Combustion Modelling

Assumptions, Models and Consequences

Content

Averaging/Filtering in CFD

In RANS Reynolds averaging is used: time averaging at a given position x

$$\overline{f(x)} = \frac{1}{\tau}\int_{0}^{\tau} f(x)dt;$$

Variable densities: Reynolds averaging yields

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0; \quad \rho = \bar{\rho} + \rho';\ u_i = \bar{u}_i + u_i'$$

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i}\left(\bar{\rho} u_{\bar{i}} + \overline{\rho' u_i'}\right) = 0;$$

and this formulation unfortunately doesn’t conserve mass

For combustion simulations where variations of density are essential, Favre averaging is applied

$$\tilde{f} = \frac{1}{\bar{\rho}} \lim_{T\to\infty} \frac{1}{T}\int_{t}^{t+T} \rho(\tau) f(\tau) d\tau \qquad \tilde{f} = \frac{\overline{\rho f}}{\bar{\rho}}$$

and Favre averaging leads to

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i}\left(\bar{\rho}\tilde{u}_i\right) = 0;$$

Favre averaging conserves continuity at least for the averaged quantities.

Averaging/Filtering in CFD

Looking in more detail at this relation
we see that we still
have the unresolved term

$$\tilde{f}\bar{\rho} = \bar{\rho}\bar{f} + \overline{\rho' f'}$$

$$\overline{\rho' f'}$$

So what does this average mean ?

We need to know the answer, if we want to compare CFD results with experiments and here the question arises which average value do the experimenters measure ?

Let’s look at temperature measurements:

a) Thermocouple

Probe with a diameter ***d*** which sits in a turbulent flow represents a volumetric average (stream tube with diameter ***d + Δd*** to account for turbulence), length o the volume depends on measuring time.

What average is it ?

b) CARS (Coherent Anti-Stokes Raman Scattering)

Signal is generated within a small volume (L ~1 mm, D ~ 0.3 mm) generated by laser beams within a few nanoseconds (frozen flow) and typically represents a vibrational molecule temperature.

What average is this ?

