf{u}^i)^n_{c_0}-(\alpha_k)^n_{c_0}\nabla P^{n+1}_{c_0}+(\mathbf{M}_{ik})^{n+1}_{c_0}. \quad (4)$$

- The discretized mass and energy equations for phase k (we adopt the notation $\Delta(\cdot)=(\cdot)^{n+1}-(\cdot)^n$):

$$\frac{(\Delta\alpha_k\rho_k)_{c0}}{\Delta t}+\frac{\sum_f(\alpha_k\rho_k)^n_f(\Phi_k)^{n+1}_f}{V_{c_0}}=(\Gamma_k)^{n+1}_{c_0}, \quad (5)$$

$$\frac{(\Delta\alpha_k\rho_k h_k)_{c0}}{\Delta t}+\frac{\sum_f(\alpha_k\rho_k e_k)^n_f(\Phi_k)^{n+1}_f}{V_{c_0}}=(\alpha_k)^n_{c_0}\frac{(\Delta P)_{c_0}}{\Delta t}-(P)^n_{c_0}\frac{\sum_f(\alpha_k)^n_f(\Phi_k)^{n+1}_f}{V_{c_0}}$$
$$+(Q_{ik}+\Gamma_k h_{ik})^{n+1}_{c_0}. \quad (6)$$

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$$= (\alpha_k \rho_k)^n_{c_0} \mathbf{g} - (\mathbf{u}_k \Gamma_k)^n_{c_0} + (\Gamma_k \mathbf{u}^i)^n_{c_0} - (\alpha_k)^n_{c_0} \nabla P^{n+1}_{c_0} + (\mathbf{M}_{ik})^{n+1}_{c_0}. \quad (4)$$

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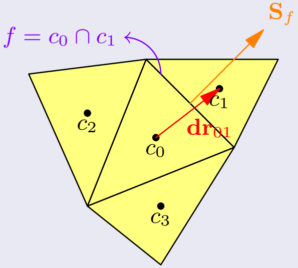

- Volumetric flow:
  $(\Phi_k)_f^m = (\mathbf{u}_k)_f^m \cdot \mathbf{S}_f$, where $m \in \{n, n+1\}$.

Semi-implicit method

Phasic velocity at cell center

Linearisation of the implicit term: $\mathbf{M}_{ik}^{n+1} = \mathbf{M}_{ik}^{n} + \left(\frac{\partial \mathbf{M}_{ik}}{\partial \mathbf{u}_k}\right)^n \cdot (\mathbf{u}_k^{n+1} - \mathbf{u}_k^n)$. The velocity at cell center in compact form:

$$(\mathbf{u}_k)_{c_0}^{n+1} = (\gamma_k)_{c_0}^n - (\beta_k)_{c_0}^n \nabla P_{c_0}^{n+1}. \quad (7)$$

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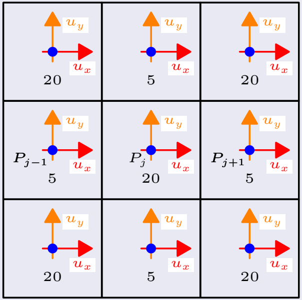
Phasic velocity at cell face

Centered scheme : $(\mathbf{u}_k)_f^{n+1} = \frac{1}{2}(\mathbf{u}_k)_{c0}^{n+1} + \frac{1}{2}(\mathbf{u}_k)_{c1}^{n+1}$.



2 : A structured grid with colocated variables (checker-board problem).

Semi-implicit method

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Phasic velocity at cell face

Rhie and Chow's interpolation to calculate the velocity at cell face[3]

- Adding a dissipation term

$$(\mathbf{u}_k)_f^{n+1} = \frac{1}{2}(\mathbf{u}_k)_{c0}^{n+1} + \frac{1}{2}(\mathbf{u}_k)_{c1}^{n+1} - (\beta_k)_f^n \frac{P_{c1}^{n+1} - P_{c0}^{n+1}}{|\mathbf{dr}_{01}|}\mathbf{n}_f + \frac{1}{2}(\beta_k)_{c0}^n \nabla P_{c0}^{n+1} + \frac{1}{2}(\beta_k)_{c1}^n \nabla P_{c1}^{n+1}. \tag{8}$$

- Analogy to the calculation of the velocity at cell center

$$(\mathbf{u}_k)_f^{n+1} = (\gamma_k)_f^n - (\beta_k)_f^n \nabla P_f^{n+1} = \frac{1}{2}\left[(\gamma_k)_{c0}^n + (\gamma_k)_{c1}^n\right] - (\beta_k)_f^n \frac{P_{c1}^{n+1} - P_{c0}^{n+1}}{|\mathbf{dr}_{01}|}\mathbf{n}_f. \tag{9}$$

These two formulations (8) and (9) are equivalent considering the formula (7).

