

# Multiphase and Reactive Flow Modelling

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Part 1

K. G. Szabó

Dept. of Hydraulic and Water Management  
Engineering,  
Faculty of Civil Engineering

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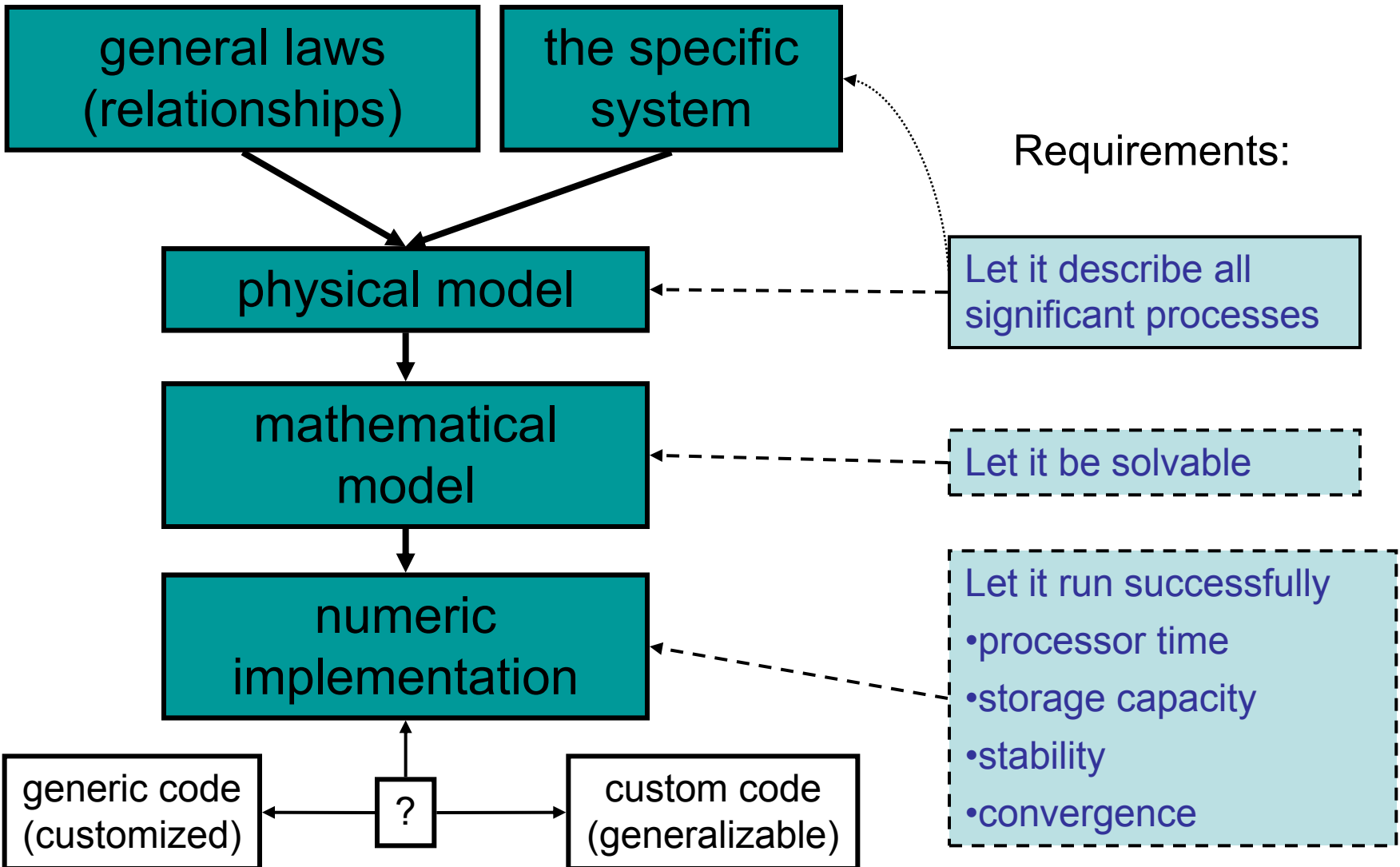
1. Modelling concepts
2. Basic notions and terminology
3. Multi-component fluids
4. Multi-phase fluids
  1. Phases
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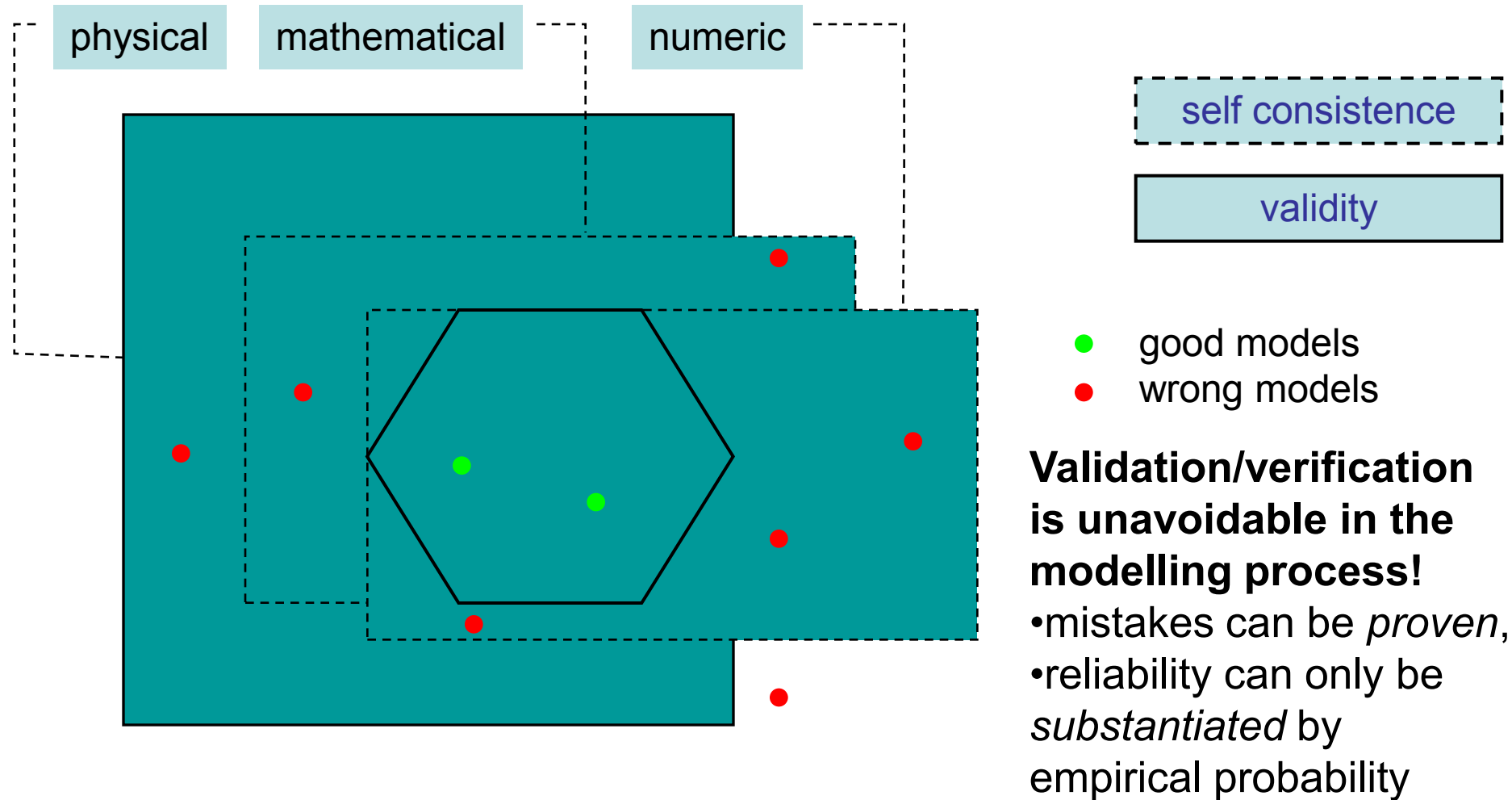
# What is modelling?

