A non-equilibrium multi-component model with miscible conditions

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Motivations

- Multiphase flow modelling
- Industrial applications : nuclear safety (loss of coolant scenario in pressurized water reactors, vapor explosion...)

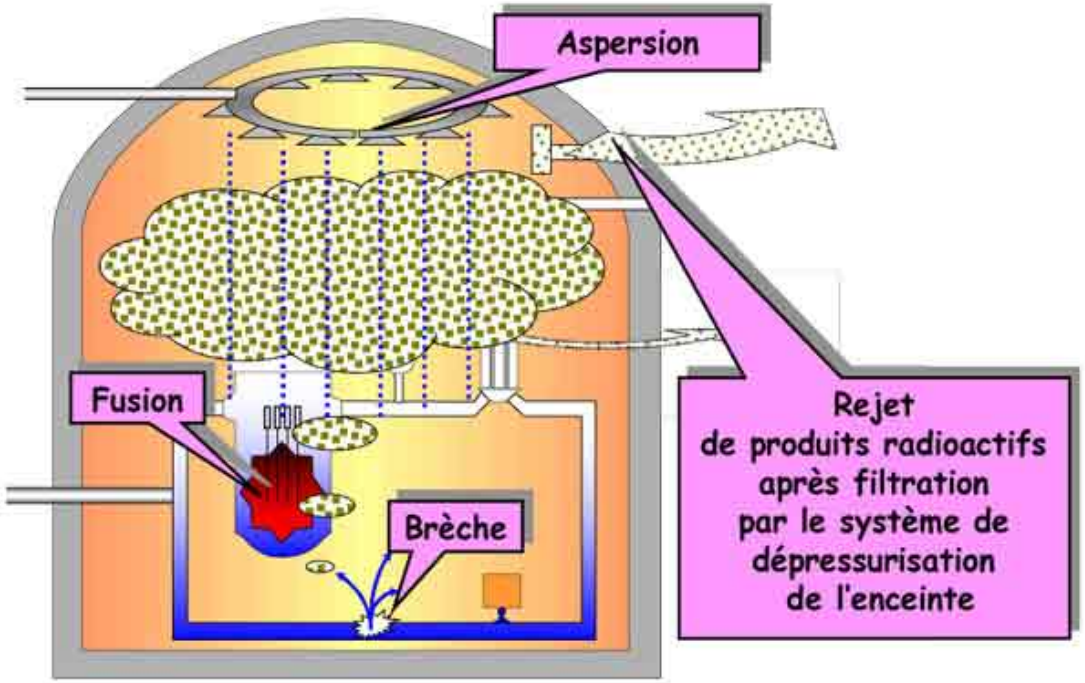

Figure: LOCA scenario (IRSN)

A brief and non-exhaustive historical review

- 1986, Baer and Nunziato: model for a two-phase compressible mixture
- 1992, Embid and Baer: analysis of this latter model
- 2002, Coquel, Gallouet, Hérard and Seguin: (P_I, V_I) entropy-consistent closure, and jump conditions for a class of two-phase flow models
- 2007, Hérard: three-phase flow model
- 2014, Coquel, Hérard, Saleh and Seguin: deeper analysis of the two-phase model (convexity of the entropy, symmetrization)
- 2016, Müller, Hantke and Richter: generalization for a mixture of N immiscible phases
- 2019, Hérard and Mathis: two-phase flow model with a miscible condition (three fields)
- 2021, Hérard, Hurisse and Quibel: three-phase flow model with a miscible condition (four fields)

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Objective

Generalizing these latter works that include the miscible hypothesis to any number of phases.

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2. Definition of the interfacial pressures
3. Analysis of the convective part
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The mixture

- Mixture of N phases and M fields
  - "phase" means a state of the matter and "field" a component in a given phase
- All the miscible components are contained in the Nth phase
- $K = M - N + 1$ miscible components