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[3] J. J. Jeong et al. A semi-implicit numerical scheme for a transient two-fluid three-field model on an unstructured grid. Int. Comm. in Heat and Mass Transfer,

Semi-implicit method (discretization of the scalar equations)

The discretized mass and energy equations for phase k ($\Delta(\cdot) = (\cdot)^{n+1} - (\cdot)^n$):

$$\frac{(\Delta\alpha_k\rho_k)_{c0}}{\Delta t} + \frac{\sum_f (\alpha_k\rho_k)_f^n (\Phi_k)_f^{n+1}}{V_{c_0}} = (\Gamma_k)_{c_0}^{n+1}, \tag{10}$$

$$\frac{(\Delta\alpha_k\rho_k h_k)_{c0}}{\Delta t} + \frac{\sum_f (\alpha_k\rho_k e_k)_f^n (\Phi_k)_f^{n+1}}{V_{c_0}} = (\alpha_k)_{c_0}^n \frac{(\Delta P)_{c_0}}{\Delta t} - (P)_{c_0}^n \frac{\sum_f (\alpha_k)_f^n (\Phi_k)_f^{n+1}}{V_{c_0}} + (Q_{ik} + \Gamma_k h_{ik})_{c_0}^{n+1}. \tag{11}$$

Linearisations:

- Product terms: $\Delta(\alpha_k\rho_k) = (\rho_k)_{c_0}^n(\Delta\alpha_k)_{c0} + (\alpha_k)_{c0}^n(\Delta\rho_k)$,
  $\Delta(\alpha_k\rho_k h_k) = (\rho_k)_{c_0}^n (h_k)_{c_0}^n (\Delta\alpha_k)_{c0} + (\alpha_k)_{c0}^n (\rho_k)_{c_0}^n (\Delta h_k)_{c_0} + (\alpha_k)_{c0}^n (h_k)^n (\Delta\rho_k)_{c_0}$
- Density: $\Delta\rho_k = \left(\frac{\partial\rho_k}{\partial P}\right)^n \Delta P + \left(\frac{\partial\rho_k}{\partial h_k}\right)^n \Delta h_k$.
- Source terms: $(q_k)^{n+1} - (q_k)^n = \left(\frac{\partial q_k}{\partial P}\right)^n \Delta P + \left(\frac{\partial q_k}{\partial h_v}\right)^n \Delta h_v + \left(\frac{\partial q_k}{\partial h_l}\right)^n \Delta h_l$,
  where $q_k \in \{\Gamma_k, Q_{ik} + \Gamma_k h_{ik}\}$.

Discretization of the scalar equations

The discretized scalar equations in matrix form :

$$\mathcal{A}_{c_0}\mathbf{x}_{c_0} = (\mathbf{s})^n_{c_0} - \sum_f (\mathbf{g})^n_f (\Phi_v)^{n+1}_f - \sum_f (\mathbf{l})^n_f (\Phi_l)^{n+1}_f, \tag{12}$$

where $\mathbf{x}$ is the vector of unknowns, $\mathbf{x} = (\Delta h_v, \Delta h_l, \Delta \alpha_v, \Delta P)^T$. By inverting the system of scalar equations we obtain

$$\mathbf{x} = \mathcal{A}^{-1}(\mathbf{s})^n_{c_0} - \mathcal{A}^{-1}\sum_f (\mathbf{g})^n_f (\Phi_v)^{n+1}_f - \mathcal{A}^{-1}\sum_f (\mathbf{l})^n_f (\Phi_l)^{n+1}_f. \tag{13}$$

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- A relation between $P^{n+1}_{c_0}$ and $(\Phi_k)^{n+1}_f$ resulting from the fourth equation of the preceding system:

$$P^{n+1}_{c_0} = P^n_{c_0} + \mathbf{A}_4 \cdot \left[(\mathbf{s})^n_{c_0} - \sum_f (\mathbf{g})^n_f (\Phi_v)^{n+1}_f - \sum_f (\mathbf{l})^n_f (\Phi_l)^{n+1}_f\right], \tag{14}$$

where $\mathbf{A}_4$ is the fourth row of the matrix $\mathcal{A}^{-1}$.

