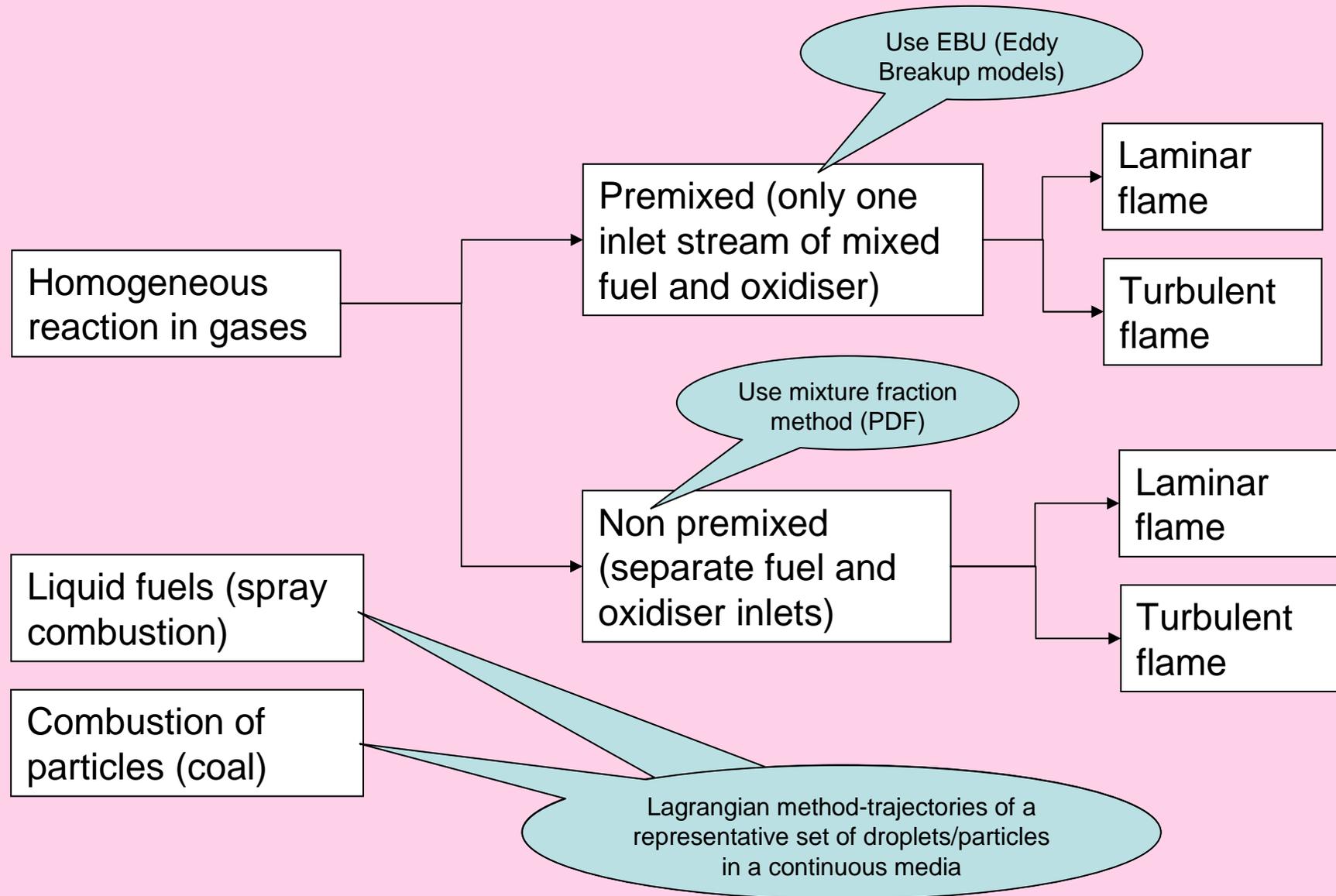


Combustion, multiphase flows

Remark: foils with „black background“
could be skipped, they are aimed to the
more advanced courses

COMBUSTION



COMBUSTION aims

Primary purpose of CFD analysis is to evaluate

- Temperature field (therefore thermal power, heat fluxes through wall...)
- Composition of flue gas (environmental requirements, efficiency of burning)

To do this it is necessary to calculate

- Velocities and turbulent characteristics (mixing intensity) – NS equations
- Transport of individual components (mass balances of species)
- Chemical reactions (reaction rates)
- Energy balances (with special emphasis to radiation energy transfer)

