Multiphase and Reactive Flow Modelling

BMEGEÁTMW07

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Basic notions and terminology

Ordinary phases:

preserve volume

Condensed phases

– Solid ← preserves shape

– Liquid

expands → – Gaseous

Fluid phases

deform

There also exist extraordinary phases, like plastics and similarly complex materials

The property of *fluidity* serves in the definition of fluids

Properties and models of solids

Properties of solids:

- Mass (inertia), position, translation → Mass point model
- Extension (density, volume), rotation, inertial momentum → Rigid body model
- Elastic deformations (small, reversible and linear), deformation and stress fields ↔ The simplest continuum model
- Inelastic deformations (large, irreversible and nonlinear), dislocations, failure etc. ↔ Even more complex models

Modelled features:

1. Mechanics
   - Statics: mechanical equilibrium is necessary
   - Dynamics: governed by deviation from mechanical equilibrium
2. Thermodynamics of solids

Models and properties of fluids

Key properties of fluids:

- Large, irreversible deformations
- Density, pressure, viscosity, thermal conductivity, etc. (are these properties or states?)

Features to be modelled:

1. Statics
   - Hydrostatics: definition of fluid (inhomogeneous [pressure and density])
   - Thermostatics: thermal equilibrium (homogenous state)
2. Dynamics
   1. Mechanical dynamics: motion governed by deviation from equilibrium of forces
   2. Thermodynamics of fluids:
      - Deviation from global thermodynamic equilibrium often governs processes multiphase, multi-component systems
      - Local thermodynamic equilibrium is (almost always) maintained

Only continuum models are appropriate!

Modelling Simple Fluids

- Inside the fluid:
  - Transport equations

    Mass, momentum and energy balances

    5 PDE's for $p(t,\vec{\mathbf{r}})$, $\vec{\mathbf{u}}(t,\vec{\mathbf{r}})$ a $T(t,\vec{\mathbf{r}})$ ← Primary (direct) field variables
  - Constitutive equations

    Algebraic equations for $\rho(p,T)$, $\mu(p,T)$, $k(p,T)$, …
- Boundary conditions ← Secondary (indirect) field variables

  On explicitly or implicitly specified surfaces
- Initial conditions

Thermodynamical representations

Representation (independent variables)	TD potential
enthropy and volume (s,1/ρ)	internal energy
temperature and volume (T,1/ρ)	free energy
enthropy and pressure (s,p)	enthalpy
temperature and pressure (T,p)	free enthalpy

- All of these are equivalent: can be transformed to each other by appropriate formulæ
- Use the one which is most practicable: e.g., (s,p) in acoustics: $s = const \Rightarrow \rho(s,p) \to \rho(p)$.

  We prefer (T,p)

Note

Some models of fluids

- $\rho = const,\ \mu = const$ → Stoksean fluid
- $\rho(\,p\,),\ \mu = const$ → compressible (or barotropic) fluid

  In both of these, the heat transport problem can be solved separately (one-way coupling):

  fluid dynamical equations → heat transport equation (1 PDE)
- $\rho(p,T),\ \mu(p,T),\ k(p,T),\ \ldots$ → general simple fluid

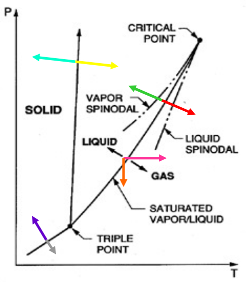
  Mutually coupled thermo-hydraulic equations:

  fluid dynamical equations ↔ heat transport equation
- Non-Newtonian behaviour etc. → models for complex fluids

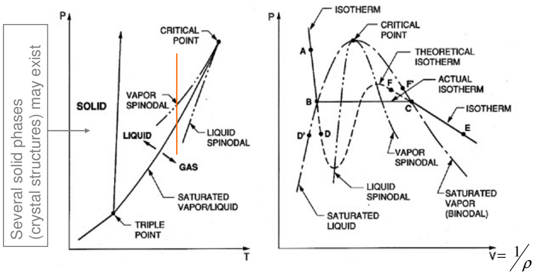
Phase transitions

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

All phase transitions involve <u>latent heat</u> deposition or release



Typical phase diagrams of a *pure* material:



In equilibrium 1, 2 or 3 phases can exist together

Complete mechanical and thermal equilibrium

Conditions of local phase equilibrium in a contact point in case of a pure material

- 2 phases:

  $T^{(1)}=T^{(2)}=:T$

  $p^{(1)}=p^{(2)}=:p$

  $\mu^{(1)}(T,p)=\mu^{(2)}(T,p)$

  Locus of solution:

  a line $T_s(p)$ or $p_s(T)$, the saturation temperature or pressure (e.g. 'boiling point').
- 3 phases:

  $T^{(1)}=T^{(2)}=T^{(3)}=:T$

  $p^{(1)}=p^{(2)}=p^{(3)}=:p$

  $\mu^{(1)}(T,p)=\mu^{(2)}(T,p)=\mu^{(3)}(T,p)$

  Locus of solution:

  a point (T_t,p_t), the triple point.

