A two-phase flow model with surface tension

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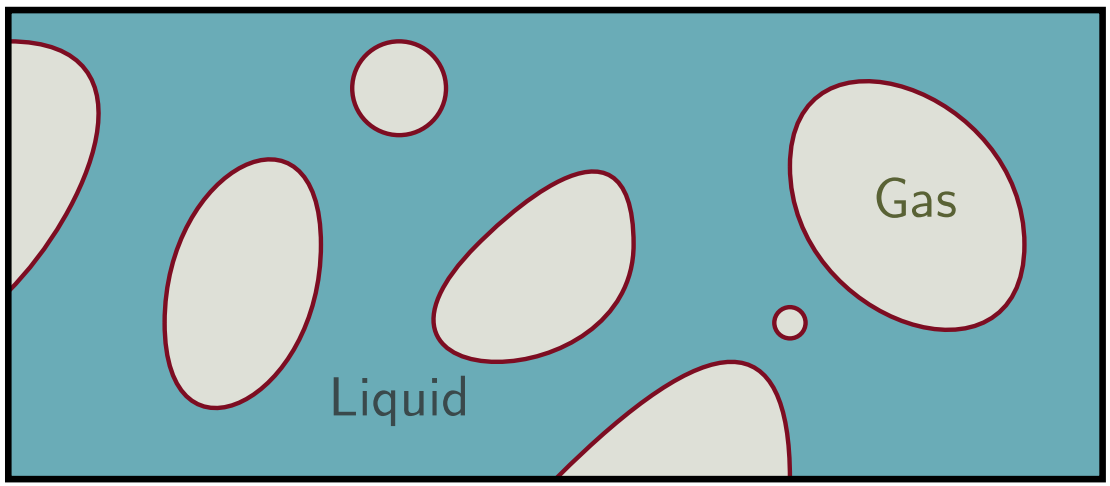
Modélisation et simulation des effets multi-échelles
dans les écoulements diphasiques

Context

- Compressible multiphase flows with heterogeneities (bubbles, droplets)
- Safety issues in nuclear power plants



- Average model, macroscopic description
- Exchanges through the interface, interfacial area density

Derivation of averaged models (1/3)

- **Averaging approach**

  [Drew & Passman '98, Ishii & Hibiki '06...]

  - Microscopic description
    - Instantaneous local conservation laws for each separated phase
    - Jump conditions through the interface
  - Averaging process
    - Introduce time and/or volume scales, or random disturbances
    - Average the microscopic model wrt the small scales
  - ✓ Bear-Nunziato type model
  - ✗ Closure laws
  - ✗ Definition of the averaging operators

- **Homogenization approach**

  [Serre '91 & '01, E '92, Hillairet '07, Bresch & Huang '11, Bresch, Hillairet '15 & '19, Hillairet '18, Bresch, Burtea & Lagoutière '20, Hillairet, M., Seguin '22,...]

  - N bubbles of size $1/N$, $N \to \infty$
  - Mathematical theory, rigorous derivation
  - ✗ One-velocity, no phase transition

Derivation of averaged models (2/3)

- **Least Action Principle**

  [Bedford '85, Gavrilyuk, Gouin '99, Gavrilyuk, Saurel '02, Berdichevsky '09, Drui '17, Essadki '18, Cordesse '20, Di Battista '21, Kokh '21, Loison '23...]

  - Set up the assumptions that govern the physical phenomenon

  $\rightsquigarrow$ Kinetic and potential energies

  - Lagrangian L whose integral over space-time gives the Hamiltonian Action of the system

  - Evolution of the system along possible trajectories
  - LAP postulate: the physical trajectory optimizes the Action

  $\rightsquigarrow$ Conservative equations (momentum, energy)

  ✗ Lack of dissipative behavior, need to ensure the second principle of thermodynamics

Derivation of averaged models (3/3)

Two main ingredients

- Kinetic energy
  [Drui '17, Essadki '18, Cordesse '20, Di Battista '21, Kokh '21, Loison '23...]
  - Modeling the interface behavior
  - Two-scale modeling: keep geometrical informations related to small scale interface features
  - ✓ Interfacial area, Gauß mean curvature, pulsating energy

- Potential energy
  [Smai '20, Laudau, Lifshitz '78...]
  - Thermodynamical behavior of the mixture
  - Each phase is depicted by its own Equation of State (EoS)
  - ✓ Accounting for interfacial energy $\rightsquigarrow$ interfacial state law
  - ✓ Fluid-interface energy

Outline

1. Potential energy
2. Lagrangian and Least Action Principle
3. Final set of equations and properties

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1. **Potential energy**
2. Lagrangian and Least Action Principle
3. Final set of equations and properties

How to compute the potential energy?