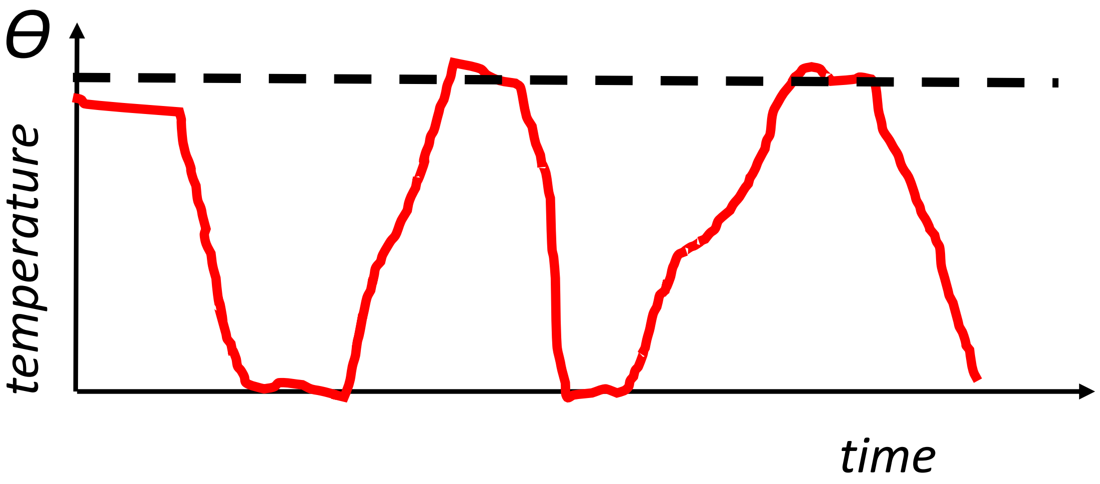
Averaging/Filtering in Combustion

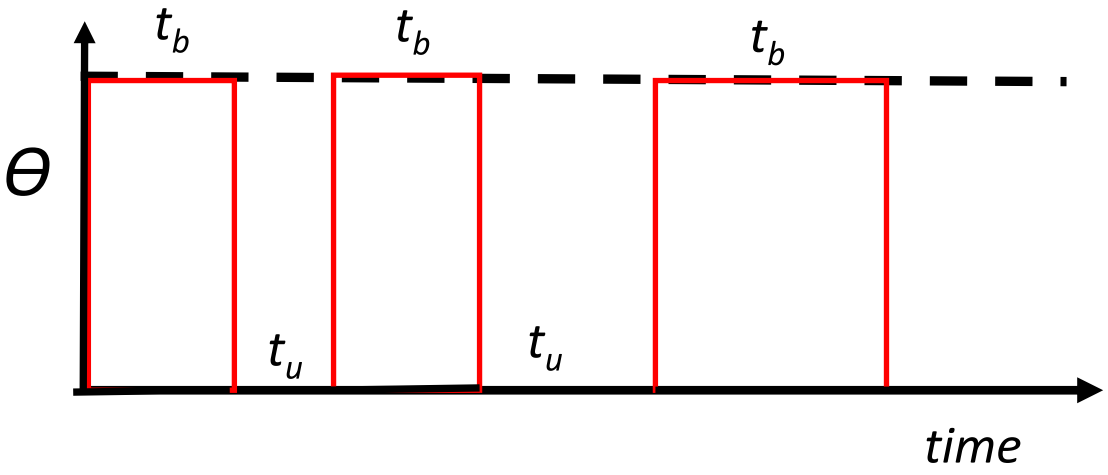
Assumption:

Infinitely thin flame (equivalent to the assumption of very fast chemistry)

→ the flame passage time becomes zero

→ the reduced temperature *Θ* a bimodal function.





Reynolds averaging then yields

$$\bar{\theta} = \frac{t_u \cdot 0 + t_b \cdot 1}{t_u + t_b} = \frac{t_b}{t_u + t_b}$$