Discretization of the scalar equations

The discretized scalar equations in matrix form :

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  where $\mathbf{A}_4$ is the fourth row of the matrix $\mathcal{A}^{-1}$.
- Another relation between the volumetric flow and the pressure resulting from the discretization of the momentum equation:

$$(\Phi_k)^{n+1}_f = (\mathbf{u}_k)^{n+1}_f \cdot \mathbf{S}_f = \frac{1}{2}\left[(\gamma_k)^n_{c_0} + (\gamma_k)^n_{c_1}\right] \cdot \mathbf{S}_f - (\beta_k)^n_f \frac{P^{n+1}_{c_1} - P^{n+1}_{c_0}}{|\mathbf{dr}_{01}|} |\mathbf{S}_f|. \tag{15}$$

Semi-implicit method (system resolution)

The combination of the equations (14) and (15) leads to an equation in which the pressure at time $n+1$ is the only unknown:

$$\left(1+\mathbf{A}_4\cdot\sum_f \mathbf{C}_f\right)P_{c_0}^{n+1}-\mathbf{A}_4\cdot\sum_f \mathbf{C}_f P_{c_1}^{n+1}=P_{c_0}^{n}+\mathbf{A}_4\cdot\left\{(\mathbf{s})_{c_0}^n-\frac{1}{2}\sum_f(\mathbf{g})_f^n\left[(\gamma_v)_{c_0}^n+(\gamma_v)_{c_1}^n\right]\cdot\mathbf{S}_f\right.$$
$$\left.-\frac{1}{2}\sum_f(\mathbf{l})_f^n\left[(\gamma_l)_{c_0}^n+(\gamma_l)_{c_1}^n\right]\cdot\mathbf{S}_f\right\}, \tag{16}$$

where $\mathbf{C}_f=\frac{|\mathbf{S}_f|}{|\mathbf{dr_{01}}|}\left[(\mathbf{g})_f^n(\beta_v)_f^n+(\mathbf{l})_f^n(\beta_l)_f^n\right]>0$.

Conservative semi-implicit method

Why the semi-implicit method is not conservative (e.g. Euler's equations)

- Use of non-conservative variables the velocity and enthalpy in the discretization of momentum and energy equations respectively.
- Linearization of the density using equations of state.

Semi-implicit method for Euler equations

$$\frac{(\Delta\rho)_{c_0}}{\Delta t} + \frac{\sum_f (\rho)_f^n (\Phi)_f^{n+1}}{V_{c_0}} = 0, \tag{17}$$

$$\rho_{c_0}^n \frac{\mathbf{u}_{c_0}^{n+1} - \mathbf{u}_{c_0}^n}{\Delta t} = \frac{\mathbf{u}_{c_0}^n}{V_{c_0}} \sum_f (\rho)_f^n (\Phi)_f^n - \frac{1}{V_{c_0}} \sum_f (\rho\mathbf{u})_f^n (\Phi)_f^n - \nabla P_{c_0}^{n+1} + \rho_{c_0}^n \mathbf{g}, \tag{18}$$

$$\frac{\rho_{c_0}^n (\Delta h)_{c_0} + h_{c_0}^n (\Delta\rho)_{c_0}}{\Delta t} + \frac{\sum_f (\rho e)_f^n (\Phi)_f^{n+1}}{V_{c_0}} = \frac{(\Delta P)_{c_0}}{\Delta t} - \frac{P_{c_0}^n}{V_{c_0}} \sum_f (\Phi)_f^{n+1}, \tag{19}$$

where

$$\Delta\rho = \left(\frac{\partial\rho}{\partial P}\right)^n \Delta P + \left(\frac{\partial\rho}{\partial h}\right)^n \Delta h. \tag{20}$$

Conservative semi-implicit method

Conservative semi-implicit method

$$\frac{(\alpha_k\rho_k)_{c_0}^{n+1}-(\alpha_k\rho_k)_{c_0}^{n}}{\Delta t}+\frac{\sum_f(\alpha_k\rho_k)_f^n(\Phi_k)_f^{n+1}}{V_{c_0}}=0, \tag{21}$$