- Go back to classical thermodynamics [Gibbs '48, Landau, Lifshitz '78, Callen '85]
  - Distinguish the fluid phases $k = 1, 2$ and the interface i
  - Local thermodynamical equilibrium is reached at each point of the system
  - Each part is described by its own EoS
  - From extensive to intensive description (accounting for fractions)
  - ✓ Thermodynamical equilibrium and fluid-interface energy

Fluid phases

Extensive description

- Volume $V_k \geq 0$, entropy $S_k \geq 0$, mass $M_k \geq 0$
- Internal energy $(M_k, V_k, S_k) \mapsto E_k(M_k, V_k, S_k) \in C^2((\mathbb{R}_+)^3)$
  - Convex and positively homogeneous: $\forall \lambda \in \mathbb{R}_+^*$

$$E_k(\lambda M_k, \lambda V_k, \lambda S_k) = \lambda E_k(M_k, V_k, S_k)$$

  - Gibbs form

$$\mathrm{d}E_k = T_k \mathrm{d}S_k - p_k \mathrm{d}V_k + \mu_k \mathrm{d}M_k$$

    - Pressure p_k, temperature $T_k > 0$, chemical potential μ_k

Intensive form : intensive variables relatively to the mass of the phase k

- Specific volume $\tau_k = V_k/M_k$ and entropy $s_k = S_k/M_k$
- Specific internal energy $e_k(\tau_k, s_k) = 1/M_k \, E_k(M_k, V_k, S_k)$

$$\mathrm{d}e_k = T_k \mathrm{d}s_k - p_k \mathrm{d}\tau_k$$

The interface (1/2)

Assumptions

- Sharp, no volume, no mass

Extensive description

- Entropy $S_i \geq 0$, area $A_i \geq 0$
- Internal energy E_i

$$\mathrm{d}E_i = T_i \mathrm{d}S_i + \gamma_i \mathrm{d}A_i$$

  - Surface tension $\gamma_i(S_i, A_i)$, interfacial temperature $T_i(S_i, A_i)$

- Gibbs-Duhem relation

$$0 = S_i \mathrm{d}T_i + A_i \mathrm{d}\gamma_i$$

The interface (2/2)

Intensive description

- Intensive variables relatively to the volume V of the mixture
  - Interfacial area density $a_i = A_i/V$
- Intensive variables relatively to the interfacial area A_i
  - Interfacial intensive entropy $s_i = S_i/A_i$
  - Interfacial intensive energy $e_i = E_i/A_i$

Consequences

$$\mathrm{d}(a_i e_i) = T_i \mathrm{d}(a_i s_i) + \gamma_i \mathrm{d}a_i$$

$$e_i = T_i s_i + \gamma_i \qquad \text{and} \qquad \gamma_i'(T_i) = -s_i(T_i)$$

The fluid-interface system

For a given state (M, V, E, A_i) of the system

Extensive constraints

- Fluid phases are immiscible, no vacuum, interface has no volume

$$V = V_1 + V_2$$

- Mass conservation, interface has no mass

$$M = M_1 + M_2$$

- Entropy conservation (homogeneity)

$$S = S_1 + S_2 + S_i$$

System extensive internal energy

$$E(M, V, S, A_i) = E_1(M_1, V_1, S_1) + E_2(M_2, V_2, S_2) + E_i(S_i, A_i)$$

Intensive constraints

$$1 = \alpha_1 + \alpha_2 \qquad 1 = y_1 + y_2 \qquad 1 = z_1 + z_2 + z_i$$

- Fractions of entropy $z_k = S_k/S \in [0, 1]$ $(k = 1, 2, i)$, volume $\alpha_k = V_k/V \in [0, 1]$ and mass $y_k = M_k/M \in [0, 1]$ $(k = 1, 2)$