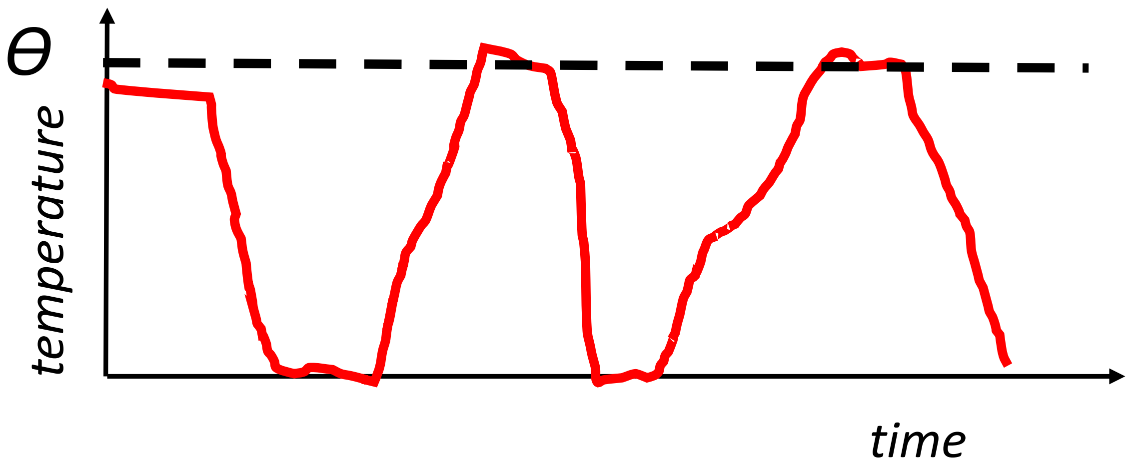
Averaging/Filtering in Combustion

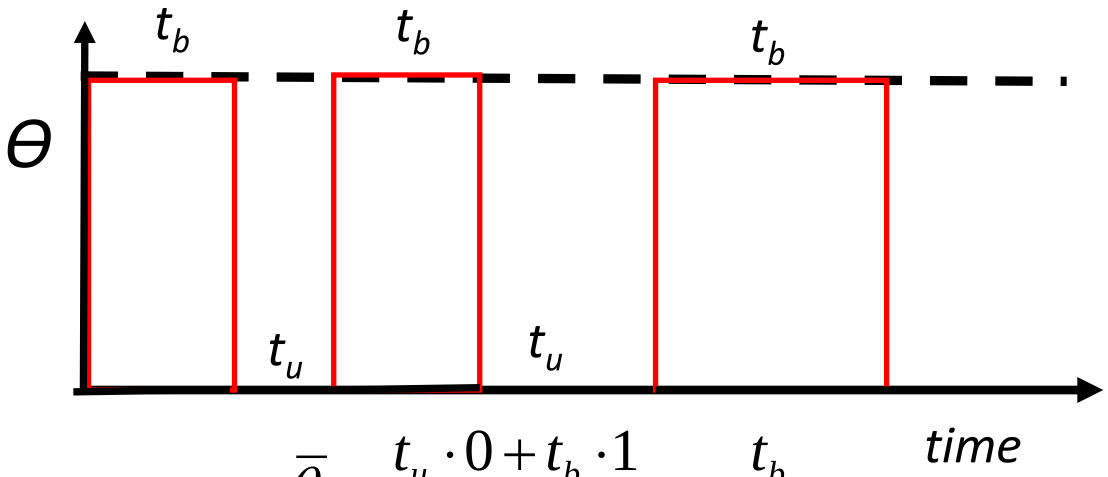
Combustion Modeling

If the RANS CFD computes an average temperature of 1800 K in a turbulent flame and the unburnt temperature is 300 K, then this result actually means that the probability of having locally this temperature is about 47%.

$$\frac{1800-300}{3500-300}=47\%$$

How would you compare this result with an experimentally determined temperature ?





