Lecture 18 - Eulerian Flow Modeling

Applied Computational Fluid Dynamics

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Contents

- Overview of Eulerian-Eulerian multiphase model.
- Spatial averaging.
- Conservation equations and constitutive laws.
- Interphase forces.
- Heat and mass transfer.
- Discretization.
- Solver basics.

Eulerian-Eulerian multiphase - overview

- Used to model droplets or bubbles of secondary phase(s) dispersed in continuous fluid phase (primary phase).
- Allows for mixing and separation of phases.
- Solves momentum, enthalpy, and continuity equations for each phase and tracks volume fractions.
- Uses a single pressure field for all phases.
- Uses interphase drag coefficient.
- Allows for virtual mass effect and lift forces.
- Multiple species and homogeneous reactions in each phase.
- Allows for heat and mass transfer between phases.
- Can solve turbulence equations for each phase.

Methodology

- A general multiphase system consists of interacting phases dispersed randomly in space and time. Interpenetrating continua.
- Methods:
  - Use of continuum theory and thermodynamical principles to formulate the constitutive equations (ASMM).
  - Use of microstructural model in which macroscopic behavior is inferred from particle interaction: Eulerian-Granular.
  - Use of averaging techniques and closure assumptions to model the unknown quantities:
    - Space averaging with no time averaging.
    - Time averaging with no space averaging.
    - Ensemble averaging with no space averaging.
    - space/time or ensemble/space averaging: Eulerian-Eulerian.

Two-fluid model (interpenetrating continua)

- Deductive approach:
  - Assume equations for each pure phase.
  - Average (homogenize) these equations.
  - Model the closure terms.
- Inductive approach:
  - Assume equations for interacting phases.
  - Model the closure terms.

Spatial averaging: basic equations

- Application of the general transport theorem to a property Ψ_k gives the general balance law and its jump condition:

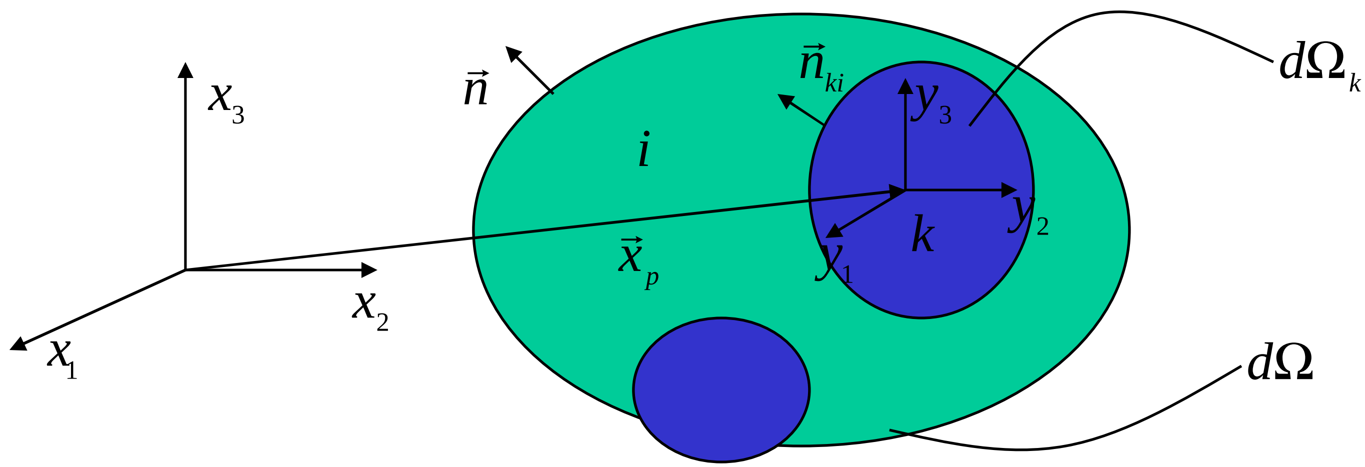
$$\frac{\partial \psi_k}{\partial t} + \nabla \cdot \vec{u}_k \psi_k + \nabla \cdot \vec{J}_k = \dot{\varphi}_k \qquad \sum_{i=1, k \neq i}^{n} (\psi_k (\vec{u}_k - \vec{u}_i) \cdot n_{ki} + n_{ki} \cdot \vec{J}_k) = 0$$

- Continuity equation: $\psi_k = \rho_k, \vec{J}_k = 0, \dot{\varphi}_k = 0$

- Momentum equation: $\psi_k = \rho_k \vec{u}_k, \bar{J}_k = P_k \bar{I} - \bar{\tau}_k, \dot{\varphi}_k = \rho_k \vec{F}_k$