- Experimental modelling
- Theoretical modelling
  - Physical model layer
  - Mathematical model layer
- Numerical model

# Model layers



# Relating model layers properly



# Creating a physical model

What are the significant processes?

- Include all
- Get rid of non-significant ones

The dimensionless numbers help us with these!

- Classify the system based on the above

# Basic notions and terminology

Ordinary phases:

preserve volume

Condensed phases

– Solid

preserves shape

– Liquid

Fluid phases

expands

– Gaseous

deform

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

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

# Properties and physical models of solids

Properties of solids:

- Mass (inertia), position, translation
- Extension (**density**, volume), rotation, inertial momentum
- Elastic **deformations** (small, reversible and linear), deformation and stress fields
- Inelastic deformations (large, irreversible and nonlinear), dislocations, failure etc.

Mass point model

Rigid body model

The simplest **continuum** model

Even more complex models

Modelled features:

## 1. Mechanics

- Statics: **mechanical equilibrium** is necessary
- Dynamics: governed by deviation from mechanical equilibrium

## 2. Thermodynamics of solids



# Properties and physical models of fluids

Key properties of fluids:

- Large, irreversible deformations
- Density, pressure, viscosity, thermal conductivity, etc.

Only continuum models are appropriate!

Features to be modelled:

## 1. Statics

- Hydrostatics: definition of fluid (pressure and density can be inhomogeneous)
- 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

# Mathematical model of simple fluids

- Inside the fluid:

- Transport equations

Mass, momentum and energy balances

5 PDE's for  $p(t, \vec{r})$ ,  $\vec{u}(t, \vec{r})$  and  $T(t, \vec{r})$  ← 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

Expressing local thermodynamic equilibrium in fluid dynamics:  
the use of intensive and extensive state variables

- Integral forms: intensive and extensive ( $X$ )
- Differential forms (PDE's):
  - fixed control volume ( $V=\text{const}$ ):  
intensive and densities of the extensive ones ( $x=X/V$ )
  - advected fluid parcel ( $m=\text{const}$ ):  
intensive and specific values of the extensive ones ( $x=X/m$ )



# Thermodynamical representations

Representation (independent variables)	TD potential
entropy and volume ( $s, 1/\rho$ )	internal energy
temperature and volume ( $T, 1/\rho$ )	free energy
entropy 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:  $s = \text{const} \Rightarrow \rho(s, p) \rightarrow \rho(p)$ .

We prefer ( $T, p$ )

Note



# Some models of simple fluids

- $\rho = \text{const}, \mu = \text{const}$

Stoksean fluid

- $\rho(p), \mu = \text{const}$

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)

- $\rho(p, T), \mu(p, T), k(p, T), \dots$

general simple fluid

Mutually coupled thermo-hydraulic equations:

fluid dynamical  
equations

heat transport  
equation

- Non-Newtonian behaviour etc.

models for complex fluids

# Phase transitions

## in case of a single compound

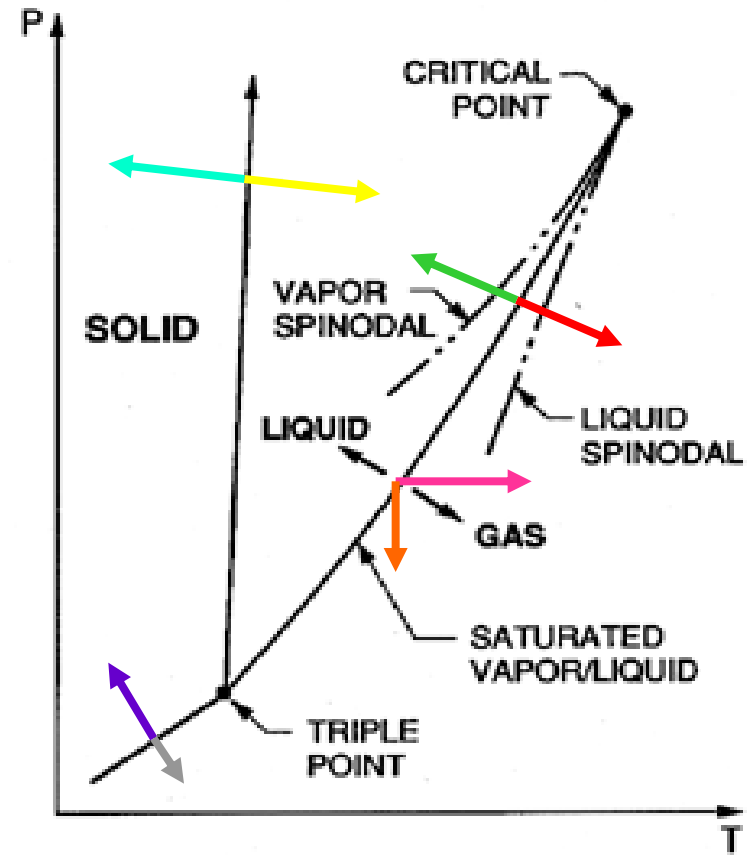
- Evaporation, incl.
  - Boiling
  - Cavitation
- Condensation, incl.
  - Liquefaction
  - Solidification