$$\overline{\theta}=\frac{t_u\cdot 0+t_b\cdot 1}{t_u+t_b}=\frac{t_b}{t_u+t_b}$$

Averaging/Filtering in Combustion

Combustion Modeling

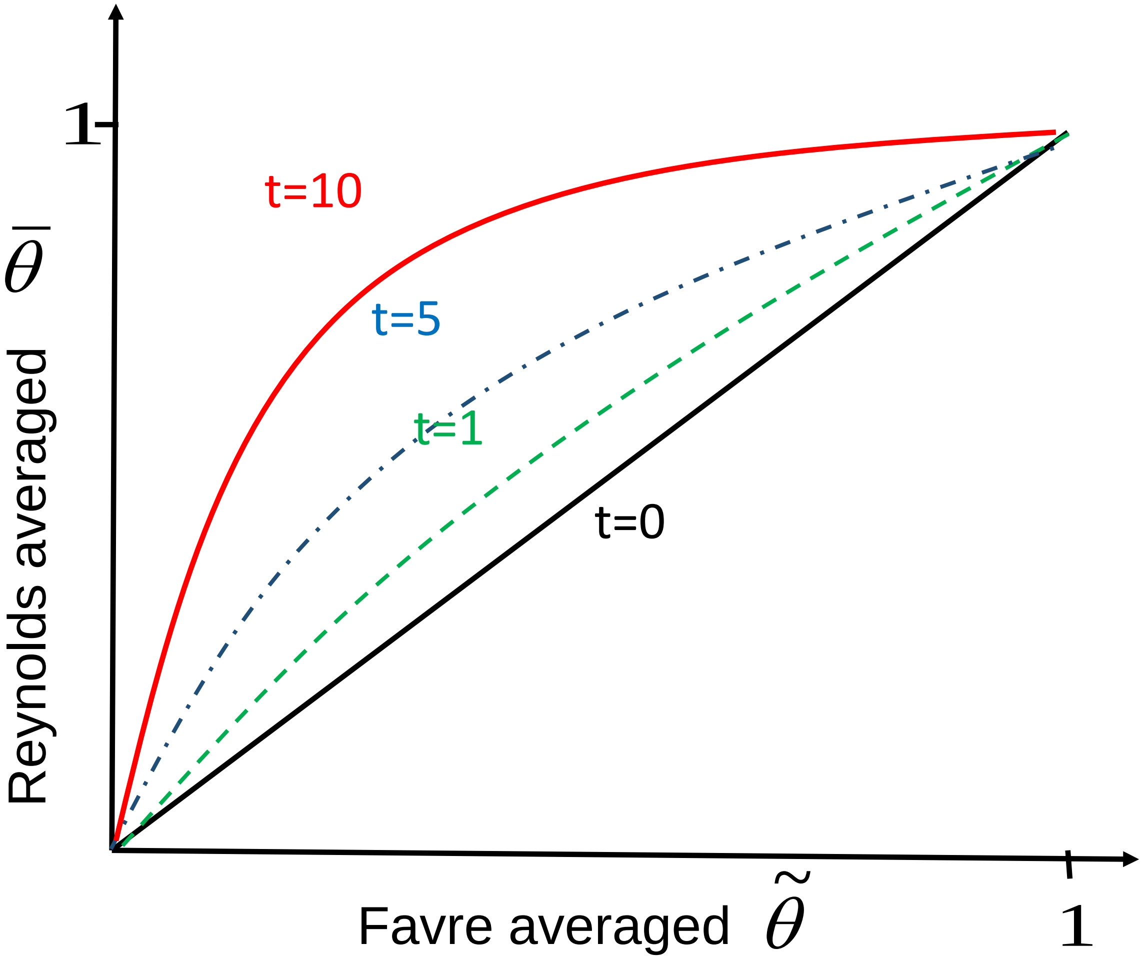
Differences between Reynolds and Favre averaged Quantities

$$\overline{\rho} = \frac{t_u \cdot \rho_u + t_b \cdot \rho_b}{t_u + t_b} = \rho_b \overline{\theta} + \rho_u \left(1 - \overline{\theta}\right)$$

$$\overline{\rho\theta} = \frac{t_u \cdot \rho_u \cdot 0 + t_b \cdot \rho_b \cdot 1}{t_u + t_b} = \rho_b \overline{\theta}$$

$$\tilde{\theta} = \frac{\overline{\theta}}{\tau\left(1 - \overline{\theta}\right) + 1}$$

$$\overline{\theta} = \overline{\theta}\,\frac{\left(1 + \tau\right)\tilde{\theta}}{1 + \tau\tilde{\theta}}$$



Modeling Combustion

Basic Equations (1)

Let’s start with the conservation of momentum

τ'_{ik} shear stress in the *i*-th direction on a surface whose normal is in the *k*-th direction

g_i, body force in *i*-th direction

$$\frac{\partial}{\partial t}\rho u_i + \frac{\partial}{\partial x_k}\left(\rho u_k u_i\right) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_k}\tau_{ik} + g_k;$$

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right);$$

When bulk viscosity is neglected.

Continuity (supplemented by species conservation)

J_{ki}, mass molecular flux of species *k* in the *i*-th coordinate direction

$\dot{w}_k$ mass rate of creation of species k

$$\boxed{\frac{\partial \rho}{\partial t}Y_k + \frac{\partial}{\partial x_i}\left(\rho u_i Y_k\right) = -\frac{\partial}{\partial x_i}J_{ki} + \dot{w}_k;}$$

Eqn (1)

Modeling Combustion

Basic Equations (2)