COMBUSTION balances

m_i mass fraction of specie i in mixture [kg of i]/[kg of mixture]

ρm_i mass concentration of specie [kg of i]/[m³]

Mass balance of species (for each specie one transport equation)

$$\frac{\partial}{\partial t}(\rho m_i) + \nabla \cdot (\rho m_i \vec{u}) = \nabla \cdot (\Gamma_i \nabla m_i) + S_i$$

Production of species is controlled by

Because only micromixed reactants can react

Rate of production of specie i [kg/m³s]

➤ Diffusion of reactants (micromixing) – $t_{\text{diffusion}}$ (diffusion time constant)

➤ Chemistry (rate equation for perfectly mixed reactants) – t_{reaction} (reaction constant)

Damkohler number $Da = \frac{t_{\text{diffusion}}}{t_{\text{reaction}}}$

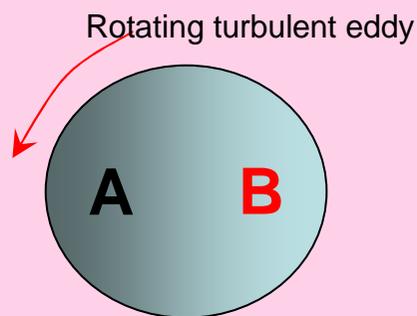
$Da \ll 1$ $S_i = \rho A \exp\left(-\frac{E}{RT}\right) m_i^a$ Reaction controlled by kinetics (Arrhenius)

$Da \gg 1$ $S_i = \rho C m_i \frac{\varepsilon}{k}$ Turbulent diffusion controlled combustion

COMBUSTION problems

Specific problems related to combustion (two examples A and B)

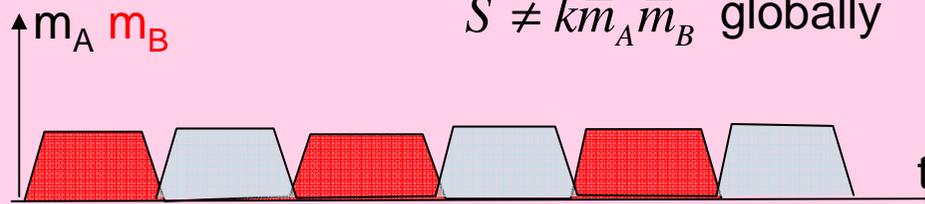
A) It is not correct to use **mean concentrations** in reaction rate equation



Bimolecular reaction $A+B \rightarrow C$

Production rate $S = km_A m_B$ locally

$\bar{S} \neq k\bar{m}_A \bar{m}_B$ globally



$\bar{m}_A > 0, \bar{m}_B > 0$ but $\overline{m_A m_B} = 0$

Actual reaction rate is zero even if the mean concentrations are positive

COMBUSTION problems

Specific problems related to combustion (example B)

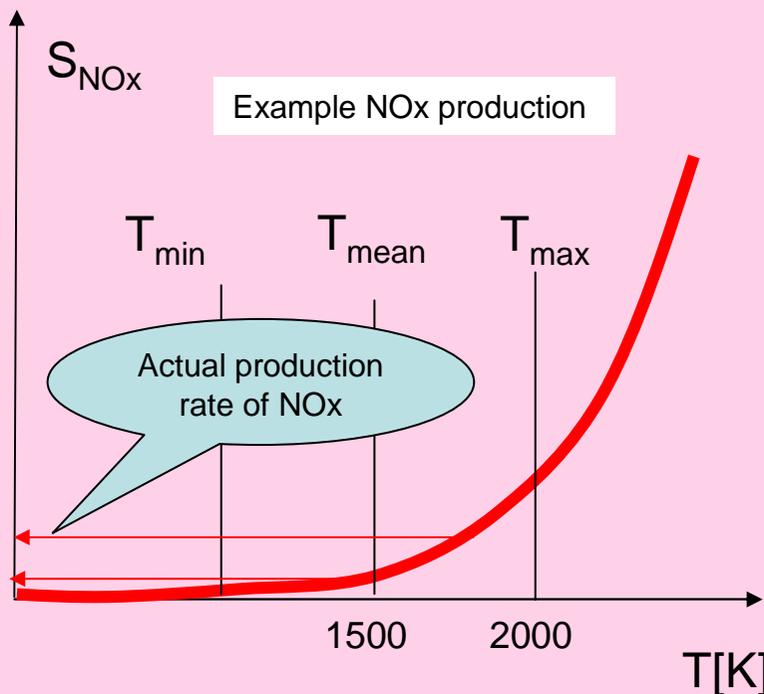
B) It is not correct to use **mean temperatures** in reaction rate equation