Mixture potentials

Variation of the system extensive energy

$$\begin{aligned}\mathrm{d}E = &(z_1T_1 + z_2T_2 + z_iT_i)\mathrm{d}S - (\alpha_1p_1 + \alpha_2p_2 - a_i\gamma_i)\mathrm{d}V \\ &+ (y_1\mu_1 + y_2\mu_2)\mathrm{d}M + \gamma_i V\mathrm{d}a_i \\ &+ S(T_1\mathrm{d}z_1 + T_2\mathrm{d}z_2 + T_i\mathrm{d}z_i) \\ &- V(p_1\mathrm{d}\alpha_1 + p_2\mathrm{d}\alpha_2) \\ &+ M(\mu_1\mathrm{d}y_1 + \mu_2\mathrm{d}y_2).\end{aligned}$$

Consequences

- Definitions of the mixture potentials

$$\begin{cases} T := z_1T_1 + z_2T_2 + z_iT_i \\ p := \alpha_1p_1 + \alpha_2p_2 - a_i\gamma_i \\ \mu := y_1\mu_1 + y_2\mu_2 \end{cases}$$

Thermodynamical equilibrium

At thermodynamical equilibrium, for a given state (M, V, E, A_i), the mixture energy E reaches a minimum

$$\begin{cases} \mu_1 = \mu_2 \\ T_1 = T_2 = T_i \\ \gamma_i \mathrm{d}a_i - (p_1 - p_2)\mathrm{d}\alpha_1 = 0 \end{cases}$$

Some comments

- Planar interface: $\gamma_i = 0$
  - Mechanical equilibrium corresponds to the saturation of the phasic pressures $p_1 = p_2$
- One gas bubble of radius R
  - Volume $V_1 = 4\pi R^3/3$, interfacial area density $a_i = A_i/V = \pi R^2/V$
  - Linked to the volume fraction

$$\alpha_1 = V_1/V = 4\pi R^2 R/3V = a_i R/3$$

  - From the mechanical equilibrium

$$\frac{\partial a_i}{\partial \alpha_1} = \frac{p_1 - p_2}{\gamma_i} = \frac{2}{R}$$ Young-Laplace law

Potential energy candidate

Intensive form of the system internal energy

✗ Choose the appropriate variables

$$\tilde{\mathbf{B}} = (\tau, s, s_1, s_2, \alpha, a_i, y)$$

where

- s is the system specific entropy

$$s = y_1 s_1 + y_2 s_2 + a_i \tau s_i$$

- $\alpha := \alpha_1$ and $y := y_1$

Potential energy accounting for interfacial information

$$e(\tau, s, s_1, s_2, a_i, \alpha, y) = y e_1 \left(\frac{\alpha}{y} \tau, s_1 \right) + (1-y) e_2 \left(\frac{1-\alpha}{1-y} \tau, s_2 \right) + a_i \tau e_i \left(\frac{s - y s_1 - (1-y) s_2}{a_i \tau} \right)$$

Outline

1. Potential energy
2. **Lagrangian and Least Action Principle**
3. Final set of equations and properties

Least Action Principle (1/2)

Some assumptions

- Single velocity kinematic: $\mathbf{u}_1 = \mathbf{u}_2 =: \mathbf{u}$
- Mass conservations
  - Density of the system $\rho = 1/\tau$: $\partial_t \rho + \mathrm{div}(\rho \mathbf{u}) = 0$
  - Mass fraction y: $D_t y = 0$ with $D_t \cdot = \partial_t \cdot + \mathbf{u} \cdot \nabla \cdot$
- Specific entropy conservation along trajectories:

$$D_t s = 0 \qquad D_t s_k = 0 \qquad k = 1, 2$$

Lagrangian

$$L(\mathbf{B}) = \text{kinetic energy} - \rho e(\tilde{\mathbf{B}})$$

- [Drui '17, Cordesse '18...] with

$$\text{kinetic energy} = \frac{1}{2}\rho |\mathbf{u}|^2 + \frac{1}{2}\nu(a_i)\,|D_t \alpha|^2$$

- Choice of variables to depict the system:

$$(x, t) \mapsto \mathbf{B} = (\rho, s, s_1, s_2, a_i, \alpha, y, \mathbf{u}, D_t \alpha)$$

Stationary Action Principle (2/2)

- Action of a transformation acting on a volume $\mathcal{C} \in \mathbb{R}^3$ for $t_1 < t < t_2$

$$\mathcal{A}(\mathbf{B}) = \int_{t_1}^{t_2} \int_{\mathcal{C}(t)} L(\mathbf{B}) \mathrm{d}x \mathrm{d}t$$

