Multiphase Flows

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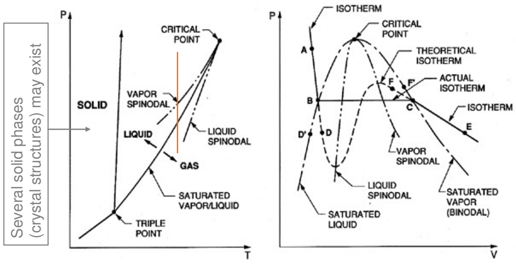
Typical phase diagrams of a *pure* material:



In equilibrium 1, 2 or 3 phases can exist together

Complete mechanical and thermal equilibrium

Outline

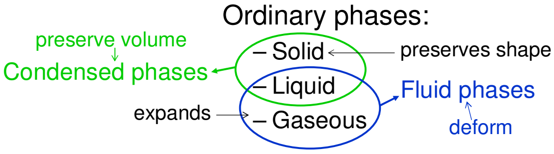
- Basic notions and terminology
- Inter-phase processes
- Modelling strategies
- Computational Multi-Fluid dynamics (CMFD) models in detail
  1. VOF and friends
  2. One-fluid models
  3. Multi-fluid models
  4. Dispersed phase modelling

Multiple components

- Almost all systems have more than 1 chemical components
  - Gibbs' Rule of Phases: *in equilibrium*
    $$\#\text{phases} \equiv N_p \le \#\text{components} + 2 \equiv N_c + 2$$
  - Phases are typically *multi-component mixtures*
- Miscibility
  - Gases always mix →
    Typically there is at most 1 contiguous gas phase
  - Liquids maybe miscible or immiscible →
    Liquids may separate into more than 1 phases
    (e.g. polar water + apolar oil)

Basic notions and terminology

Ordinary phases:



Topology of phases and interfaces

A phase may be

- *Contiguous*
  (more than 1 contiguous phases can coexist)
- *Dispersed:*
  - solid particles, droplets or bubbles
  - of small size
  - usually surrounded by a contiguous phase

Interfaces are

- 2D interface surfaces separating 2 phases
  - gas-liquid: *surface*
  - liquid-liquid: *interface*
  - solid-liquid: *wall*
- 1D contact lines separating 3 phases and 3 interfaces
- 0D contact points of 4 phases, 6 interfaces and 4 contact lines

Special Features to Be Modelled

- Multiple components →
  - Chemical reactions
  - Molecular diffusion of constituents
- Multiple phases → inter-phase processes
  - momentum transport,
  - mass transport and
  - energy (heat) transfer

  across interfaces.

  (Deviations from local equilibrium are possible)

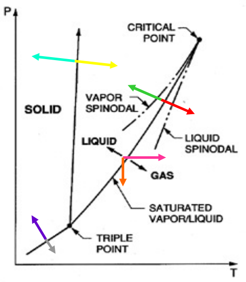
Modelling Strategies for Multiphase Problems

1. Fine resolution models (expensive)
   - The location, motion and dynamics of each interface is resolved
   - The fluid inside each phase is treated as a single-phase homogenous (but multi-component) fluid
2. Coarse resolution models (cheap)
   - Interfaces are not resolved
   - Inter-phase processes are described via subscale parameterisation
   - fluid is treated as a mixture of phases
   1. One-fluid models (good for dispersed phases)
   2. Multi-fluid models (for separated contiguous phases)

Phase transitions

- Evaporation, incl.
  - Boiling
  - Cavitation
- Condensation
- Freezing
- Melting
- Solidification
- Sublimation

All phase transition involve latent heat deposition or release



Notations

- Phase index (upper):
  - (p) or
  - (s), (l), (g), (v), (f) for solid, liquid, gas, fluid, vapour
- Component index (lower): k
- Coordinate index (lower): i, j or t
- Partial differentiation: $\partial_t,\ \partial_i\,(\partial_1=\partial_x, \partial_2=\partial_y, \partial_3=\partial_z)$

$\rho^{(s)},\ c_k^{(p)},\ u_i^{(p)}$

Modelling Simple Fluids

- Inside the fluid:
  - Transport equations

    Mass, momentum and energy balances

    5 PDE's for $p(t,\vec{\mathbf{r}}),\ \vec{\mathbf{u}}(t,\vec{\mathbf{r}})\quad T(t,\vec{\mathbf{r}})$
  - Constitutive equations

    Algebraic equations for $\rho(p,T),\ \mu(p,T),\ k(p,T),\ \ldots$
- Boundary conditions