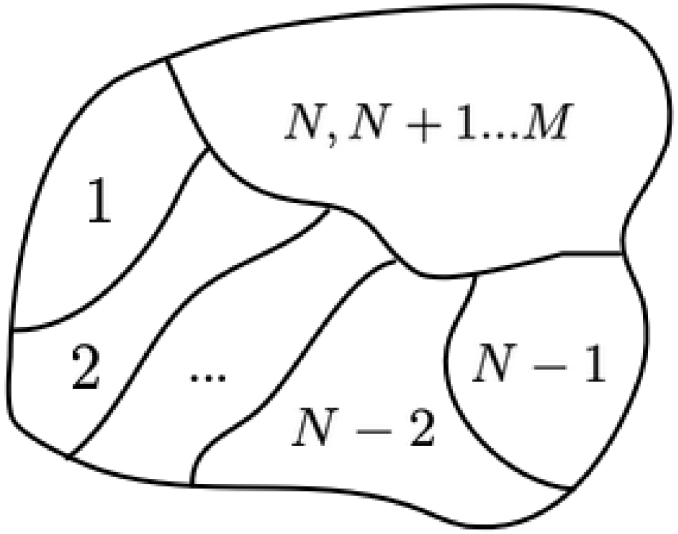

Figure: N phases and M fields mixture

Mixture description

- We note $\mathcal{K}$ the set of fields, and each field k is depicted by its state vector $\mathbf{Y}_k = (\alpha_k, \rho_k, v_k, e_k)$, where
  - α_k is the volume fraction
  - ρ_k is the phasic density
  - v_k is the phasic speed
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$$\left\{ \begin{array}{l} \sum_{k=1}^{N} \alpha_k = 1 \\ \alpha_k = \alpha_N \text{ for } k \geq N \end{array} \right. .$$

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- By introducing $m_k = \alpha_k \rho_k$, we define the mixture entropy

$$\sigma(\mathbf{Y}) = \sum_{k \in \mathcal{K}} m_k \sigma_k(\mathbf{Y}_k),$$

where σ_k is the specific entropy of the phase k.

System of equations

For $k = 1, ..., N$

$$\partial_t \alpha_k + V_I(\mathbf{Y})\partial_x \alpha_k = \Phi_k(\mathbf{Y}).$$

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$$\partial_t(m_k) + \partial_x(m_k v_k) = \Gamma_k(\mathbf{Y}),$$

$$\partial_t(m_k v_k) + \partial_x(m_k v_k^2 + \alpha_k p_k) + \sum_{l=1,\neq k}^{M} P_{k,l}(\mathbf{Y})\partial_x \alpha_l = S_{q,k}(\mathbf{Y}),$$

$$\partial_t(m_k E_k) + \partial_x(m_k v_k(E_k + \frac{p_k}{\rho_k})) + \sum_{l=1,\neq k}^{M} P_{k,l}(\mathbf{Y})V_I(\mathbf{Y})\partial_x \alpha_l = S_{E,k}(\mathbf{Y}),$$

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$\rightsquigarrow$ Closure laws: nonconservative interfacial terms $P_{k,l}(\mathbf{Y})$ and $V_I(\mathbf{Y})$ + source terms

Several constraints

Since the system is isolated, the source terms must verify

$$\sum_{k\in\mathcal{K}} \Gamma_k(\mathbf{Y}) = 0, \quad \sum_{k\in\mathcal{K}} S_{q,k}(\mathbf{Y}) = 0, \quad \sum_{k\in\mathcal{K}} S_{E,k}(\mathbf{Y}) = 0.$$

Moreover, as we consider no vacuum occurrence

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Besides, the interfacial quantities $P_{k,l}$ should cancel each other

$$\sum_{k\in\mathcal{K}} \sum_{\substack{l\in\mathcal{K} \\ l\neq k}} P_{k,l}(\mathbf{Y})\partial_x \alpha_l = 0,$$

to preserve the mixture conservative equations on momentum and energy.

Entropy equation

The mixture entropy verifies the following equation

$$\partial_t \sigma(\mathbf{Y}) + \partial_x f_\sigma(\mathbf{Y}) = \mathcal{A}_\sigma(\mathbf{Y}, \partial_x \mathbf{Y}) + RHS_\sigma(\mathbf{Y}),$$

where

- $f_\sigma(\mathbf{Y}) = \sum_{k \in \mathcal{K}} m_k \sigma_k v_k$ is the entropy flux
- $\mathcal{A}_\sigma(\mathbf{Y}, \partial_x \mathbf{Y})$ contains the interfacial contribution
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$\rightsquigarrow$ These production terms have to be non-negative to satisfy the second law of thermodynamics

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Approach

The proof relies on the previous ones in different situations: immiscible two, three and then N-phase flow [Coq+02; Hér07; MHR16], or more recently for hybrid mixtures in [HM19; HHQ21].