Bimolecular reaction $A+B \rightarrow C$

Production rate $S = Am_A m_B \exp\left(-\frac{E}{RT}\right)$ locally

$\bar{S} > \overline{Am_A m_B \exp\left(-\frac{E}{RT}\right)}$ globally

Underestimated reaction rate follows from nonlinear temperature dependence of reaction constant



$$\overline{\exp\left(-\frac{E}{RT}\right)} \gg \exp\left(-\frac{E}{\bar{T}}\right)$$

COMBUSTION enthalpy

Enthalpy balance is written for mixture of all species (result-temperature field)

$$\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho h \vec{u}) = \nabla \cdot (\Gamma \nabla h) + S_h$$

Sum of all reaction enthalpies of all reactions

$$S_h = \sum_i S_i \Delta h_{ri}$$

It holds only for reaction without
phase changes $h \sim c_p T$

Energy transport must be solved together with the fluid flow equations (usually using turbulent models, $k-\varepsilon$, RSM,...). Special attention must be paid to radiative energy transport (not discussed here, see e.g. [P1-model](#), [DTRM](#)-discrete transfer radiation,...). For modeling of chemistry and transport of species there exist many different methods and only one - mixture fraction method will be discussed in more details.

MIXTURE Fraction method

Non-premixed combustion, and assumed fast chemical reactions (paraphrased as “**What is mixed is burned** (or is at equilibrium)”)



Calculation of fuel and oxidiser consumption is the most difficult part. Mixture fraction method is the way, how to avoid it

Mass balance of fuel

Mass fraction of fuel
(e.g.methane)

$$\frac{\partial}{\partial t}(\rho m_{fuel}) + \nabla \cdot (\rho m_{fuel} \vec{u}) = \nabla \cdot (\Gamma \nabla m_{fuel}) + S_{fuel}$$

Mass balance of oxidant

$\left[\frac{\text{kg of produced fuel}}{\text{s} \cdot \text{m}^3} \right]$

$$\frac{\partial}{\partial t}(\rho m_{ox}) + \nabla \cdot (\rho m_{ox} \vec{u}) = \nabla \cdot (\Gamma \nabla m_{ox}) + S_{ox}$$

Mass fraction of
oxidiser (e.g.air)

MIXTURE Fraction method

Stoichiometry

1 kg of fuel + **s** kg of oxidiser → (1+s) kg of product

Introducing new variable

$$\Phi = sm_{fuel} - m_{ox}$$

and subtracting previous equations

$$\frac{\partial}{\partial t}(\rho sm_{fuel}) + \nabla \cdot (\rho sm_{fuel} \vec{u}) = \nabla \cdot (\Gamma \nabla sm_{fuel}) + sS_{fuel}$$

$$\frac{\partial}{\partial t}(\rho m_{ox}) + \nabla \cdot (\rho m_{ox} \vec{u}) = \nabla \cdot (\Gamma \nabla m_{ox}) + S_{ox}$$

$$\frac{\partial}{\partial t}(\rho \Phi) + \nabla \cdot (\rho \Phi \vec{u}) = \nabla \cdot (\Gamma \nabla \Phi) + sS_{fuel} - S_{ox}$$

This term is ZERO
due to stoichiometry

MIXTURE Fraction method

Mixture fraction f is defined as linear function of Φ normalized in such a way that $f=0$ at oxidising stream and $f=1$ in the fuel stream

$$f = \frac{\Phi - \Phi_0}{\Phi_1 - \Phi_0} = \frac{s m_{fuel} - m_{ox} + m_{ox,0}}{s m_{fuel,1} + m_{ox,0}}$$

m_{ox} is the mass fraction of oxidiser at an arbitrary point x,y,z , while $m_{ox,0}$ at inlet (at the stream 0)

Resulting transport equation for the mixture fraction f is without any source term

$$\frac{\partial}{\partial t} (\rho f) + \nabla \cdot (\rho f \vec{u}) = \nabla \cdot (\Gamma \nabla f)$$

Mixture fraction is property that is CONSERVED, only dispersed and transported by convection. f can be interpreted as a concentration of a key element (for example carbon). And because it was assumed that „what is mixed is burned“ the information about the carbon concentration at a place x,y,z bears information about all other participating species.