  On explicitly or implicitly specified surfaces
- Initial conditions

Equations inside the phase domains

- Constitutional equations

  For each phase (p) one needs to know

  $\rho^{(p)}(p,T,c_1^{(p)},c_2^{(p)},\ldots)$

  $\mu^{(p)}(p,T,c_1^{(p)},c_2^{(p)},\ldots)$

  $k^{(p)}(p,T,c_1^{(p)},c_2^{(p)},\ldots)$

  $D_{k,\ell}^{(p)}(p,T,c_1^{(p)},c_2^{(p)},\ldots)$
- Primary field variables:

  $p(t,\vec{\mathbf{r}}),\ \vec{\mathbf{u}}(t,\vec{\mathbf{r}}),\ T(t,\vec{\mathbf{r}})\quad c_k(t,\vec{\mathbf{r}})$

  for all k components
- Marker functions for each (p) phase

  $\chi^{(p)}(t,\vec{\mathbf{r}})=1$ or 0

  $\sum_p \chi^{(p)}(t,\vec{\mathbf{r}})=1$

$$\rho = \sum_p \chi^{(p)} \cdot \rho^{(p)}$$
$$\mu = \sum_p \chi^{(p)} \cdot \mu^{(p)}$$
$$k = \sum_p \chi^{(p)} \cdot k^{(p)}$$

Pros and Cons

TOO FEW EQUATIONS
- Do not describe small-scale phenomena at all
- The external constitutive equations must be based on empirical correlations
- Not even the intrinsic constitutive equations are general, they are problem-dependent
- Too much constrained to describe adequately the flow phenomena
- Lowest computational demand (w.r.t. fine models)

Interface Processes

- Interphase processes are included as source terms in the balance equations
- The source terms are concentrated in cells which are cut by interfaces

Remedies

It is possible to extend the model by adding new primary fields to the model in addition to $p(t,\vec{\mathbf{r}})$, $\vec{\mathbf{u}}(t,\vec{\mathbf{r}})$ $T(t,\vec{\mathbf{r}})$

Example: volume fraction field, $\alpha^{(p)}$

$$\alpha^{(p)}(t,\vec{\mathbf{r}}) \equiv \left\langle \chi^{(p)} \right\rangle = \left(\iiint \sum_p \chi^{(p)}(t,\vec{\mathbf{r}})\, dV \right) \Big/ \left(\iiint dV \right)$$

1. Homogenous model
2. Generalised homogenous model
3. Slip model
4. Non-equilibrium model
5. Diffusion model

- These include more constitutive equations and thus need more correlations
- The consistency of the system cannot be assured

One-Fluid Models

- Derived by averaging and using simplifying assumptions
- The mixture is considered as a single fluid
- Common T and p
- The interfaces are ignored
- All interface processes are transferred to constitutive laws

$$\rho(t,\vec{\mathbf{r}}) \equiv \langle \rho \rangle = \left(\iiint \sum_p \chi^{(p)}(t,\vec{\mathbf{r}}) \rho^{(p)}(t,\vec{\mathbf{r}})\, dV \right) \Big/ \left(\iiint dV \right)$$

$$\vec{\mathbf{u}}(t,\vec{\mathbf{r}}) \equiv \langle \rho \vec{\mathbf{u}} \rangle / \rho(t,\vec{\mathbf{r}}) = \left(\iiint \sum_p \chi^{(p)}(t,\vec{\mathbf{r}}) \rho^{(p)}(t,\vec{\mathbf{r}}) \vec{\mathbf{u}}(t,\vec{\mathbf{r}})\, dV \right) \Big/ \rho(t,\vec{\mathbf{r}})$$

$$e(t,\vec{\mathbf{r}}) \equiv \langle \rho e \rangle / \rho(t,\vec{\mathbf{r}}) = \left(\iiint \sum_p \chi^{(p)}(t,\vec{\mathbf{r}}) \rho^{(p)}(t,\vec{\mathbf{r}})\, e(t,\vec{\mathbf{r}})\, dV \right) \Big/ \rho(t,\vec{\mathbf{r}})$$

Multi-fluid models

- Fluid elements (computational cells) are large, typically contain both/several phases
- This is described by volume fraction fields, $\alpha^{(p)}$
- Each phase is described by its own phasic transport equations
- A common pressure field is shared
- There is no thermal equilibrium
- The interfaces are not resolved, but inter-phase processes must be parameterised and included in constitutional relations