- Sublimation

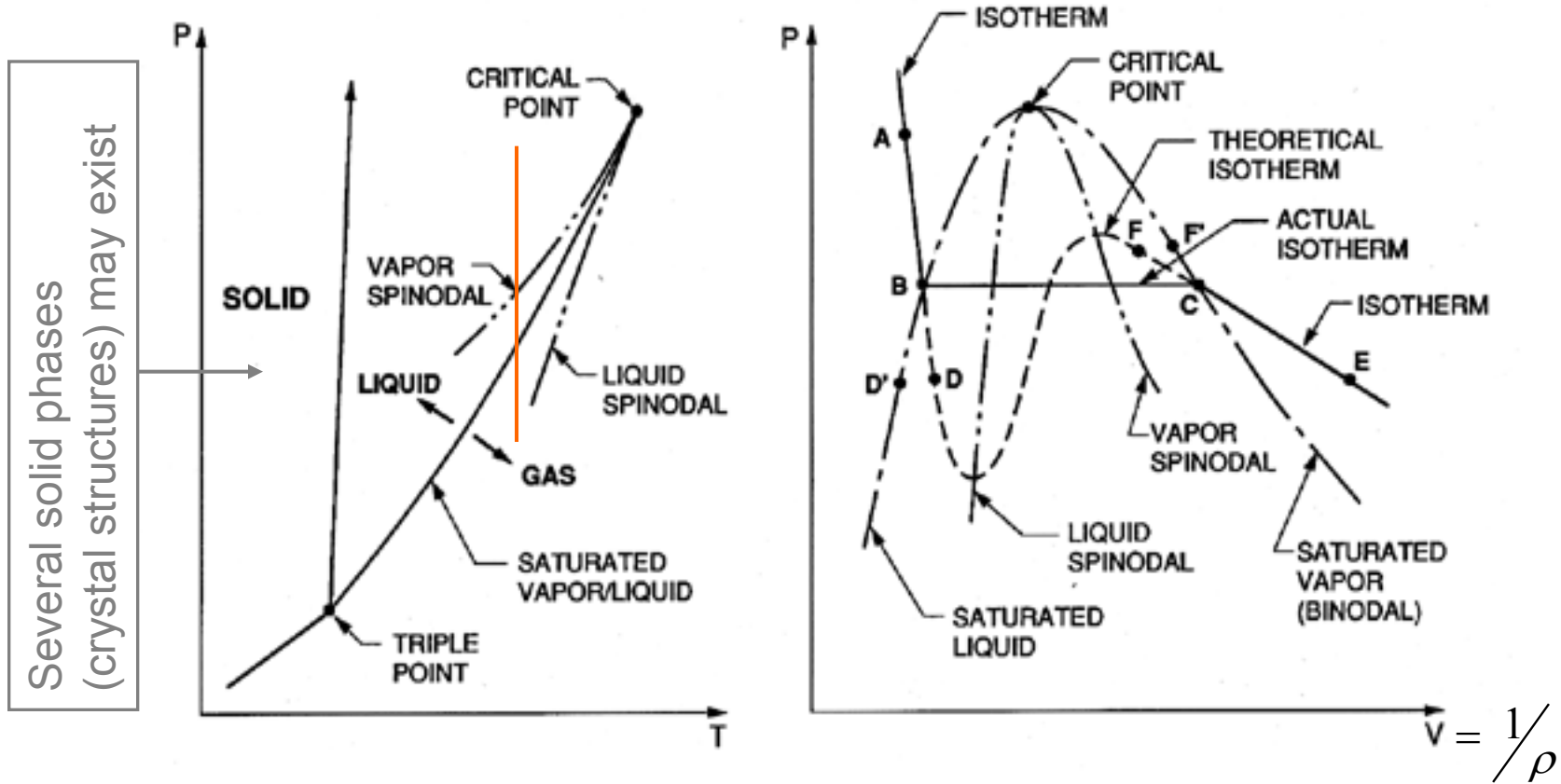
- Freezing

- Melting

All phase transitions involve latent heat 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*

## Concentration(s): measure(s) of composition

There are lot of practical concentrations in use, e.g.

- Mass fraction (we prefer this!)

$$c_1 = m_1/m, \quad c_2 = m_2/m, \quad \dots \quad c_k = m_k/m, \quad \dots \quad \sum_k c_k = \sum_k m_k/m = 1$$

- Volume fraction (good only if volume is conserved upon mixing!)

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

- Mole fraction (used in case of chemical reactions and diffusion)

$$y_1 = n_1/n, \quad y_2 = n_2/n, \quad \dots \quad y_k = n_k/n, \quad \dots \quad \sum_k y_k = \sum_k n_k/n = 1$$

# Multiple components

Concentration fields appear as new primary field variables in the equation:

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

$$c_k(t, \vec{\mathbf{r}}) \text{ for } k = 2, \dots, K$$

# Notations to be used (or at least attempted)

- Phase index (upper):
  - $(p)$  or
  - $(s)$ ,  $(l)$ ,  $(g)$ ,  $(v)$ ,  $(f)$  for solid, liquid, gas, vapour, fluid
- 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 multi-component 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  $\rho^{(p)}(p, T, c_1^{(p)}, c_2^{(p)}, \dots)$
- the heat capacity  $c_p^{(p)}(p, T, c_1^{(p)}, c_2^{(p)}, \dots)$
- the viscosity  $\mu^{(p)}(p, T, c_1^{(p)}, c_2^{(p)}, \dots)$
- the thermal conductivity  $k^{(p)}(p, T, c_1^{(p)}, c_2^{(p)}, \dots)$
- the diffusion coefficients  $D_{k,\ell}^{(p)}(p, T, c_1^{(p)}, c_2^{(p)}, \dots)$

# 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:

$$T^{(1)}=T^{(2)} = \dots = T^{(N)}=:T$$

$$p^{(1)}=p^{(2)} = \dots = p^{(N)}=:p \quad 2N \rightarrow \text{only 2 independent unknowns}$$

- Mass balance for each component among all phases:

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

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

⋮

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

$K(N-1)$  independent equations for  $2+N(K-1)$  independent unknowns



# Phase equilibrium in a multi-component mixture

Gibbs' Rule of Phases, *in equilibrium*:

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

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 (at least)
- 0D contact points with 4 phases, 6 interfaces and 4 contact lines (at least)



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** and within each phase.

(Local deviation from total TD equilibrium is typical)

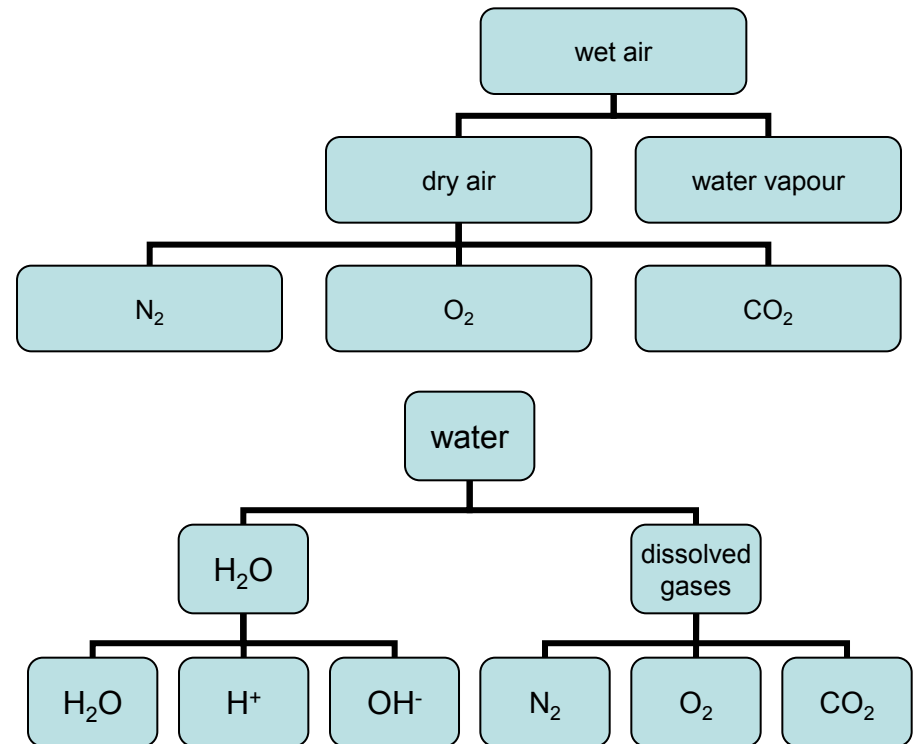
# Are components = chemical species?