Spatial averaging

- Consider an elementary control volume $d\Omega$ bounded by the surface *dS.*
  - Length scales: $L >> l >> d_k \sim l_t$
  - Volumes: $d\Omega = \sum_{i=1}^{n} d\Omega_i(t)$
  - Averaging volume and coordinate system:



Space averaging: basic equations

- Definitions:
  - Volume average   Intrinsic phasic average.

$$< f >= \frac{1}{d\Omega} \int_{d\Omega_i} f(\vec{x}+\vec{y},t) d^{'}\Omega$$

$$< f >_k = \frac{1}{d\Omega_k} \int_{d\Omega_k} f(\vec{x}+\vec{y},t) d^{'}\Omega$$

  - Volume phase fraction:

$$\alpha_k = \frac{d\Omega_k(\vec{x}_p,t)}{d\Omega} \qquad \sum_{k=1}^{n} \alpha_k = 1 \qquad < f >= \alpha_k < f >_k$$

Space averaging: averaging theorems

- For all k-volumes that are differentiables, (Gray and Lee (1977), Howes and Whitaker (1985)).
  - Temporal derivative: $<\frac{\partial f}{\partial t}> \neq \frac{\partial}{\partial t} < f >$

$$<\frac{\partial f}{\partial t}> = \frac{\partial}{\partial t} < f > - \frac{1}{d\Omega} \int_{dS_{ki}} f \vec{u}_{ki} \cdot \vec{n}_{ki} d^{'} S$$

  - Spatial derivative: $< \nabla f > \neq \nabla < f >$

$$< \nabla f > = \nabla < f > + \frac{1}{d\Omega} \int_{dS_{ki}} f \vec{n}_{ki} d^{'} S$$

  - Next, apply averaging to the conservation equations.

Space averaging: conservation equations

- Continuity equation:

$$\frac{\partial}{\partial t}\alpha_k < \rho_k >_k + \nabla \cdot \alpha_k < \rho_k \vec{u}_k >_k = -\frac{1}{d\Omega}\int_{dS_{ki}} \rho_k (\vec{u}_k - \vec{u}_{ki}) \cdot \vec{n}_k d^{'} S$$

mass transfer term

- Momentum equation:

$$\frac{\partial}{\partial t}\alpha_k < \rho_k \vec{u}_k >_k + \nabla \cdot \alpha_k < \rho_k \vec{u}_k \vec{u}_k >_k = -\nabla \alpha_k < P_k >_k + \nabla \cdot \alpha_k < \bar{\tau}_k >_k + \alpha_k < \rho_k F_k >_k$$

$$+ \frac{1}{d\Omega}\int_{dS_{ki}} \{\rho_k \vec{u}_k (\vec{u}_{ki} - \vec{u}_k) - P_k + \bar{\tau}_k\} \cdot \vec{n}_{ki} d^{'} S$$

