Brief course outline

- **Introduction**
  - reactor systems applications
  - two-phase flow regimes
- **Direct numerical simulation (DNS)**
  - Navier-Stokes equations
  - Conservation of mass, momentum, energy
  - incompressible flows
  - Turbulence resolution requirements
- **Interface capturing methods (ICM)**
  - Overview of modeling approaches at various scales
  - One-fluid approach: incompressible N.S. incorporating interface treatment
  - Surface tension
  - Dimensionless groups
- **Numerical considerations:**
  - Overview of ICM methods
  - Time integration (explicit and implicit methods)
  - Spatial discretization
  - Boundary conditions
  - One-fluid approach:
    - Volume of Fluid method
    - Front-tracking method
    - Level-Set method
- **Computational Multiphase Fluid Dynamics (CMFD)**
  - Reynolds-averaged Navier-Stokes equations (RANS)
  - Turbulence modeling:
    - Gradient-diffusion and turbulent viscosity hypothesis
    - Shear stress and turbulent shear stress
    - law of the wall
    - turbulence models
  - two-phase modeling approach
  - interfacial forces
  - interfacial area density evolution
  - subcooled boiling modeling
  - critical heat flux

Interface tracking methods (ITM)

1. **Introduction**
2. **Direct numerical simulation (DNS)**
3. **Interface tracking methods (ITM)**
   - Overview of modeling approaches at various scales
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   - Surface tension
   - Dimensionless groups
4. **Numerical considerations**
5. **Computational Multiphase Fluid Dynamics (CMFD)**

Simulation scales

Level	Single-phase	Multi-phase
Macro scale	System level, e.g. pressure drop estimate	1d drift flux models, area averaged models
Meso scale	RaNS-type CFD models	3D ensemble-averaged models: predicting void fraction distribution in 3D domains
Micro scale	LES, DNS	Interface tracking simulations (with DNS in the carrier phase)

We will concentrate on Micro and Meso scales for both single and two-phase flows

Interface tracking methods (ITM)

- Non-conservative form of N.S.
- General Interface representation
- Interface mass flux
- Interface boundary conditions
- Surface tension treatment
- Dimensionless groups

Non-conservative form of N.S.

Starting with Eq. (9) (Chapter 2), dividing by ρ and using material derivative definition:

$$\frac{\partial \underline{u}}{\partial t} + (\underline{u} \cdot \nabla)\underline{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \underline{u} + \underline{f} \qquad (17)$$

Note on vector notation:

$$[(\underline{u} \cdot \nabla)\underline{u}]_i = \sum_{j=1}^{3} u_j \frac{\partial u_i}{\partial x_j} = u_j u_{i,j} \qquad (18)$$

If the force field, $\underline{f}$, can be expressed through a potential, $\mathcal{U}$: $\underline{f} = -\nabla \mathcal{U}$, one can introduce a <u>reduced</u>, or <u>modified</u> <u>pressure</u>:

$$p^r = p + \rho \mathcal{U} \qquad (19)$$

Non-conservative form of N.S.

Thus, Eq. (17) can be written as:

$$\frac{\partial \underline{u}}{\partial t} + \left(\underline{u} \cdot \nabla\right)\underline{u} = -\frac{1}{\rho}\nabla p^r + \nu \nabla^2 \underline{u} \qquad (20)$$

As an example, for a gravitational force: $\mathcal{U} = -\underline{g} \cdot \underline{x}$

Note that multiphase flows characterized by the presence of interfaces.

During boiling, chemical reactions a mass flux, $\dot{m}$, across the interface S can occur.

Conservation of mass requires that:

$$\dot{m} \equiv \rho_2\left(\underline{u}_2 - \underline{w}\right) \cdot \underline{n} = \rho_1\left(\underline{u}_1 - \underline{w}\right) \cdot \underline{n} \qquad (21)$$

where $\underline{n}$ is the unit normal and $\underline{w} \cdot \underline{n}$ is the normal velocity of the interface.

General interface representation

If the interface is represented by the equation:

$$S(\underline{x}, t) = 0 \tag{22}$$

we can determine both $\underline{n}$ and $\underline{w} \cdot \underline{n}$.

Consider Eq. (22) evaluated at $t + dt$:

$$S(\underline{x} + \underline{w}dt, t + dt) = 0$$

Use Taylor's series expansion:

$$\frac{\partial S}{\partial t} + \underline{w} \cdot \nabla S = 0 \text{ on } S = 0 \tag{23}$$

Note:

$$S(\underline{x} + \underline{w}dt, t + dt) - S(\underline{x}, t) = dS = \frac{dS}{dt}dt = \left(\frac{\partial S}{\partial t} + \cdots\right)dt$$

Interface mass flux

The unit normal is directed from the region with $S < 0$ to the region of $S > 0$:

$$\underline{n} = \frac{\nabla S}{|\nabla S|} \tag{24}$$

so that

$$\underline{w} \cdot \underline{n} = -\frac{1}{|\nabla S|} \cdot \frac{\partial S}{\partial t} \tag{25}$$

If $S = 0$ denotes an impermeable surface (such as solid wall), $\dot{m} = 0$, so that

$$\underline{n} \cdot \underline{u} = \underline{n} \cdot \underline{w}$$

In this case Eq. (23) (using (21)) becomes “kinematic boundary condition”:

$$\frac{\partial S}{\partial t} + \underline{u} \cdot \nabla S = 0 \text{ on } S = 0 \tag{26}$$

Interface boundary conditions

At solid surfaces, for viscous flow, one usually imposes the **no-slip** condition:

$$\underline{n} \times \left(\underline{u} - \underline{w}\right) = 0 \text{ on } S = 0 \tag{27}$$

Note: no-slip condition is not always physical: e.g. contact line motion.