Not always:

- Major reagents in chemical reactions has to be modelled separately,
- but similar materials can be grouped together and treated as a single component
  - The grouping can be refined in the course of the modelling

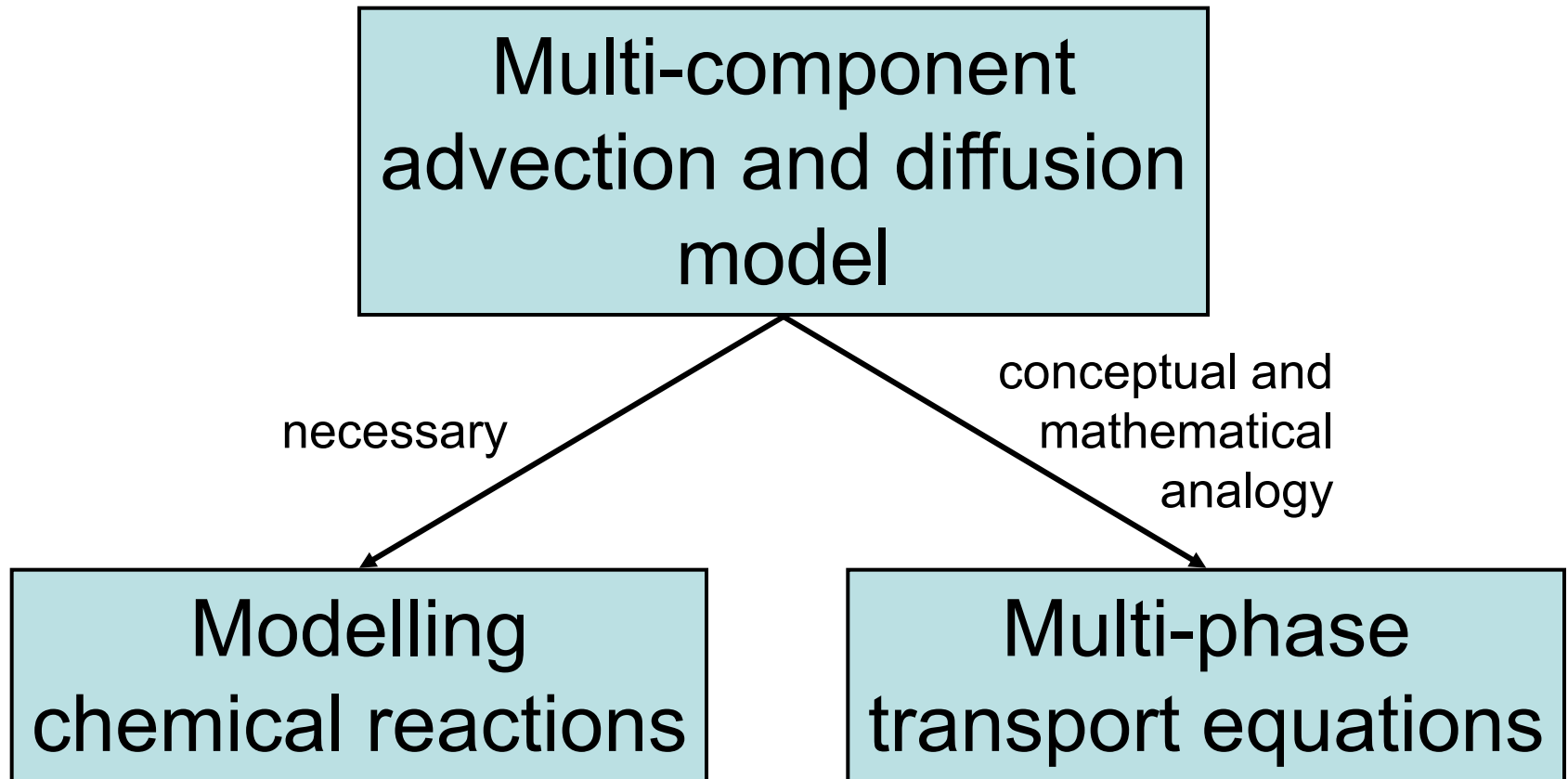
Example:

components in an air-water two phase system



# Multi-component transport

We set up transport equations for single-phase multi-component fluids



# Multi-component transport Outline

- Balance equations
- Mass balance — equation of continuity
- Component balance
- Advection
- Molecular diffusion
- Chemical reactions



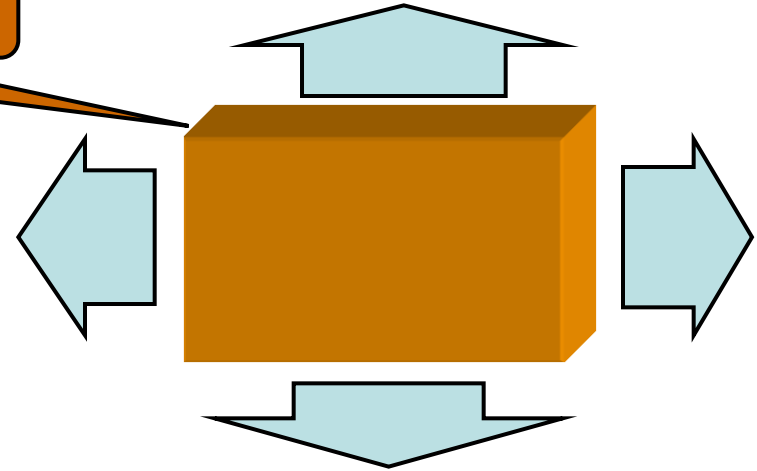
# Mass balance for a control volume

Eulerian (fixed) control volume in 3D

Mass inside:  $m(t) = \iiint \rho(t, \vec{r}) dV$

Outflow rate:  $J(t) = \oiint \vec{j}(t, \vec{r}) \cdot d\vec{A}$

Mass production rate:  $Q(t) = 0$



Mass is a conserved quantity (in 3D):  
no production (sources) and decay (sinks) inside

This is a conservation law

Integral form:  $\frac{dm}{dt} = -J(t) + Q(t)$

**Mass balance equation**

Differential form:  $\partial_t \rho + \vec{\nabla} \cdot (\rho \vec{u}) = 0$

By definition:

