A thermodynamically consistent model of a liquid-vapor fluid with a gas

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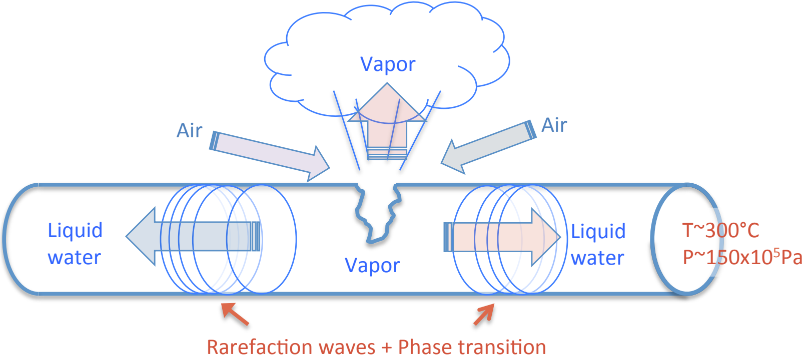
Context and motivations

- Modelling compressible multiphase flows
- Applications in nuclear industry, water circuit of pressurized water reactors

⇝ Loss-of-coolant accident Bartak, 90



✓ Three-phase mixture: a liquid, its vapor and a gas

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- Mixture of A and B in a total volume V
  - Immiscible mixture: phases A and B are separated, case of liquid+gas

$$V_A + V_B = V, \quad p = p_A = p_B \quad \text{(Pressures equality at equilibrium)}$$

  - Miscible mixture: phases A and B are intimate, case of gases

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- Difficulty of the three-phase mixture:
  - Gas (g) and vapor (v) are miscible
  - Liquid (l) immiscible with the 2 gaseous phases
  - Mass transfer between the liquid and its vapor
  - No mass transfer between the gas and the liquid/vapor phase

State of art

- Huge literature for two-phase flows Flåtten, Lund, 11
  - Two-fluid models Baer, Nunziato, 86
    coupled Euler systems, volume fraction equation, nonconservative terms, relaxation source terms
  - Homogeneous Equilibrium models Dias *et al*, 10 ; Faccanoni *et al*, 12
    Euler type system, EoS of the mixture at thermo. equilibrium
  - Homogeneous Relaxation models Hurisse, 17
    Relaxation towards the equilibrium EoS, source terms on fractions equations

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- Works about multicomponents and 3-phase flows Müller *et al*, 16-17
  - Models "*à la* Baer-Nunziato": mathematical structure (hyperbolicity,..), robust numerical schemes
  - ✗ Perfectly immiscible or miscible mixtures

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✓ Provide a consistent mathematical model, guarantees the volume constraint, distinguish whether phase transition occurs or not, valid for any EoS

Outline

1. Thermodynamical model - Gibbs' formalism
   - Extensive constraints
   - Characterization of the thermodynamical equilibrium: partial Dalton's law, mixture entropy
   - Intensive constraints and entropies
2. Homogeneous Equilibrium/Relaxation Models
   - Closure laws, hyperbolicity
   - Relaxation process, source terms, some numerics
3. Conclusion - perspectives

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Single fluid - extensive description, assumptions Callen, 85

Fluid of mass M, energy E, occupying the volume V, described by its entropy function

$$S : W = (M, V, E) \to S(W)$$

- Concave on $C := \{W \in (\mathbb{R}^+)^3,\ S(W) > -\infty\}$
- PH1 (*extensive*)

$$\forall \lambda \in \mathbb{R}_*^+, \forall W \in C, \quad S(\lambda W) = \lambda S(W)$$

- S of class $\mathcal{C}^1$ s.t.

$$\forall W \in C, \quad \frac{\partial S}{\partial E} = \frac{1}{T} > 0$$

- Intensive potentials: temperature T, pressure p, chemical potential μ

$$TdS = dE + pdV - \mu dM \quad \text{(Gibbs' relation)}$$

Three-phase model - extensive constraints

Mass $M_k \geq 0$, volume $V_k \geq 0$ and energy $E_k \geq 0$ of the phase $k = l, g, v$