- Family of transformations: $\lambda \in [0,1] \mapsto \hat{\mathbf{B}}(\lambda; \cdot, \cdot)$ such that the constraints hold and

$$\hat{\mathbf{B}}(\lambda; x, t)_{|\lambda=0,1} = \mathbf{B}(x,t) \qquad \hat{\mathbf{B}}(\lambda; x, t)_{|(x,t)\in\partial(\mathcal{C}(t)\times(t_1,t_2))} = \mathbf{B}(x,t)$$

- Physically relevant transformation verifies

$$\frac{\mathrm{d}\mathcal{A}(\mathbf{B}(\hat{\lambda}))}{\mathrm{d}\lambda}(\lambda = 0) = 0$$

Some computations

It remains to compute the infinitesimal variations of the action namely

$$\frac{\mathrm{d}\mathcal{A}}{\mathrm{d}\xi}(0) = \int_{t_1}^{t_2} \int_{\mathcal{C}(t)} \sum_{b \in \mathbf{B}} \frac{\partial L}{\partial b} \delta b \, \mathrm{d}x \mathrm{d}t = 0$$

- Using the conservation constraints

$$\delta\rho = -\mathsf{div}(\rho \delta x) \qquad \delta b = -\nabla b \cdot \delta x$$

- Using the velocity variation

$$\delta \mathbf{u} = D_t(\delta x) - \nabla \mathbf{u} \cdot \delta x$$

- At the end

$$\frac{\mathrm{d}\mathcal{A}}{\mathrm{d}\xi}(0) = \int_{t_1}^{t_2} \int_{\mathcal{C}(t)} \{[\ldots] \cdot \delta x + [\ldots] \, \delta\alpha + [\ldots] \, \delta a_i\} \, \mathrm{d}x \mathrm{d}t = 0$$

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Set of equations (1/2)

- Cancel the $[\ldots]$ terms
- Term in δx

$$\partial_t K + \mathrm{div}(K\mathbf{u}) - \nabla L^* = 0$$

  with $K = \dfrac{\partial L}{\partial u}$ and $L^* = \rho \dfrac{\partial L}{\partial \rho} - L$

- Term in $\delta \alpha$

$$\partial_t M + \mathrm{div}(M\mathbf{u}) - \frac{\partial L}{\partial \alpha} = 0$$

  with $M = \dfrac{\partial L}{\partial D_t \alpha}$

- Term in δa_i

$$\frac{\partial L}{\partial a_i} = 0$$

  - In agreement with [Di Battista '21]
  - Additional constraint in a_i

- Full system accounting for the conservation constraints

Set of equations (2/2)

- By definition of $L(\mathbf{B})$
- Equation on $K = \partial L / \partial u$ gives the momentum equation

$$\partial_t(\rho \mathbf{u}) + \mathrm{div}(\rho \mathbf{u}^\top \mathbf{u}) + \nabla \left((\alpha p_1 + (1-\alpha) p_2 - a_i \gamma_i) + \frac{1}{2} \nu(a_i) |D_t \alpha|^2 \right) = 0$$

  - Similar to [Drui '17]

- Constraint $\dfrac{\partial L}{\partial a_i} = 0$ gives

$$\partial_t \alpha + \mathbf{u} \cdot \nabla \alpha = \sqrt{-\frac{2\gamma_i}{\nu'(a_i)}}$$

  - Constraint on $\nu(a_i)$ to be well-defined
  - ✓ [Cordesse *et al* '19] : $\nu(a_i) = 2/a_i^2$

- Equation on $M = \partial L / \partial D_t \alpha$ gives

$$\partial_t \left(\nu(a_i) D_t \alpha \right) + \mathrm{div} \left(\mathbf{u} \nu(a_i) D_t \alpha \right) = \tau(p_2 - p_1)$$

  - Depending on $\nu(a_i)$, gives an equation on a_i...

Concluding/opening remarks

- Propose to integrate the interfacial properties into the potential energy
- Coherent structure with the existent models

A lot to do...

- ✗ Compare to existing $\nu(a_i)$ or $\nu(a_i, \alpha)$
- Dissipative structure, hyperbolicity...
- Compare to bubbly flow models [Plesset, Prosperetti '77]

Thank you for your attention!