Balance Equations

$$\sum_p \alpha^{(p)} = 1$$

$$\forall p: \quad \partial_t\left(\alpha^{(p)}\rho^{(p)}\right) + \vec{\nabla}\cdot\left(\alpha^{(p)}\rho^{(p)}\vec{\mathbf{u}}^{(p)}\right) = \boxed{\sum_{p'}\left(\dot{\rho}^{(p'\to p)} - \dot{\rho}^{(p\to p')}\right)}$$

$$\forall p,i: \ \partial_t\left(\alpha^{(p)}\rho^{(p)}u_i^{(p)}\right) + \vec{\nabla}\cdot\left(\alpha^{(p)}\rho^{(p)}u_i^{(p)}\vec{\mathbf{u}}^{(p)}\right) =$$
$$= \alpha^{(p)}\rho^{(p)}g_i - \alpha^{(p)}\vec{\nabla}p + \vec{\nabla}\cdot\left(\alpha^{(p)}\hat{\boldsymbol{\tau}}^{(p)}\right)$$
$$+ \boxed{\sum_{p'}\left(\dot{\rho}^{(p'\to p)}u_i^{(p'\to p)} - \dot{\rho}^{(p\to p')}u_i^{(p\to p')} + g_i^{(p\to p')}\right)}$$

$$\forall p: \quad \partial_t\left(\alpha^{(p)}\rho^{(p)}h^{(p)}\right) + \vec{\nabla}\cdot\left(\alpha^{(p)}\rho^{(p)}h^{(p)}\vec{\mathbf{u}}^{(p)}\right) =$$
$$= \alpha^{(p)}\partial_t p - \boxed{\vec{\nabla}\cdot\vec{\mathbf{j}}_h^{(p)} + \dot{q}_h^{(p)}} + \left(\alpha^{(p)}\hat{\boldsymbol{\tau}}^{(p)}\right)\bullet\left(\vec{\nabla}\vec{\mathbf{u}}^{(p)}\right)$$
$$+ \boxed{\sum_{p'}\left(\dot{\rho}^{(p'\to p)}h^{(p'\to p)} - \dot{\rho}^{(p\to p')}h^{(p\to p')} + \dot{q}_h^{(p\to p')}\right)}$$

Inter-phase processes

Modelling Discrete Phases

The previous models were based on the 'Eulerian' approach (time- and position-dependent fields)

- Ambient fluid: single-phase 'Eulerian' model
- Disperse phase — 'Lagrangian' model:
  - Establish equation of motion of particles subject to fluid forces
  - Solve this for each particle, and follow their path in the fluid
  - Draw conclusions from statistics upon particles

Mixed 'Eulerian–Lagrangian' approach

Constitutive Relations

- Primary field varaibles:

  $\alpha^{(p)}(t,\vec{\mathbf{r}}),\ \vec{\mathbf{u}}^{(p)}(t,\vec{\mathbf{r}}),\ p(t,\vec{\mathbf{r}}),\ h^{(p)}(t,\vec{\mathbf{r}})$
- Constitutive equations
  - Intrinsic:

    $\rho^{(p)}(p,h^{(p)})$

    $\mu^{(p)}(p,h^{(p)})$

    $k^{(p)}(p,h^{(p)})$
  - Heat sources: $\dot{q}_h^{(p)}$
  - Phase transition fluxes
    - Inter-phase processes: $\dot{\rho}^{(p'\to p)}, \vec{\mathbf{u}}^{(p'\to p)}, h^{(p\to p')}$,
    - Work $g_i^{(p\to p')}$,
    - Heat transfer $\dot{q}_h^{(p\to p')}$

It is possible to generalise to multi-component phases

Degrees of Disperse Phase Modelling

Increasing particle loading

1. Flow→particle: Track individual particles subject to ambient flow
2. Particle↔particle coupling: include interactions
3. Flow↔particles coupling: include effect of particles on the ambient flow
4. Consider particle–particle contacts

Pros and Cons

TOO MANY EQUATIONS

- Intrinsic constitutive equations are the same as the single-phase ones
- One needs a lot of external constitutive equations
- Some of these require empirical correlations
- Sometimes there is not enough experimental data to establish such correlations
- Risk of unsubstantiated assumptions
- High computational demand (w.r.t. the one-fluid models)
- Low computational demand (w.r.t. fine models)
- Flexibility

Features of Disperse Phase Modelling

- Effects of various fluid dynamical actions
- Particle-wall interactions, depositions
- Sedimentation
- Bubbles and drops:
  - Growth and collapse
  - Coalescence and breakup
- Studying varying particle size distribution