$\vec{u}(t, \vec{r}) := \vec{j} / \rho$

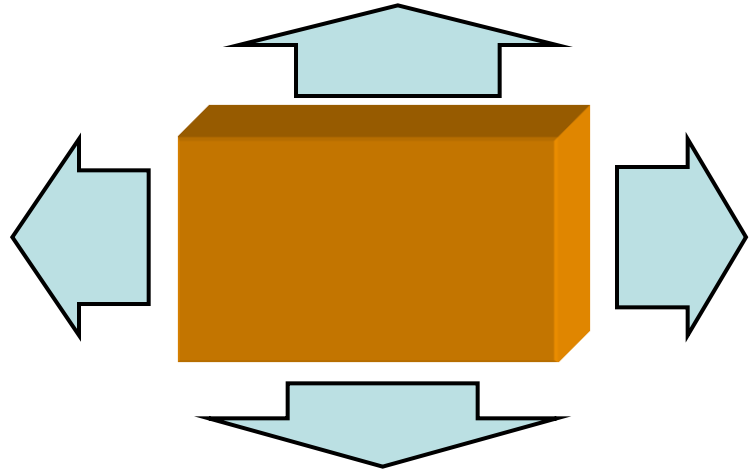
# Component mass balance

For each component:

Mass inside:  $m_k(t) = \iiint \rho_k(t, \vec{r}) dV$

Outflow rate:  $J_k(t) = \oiint \vec{j}_k(t, \vec{r}) \cdot d\vec{A}$

Mass production rate:  $Q_k(t) = 0$



**If** component masses are also conserved, **then** no production (sources) and decay (sinks) inside

These are also conservation laws

Integral form:  $\frac{dm_k}{dt} = -J_k(t) + Q_k(t)$

**Mass balance equations**

By definition:

Differential form:  $\partial_t \rho_k + \vec{\nabla} \cdot (\rho_k \vec{u}_k) = 0 \leftarrow \vec{u}_k(t, \vec{r}) := \vec{j}_k / \rho_k$



# The mass transport equations

$$\partial_t \rho + \vec{\nabla}(\rho \vec{u}) = 0$$

$$\sum_k \uparrow$$

$$\forall k: \partial_t \rho_k + \vec{\nabla}(\rho_k \vec{u}_k) = 0$$



$$\partial_t(c_k \rho) + \vec{\nabla}(c_k \rho \vec{u}) = -\vec{\nabla}(\rho_k \vec{w}_k) = -\vec{\nabla} \vec{j}_{\text{diff } k} \quad \Leftarrow \quad \vec{j}_{\text{diff } k} := \rho_k \vec{w}_k$$

**advection**

**diffusion**

$$c_k [\cancel{\partial_t \rho + \vec{\nabla}(\rho \vec{u})}] + \rho [\partial_t c_k + \vec{u} \vec{\nabla} c_k] = -\vec{\nabla} \vec{j}_{\text{diff } k}$$

$$\forall k: D_t c_k = \partial_t c_k + \vec{u} \vec{\nabla} c_k = -\frac{1}{\rho} \vec{\nabla} \vec{j}_{\text{diff } k}$$



$$\sum_k \rho_k = \rho, \quad \sum_k \vec{j}_k = \sum_k \rho_k \vec{u}_k = \vec{j}$$

$$\rho_k = c_k \rho, \quad \vec{j}_k = \rho_k \vec{u}_k = c_k \rho \vec{u}_k$$

$$\vec{u}_k = \vec{u} + (\vec{u}_k - \vec{u}) = \vec{u} + \vec{w}_k$$

$$\sum_k \vec{j}_{\text{diff } k} = \sum_k \rho_k \vec{w}_k = \vec{0}$$



# Notations to be used (or at least attempted)

- Material derivative of a specific quantity:

$$\frac{Df}{Dt} := \frac{\partial f}{\partial t} + (\vec{\mathbf{u}} \cdot \vec{\nabla})f \rightarrow D_t f := \partial_t f + (\vec{\mathbf{u}} \cdot \vec{\nabla})f$$

Note





# Two ways of resolving redundancy

- Pick exactly  $K$  mass transport equations and choose the  $K$  primary variables as follows:

$$k = 1, \dots, K : \partial_t \rho_k + \vec{\nabla}(\rho_k \vec{u}) = -\vec{\nabla} \cdot \vec{j}_{\text{diff } k} \quad \partial_t \rho + \vec{\nabla}(\rho \vec{u}) = 0$$

$$k = 2, \dots, K : D c_k = -(1/\rho) \vec{\nabla} \cdot \vec{j}_{\text{diff } k}$$

- If needed, calculate the remaining secondary variable fields from the algebraic relations:

$$\rho(t, \vec{x}) = \sum_k \rho_k(t, \vec{x})$$

$$c_k(t, \vec{x}) = \rho_k(t, \vec{x}) / \rho(t, \vec{x})$$

$$c_1(t, \vec{x}) = 1 - \sum_{k=2}^K c_k(t, \vec{x})$$

$$\rho_k(t, \vec{x}) = \rho(t, \vec{x}) \cdot c_k(t, \vec{x})$$

Typically,  
this is the  
solvent

For a binary mixture:

$$c_2(t, \vec{x}) = c(t, \vec{x})$$

$$c_1(t, \vec{x}) = 1 - c(t, \vec{x})$$



# Differential forms in balance equations



Conservation of  $F$ :  $F(t) = \iiint \varphi(t, \vec{r}) dV = \iiint f(t, \vec{r}) \cdot \rho(t, \vec{r}) dV$

- equations for the density ( $\varphi$ )
  - general
  - only convective flux
- equation for the specific value ( $f$ )



$$\partial_t \varphi + \vec{\nabla} \cdot \vec{j}_F = 0$$

$$\Downarrow \text{if } \vec{j}_F = \vec{u} \cdot \varphi$$

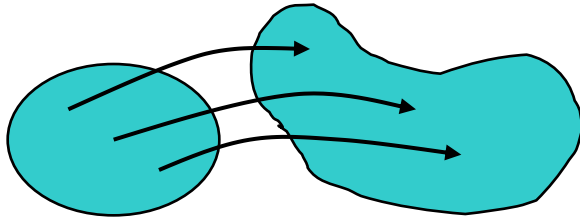
$$\partial_t \varphi + \vec{\nabla}(\vec{u} \cdot \varphi) = 0$$

$$\Downarrow \text{if } m \text{ is conserved}$$

$$D_t f \equiv \partial_t f + (\vec{u} \cdot \vec{\nabla}) f = 0$$

These forms describe passive advection of  $F$

# Passive advection



- The concentrations of the fluid particles do not change with time:

$$D_t c_k \equiv \partial_t c_k + (\vec{\mathbf{u}} \cdot \vec{\nabla}) c_k = 0$$

- The component densities vary in fixed proportion to the overall density:

$$\partial_t \rho_k + \vec{\nabla}(\rho_k \vec{\mathbf{u}}) = 0$$

- Computational advantage: The component transport equations uncouple from the basic fluid dynamical problem and can be solved separately and *a posteriori*
- The solution requires
  - Lagrangian particle orbits
  - Initial conditions (hyperbolic equations)

# Simple diffusion models

- No diffusion → pure advection



$$\vec{\mathbf{j}}_{\text{diff } k} = \vec{\mathbf{0}}$$

$$\begin{cases} \partial_t \rho_k + \vec{\nabla}(\rho_k \vec{\mathbf{u}}) = 0 \\ D_t c_k = 0 \end{cases}$$