$$\frac{(\alpha_k\rho_k\mathbf{u}_k)_{c_0}^{n+1}-(\alpha_k\rho_k\mathbf{u}_k)_{c_0}^{n}}{\Delta t}+\frac{\sum_f(\alpha_k\rho_k\mathbf{u}_k)_f^n(\Phi_k)_f^{n+1}}{V_{c_0}}+(\alpha_k)_{c_0}^n\frac{\sum_f P_f^*\mathbf{S}_f}{V_{c_0}}=(\alpha_k\rho_k)_{c_0}^n\mathbf{g}, \tag{22}$$

$$\frac{(\alpha_k\rho_k E_k)_{c_0}^{n+1}-(\alpha_k\rho_k E_k)_{c_0}^{n}}{\Delta t}+\frac{\sum_f\left[(\alpha_k\rho_k E_k)_f^n+(\alpha_k)_f^nP_f^*\right](\Phi_k)_f^{n+1}}{V_{c_0}}+(P)_{c_0}^*\frac{(\alpha_k)_{c_0}^*-(\alpha_k)_{c_0}^n}{\Delta t}=(\alpha_k\rho_k)_{c_0}^n\mathbf{g}\cdot(\mathbf{u}_k)_{c_0}^n, \tag{23}$$

where P_f^* and $(\alpha_k)_{c_0}^*$ are obtained by the non-conservative semi-implicit method.

Advantages of a conservative method

- Exact shock capture in single-phase flows.
- Exact conservation of mass, momentum and total energy of the mixture in two-phase flows.

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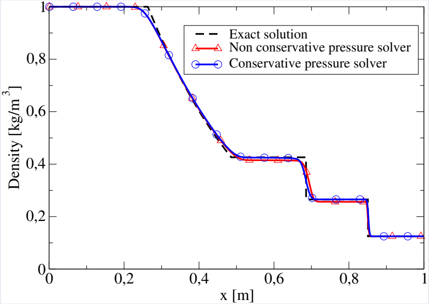
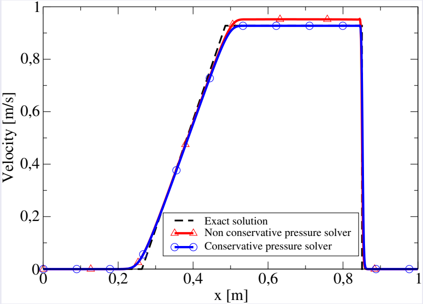
- Riemann problem (ideal gas for the fluid).
- Exact shock capture by the conservative semi-implicit method.



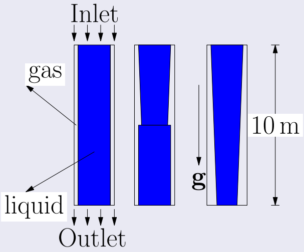
2 : Density comparison at $t = 0.2$s.



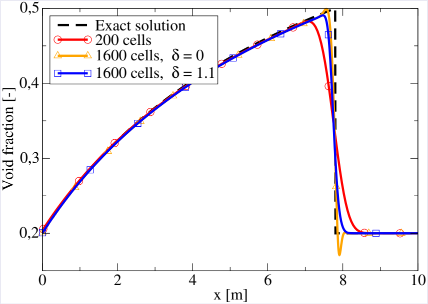
3 : Velocity comparison at $t = 0.2$s.

Ransom's faucet

- Capture of a void fraction front.
- Convergence study with an interfacial pressure default model.



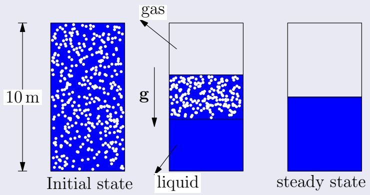
4 : Ransom's water faucet at $t = 0$, $0 < t < t_{\text{converge}}$ and $t = t_{\text{converge}}$ (the time to reach the steady state).



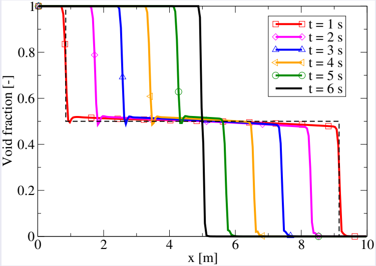
5 : Ransom's faucet : void fraction at $t = 0.6\,\text{s}$.

Sedimentation

- Phase separation by gravity.
- Cover the full range of void fraction from 0 to 1.



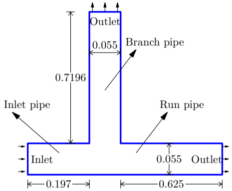
6 : Illustration of the sedimentation test case.



