Combustion, multiphase flows

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

**Homogeneous reaction in gases**
- Premixed (only one inlet stream of mixed fuel and oxidiser)
  - Laminar flame
  - Turbulent flame
- Non premixed (separate fuel and oxidiser inlets)
  - Use mixture fraction method (PDF)
  - Laminar flame
  - Turbulent flame

**Liquid fuels (spray combustion)**
- Lagrangian method-trajectories of a representative set of droplets/particles in a continuous media

**Combustion of particles (coal)**
- Use EBU (Eddy Breakup models)
  - Laminar flame
  - Turbulent flame
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 \([\text{kg of } i]/[\text{kg of mixture}]\)
- $\rho m_i$ mass concentration of specie \([\text{kg of } i]/[\text{m}^3]\)

**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

- Diffusion of reactants (micromixing) – $t_{\text{diffusion}}$ (diffusion time constant)
- Chemistry (rate equation for perfectly mixed reactants) – $t_{\text{reaction}}$ (reaction constant)

**Damkohler number**

\[Da = \frac{t_{\text{diffusion}}}{t_{\text{reaction}}}\]

Da<<1 \hspace{1cm} \[S_i = \rho A \exp(-\frac{E}{RT}) m_i^a\] Reaction controlled by kinetics (Arrhenius)

Da>>1 \hspace{1cm} \[S_i = \rho C m_i \frac{\varepsilon}{k}\] Turbulent diffusion controlled combustion
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 \( \bar{m}_A \bar{m}_B = 0 \)

Actual reaction rate is zero even if the mean concentrations are positive
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 $S = A m_A m_B \exp(-\frac{E}{RT})$ locally

$\bar{S} > \overline{A m_A m_B \exp(-\frac{E}{RT})}$ globally

Underestimated reaction rate follows from nonlinear temperature dependence of reaction constant

$\exp(-\frac{E}{RT}) \gg \exp(-\frac{E}{RT})$
Enthalpy balance is written for mixture of all species (result-temperature field)

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

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)”)

\[
\frac{\partial}{\partial t} (\rho m_{\text{fuel}}) + \nabla \cdot (\rho m_{\text{fuel}} \bar{u}) = \nabla \cdot (\Gamma \nabla m_{\text{fuel}}) + S_{\text{fuel}}
\]

Mass balance of fuel

Mass fraction of fuel (e.g. methane)

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

\[
\frac{\partial}{\partial t} (\rho m_{\text{ox}}) + \nabla \cdot (\rho m_{\text{ox}} \bar{u}) = \nabla \cdot (\Gamma \nabla m_{\text{ox}}) + S_{\text{ox}}
\]

Mass balance of oxidant

Mass fraction of oxidiser (e.g. air)
MIXTURE Fraction method

Stoichiometry

1 kg of fuel + $s$ kg of oxidiser $\rightarrow$ $(1+s)$ kg of product

Introducing new variable

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

and subtracting previous equations

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

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

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

This term is ZERO due to stoichiometry
Mixture fraction $f$ is defined as linear function of $\Phi$ normalized in such a way that $f=0$ at oxidising stream and $f=1$ in the fuel stream.

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

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

\[
f_{\text{stoichio}} = \frac{m_{\text{oxygen},0}}{s m_{\text{fuel},1} + m_{\text{oxygen},0}}
\]

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

For example the mass fraction of fuel is calculated as

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

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

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

\[
f \rightarrow m_i \quad \text{mass fraction of species is calculated from equilibrium constants (evaluated from Gibbs energies)}
\]
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.

\[
\bar{m}_{\text{fuel}} = \int_{0}^{1} m_{\text{fuel}}(f) p(f) df
\]

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 \( f \):

\[
p(f) = \frac{f^{p-1}(1-f)^{q-1}}{\int_{0}^{1} f^{p-1}(1-f)^{q-1} df}
\]

Frequently used \( \beta \) distribution

Variance of \( f \) is calculated from another transport equation

\[
\frac{\partial}{\partial t} \left( \rho \bar{f}^{\prime 2} \right) + \nabla \cdot (\rho \bar{f}^{\prime 2} \bar{u}) = \nabla \cdot (\Gamma_f \nabla \bar{f}^{\prime 2}) + C_g \mu_t (\nabla \bar{f})^2 - C_d \frac{\varepsilon}{k} \rho \bar{f}^{\prime 2}
\]
Final remark: In the case, that $m_{\text{fuel}}$ is a linear function of $f$, the mean value of mass fraction $m_{\text{fuel}}$ 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.

$$
\bar{m}_{\text{fuel}} = \frac{1}{0} \int m_{\text{fuel}}(f) p(f) df \neq m_{\text{fuel}}(\bar{f})
$$
COMBUSTION of liquid fuel

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

\[
m \frac{d\vec{u}}{dt} = \vec{F}
\]

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

Drag coefficient \( c_D \)
depends upon Reynolds number

\[
c_D = \frac{24}{Re} (1 + \frac{3}{16} \text{Re}) \quad \text{Re} < 5 \quad \text{Oseen}
\]

\[
c_D = \frac{24}{Re} (1 + 0.15 \text{Re}^{0.687}) \quad \text{Re} < 800 \quad \text{Schiller Nauman}
\]

\[
c_D = 0.4 \quad 1000 \leq \text{Re} < 3 \times 10^5 \quad \text{Newton}
\]

Effect of cloud (\( \alpha_c \) volume fraction of dispersed phase-gas)

\[
c_D = c_{D0} / \alpha_c^{3.7}
\]

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)

Drag force
Evaporation of fuel droplet

Diffusion from droplet surface to gas:

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

Ranz Marshall correlation for mass transport

\[
Sh = 2 + 0.6 \text{Re}^{0.05} \text{Sc}^{0.33}
\]

Sherwood number

Mass fraction of fuel at surface

Schmidt number = \( \nu/D_{dif} \)
MULTIPHASE flows examples

- Fluidised bed reactor or combustor
- Mixer (draft tube)
- Spray dryer
- Flow boiling

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

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…)
For each phase $q$ are separately solved

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

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

- $\alpha_q$ : Volumetric fraction of phase $q$
- $\rho_q$ : Density of phase $q$
- $\vec{v}_q$ : Velocity of phase $q$
- $m_{pq}$ : 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)

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

- $\vec{\tau}_q$ : Stresses of phase $q$
- $\vec{R}_{pq}$ : Interphase forces

Stresses are calculated in the same way like in one phase flows
Specific semiemprical correlations describe interaction terms

**Mass transfer**
for example Ranz Marschall correlation for Sh=2+…

**Momentum exchange**

\[ \vec{R}_{pq} = k_{pq} \left( \vec{v}_q - \vec{v}_p \right) \]

Special models for \( k_{pq} \) are available for liquid-liquid, liquid-solid, and also for solid-solid combinations
Mixture model solves in principle one-phase flow with mean density $\rho_m$, mean velocity $v_m$

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)

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

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 ($p$)

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

\[
\frac{\partial \epsilon}{\partial t} + \bar{u} \cdot \nabla \epsilon = 0
\]

Dissadvantage: initially sharp interface is blurred due to numerical diffusion