Extensive constraints

- Mass conservation: $M = M_l + M_g + M_v$
- Energy conservation: $E = E_l + E_g + E_v$
- Immiscibility/miscibility constraints

$$\begin{cases} V = V_l + V_g \\ V_v = V_g \end{cases}$$

Three-phase model - mixture entropy

Let S_k, $k = l, g, v$ satisfying the previous assumptions
Out equilibrium :

$$\Sigma(W_l, W_g, W_v) = S_l(W_l) + S_g(W_g) + S_v(W_v)$$

According to the second principle of Thermodynamics

Mixture entropy at equilibrium - without phase transition

Fix $M_g \geq 0$. Let $W = (M, V, E)$ be the state vector of the 3-phase system. The equilibrium entropy of the mixture is:

- with fixed M_l and M_v

$$S_{NPT}(M, V, E, M_l, M_g) = \max_{(W_l, W_g, W_v)} \Sigma(W_l, W_g, W_v)$$

under the energy and volume constraints

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Mixture entropy at equilibrium - with phase transition

Fix $M_g \geq 0$. Let $W = (M, V, E)$ be the state vector of the 3-phase system. The equilibrium entropy of the mixture is:

$$S_{PT}(M, V, E, M_g) = \max_{(W_l, W_g, W_v)} \Sigma(W_l, W_g, W_v)$$

under the energy and volume constraints and $M - M_g = M_l + M_v$

Three-phase model - characterization of the equilibrium

The thermodynamical equilibrium corresponds to

- The equality of the temperatures

$$T_l = T_g = T_v$$

- The Dalton's law on the pressures of the gas and the vapor phases

$$p_l = p_g + p_v$$

If phase transition is allowed between the liquid and its vapor then

$$\mu_l = \mu_v$$

Intensive variables and constraints

- System of specific volume $\tau = V/M > 0$ and internal energy $e = E/M > 0$
  - Specific entropy: $s(\tau, e) = S(1, V/M, E/M)$
- Phase $k = l, g, v$ described by
  - Fractions of mass $\varphi_k = M_k/M$, volume $\alpha_k = V_k/V$ and energy $z_k = E_k/E \in [0, 1]$
  - Specific entropy: $s_k(\tau_k, e_k) = S_k(1, \tau_k, e_k)$

Intensive constraints

- Mass conservation: $1 = \varphi_l + \varphi_g + \varphi_v$
- Energy conservation: $1 = z_l + z_g + z_v$
- Immiscibility/miscibility constraints

$$\begin{cases} 1 = \alpha_l + \alpha_g \\ \alpha_v = \alpha_g \end{cases}$$

Intensive entropy

Out equilibrium:

$$\sigma(\tau, e, (\varphi_k)_k, (\alpha_k)_k, (z_k)_k)$$
$$= \varphi_l s_l \left(\frac{\alpha_l}{\varphi_l} \tau, \frac{z_l}{\varphi_l} e \right) + \varphi_g s_g \left(\frac{\alpha_g}{\varphi_g} \tau, \frac{z_g}{\varphi_g} e \right) + \varphi_v s_v \left(\frac{\alpha_v}{\varphi_v} \tau, \frac{z_v}{\varphi_v} e \right)$$

Intensive entropy

At thermodynamical equilibrium - without phase transition

Fix $\varphi_g \in [0,1]$. Let (τ, e) be the specific state vector of the system. The mixture entropy is given by

$$s_{NPT}(\tau, e, \varphi_l, \varphi_g) = \max_{((\alpha_k)_k,(z_k)_k)} \sigma(\tau, e, (\varphi_k)_k, (\alpha_k)_k, (z_k)_k)$$

under energy and volume constraints with fixed φ_l and φ_v

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Properties

For fixed $\varphi_k, k = l, g, v$

- s_{NPT} is strictly concave wrt (τ, e)
- Gibb's relation: $T ds_{NPT} = de + p d\tau$

Equilibrium

- $T := T_l = T_g = T_v$ and $p := p_l = p_v + p_g$

Intensive entropy

At thermodynamical equilibrium - with phase transition

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under energy and volume constraints and $1 - \varphi_g = \varphi_l + \varphi_v$