- Equimolecular counter-diffusion

$$\vec{\mathbf{j}}_{\text{diff } k} = -\rho D \vec{\nabla} c_k$$

for constant  $D$  and  $\rho \rightarrow$

$$\begin{cases} \partial_t \rho_k + \vec{\nabla}(\rho_k \vec{\mathbf{u}}) = D \nabla^2 \rho_k \\ D_t c_k = D \nabla^2 c_k \end{cases}$$

- Fick's 1st Law

for each solute if  $c_k \ll 1$  ( $k = 2, \dots, K$ )

$$\vec{\mathbf{j}}_{\text{diff } k} = -\rho D_k \vec{\nabla} c_k$$

constant  $D_k$  and  $\rho \rightarrow$

$$\begin{cases} \partial_t \rho_k + \vec{\nabla}(\rho_k \vec{\mathbf{u}}) = D_k \nabla^2 \rho_k \\ D_t c_k = D_k \nabla^2 c_k \end{cases}$$

but note that  $\sum_{k=1}^K \vec{\mathbf{j}}_{\text{diff } k} \neq \vec{\mathbf{0}}$

Fick's 2nd Law:

$$\partial_t c_k = D_k \nabla^2 c_k$$

Turbulent mixing

# Further diffusion models

## Thermodiffusion and/or barodiffusion

Occur(s) at

- high concentrations
- high T and/or p gradients

For a binary mixture:

$$\vec{j}_{\text{diff}} = -\rho D \left( \nabla c + (k_T / T) \nabla T + (k_p / p) \nabla p \right)$$

$D \cdot k_T$  : coefficient of thermodiffusion

$D \cdot k_p$  : coefficient of barodiffusion

Analogous cross effects  
appear in the heat  
conduction equation

# Further diffusion models

## Nonlinear diffusion model

Cross effect among species' diffusion

Valid also at

- high concentrations
- more than 2 components
- low  $T$  and/or  $p$  gradients

(For a binary mixture it falls back to Fick's law.)

$$\vec{\mathbf{j}}_{\text{diff } k} = \rho \cdot \sum_{\ell \neq k} \frac{M_k}{M} \cdot \frac{\tilde{K}_{\ell k} - \tilde{K}_{kk}}{\det(\mathbf{K})} \cdot \vec{\nabla} y_k$$

$$\tilde{\mathbf{K}} = \text{adj}(\mathbf{K})$$

$$K_{k\ell} = \frac{y_k}{D_{k\ell}} + \frac{M_\ell}{M_k} \cdot \sum_{s \neq k} \frac{y_s}{D_{ks}} \quad \text{if } k \neq \ell$$

$$K_{kk} = 0$$

$$y_k = \frac{M}{M_k} \cdot c_k : \text{mole fraction}$$

$$M = \sum_k y_k M_k : \text{mean molar mass}$$

$D_{k\ell}$  : binary diffusion coefficient

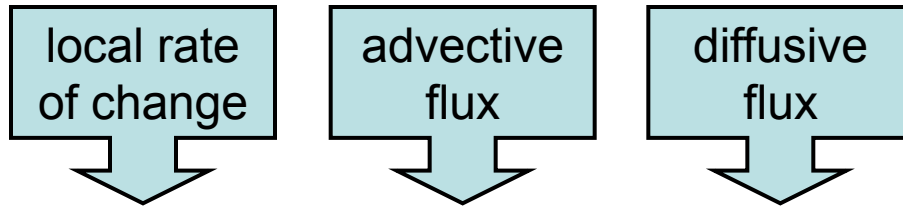
$$D_{k\ell}(T, n, M_k, M_\ell) = D_{\ell k}$$

# Further notes on diffusion modelling

- For internal consistency of the whole model
  - $D$  has to be changed in accordance to the turbulence model ('turbulent diffusivity')
  - Diffusive heat transfer has to be included in the heat transport equation
- In the presence of multiple phases, the formulation can be straightforwardly generalised by introducing the phasic quantities

$$c_k \rightarrow c_k^{(p)}, \rho_k \rightarrow \rho_k^{(p)}, \vec{j}_k \rightarrow \vec{j}_k^{(p)}, \vec{j}_{\text{diff } k} \rightarrow \vec{j}_{\text{diff } k}^{(p)}, D_k \rightarrow D_k^{(p)} \dots$$

# The advection–diffusion equations



$$\partial_t(\rho \cdot c_k) + \vec{\nabla}(\vec{\mathbf{u}} \cdot \rho \cdot c_k) = -\vec{\nabla} \cdot \vec{\mathbf{j}}_k$$

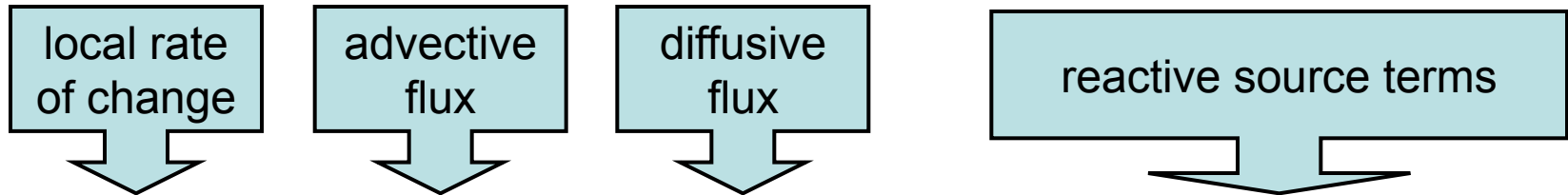
↕ since  $m$  is conserved

$$D_t c_k \equiv \partial_t c_k + (\vec{\mathbf{u}} \cdot \vec{\nabla}) c_k = -\frac{1}{\rho} \vec{\nabla} \cdot \vec{\mathbf{j}}_k \quad \leftarrow \text{e.g. } D \cdot \nabla^2 c_k$$

The component masses are *conserved* but *not passive* quantities



# The advection–diffusion–reaction equations



$$\partial_t(\rho \cdot c_k) + \vec{\nabla}(\vec{\mathbf{u}} \cdot \rho \cdot c_k) = -\vec{\nabla} \cdot \vec{\mathbf{j}}_k + (\text{mass production rate density})$$

⇕ since  $m$  is conserved



$$D_t c_k \equiv \partial_t c_k + (\vec{\mathbf{u}} \cdot \vec{\nabla}) c_k = -\frac{1}{\rho} \vec{\nabla} \cdot \vec{\mathbf{j}}_k + (\text{local specific production rate})$$

The component masses are *not conserved* quantities

# Reaction modelling OUTLINE



1. Reaction stoichiometry
2. Reaction energetics
3. Reaction kinetics

Effects in the model equations:

- reactive source terms in the advection–diffusion–reaction equations
- reaction heat source terms in the energy (=heat conduction) equation

# A template reaction

## Stoichiometry

forward reaction

reactants  $\rightarrow$  product



products  $\leftarrow$  reactant

reverse reaction

Reagents and reaction products	
$k$	species
1	$\text{H}_2\text{O}$
2	$\text{O}_2$
3	$\text{H}_2$