- To reduce complexity, J_{ki} is often simplified although this may cause erroneous results with molecules which are more agile than others such as hydrogen or in areas where turbulent mixing isn't dominant such as in boundary layers;

$$\boxed{J_{ki} = -\rho D_k \frac{\partial Y_k}{\partial x_i};}$$

Eqn (2)

- In air-breathing combustion, nitrogen is often considered as background fluid and the individual diffusion coefficients D_k will become the binary diffusion coefficient of nitrogen and the fluid of interest

→ and then the continuity equation becomes its simpler form

$$\frac{\partial \rho}{\partial t} Y_k + \frac{\partial}{\partial x_i}\left(\rho u_i Y_k\right) = \frac{\partial}{\partial x_i} \rho D_k \frac{\partial Y_k}{\partial x_i} + \dot{w}_k;$$

Modeling Combustion

Basic Equations (3)

Implementing the mass fraction μ_{ik} of element *i* in species *k* with $Z_i = \sum_{i=1}^{N} \mu_{ik} Y_k$ and $\sum_{i=1}^{M} Z_i = 1$ yields finally the conservation equation of elements

$$\frac{\partial \rho}{\partial t} \rho Z_k + \frac{\partial}{\partial x_i}\left(\rho u_i Z_k\right) = \frac{\partial}{\partial x_i} \sum_{l=1}^{N} \rho \mu_{il} D_l \frac{\partial Y_l}{\partial x_i};$$

Generally, this equation is too complicated due to the species diffusion coefficients and therefore it is assumed that diffusion can be described sufficiently by a single coefficient *D*

$$\boxed{\frac{\partial \rho}{\partial t} \rho Z_k + \frac{\partial}{\partial x_i}\left(\rho u_i Z_k\right) = \frac{\partial}{\partial x_i} \rho D \frac{\partial Z_k}{\partial x_i};}$$

Eqn (3)

This conservation of element formulation is useful for laminar flows and simple chemical systems. If *M* is the number of elements and *N* the number of species, we have to take into account *M-1* times Eqn (3) and N-M times Eqn (2) and this approach isn’t feasible anymore and the species conservation form (Eqn (1)) is applied.

Modeling Combustion

Basic Equations (4)

Energy (various formulations depending on application)

Low speed turbulent flow (M<<1)

$$\frac{\partial \rho}{\partial t}\rho h+\frac{\partial}{\partial x_i}(\rho u_i h)=\frac{\partial p}{\partial t}+\frac{\partial}{\partial x_i}\left[\frac{\mu}{Pr}\frac{\partial h}{\partial x_i}+\mu\sum_{l=1}^{N}\left(\frac{1}{Sc_k}-\frac{1}{Pr}\right)h_k\frac{\partial Y_l}{\partial x_i}\right];$$

Radiation is neglected here

h, static enthalpy of the mixture and h_i that of species *i* ; *Pr*, Prandtl number of the mixture and Sc_i, Schmidt number of species *i.*

with the definition $Sc_i=\frac{\eta}{\rho D_i}$ the importance of the single diffusion coefficient $D \approx D_i$ becomes obvious.

→ $\boxed{Sc_i = Sc \quad \text{and} \quad Sc = Pr}$

and then

$$\frac{\partial \rho}{\partial t}\rho h+\frac{\partial}{\partial x_i}(\rho u_i h)=\frac{\partial p}{\partial t}+\frac{\partial}{\partial x_i}\frac{\mu}{Pr}\frac{\partial h}{\partial x_i};$$