Intensive entropy

At thermodynamical equilibrium - with phase transition

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under energy and volume constraints and $1 - \varphi_g = \varphi_l + \varphi_v$

Properties

For fixed $\varphi_k, k = l, g, v$

- s_{PT} isn't strictly concave wrt (τ, e) (Bachmann *et al*, 10)
- Gibb's relation: $T ds_{PT} = de + p d\tau$

Equilibrium

- $T := T_l = T_g = T_v$ and $p := p_l = p_v + p_g$, and $\mu_l = \mu_v$

Outline

Homogeneous Equilibrium Model - without phase transition

Dellacherie, 03

$$\begin{cases} \partial_t(\varphi_l\rho) + \partial_x(\varphi_l\rho u) = 0 \\ \partial_t(\varphi_g\rho) + \partial_x(\varphi_g\rho u) = 0 \\ \partial_t\rho + \partial_x(\rho u) = 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p) = 0 \\ \partial_t(\rho E) + \partial_x((\rho E + p)u) = 0 \\ E = \dfrac{1}{2}u^2 + e \\ \forall k \in \{l, g, v\} :\ p_k = p_k(\tau_k, e_k),\ \tau_k = \rho_k^{-1} \\ \varphi_l + \varphi_g + \varphi_v = 1 \end{cases}$$

- 10 equations
- 17 unknowns:
  $\rho, u, E, p, e, (\varphi_k)_{k\in\{l,g,v\}}, (\tau_k)_{k\in\{l,g,v\}}, (e_k)_{k\in\{l,g,v\}}, (p_k)_{k\in\{l,g,v\}}$

Homogeneous Equilibrium Model - closure laws

⇝ 7 closure laws

1. Internal energy e, energy constraint: $e = \sum_k \varphi_k e_k$
2. Density $\rho = 1/\tau$, volume constraint:

$$\begin{cases} \tau = \varphi_l \tau_l + \varphi_v \tau_v \\ \varphi_g \tau_g = \varphi_v \tau_v \end{cases}$$

3. Mass conservation: $1 = \varphi_l + \varphi_g + \varphi_v$ with fixed φ_g

⇝ Remains 4, given by the equilibrium characterization

$$\begin{cases} T(1/\rho, e, \varphi_l, \varphi_g) := T_l = T_g = T_v \\ p(1/\rho, e, \varphi_l, \varphi_g) := p_l = p_g + p_v \end{cases}$$

Homogeneous Equilibrium Model - entropy, hyperbolicity

Stability theorem (Mathis, 17)

The three-phase homogeneous model at equilibrium is hyperbolic

- Based on an Godunov-Mock like result

⇝ Prove that the system is symmetrizable with symmetric positive-definite matrix P and a symmetric matrix Q

$$P(w)\partial_t w + Q(w)\partial_x w = 0$$

- Lagrangian coordinates
- $\eta : (\varphi_l, \varphi_g, \tau, u, E) \to -s_{NPT}(\tau, E - u^2/2, \varphi_l, \varphi_g)$ is an entropy of the system

Homogeneous Relaxation Model

- ✗ Mixture pressure law p not explicit (even for simple EoS)
- ✓ Relaxation model towards thermodynamical equilibrium
- ✓ Add fraction $Y = (\alpha_l, z_l, z_g)$ equations: $\partial_t Y + u\partial_x Y = Q$

$$
\begin{cases}
\partial_t(\varphi_k \rho) + \partial_x(\varphi_\rho u) = 0, \quad k = l, g \\
\partial_t z_k + u\partial_x z_k = ..., \quad k = l, g \\
\partial_t \alpha_l + u\partial_x \alpha_l = ... \\
\partial_t \rho + \partial_x(\rho u) = 0 \\
\partial_t(\rho u) + \partial_x(\rho u^2 + p) = 0 \\
\partial_t(\rho E) + \partial_x((\rho E + p)u) = 0
\end{cases}
$$

Homogeneous Relaxation Model

- Relaxation pressure: $p = p(1/\rho, e, (\varphi)_{l,g}, \alpha_l, (z)_{l,g})$
- Weak solutions satisfy

$$\partial_t(\rho\sigma) + \partial_x(\rho u\sigma) \geq 0$$

with $\sigma(\tau, e, \varphi_l, \varphi_g, \alpha_l, z_l, z_g)$ s.t.