MIXTURE Fraction method

Knowing f we can calculate mass fraction of fuel and oxidiser at any place x,y,z

$$f_{stoichio} = \frac{m_{ox,0}}{sm_{fuel,1} + m_{ox,0}}$$

At the point x,y,z where $f=f_{stoichio}$
are all reactants consumed
(therefore $m_{ox}=m_{fuel}=0$)

For example the mass fraction of fuel is calculated as

$$f_{stoichio} < f \leq 1 \quad (\text{fuel rich region, oxidiser is consumed } m_{ox}=0) \quad m_{fuel} = \frac{f - f_{stoichio}}{1 - f_{stoichio}} m_{fuel,1}$$

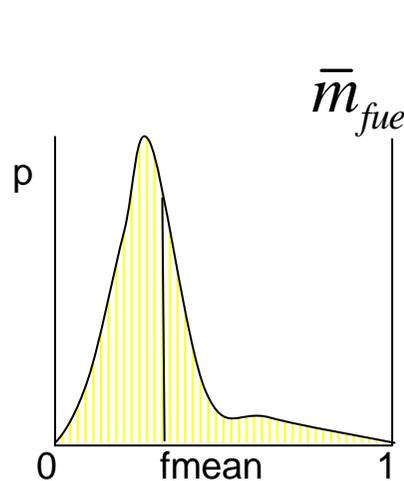
$$0 < f < f_{stoichio} \quad (\text{fuel lean region}) \quad m_{fuel} = 0$$

The concept can be generalized assuming that chemical reactions are at equilibrium

$f \rightarrow m_i$ mass fraction of species is calculated from equilibrium constants
(evaluated from Gibbs energies)

MIXTURE Fraction method

Equilibrium depends upon concentration of the key component (upon f) and temperature. Mixture fraction f undergoes turbulent fluctuations and these fluctuations are characterized by probability density function $p(f)$. Mean value of mass fraction, for example the mass fraction of fuel is to be calculated from this distribution



$$\bar{m}_{fuel} = \int_0^1 m_{fuel}(f) p(f) df$$

Mass fraction corresponding to an arbitrary value of mixture fraction is calculated from equilibrium constant

Probability density function, defined in terms of **mean and variance of f**

Frequently used β distribution

$$p(f) = \frac{f^{p-1} (1-f)^{q-1}}{\int_0^1 f^{p-1} (1-f)^{q-1} df}$$

Variance of f is calculated from another transport equation

$$\frac{\partial}{\partial t} (\overline{\rho f'^2}) + \nabla \cdot (\overline{\rho f'^2 \vec{u}}) = \nabla \cdot (\Gamma_f \nabla \overline{f'^2}) + C_g \mu_t (\nabla \bar{f})^2 - C_d \frac{\epsilon}{k} \overline{\rho f'^2}$$

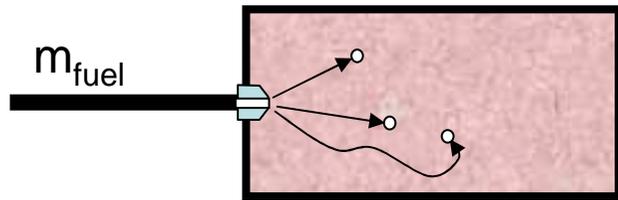
MIXTURE Fraction method

Final remark: In the case, that m_{fuel} is a linear function of f , the mean value of mass fraction m_{fuel} can be evaluated directly from the mean value of f (and it is not necessary to identify probability density function $p(f)$, that is to solve the transport equation for variation of f). Unfortunately the relationship $m_{\text{fuel}}(f)$ is usually highly nonlinear.

$$\bar{m}_{\text{fuel}} = \int_0^1 m_{\text{fuel}}(f) p(f) df \neq m_{\text{fuel}}(\bar{f})$$

COMBUSTION of liquid fuel

Lagrangian method: trajectories, heating and evaporation of droplets injected from a nozzle are calculated.