Modeling Combustion

Favre-averaged Navier-Stokes Energy Equation

$$\frac{\partial \tilde{e}}{\partial t}+\frac{\partial}{\partial x_j}\left[\left(\tilde{e}+\bar{p}\right)\tilde{u}_j\right]=\frac{\partial}{\partial x_j}\left[\left(\bar{\tau}_{ij}-\overline{\rho u_i'' u_j''}\right)\tilde{u}_i\right]-\frac{\partial}{\partial x_j}\left[\bar{q}_j+\overline{\rho u_i'' h''}-\overline{\tau_{ij} u_i''}+\overline{\frac{1}{2}\rho u_j'' u_i'' u_i''}\right]$$

$$\text{with}\;\; \bar{\tau}_{ij}=2\bar{\mu}\bar{S}_{i\,ij};\;\; \bar{\mu}=\mu_{ref}\left(\frac{\rho_{ref}}{p_{ref}}\frac{\bar{p}}{\bar{\rho}}\right)^{3/4};\;\; \bar{S}_{ij}=\frac{1}{2}\left(\frac{\partial \tilde{u}_i}{\partial x_j}+\frac{\partial \tilde{u}_j}{\partial x}-\frac{2}{3}\delta_{ij}\frac{\partial \tilde{u}_k}{\partial x_k}\right);\;\; \bar{q}_j=-\frac{\kappa}{\kappa-1}\frac{\bar{\mu}}{\Pr}\left(\frac{\bar{p}}{\bar{\rho}}\right)$$

To close the system we need an equation of state
Assuming a perfect gas we may derive

$$\bar{p}=\left(\kappa-1\right)\left[\tilde{e}-\frac{1}{2}\bar{\rho}\tilde{u}_j\tilde{u}_j-\bar{\rho}k\right]\quad \text{with}\quad k=\frac{1}{2}\overline{u_i'' u_i''}$$

Modeling Combustion

Basic Equations (5)

Hence, this energy equation has the form of a standard convection-diffusion one except the pressure term $\frac{\partial p}{\partial t}$.

Look at the two time derivate terms $\frac{\partial \rho}{\partial t}\rho h$ and $\frac{\partial p}{\partial t}$ and argue that a velocity fluctuation u' is associated with a pressure fluctuation $\rho u'^2$ and an enthalpy fluctuation $c_p T'$, then we can show that the ratio of pressure and enthalpy terms is similar to the square of Mach number fluctuation $\frac{u'^2}{c_p T'} \approx M'^2$ and with M << 1 we can neglect the pressure term.

Equation of State

For combustion studies it is often sufficient to assume of ideal gas (this isn't applicable if propellant injection is included where you have to deal with liquids and in case of rocket engines the liquids may be at cryogenic temperatures and even at trans-critical conditions.

$$p = \rho \frac{R_0 T}{W} = \rho R_0 T \sum_{k=1}^{N} \frac{Y_k}{W_k};$$

with *W*, the mixture molecular weight and W_i that of the species *i.*

For many applications it is acceptable to assume *p = const.,* except high speed flows and rocket engines.

Modeling Combustion

Basic Equations (6)

Thermo-physical Properties

$h = \sum_{k=1}^{N} Y_k h_k;\ \text{with}\ h_i = h_i(T)$ for turbulent flows the accuracy of $h_i = c_{p_i} T + \Delta_i$ is usually sufficient.

c_{p_i} and Δ_i are chosen such that this equation accurately predicts the static enthalpy for the desired range of temperature.

$$h = c_p T + \sum_{k=1}^{N} Y_k \Delta_k; \quad \text{with}\ c_p = \sum_{k=1}^{N} c_{p_k} Y_k$$

and now we have a relation to predict the temperature.

c_p is the mixture heat capacity at constant pressure (Prandtl number)

$$T = \frac{h - \sum_{k=1}^{N} Y_k \Delta_k}{c_p}$$

Basic Equations (7)

Chemical Source Terms

Let’s consider *N* species are destroyed and generated in *R* elementary reactions

$$\sum_{k=1}^{N} \nu'_{ij} M_i \underset{k_{\mathrm{bj}}}{\overset{k_{\mathrm{fj}}}{\rightleftarrows}} \sum_{k=1}^{N} \nu''_{ij} M_i$$

M_i is the symbol for the *i*-th species, ν'_i and ν''_i are the stoichiometric coefficients for species *i* in reaction *j*.

The chemical source term $\dot{w}_i$ accounts for generation and consumption of species *i* due to each reaction step.