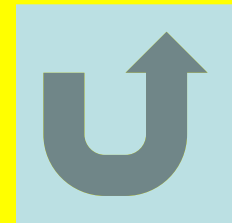
## Energetics

forward reaction:  $\Delta E > 0$  energy released  $\rightarrow$  exothermic

reverse reaction:  $-\Delta E > 0$  energy consumed  $\rightarrow$  endothermic

# Notational system for local extensive quantities

- For integral description (in control volumes):
  - extensive quantity:  $F$
- For differential description (local values):
  - density:  $\varphi = F/V = \rho \cdot f$
  - specific value  $f = F/m$
  - molar value  $f = F/n$
  - molecular value  $F^* = F/N$



# Modelling multiple phases in fluids

# Phases



## Mathematical description

using characteristic functions:

$$\chi^{(p)}(t, \vec{\mathbf{r}}) = \begin{cases} 1 & \text{if } \vec{\mathbf{r}} \text{ is in phase } p \text{ at time } t, \\ 0 & \text{if } \vec{\mathbf{r}} \text{ is in another phase at time } t. \end{cases}$$

They resemble concentrations since one of them is redundant:

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

but they are discreet and not continuous  
(either 0 or 1, but not in between)



# Phasic volume fractions

More practical description by averaging:

- Time averaged local volume fraction:

$$\frac{1}{T} \int_{t-T/2}^{t+T/2} \chi^{(p)}(\tau, x, y, z) d\tau = \alpha^{(p)}(t, x, y, z; T) \xrightarrow{T \rightarrow \infty} \alpha^{(p)}(x, y, z)$$

$$\frac{1}{V} \iiint \chi^{(p)}(t, x, y, z) dV = \alpha^{(p)}(t; V)$$

- Volume averaged volume fraction

$$\frac{1}{A} \iint \chi^{(p)}(t, x, y, z) dy dz = \alpha^{(p)}(t, x)$$

- Cross-sectional averaged volume fraction

$$\frac{1}{L} \int \chi^{(p)}(t, x, y, z) dz = \alpha^{(p)}(t, x, y)$$

- Chordal/vertical averaged volume fraction



# Phasic volume fractions 2

- Averaging in time and space can be combined using appropriate averaging windows
- Such averages are directly related to measurement processes
- Running averaging can produce smooth functions
- Volume fractions resemble much more to concentrations:

## Measurement methods:

- Optical fibre probe
- gamma-ray absorption
- X-ray absorption
- neutron scattering
- optical image processing
- etc.

$$0 \leq \alpha^{(p)} \leq 1$$
$$\sum_p \alpha^{(p)} = 1$$





# Volume fractions in gas—liquid two-phase systems

- If the volume fraction of the gas phase is used, it is often called void fraction:

frequently used alternative notations →

$$\varepsilon = \varepsilon_G = \alpha = \alpha^{(g)}, \alpha^{(\ell)} = 1 - \alpha$$

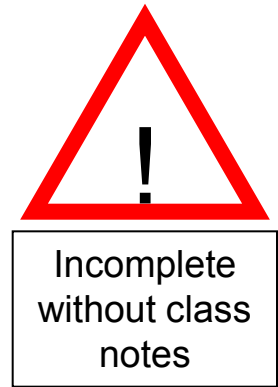
- If the volume fraction of the liquid phase is used, it is often called liquid holdup:

frequently used alternative notations →

$$h = h_L = \alpha = \alpha^{(\ell)}, \alpha^{(g)} = 1 - \alpha$$



# Interfaces

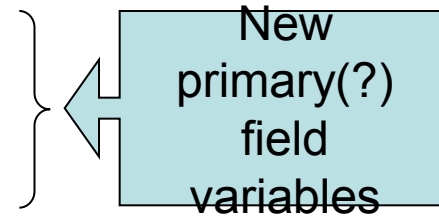


- Mathematical description of interfaces
  - normal, tangent, curvature
  - implicit description
  - parametric description
  - interface motion
- Transport through interfaces
  - Continuity and jump conditions:
    - mass balance
    - force balance
    - heat balance

# Interfaces and their motion

- Description of interface surfaces:

- parametrically
- by implicit function
- (the explicit description is the common case of the previous two)



- Moving phase interface:  
(only!) the normal velocity component makes sense



# Description of an interface by an implicit function

$$F(t, x, y, z) = 0$$

$$\mathbf{n} = \nabla F / |\nabla F| \quad (\text{unit normal})$$

$$\kappa = \frac{1}{2} \cdot \left( \frac{1}{R_1} + \frac{1}{R_2} \right) = \nabla \cdot \mathbf{n} \quad (\text{mean curvature})$$

Type I surface integrals  $\leftrightarrow$  volume integrals :

$$\iint f(t, x, y, z) \cdot dA = \iiint f(t, x, y, z) \cdot \delta(F(t, x, y, z)) \cdot |\nabla F(t, x, y, z)| \cdot dV$$

Type II surface integrals  $\leftrightarrow$  volume integrals :

$$\iint \mathbf{v}(t, x, y, z) \cdot d\mathbf{A} = \iiint \mathbf{v}(t, x, y, z) \cdot \delta(F(t, x, y, z)) \cdot \nabla F(t, x, y, z) \cdot dV$$



# Equation of motion of an interface given by implicit function

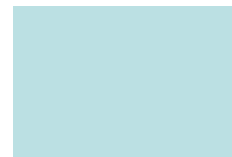
- Equation of interface
- Path of the point that remains on the interface (but not necessarily a fluid particle)
- Differentiate
- For any such point the normal velocity component must be the same
- Propagation speed and velocity of the interface

$$F(t, \mathbf{r}) = 0$$

$$\mathbf{r}(t)$$

$$F(t, \mathbf{r}(t)) = 0$$

$$\frac{d}{dt} F(t, \mathbf{r}(t)) = \partial_t F + \dot{\mathbf{r}}(t) \cdot \nabla F = 0$$



$$\partial_t F + u_{\perp}^* \cdot \mathbf{n} \cdot \nabla F = 0$$

$$u_{\perp}^* = \mathbf{n} \cdot \dot{\mathbf{r}}(t)$$

$$\mathbf{u}_{\perp}^* = \mathbf{n} \cdot \mathbf{u}_{\perp}^*$$

Only the normal component makes sense



# Parametric description of interface motion

- Functional form of the surface:  $\mathbf{r}(t, a, b)$
- Curvilinear coordinates and  $a(t), b(t)$
- path of a point that remains on the interface  $\mathbf{r}(t, a(t), b(t))$   
(not necessarily a fluid particle)
- Differentiate:  $\frac{d}{dt} \mathbf{r}(t, a(t), b(t)) =$   

$$= \partial_t \mathbf{r} + \partial_a \mathbf{r} \cdot \dot{a}(t) + \partial_b \mathbf{r} \cdot \dot{b}(t)$$
- Take the normal velocity component to get  $\mathbf{n} = \frac{\partial_a \mathbf{r} \times \partial_b \mathbf{r}}{|\partial_a \mathbf{r} \times \partial_b \mathbf{r}|}$
- the propagation speed and velocity of the interface:  $u_{\perp}^* = \mathbf{n} \cdot \dot{\mathbf{r}}(t) = \mathbf{n} \cdot \partial_t \mathbf{r}(t, a(t), b(t))$   

$$\mathbf{u}_{\perp}^* = \mathbf{n} \cdot u_{\perp}^*$$



# Mass balance through an interface

Steps of the derivation:

1. Describe in a reference frame that moves with the interface (e.g. keep the position of the origin on the interface)
2. Describe velocities inside the phases in the moving frame
3. Match mass fluxes



Incomplete  
without class  
notes

# The kinematical boundary conditions

The net mass flux through the interface :

$$j_{\text{mass}}^* \stackrel{\text{def}}{=} \rho^{(1)}(\mathbf{u}^{(1)} - \mathbf{u}_{\perp}^*) \cdot \mathbf{n} \equiv \rho^{(2)}(\mathbf{u}^{(2)} - \mathbf{u}_{\perp}^*) \cdot \mathbf{n}$$

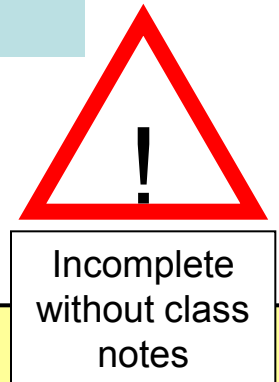
$$[\rho(\mathbf{u} - \mathbf{u}_{\perp}^*) \cdot \mathbf{n}] = 0$$

For the tangential components:

$$[\mathbf{u} \times \mathbf{n}] = \mathbf{0} \text{ (no slip condition)}$$

$$\partial_t F + \mathbf{u}_{\perp}^* \cdot \nabla F = 0$$

This condition does not follow from mass conservation



Without (net) mass transfer:

$$j_{\text{mass}}^* = 0 \Rightarrow \mathbf{u}^{(1)} \cdot \mathbf{n} = \mathbf{u}^{(2)} \cdot \mathbf{n} = \mathbf{u}_{\perp}^* \cdot \mathbf{n} \equiv u_{\perp}^*$$

$$[\mathbf{u} \cdot \mathbf{n}] = 0$$

tangential components:

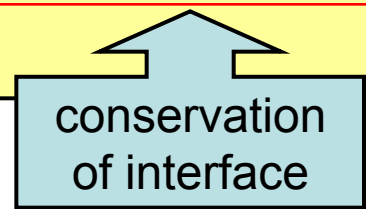
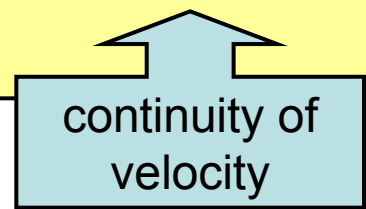
$$[\mathbf{u} \times \mathbf{n}] = \mathbf{0}$$

$$\Rightarrow [\mathbf{u}] = \mathbf{0}$$

$$\partial_t F + \mathbf{u} \cdot \nabla F = 0$$

continuity of velocity

conservation of interface





# Diffusion through an interface

Mass flux of component  $k$  in the co-moving reference frame:

$$\rho_k(\mathbf{u}_k - \mathbf{u}_\perp^*) = c_k \rho(\mathbf{u} - \mathbf{u}_\perp^* + \mathbf{u}_k - \mathbf{u}) = c_k \rho(\mathbf{u} - \mathbf{u}_\perp^*) + \mathbf{j}_k$$



Case of conservation of component mass:

- on a pure interface (no surface phase, no surfactants)
- without surface reactions (not a reaction front)

$$\left. \begin{array}{l} \bullet \text{ on a pure interface (no surface phase, no surfactants)} \\ \bullet \text{ without surface reactions (not a reaction front)} \end{array} \right\} \Rightarrow \left\{ \begin{array}{l} [\rho_k(\mathbf{u}_k - \mathbf{u}_\perp^*) \cdot \mathbf{n}] = 0 \\ \Downarrow \\ [c_k] \cdot j_{\text{mass}}^* + [\mathbf{j}_k \cdot \mathbf{n}] = 0 \end{array} \right.$$

The component flux through the interface:

$$\begin{aligned} j_k^* &\stackrel{\text{def}}{=} \rho_k^{(1)}(\mathbf{u}_k^{(1)} - \mathbf{u}_\perp^*) \cdot \mathbf{n} \equiv \rho_k^{(2)}(\mathbf{u}_k^{(2)} - \mathbf{u}_\perp^*) \cdot \mathbf{n} \\ &= c_k^{(1)} \cdot j_{\text{mass}}^* + \mathbf{j}_k^{(1)} \cdot \mathbf{n} \equiv c_k^{(2)} \cdot j_{\text{mass}}^* + \mathbf{j}_k^{(2)} \cdot \mathbf{n} \end{aligned}$$



# Examples

Impermeability condition

Surface reaction



# Momentum balance through an interface

Effects due to

- surface tension ( $S$ )
- surface viscosity
- surface compressibility
- mass transfer

# Surface tension

- The origin and interpretation of surface tension



# Dynamical boundary conditions with surface/interfacial tension

- Fluids in rest
  - normal component:
- Moving fluids without interfacial mass transfer

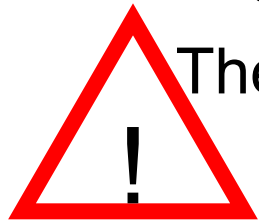


$$[p] = 2 S \kappa$$

Modifies the thermodynamic phase equilibrium conditions

- normal component:  $[p - \mathbf{n} \cdot (\boldsymbol{\tau} \mathbf{n})] = 2 S \kappa$
- tangential components:  $[-\mathbf{t} \cdot (\boldsymbol{\tau} \mathbf{n})] = \mathbf{t} \cdot \nabla S \quad (\mathbf{t} \perp \mathbf{n})$

The viscous stress tensor:  $\tau_{ij} = \mu \cdot (\partial_i u_j + \partial_j u_i)$



Incomplete without class notes



# The heat conduction equation

## Transport equation in the bulk

- Fourier's formula
  - (thermodiffusion not included!)
- Volumetric heat sources:
  - viscous dissipation
  - direct heating
  - heat released in chemical reactions

$$\rho c_p (\partial_t T + \mathbf{u} \cdot \nabla T) = -\nabla \cdot \mathbf{j}_{\text{heat}} + \dot{q}_{\text{heat}}$$

$$\mathbf{j}_{\text{heat}} = -\lambda \cdot \nabla T$$

## Conditions on the interfaces

- Thermal equilibrium
  - Heat flux:
    - continuity (simplest)
    - latent heat (phase transition of pure substance)
- Even more complex cases:
- chemical component diffusion
  - chemical reactions on surface
  - direct heating of surface

$$[T] = 0$$

$$[\mathbf{n} \cdot \mathbf{j}_{\text{heat}}] = 0$$

$$[\mathbf{n} \cdot \mathbf{j}_{\text{heat}}] = L \cdot j_{\text{mass}}^*$$

$$[\mathbf{n} \cdot \mathbf{j}_{\text{heat}}] = \dots$$

Jump conditions



# Summary of boundary conditions on moving interfaces

Physical balance equations imply conditions  
on the interface elements:

- continuity conditions
- jump conditions

These are different

- with and without mass transfer
- in case of special interfacial properties  
(`active interfaces')