interaction term

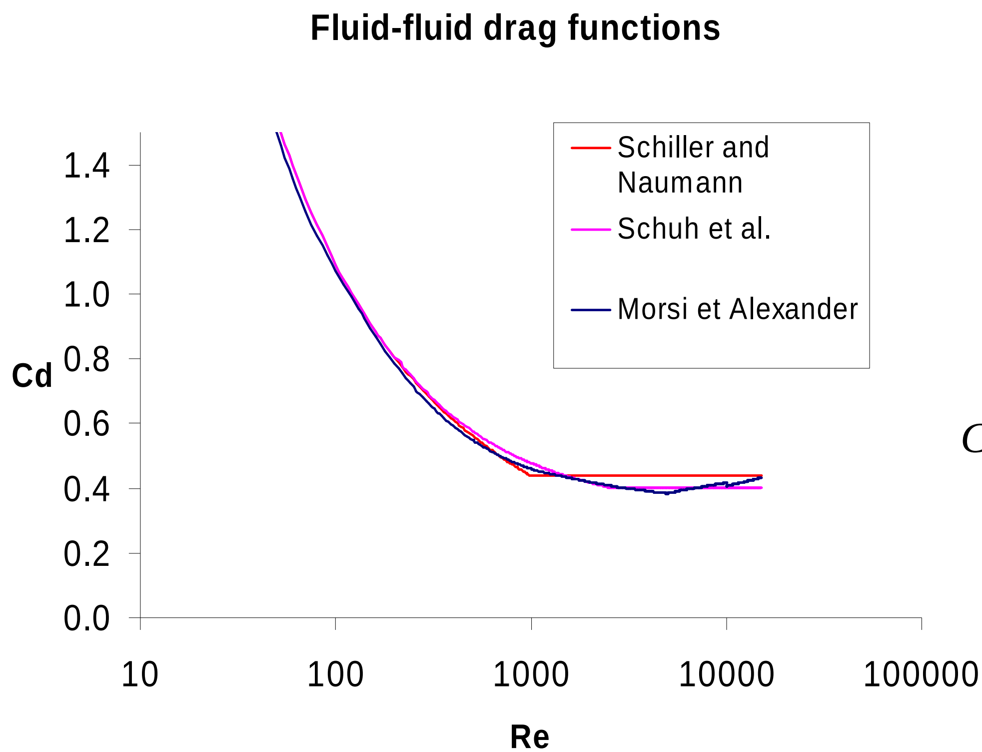
Interphase forces

- Drag is caused by relative motion between phases.

$$\sum_{i=1}^{n} K_{ik}(\vec{u}_i - \vec{u}_k) = 0, \qquad K_{ik} = \alpha_k \rho_k \frac{f_{drag}}{\tau_{ik}} \qquad \tau_{ik} = \frac{\rho_k d^2{}_k}{18\mu_i}$$

- Commonly used drag models (fluid-fluid multiphase).
  - Schuh et al. (1989).
  - Schiller and Naumann (1935).
  - Morsi and Alexander (1972).
  - Schwarz and Turner (1988; for bubble columns).
  - Symmetric law.
- Many researchers devise and implement their own drag models for their specific systems.

Interphase forces: drag force models



Schiller and Naumann

$$C_D = \begin{cases} 24\left(1+0.15\mathrm{Re}^{0.687}\right) & \mathrm{Re} \leq 1000 \\ 0.44 & \mathrm{Re} > 1000 \end{cases}$$

Schuh et al.

$$C_D = \begin{cases} 24\left(1+0.15\mathrm{Re}^{0.687}\right) & 0 < \mathrm{Re} \leq 200 \\ 24\left(0.914\mathrm{Re}^{0.282}+0.0135\mathrm{Re}\right)/\mathrm{Re} & 200 \leq \mathrm{Re} > 2500 \\ 0.4008 & \mathrm{Re} > 2500 \end{cases}$$

Morsi and Alexander

$$C_D = a_1 + \frac{a_2}{\mathrm{Re}} + \frac{a_3}{\mathrm{Re}^2} \quad \text{where} \quad a_1, a_2, a_3 \quad \text{are} \quad f(\mathrm{Re})$$

Interphase forces: virtual mass and lift

- Virtual mass effect: caused by relative acceleration between phases Drew and Lahey (1990).

$$K_{vm,fs} = C_{vm}\alpha_s\rho_f\left((\frac{\partial \vec{u}_f}{\partial t} + \vec{u}_f \cdot \nabla \vec{u}_f) - (\frac{\partial \vec{u}_s}{\partial t} + \vec{u}_s \cdot \nabla \vec{u}_s) \right)$$

  - Virtual mass effect is significant when the second phase density is much smaller than the primary phase density (i.e., bubble column).
- Lift force: caused by the shearing effect of the fluid onto the particle Drew and Lahey (1990).

$$K_{k,fs} = C_L\alpha_s\rho_f(\vec{u}_f - \vec{u}_s)\times(\nabla\times\vec{u}_f)$$

  - Lift force usually insignificant compared to drag force except when the phases separate quickly and near boundaries.

Modeling heat transfer

- Conservation equation of phase enthalpy.

Energy sources e.g., radiation

$$\frac{\partial}{\partial t}(\alpha_k \rho_k h_k) + \nabla \cdot (\alpha_k \rho_k \vec{u}_k h_k) = \alpha_k \left(\frac{\partial P_k}{\partial t} + \vec{u}_k \cdot \nabla P_k\right) + \bar{S}_k : \nabla \vec{u}_k + R_k$$

Originates from work term for volume fraction changes

$$-\nabla \vec{q}_k + \sum_{k=1}^{n} \gamma_{ki} (T_i - T_k) + \dot{m}_{ki} (h_k - h_{ik})$$

Viscous dissipation term

Modeling heat transfer

- Conservation equation of phase enthalpy.

$$\frac{\partial}{\partial t}(\alpha_k \rho_k h_k) + \nabla \cdot (\alpha_k \rho_k \vec{u}_k h_k) = \alpha_k \left(\frac{\partial P_k}{\partial t} + \vec{u}_k \cdot \nabla P_k\right) + \overline{S}_k : \nabla \vec{u}_k + R_k$$

Heat conduction

$$- \nabla \vec{q}_k + \sum_{k=1}^{n} \gamma_{ki} (T_i - T_k) + \dot{m}_{ki} (h_k - h_{ik})$$

Interphase heat transfer term

Energy transfer with mass transfer

Heat conduction

- Assume Fourier's law:

$$\vec{q} = -\alpha_k \kappa_k \nabla T_k$$

For granular flows κ_k is obtained from packed bed conductivity expression, Kuipers, Prins and Swaaij (1992).