Multiple components

Almost all systems have more than 1 chemical components

Phases are typically *multi-component mixtures*

- <u>Concentration(s)</u>: measure(s) of composition

  There are lot of practical concentrations in use, e.g.
  - <u>Mass fraction</u> (we prefer this!)

    $c_1 = m_1/m,\quad c_2 = m_2/m,\ \ldots\quad c_k = m_k/m,\ \ldots\quad \sum_k c_k = \sum_k m_k/m = 1$
  - <u>Volume fraction</u> (good only if volume is conserved upon mixing!)

    $\alpha_1 = V_1/V,\quad \alpha_2 = V_2/V,\ \ldots\quad \alpha_k = V_k/V,\ \ldots\quad \sum_k \alpha_k = \sum_k V_k/V = 1$

Concentration fields appear as new primary field variables in the equation: $c_k(\,t,\vec{\mathbf{r}}\,)$ for $k = 2,\ldots,N_p$

One of them (usually that of the solvent) is redundant, not used.

Notations to be used (or at least attempted)

- 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

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

- Partial differentiation:

  $\partial_t,\ \partial_i\ (\partial_1 = \partial_x, \partial_2 = \partial_y, \partial_3 = \partial_z)$

Note

Material properties in multicomponent mixtures

- One needs constitutional equations for each phase
- These algebraic equations depend also on the concentrations

For each phase (p) one needs to know:

- the equation of state $\rho^{(p)}\left(p,T,c_1^{(p)},c_2^{(p)},\ldots\right)$
- the viscosity $\mu_k^{(p)}\left(p,T,c_1^{(p)},c_2^{(p)},\ldots\right)$
- the thermal conductivity $k^{(p)}\left(p,T,c_1^{(p)},c_2^{(p)},\ldots\right)$
- the diffusion coefficients $D_{k,\ell}^{(p)}\left(p,T,c_1^{(p)},c_2^{(p)},\ldots\right)$

Conditions of local phase equilibrium in a contact point in case of multiple components

- Suppose N phases and K components:
- Thermal and mechanical equilibrium on the interfaces:

  $T^{(1)}=T^{(2)}=T^{(3)}=:T$

  $p^{(1)}=p^{(2)}=p^{(3)}=:p$
- Mass balance for each component among all phases:

$$\mu_1^{(1)}\left(T,p,\cancel{c_1^{(1)}},c_2^{(1)},\ldots,c_K^{(1)}\right)=\mu_1^{(2)}\left(T,p,\cancel{c_1^{(2)}},c_2^{(2)},\ldots,c_K^{(2)}\right)=\ldots=\mu_1^{(N)}\left(T,p,\cancel{c_1^{(N)}},c_2^{(N)},\ldots,c_K^{(N)}\right)$$

$$\mu_2^{(1)}\left(T,p,\cancel{c_1^{(1)}},c_2^{(1)},\ldots,c_K^{(1)}\right)=\mu_2^{(2)}\left(T,p,\cancel{c_1^{(2)}},c_2^{(2)},\ldots,c_K^{(2)}\right)=\ldots=\mu_2^{(N)}\left(T,p,\cancel{c_1^{(N)}},c_2^{(N)},\ldots,c_K^{(N)}\right)$$

$$\vdots$$

$$\mu_K^{(1)}\left(T,p,\cancel{c_1^{(1)}},c_2^{(1)},\ldots,c_K^{(1)}\right)=\mu_K^{(2)}\left(T,p,\cancel{c_1^{(2)}},c_2^{(2)},\ldots,c_K^{(2)}\right)=\ldots=\mu_K^{(N)}\left(T,p,\cancel{c_1^{(N)}},c_2^{(N)},\ldots,c_K^{(N)}\right)$$

$(N\text{-}1)K$ equations for $2+N(K\text{-}1)$ unknowns

Phase equilibrium in a multi-component mixture

Gibbs' Rule of Phases, *in equilibrium*:

$$\boxed{\#\text{phases} \equiv N \le \#\text{components} + 2 \equiv K + 2}$$

TD limit on the # of phases

If there is *no (global) TD equilibrium*: additional phases may also exist

- in transient metastable state or
- spatially separated, in distant points

Miscibility

The number of phases in a given system is also influenced by the miscibility of the components:

- 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)
  1. Surface tension (gas-liquid interface)
  2. Interfacial tension (liquid-liquid interface)

  (In general: Interfacial tension on fluid-liquid interfaces)
- Solids typically remain granular

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
- *Compound*

Interfaces are

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

Topological limit on the # of phases (always local)

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.

  (Local deviation from total TD equilibrium is typical)