$\dot{w}_i = \sum_{J=1}^{R} \dot{w}_{ij}$; with $\dot{w}_{ij} = 0$ if species *i* doesn’t participate in reaction step *j*.

$$\boxed{\dot{w}_{ij} = \left(\nu''_{ij} - \nu'_{ij}\right) k_{\mathrm{fj}} \rho^{m_{\mathrm{fj}}} \frac{W_i}{W_j} \prod_{i=1}^{N} Y_i^{\nu'_{ij}} \left[1 - \frac{\mathrm{k}_{\mathrm{bj}}}{\mathrm{k}_{\mathrm{fj}}} \rho^{\left(m_{\mathrm{bj}} - m_{\mathrm{fj}}\right)} \prod_{i=1}^{N} Y_i^{\left(m_{\mathrm{bj}} - m_{\mathrm{fj}}\right)}\right]}$$

Eqn (4)

$$\text{with } W_j = \sum_{i=1}^{N} \nu'_{ij} W_i;$$

Modelling Combustion

Basic Equations (8)

Chemical Source Terms

$m_{\mathrm{f}j} \equiv \sum_{i=1}^{N} \nu'_{ij}$ and $m_{\mathrm{b}j} \equiv \sum_{i=1}^{N} \nu''_{ij}$ the forward and backward reaction rates for reaction *j*

Setting the bracket term in Eqn 4 to zero is the condition for chemical equilibrium for the *j*-th reaction step, i.e. forward and backward reaction rates are equal and then:

$$\frac{k_{\mathrm{f}j}}{k_{\mathrm{b}j}} = K_j(T)$$

Rate constants are often expressed as:

$$k_{\mathrm{f}j} = B_{\mathrm{f}j} T^{\alpha_{\mathrm{f}j}} \exp\left(-\frac{T_{\mathrm{af}j}}{T}\right)$$

where the pre-exponential factor $B_{\mathrm{f}j}$, the temperature exponent $\alpha_{\mathrm{f}j}$ and the activation temperature $T_{\mathrm{af}j}$ are constants which characterize the rate of the *j*-th reaction in forward direction.

in general Arrhenius form:

$$k_n = A_n T^{n_\mathrm{n}} \exp\left(-\frac{E_\mathrm{n}}{RT}\right)$$

with the frequency factor A_n, the temperature exponent n_n and the activation energy E_n.

Turbulence and Combustion

Two way coupling process

- Turbulence causes intensified heat and mass transport which results in flame wrinkling which results in increased flame surface (heat release/unit volume) and thus increases flame propagation
- Temperature increase yields increase viscosities and thus dampens turbulence in the burned gases (volumetric effect)
- Thermal expansion in the flame front causes velocity gradients in both the cold and hot regions an thus generates turbulence (effect length scale limited characteristic length of wrinkles ?)

Simple gradient-like closures or averaged/filtered dependencies aren’t sufficient to resolve the highly non-linear Arrhenius terms from chemistry and the interaction with turbulence

Combustion Models

Finite Rate Chemistry Model (FRCM)

Combustion model for cases where chemistry is controlling the combustion process

- Assumes $t_{chemistry} > t_{mixing}$ (laminar and or turbulent) and is applicable for both laminar and turbulent non-premixed situations when non-equilibrium effects become important

Source term (species *i* in reaction *j*)

$$\tilde{S}_{i,j} = A\tilde{\Gamma} M_i \left(\nu''_{i,j} - \nu'_{i,j}\right)\left(k_{\mathrm{f},j} \prod_i \left(\frac{\bar{\rho}\tilde{Y}_i}{M_i}\right)^{\upsilon'_{i,j}} - k_{\mathrm{b},j} \prod_i \left(\frac{\bar{\rho}\tilde{Y}_i}{M_i}\right)^{\upsilon''_{i,j}} \right)$$