Drag force

$$m \frac{d\vec{u}}{dt} = \vec{F}$$

Sum of all forces acting to liquid droplet moving in continuous fluid (fluid velocity \vec{v} is calculated by solution of NS equations)

Relative velocity (fluid-particle)

$$\vec{F}_D = \frac{1}{2} \rho c_D A |\vec{u} - \vec{v}| (\vec{u} - \vec{v})$$

Drag coefficient c_D
depends upon Reynolds number

Effect of cloud (α_c volume fraction of dispersed phase-gas)

$$c_D = c_{D0} / \alpha_c^{3.7}$$

$$c_D = \frac{24}{Re} \left(1 + \frac{3}{16} Re\right)$$

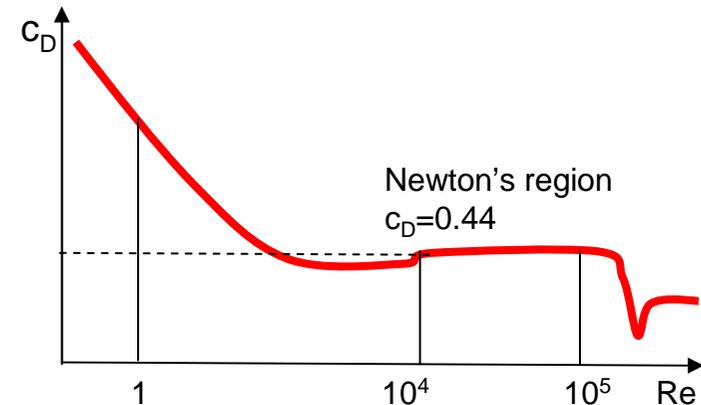
$Re < 5$ Oseen

$$c_D = \frac{24}{Re} (1 + 0.15 Re^{0.687})$$

$Re < 800$ Schiller Nauman

$$c_D = 0.4$$

$1000 < Re < 3 \cdot 10^5$ Newton



COMBUSTION of liquid fuel

Evaporation of fuel droplet

Diffusion from droplet surface to gas:

$$\frac{dm}{dt} = \frac{d}{dt} \left(\frac{\pi D^2}{6} \rho_p \right) = \pi D^2 Sh \rho_g D_{dif} (m_{fg} - m_s)$$

Sherwood number

Mass fraction of fuel at surface

Ranz Marshall correlation for mass transport

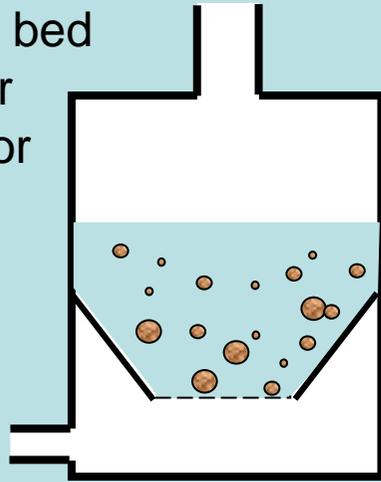
$$Sh = 2 + 0.6 Re^{0.5} Sc^{0.33}$$

Schmidt number = ν/D_{dif}

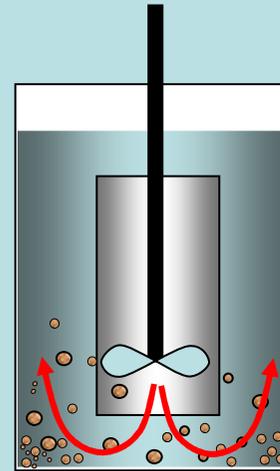
CFD8

MULTIPHASE flows examples

Fluidised bed reactor or combustor



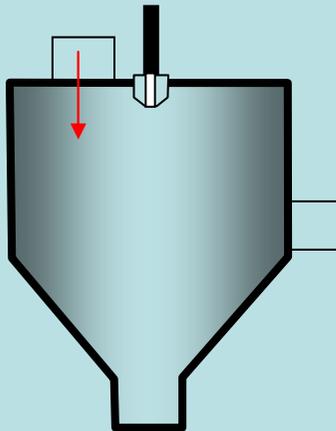
Mixer (draft tube)



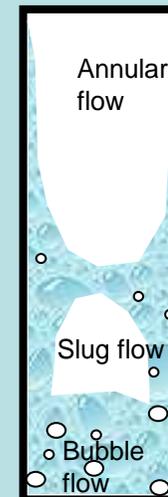
...and others

Hydrotransport, cyclones, free surfaces, breakup of liquid jets, expanding foams, aerated reactors, cavitation, mold filling...