- Near wall heat transfer is calculated as in single phase.
- All standard boundary conditions for temperature can be implemented for multiphase.

Interphase heat transfer

- The interphase heat transfer coefficient is given by.

$$\gamma_{ik} = \frac{6\kappa_k \alpha_i Nu_i}{d_i^{\,2}}$$

- Granular Model (Gunn, 1978).

$$Nu_s = (7 - 10\alpha_f + 5\alpha_f^2)(1 + 0.7\,\mathrm{Re}^{0.2}\,\mathrm{Pr}^{1/3}) + (1.33 - 2.4\alpha_f + 1.2\alpha_f^2)\,\mathrm{Re}^{0.7}\,\mathrm{Pr}^{1/3}$$

- Fluid-fluid model.

$$Nu_i = 2 + 0.6\,\mathrm{Re}^{0.5}\,\mathrm{Pr}^{0.3}$$

$$\mathrm{Re} = \frac{\alpha_k \rho_k \left|u_i - u_k\right| d_i}{\mu_k} \qquad \mathrm{Pr} = \frac{C_{p,k}\mu_k}{\kappa_k}$$

Conservation of species

- Conservation equation for the mass fraction m_k^i of the species i in the phase k:

$$\frac{\partial}{\partial t}(\alpha_k \rho_k m_k^i) + \nabla \cdot (\alpha_k \rho_k \vec{u}_k m_k^i) = \nabla \cdot (\alpha_k \rho_k D_k^i \nabla m_k^i) + \dot{m}_k^i$$

- Here D_k^i is the diffusivity of the species in the mixture of the respective phase, $\dot{m}_k^i$ is the rate of production/destruction of the species.
- Thermodynamic relations an state equations for the phase k are needed.
- When calculating mass transfer the shadow technique from Spalding is used to update diameter of the dispersed phase.

Modeling mass transfer

- Evaporation and condensation:
  - For liquid temperatures ≥ saturation temperature, evaporation rate:

$$\dot{m}_v = \frac{r_v \alpha_l \rho_l \left(T_l - T_{sat}\right)}{T_{sat}}$$

  - For vapor temperatures ≤ saturation temperature, condensation rate:

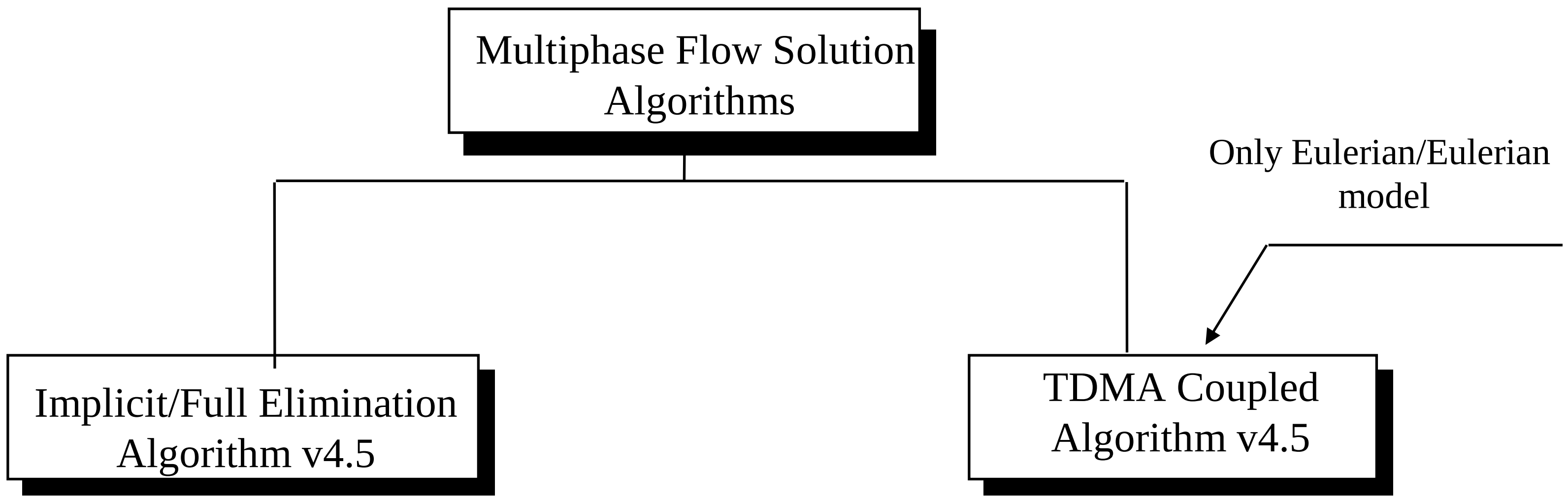
$$\dot{m}_l = \frac{r_l \alpha_v \rho_v \left(T_{sat} - T_v\right)}{T_{sat}}$$