$$Td\sigma = de + pd\tau + \sum_{k=l,g} \partial_{\varphi_k} s d\varphi_k + \partial_{\alpha_l} s d\alpha_l + \sum_{k=l,g} \partial_{z_k} s dz_k.$$

Homogeneous Relaxation Model - source terms

- As relaxation towards equilibrium is infinitely fast
  - the fractions Y at equilibrium

$$Y_{eq}^{NPT}(\tau, e, \varphi_l, \varphi_g) = \underset{(\alpha_l, z_l, z_g)}{\operatorname{argmax}}\, \sigma(\tau, e, \varphi_l, \varphi_g, \alpha_l, z_l, z_g)$$

  - Pressure p at equilibrium, partial Dalton's law

$$p_{eq}^{NPT}(\tau, e, \varphi_l, \varphi_g) := p(\tau, e, \varphi_l, \varphi_g, Y_{eq}^{NPT}(\tau, e, \varphi_l, \varphi_g))$$

- Multiple choice for $Q(Y)$ as soon as it complies with the entropy growth criterion
  - $Q = \lambda(Y_{eq}^{NPT}(\tau, e, \varphi_l, \varphi_g) - Y)$
    - ✓ Handle appearance/disappearance of phases
    - ✗ Same relaxation time for the 3 fractions
  - $Q = \nabla_Y \sigma(\tau, e, \varphi_l, \varphi_g, Y)$
    - ✓ Different relaxation time for the 3 fractions

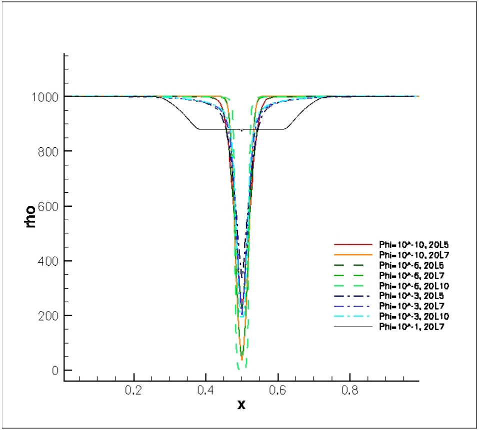
A hint towards numerical approximation

Bachmann *et al*, 2010: application to cavitation bubble simulation

- Homogeneous Equilibrium model with φ_g fixed and phase transition
- Stiffened gas EoS for the liquid, perfect gas EoS for the vapor/air
- Two rarefactions wave moving in opposite direction in water
- 1D finite volume approximation, Godunov scheme with relaxation
- Density profile for several φ_g

A hint towards numerical approximation

Bachmann *et al*, 2010: application to cavitation bubble simulation



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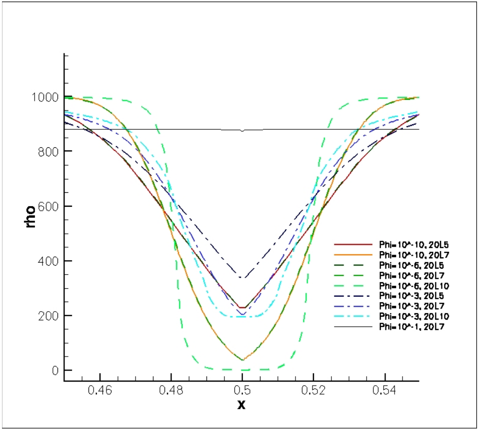

⇝ The more amount of air is important, the less is vapor in the cavitating zone

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To Finish

Conclusions

- Propose a rigorous thermodynamic framework for a liquid-vapor-gas mixture for any EoS
- Complies with the Dalton's law in the gaseous phase
- With and without phase transition between the liquid and the vapor
- Homogeneous Equilibrium models are hyperbolic and admit an entropy structure

Perspectives

- ⇝ Numerical approximation of the HRM
- ⇝ Compare the source terms properties (H. Ghazi for metastable states)
- ⇝ Relevant test cases of three-phase mixtures Bartak, 90

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Thanks for your attention !