Spray dryer



Flow boiling



Phases

Gas-liquid

Gas-solid

Liquid-liquid

MULTIPHASE flows methods

Methods

- **Lagrange** (see liquid fuel burners, suitable for low concentration of particles)
- **Mixture** (not significant difference between phases, e.g. sedimentation)
- **Euler** (the most frequently used technique for any combination of phases)
- **VOF (Volume Of Fluid)** (evolution of continuous interface, e.g. shape of free surface modeling, moving front of melted solid...)

MULTIPHASE EULER

For each phase q are separately solved

➤ **Continuity equation** (mass balance of phase)

$$\frac{\partial}{\partial t}(\alpha_q \rho_q) + \nabla \cdot (\alpha_q \rho_q \vec{v}_q) = \sum_p \dot{m}_{pq}$$

Volumetric
fraction of phase q

Velocity of
phase q

Mass transfer from
phase p to phase q

➤ **Momentum balance** (each phase is moving with its own velocity,
only pressure is common for all phases)

$$\frac{\partial}{\partial t}(\alpha_q \rho_q \vec{v}_q) + \nabla \cdot (\alpha_q \rho_q \vec{v}_q \vec{v}_q) = -\alpha_q \nabla p + \nabla \cdot (\alpha_q \vec{\tau}_q) + \sum_p \vec{R}_{pq}$$

Stresses are calculated in the
same way like in one phase flows

Interphase
forces

MULTIPHASE EULER

Specific semiempirical correlations describe interaction terms

Mass transfer

for example Ranz Marschall correlation for $Sh=2+\dots$

Momentum exchange

$$\vec{R}_{pq} = k_{pq} (\vec{v}_q - \vec{v}_p)$$

Special models for k_{pq} are available for liquid-liquid, liquid-solid, and also for solid-solid combinations

MULTIPHASE MIXTURE method

Mixture model solves in principle one-phase flow with mean density ρ_m , mean velocity \vec{v}_m

Continuity equation for mixture

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \vec{v}_m) = 0$$

Momentum balance for mixture (with corrections to drift velocities)

$$\frac{\partial}{\partial t} (\rho_m \vec{v}_m) + \nabla \cdot (\rho_m \vec{v}_m \vec{v}_m) = -\nabla p + \nabla \cdot (\mu_m (\nabla \vec{v}_m + (\nabla \vec{v}_m)^T)) + \nabla \cdot \left(\sum_p \alpha_p \rho_p \vec{v}_{dr,p} \vec{v}_{dr,p} \right)$$

Drift velocities are evaluated from algebraic models
(mixture acceleration determines for example centrifugal
forces applied to phases with different density)

$$\vec{v}_{dr,p} = \vec{v}_p - \vec{v}_m$$

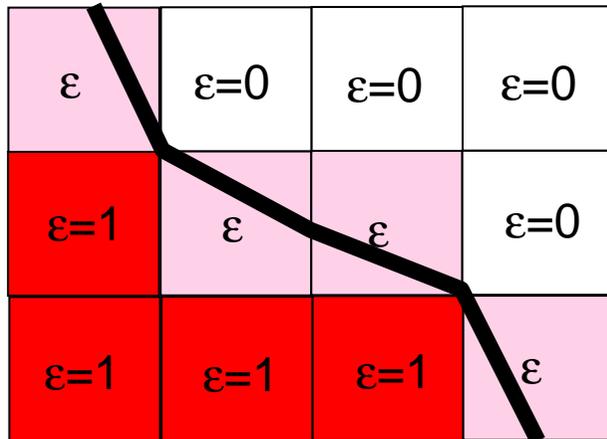
Volumetric fraction of secondary phase (p)

$$\frac{\partial}{\partial t} (\alpha_p \rho_p) + \nabla \cdot (\alpha_p \rho_p \vec{v}_m) = -\nabla \cdot (\alpha_p \rho_p \vec{v}_{dr,p})$$

MULTIPHASE VOF

Evolution of clearly discernible interface between immiscible fluids (examples: jet breakup, motion of large bubbles, free surface flow)

There exist many different methods in this category, [Level set method](#), Marker and cell, Lagrangian method tracking motion of particles at interface.



Fluent

- Donor acceptor
- Geometric reconstruction

$$\frac{\partial \varepsilon}{\partial t} + \vec{u} \cdot \nabla \varepsilon = 0$$

Dissadvantage: initially sharp interface is blurred due to numerical diffusion