$k_{f,j}$, $k_{b,j}$: rates of reaction j (forward/backward) determined by Arrhenius expressions $f(\tilde{T})$

$\tilde{\Gamma}$: models influence of third body reactions $\tilde{\Gamma} = \sum \gamma_{i,j} \frac{\bar{\rho}\tilde{Y}_i}{M_i} M_i$

- Source term linearization centered on operating point which allows for integration into species equations and realization of larger time steps

However

- Takes only mean values for temperature in the Arrhenius expression and thus ignores effect of turbulent fluctuations which yields an under-prediction of temperatures

Combustion Models

Combination of EDM and FRCM

Model computes for each cell two reaction rates, one based on EDM and the other on FRCM assumptions and the smaller rate is then used to determine the local reaction rate.

$$r_i = \min\left(r_i^{EDM}, r_i^{FRCM}\right)$$

Hence, the model automatically decides if the process is controlled by mixing or by chemistry.

Although this combined approach enlarges the range of applicability,

it still does not account for turbulence chemistry interaction.

Combustion Models

Eddy Dissipation Concept (EDC)

EDC is an extension of EDM insofar as it considers detailed chemical kinetics and it assumes that reactions take place at small scales`*´

$$\xi^* = C_\xi \left(\frac{\upsilon \bar{\varepsilon}}{\tilde{k}^2} \right)^{1/4}$$ with a volume of the order ξ^{*3}

(in Fluent $C_\xi = 2.1377$)

Reaction rates are derived from Arrhenius expression (FRCM) with a time scale of reactions:

$$\tau^* = C_\tau \left(\frac{\upsilon}{\tilde{\varepsilon}} \right)^{1/2}$$

(in Fluent $C_\tau = 0.4082$)

Combustion Models

Eddy Dissipation Concept (EDC)

Boundary/Initial conditions for reactions on small scales:

- Assumption: *p* = *const.*
- Initial condition: temperature and species concentration in a cell
- Reactions at time scale τ^*
- Numerical integration (e.g. ISAT-Algorithm) → $\tilde{Y}_{i*}$

- Source term model

$$\tilde{S}_i = \frac{\xi^{*2}}{\tau^*\left(1-\xi^{*3}\right)}\left(\tilde{Y}_{i^*} - \tilde{Y}_i\right)$$

Mass fraction of species *i* on small scales after reaction time τ^*

- However:
  - Requires processing power
  - System of differential equations very stiff

Direct Numerical Simulation (DNS)

Solution of entire set of equations down to the smallest scales and reaction zones

- Governing equations (N+5, N+4)
    - Continuity (1)
    - Momentum (3)
    - Species transport (N, number of species)
    - Enthalpy transport (1)
    - EOS (1)
    - Caloric EOS (1)
    - Transport properties (N+2)
- Independent variables to be determined (2N+9)
    - Density, pressure, temperature (3)
    - Velocity components (3)
    - Species mass fractions (N)
    - Enthalpy 8(1)
    - Transport coefficients (N+2)

Direct Numerical Simulation (DNS)

Scales to be resolved:

$$\frac{l_0}{\eta} \propto \mathrm{Re}_{l0}{}^{3/4} \qquad \frac{v_0}{v_\eta} \propto \mathrm{Re}_{l0}{}^{1/4} \qquad \frac{\tau_0}{\tau_\eta} \propto \mathrm{Re}_{l0}{}^{1/2}$$

Assume smallest grid is η and smallest time step is t:

1-D simulation cost
$$\frac{l_0}{\eta}\frac{\tau_0}{\tau_\eta} \propto \mathrm{Re}_{l0}{}^{5/4}$$

2-D Simulation cost
$$\left(\frac{l_0}{\eta}\right)^2 \propto \mathrm{Re}_{l0}{}^{2}$$

3-D Simulation cost
$$\left(\frac{l_0}{\eta}\right)^3 \frac{\tau_0}{\tau_\eta} \propto \mathrm{Re}_{l0}{}^{11/4}$$