Combining Eqs. (23) and (27):

$$\underline{u} = \underline{w} \text{ on } S = 0 \tag{28}$$

for an impermeable surface.

Question:

Do we care about tangential velocity on the interface ?

Interface boundary conditions

If we assume a purely geometrical interface, then velocity in each fluid individually satisfy Eq. (26). Thus, the proper condition for continuity of the tangential velocity is (compare to Eq. (27)):

$$\underline{n} \times \left(\underline{u}_1 - \underline{u}_2\right) = 0 \tag{29}$$

Question: what is the geometrical meaning of this ?

<u>Note</u>: if we consider inviscid fluids w/ constant surface tension, Eq. (29) is actually a consequence of tangential momentum conservation for $\dot{m} \neq 0$. If $\dot{m} = 0$, Eq. (26) for fluids 1 and 2 and Eq. (29) will result in:

$$\underline{u}_1 = \underline{u}_2 \text{ on } S = 0 \tag{30}$$

Surface tension treatment

Vector form of momentum balance across the interface:

$$(\boldsymbol{\sigma}_2 - \boldsymbol{\sigma}_1) \cdot \boldsymbol{n} - \dot{m}(\boldsymbol{u}_2 - \boldsymbol{u}_1) = -\boldsymbol{\nabla} \cdot [(\boldsymbol{I} - \boldsymbol{n}\boldsymbol{n})\gamma]$$
$$= -(\boldsymbol{I} - \boldsymbol{n}\boldsymbol{n}) \cdot \boldsymbol{\nabla}\gamma + \gamma\kappa\boldsymbol{n} \qquad (31)$$

Decomposition into normal and tangential components:

$$-p_2 + p_1 + \boldsymbol{n} \cdot (\boldsymbol{\tau}_2 - \boldsymbol{\tau}_1) \cdot \boldsymbol{n} - \dot{m}(\boldsymbol{u}_2 - \boldsymbol{u}_1) \cdot \boldsymbol{n} = \gamma\kappa$$
$$\boldsymbol{n} \times (\boldsymbol{\tau}_2 - \boldsymbol{\tau}_1) \times \boldsymbol{n} = -\boldsymbol{n} \times \boldsymbol{\nabla}\gamma \qquad (32)$$

For reduced pressure the normal part can be written as:

$$-p_2^r + p_1^r + \boldsymbol{n} \cdot (\boldsymbol{\tau}_2 - \boldsymbol{\tau}_1) \cdot \boldsymbol{n} - \dot{m}(\boldsymbol{u}_2 - \boldsymbol{u}_1) \cdot \boldsymbol{n}$$
$$= \gamma\kappa + \rho_1\mathcal{U}_1 - \rho_2\mathcal{U}_2 \qquad (33)$$

Dimensionless groups

Number/ definition	Meaning	Comments
$Sl = \frac{U\tau}{L}$	"Strouhal number" - ratio of intrinsic time scale, τ, to the convective time scale, $\frac{L}{U}$	**Vincenc Strouhal** (Čeněk Strouhal) (April 10, 1850 – January 26, 1922) was a Czech physicist specializing in experimental physics.
$Re = \frac{LU}{\nu}$	"Reynolds number" – ratio of inertial to viscous forces, OR ration of viscous diffusion time, $\frac{L^2}{\nu}$ to the convective timescale, $\frac{L}{U}$	**Osborne Reynolds** FRS (23 August 1842 – 21 February 1912) was a prominent Anglo-Irish innovator in the understanding of fluid dynamics.
$Fr = \frac{U^2}{gL}$	"Froude number" – ratio of inertial to gravitational forces	**William Froude** (/ˈfruːd/;[1] 28 November 1810 in Devon[2] – 4 May 1879 in Simonstown, South Africa) was an English engineer, hydrodynamicist and naval architect. He was the first to formulate reliable laws for the resistance that water offers to ships
$We = \frac{\rho L U^2}{\gamma}$	"Weber number" – ratio of inertial and surface-tension induced pressures	Moritz Weber (1871–1951)
$Eo = Bo = \frac{\lvert\rho - \rho'\rvert g L^2}{\gamma}$	Eotvos / Bond number is a version of Weber number for buoyancy driven characteristic velocity	**Baron Loránd Eötvös de Vásárosnamény** (27 July 1848 – 8 April 1919), more commonly called Baron Roland von Eötvös in English literature,[1] was a Hungarian physicist. **Wilfrid Noel Bond** (27 December 1897 – 25 August 1937) was an English physicist and engineer known for his work in fluid mechanics.
$Mo = \frac{g\mu^4}{\rho\gamma^3}$	Morton number	