Goal

Determine interfacial pressure and velocity terms that correspond to the minimal entropy dissipation model: $\mathcal{A}_\sigma(\mathbf{Y}, \partial_x \mathbf{Y}) = 0$.

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Determine interfacial pressure and velocity terms that correspond to the minimal entropy dissipation model: $\mathcal{A}_\sigma(\mathbf{Y}, \partial_x \mathbf{Y}) = 0$.

$\rightsquigarrow$ Define new interfacial terms $(K_{k,l})$ from $(P_{k,l})$, defined for $k = 1, ..., M$, $l = 1, ..., N-1$ to rewrite the PDE system that only use the $N-1$ first $\partial_x \alpha_k$

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- $\rightsquigarrow$ Explicit the condition $\mathcal{A}_\sigma(\mathbf{Y}, \partial_x \mathbf{Y}) = 0$ by using the independence of the $N-1$ first $\partial_x \alpha_l$, that give $N-1$ equations for each $l = 1, ..., N-1$

$$\mathcal{A}_\sigma(\mathbf{Y}, \partial_x \mathbf{Y}) = 0 \iff \forall l \leq N-1, \sum_{k=1}^{M} \frac{1}{T_k}(v_k - V_I)(K_{k,l} + \chi_{k,l} p_k) = 0$$

Approach

$\rightsquigarrow$ Assume the convex combination (galilean invariance) $V_I(\mathbf{Y}) = \sum_{k\in\mathcal{K}} \beta_i v_i$ that give the relations

$$v_k - V_I = \sum_{i=1}^{k-1}\sum_{j=1}^{i}(-\beta_j)(v_i - v_{i+1}) + \sum_{i=k}^{M-1}\sum_{j=i+1}^{M}(\beta_j)(v_i - v_{i+1})$$

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- Each of these equations can be split into $M-1$ new equations for each $i = 1, ..., M-1$ by using the independence of the $M-1$ velocities differences $v_{i+1} - v_i$

$$... \iff \forall l \leq N-1,\ i \leq M-1, \quad \sum_{k=1}^{i} c^i \frac{1}{T_k} K_{k,l} - \sum_{k=i+1}^{M} c_i \frac{1}{T_k} K_{k,l} = d_l^i$$

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- By adding the balance momentum equation, we obtain, for each $l = 1, ..., N-1$, a linear systems of size $M \times M$ and of unknowns $\boldsymbol{K}_l = (K_{1,l}, ..., K_{M,l})$

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$$\boldsymbol{d}_l = (d_l^1, d_l^2, ..., d_l^M)^\top$$

where $a_k = T_k^{-1}$, and $(\boldsymbol{d}_l)_{l=1,...,N-1}$ depends on the phasic pressures p_k, the phasic temperatures T_k, and the convex combination of coefficients β_k

Regularity of A

Proposition

We have the following expression

$$\det \boldsymbol{A} = \bar{a_1} c_1 + \bar{a_M} c^{M-1} + \sum_{i=2}^{M-1} \bar{a_i} \beta_i .$$

Moreover, if the phasic temperatures are all positive, then for any convex combination of V_I, $\det \boldsymbol{A} > 0$ and so $\boldsymbol{A}$ is regular.

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- $\rightsquigarrow$ Remark: the lack of an explicit form of the $(K_{k,l})$ has several consequences. For instance, we cannot verify that a flow initially at rest and at temperature and pressure equilibria will remain steady, (RIP condition, [HJ21])

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Analysis of the convective part

Proposition (Hyperbolicity)

The considered system is hyperbolic under the classical non-resonance condition $c_k^2 \neq (v_k - V_I)^2$.

✓ The proof is close to the immiscible case [MHR16]

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Proposition (Symmetrization)

Under the same non-resonance condition, the system is symmetrizable.

- ✓ The proof is exactly the same than in the immiscible case [MHR16]
- $\rightsquigarrow$ For a non-resonant initial data, there exists a local-in-time smooth solution to the Cauchy problem (Kato's theorem)

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- ⇝ Source terms are reorganized according to their nature contribution: mechanical, mass transfer, drag effects and thermal
- ⇝ Constraints are stated to ensure the non-negativity of RHS_σ (*i.e.* the growth of the entropy)
- ✓ Classical conditions obtained on mass transfer, drag effects and thermal contributions
- ✗ Less explicit condition on the mechanical contribution Φ due to the lack of interfacial terms expressions

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Thank you for your attention !