  - User specifies saturation temperature and, if desired, “time relaxation parameters” r_l and r_v (Wen Ho Lee (1979)).

- Unidirectional mass transfer, r is constant: $\dot{m}_{12} = r \alpha_2 \rho_1$

Solution algorithms for multiphase flows

- Coupled solver algorithms (more coupling between phases).
  - Faster turn around and more stable numerics.
- High order discretization schemes for all phases.
  - More accurate results.



Full elimination algorithm

- Momentum equation for primary and secondary phase:

$$(a_p + k)u_p - k\,u_s = \sum a_{nb,p}\,u_{nb,p} + b_p$$

$$-k\,u_p + (a_s + k)u_s = \sum a_{nb,s}\,u_{nb,s} + b_s$$

- Elimination of secondary phase gives primary phase:

$$\left(a_p + \frac{k}{a_s + k}a_s\right)u_p = \sum a_{nb,p}\,u_{nb,p} + b_p + \frac{k}{a_s + k}\left(\sum a_{nb,s}\,u_{nb,s} + b_s\right)$$

$$a_{p,eff}\,u_p = \sum a_{nb,p}\,u_{nb,p} + b_p + b_{p,s}$$

- Secondary phase has similar form.
- Applicable to N phases.

Coupled TDMA-algorithm

- Discretized equations of primary and secondary phase are in matrix form:

$$\begin{pmatrix} a_p + k & -k \\ -k & a_s + k \end{pmatrix} \begin{pmatrix} u_p \\ u_s \end{pmatrix} = \begin{pmatrix} \sum a_{nb,p} & 0 \\ 0 & \sum a_{nb,s} \end{pmatrix} \begin{pmatrix} u_{nb,p} \\ u_{nb,s} \end{pmatrix} + \begin{pmatrix} b_p \\ b_s \end{pmatrix}$$

$$\overline{\overline{\mathbf{A}}}\vec{U} = \overline{\overline{\mathbf{A}}}_{nb}\vec{U}_{nb} + \vec{B}$$

- Results in a tri-diagonal matrix consisting of submatrices

$$\left(\begin{array}{ccc:c} A_{11} & A_{12} & 0 & 0 \\ A_{21} & A_{22} & A_{23} & 0 \\ 0 & A_{32} & A_{33} & 0 \\ \hdashline 0 & 0 & 0 & A_{nn} \end{array}\right) \begin{pmatrix} \vec{U}_1 \\ \vec{U}_2 \\ \vec{U}_3 \\ \vec{U}_n \end{pmatrix} = \begin{pmatrix} \vec{C}_1 \\ \vec{C}_2 \\ \vec{C}_3 \\ \vec{C}_n \end{pmatrix}$$

- Closer coupling in each iteration gives faster convergence

Solution algorithm for multiphase

- Typical algorithm:
  - Get initial and boundary conditions.
  - Perform time-step iteration.
  - Calculate primary and secondary phase velocities.
  - Calculate pressure correction and correct phase velocities, pressure and phase fluxes. Pressure is shared by all phases.
  - Calculate volume fraction.
  - Calculate other scalars. If not converged go to step three.
  - Advance time step and go to step two.

Solution guidelines

- All multiphase calculations:
  - Start with a single-phase calculation to establish broad flow patterns.
- Eulerian multiphase calculations:
  - Copy primary phase velocities to secondary phases.
  - Patch secondary volume fraction(s) as an initial condition.
  - Set normalizing density equal to physical density.
  - Compute a transient solution.
  - Use multigrid for pressure.

Summary

- Eulerian-Eulerian is the most general multiphase flow model.
- Separate flow field for each phase.
- Applicable to all particle relaxation time scales.
- Includes heat/mass exchange between phases.
- Available in both structured and unstructured formulations.