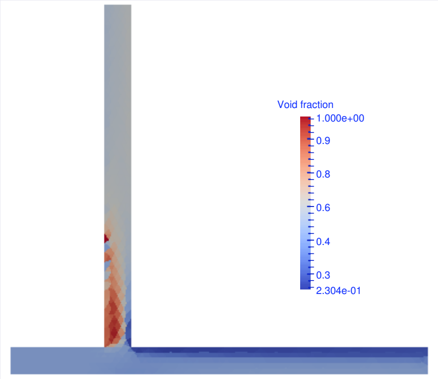
7 : Sedimentation: void fraction profile at different time instants.

Tee junction

- Dynamic separation of gas and liquid due to geometry.
- Unstructured 2D grid.



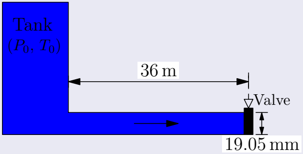
8 : Geometry of Tee junction test case, dimension in [m].



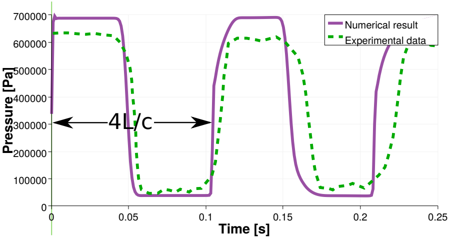
9 : T Junction: void fraction.

Water hammer

- Propagation of a pressure wave in a pipe.
- Simulation of the water hammer phenomenon for the safety study of an industrial installation.
- Validation by experimental data.



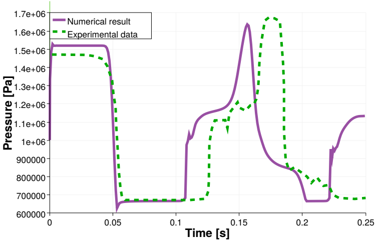
10 : Illustration of the water hammer problem.



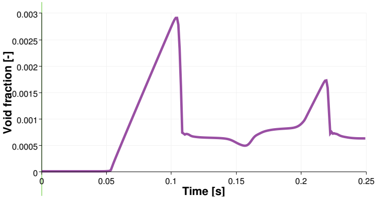
11 : Single-phase water hammer: pressure at the valve as a function of time.

Notation: c is the sound speed, L is the length of the pipe.

Water hammer



(a) Pressure at the valve $P(t)$.

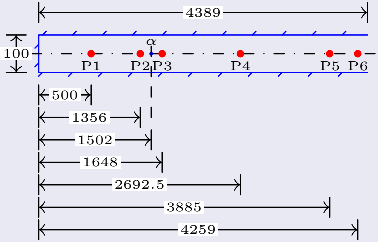


(b) Void fraction at the valve $\alpha_v(t)$.

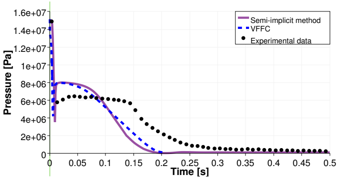
12 : Two-phase water hammer.

Rapid depressurization

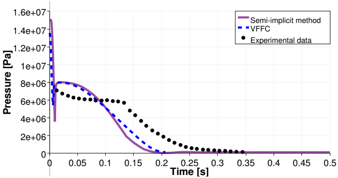
- Study of the accidental scenario of a pipe breach in the primary circuit of a nuclear reactor.
- Comparison with experimental data and numerical results of a density-based solver (VFFC[4]).



13 : Geometry of the rapid depressurization test case, all dimensions in [mm].



(a) Point P1.



(b) Point P2.

[4] J.-M. Ghidaglia, A. Kumbaro, and G. Le Coq. On the numerical solution to two fluid models via a cell centered finite volume method. Eur. J. Mech. B-Fluids, 2001.

1 Introduction
- Introduction
- Mathematical model

2 Numerical method
- Semi-implicit method
- Conservative semi-implicit method

3 Numerical results
- Application to benchmark test cases
- Application to test cases with experimental data

4 Conclusions et perspectives

General conclusions :

- Development of a pressure solver on non-structured grids with colocated variables for the bi-fluid six-equation model.
- Development of a conservative semi-implicit method.
- A battery of test cases to validate the numerical methods and to evaluate their behavior at different physical configurations.

Perspectives :

- Development of a 2nd order discretization in time and in space.
- Inclusion of more realistic interfacial terms and consideration of other physical phenomena (e.g. diffusion, turbulent effects) to have a code for industrial use.
- Improvement of code performance.
- ...