Fundamentos de Escoamentos Reativos Turbulentos

Aula 4 - 5

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Momentum Conservation Equation

For an reactive multicomponent mixture, the momentum equation reads

$$\frac{\partial \rho u_i}{\partial t}+\frac{\partial \rho u_i u_j}{\partial x_j}=-\frac{\partial p}{\partial x_i}+\frac{\partial}{\partial x_j}\left[2\mu S_{ij}-\frac{2}{3}\delta_{ij}\left(\mu\frac{\partial u_k}{\partial x_k}\right)\right]+\rho g_i+\rho\sum_{k=1}^{N} Y_k f_{k,i}, \tag{1}$$

where

$$S_{ij}=\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right), \tag{2}$$

The last term stands for the body force f_k acting over the specie k in the direction i. This could be, for example, electric/magnetic fields.

Momentum Conservation Equation

Neglecting the body forces, the averaged momentum equations reads

$$\frac{\partial \rho \overline{u}_i \overline{u}_j}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}\left(\mu \frac{\partial \overline{u}_k}{\partial x_k}\right)\right] - \frac{\partial \rho \overline{u_i^{'} u_j^{'}}}{\partial x_i}, \quad (3)$$

The last term stands for the Reynolds Stresses.

Classical Turbulence Models for the Reynolds Stresses

With the analogy to the molecular viscous tensor, the Boussinesq assumption leads to

$$\rho\overline{u_i'u_j'} = -\mu_t\left[\left(\frac{\partial\overline{u_i}}{\partial x_j} + \frac{\partial\overline{u_j}}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}\left(\frac{\partial\overline{u_k}}{\partial x_k}\right)\right] + \frac{2}{3}\delta_{ij}\rho k, \qquad (4)$$

where k is the kinetic energy of the turbulence, defined as $k = \frac{1}{2}\overline{u_i'u_i'}$

The question is, however, how to evaluate the turbulent viscosity μ_t

Classical Turbulence Models : Zero Equation or Prandtl Mixing Length

Prandtl has proposed to evaluate the turbulent viscosity based on the velocity gradient and a characteristic length l_m as

$$\mu_t = \rho {l_m}^2 |\overline{S_{ij}}| \tag{5}$$

where

$$\overline{S_{ij}} = \frac{1}{2}\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\right), \tag{6}$$

The characteristic length l_m is calculated based on empirical relations for typical flows geometry (flat plate, cylinder, sphere, jet)

Classical Turbulence Models : One Equation or Prandtl-Kolmogorov Model

The turbulent viscosity based on the turbulence kinetic energy k and a characteristic length l_m as

$$\mu_t = \rho C_\mu l_{PK} \sqrt{k} \tag{7}$$

where C_μ is a model constant (normally $C_\mu = 0.09$. The characteristic length l_m is calculated based on empirical relations for typical flows geometry (flat plate, cylinder, sphere, jet)

Transport Equation for the Reynolds Tensor

$$\underbrace{\frac{\partial}{\partial x_k}\left(\rho\overline{u_k}\overline{u_i'u_j'}\right)}_{\text{Advecção}} = \underbrace{\frac{\partial}{\partial x_k}\left[\mu\frac{\partial}{\partial x_k}\left(\overline{u_i'u_j'}\right)\right]}_{\text{Difusão molecular}} - \underbrace{\frac{\partial}{\partial x_k}\left[\rho\overline{u_i'u_j'u_k'} + \overline{p\left(\delta_{kj}u_i' + \delta_{ik}u_j'\right)}\right]}_{\text{Difusão turbulenta}}$$
$$- \underbrace{\rho\left(\overline{u_i'u_k'}\frac{\partial\overline{u_j}}{\partial x_k} + \overline{u_j'u_k'}\frac{\partial\overline{u_i}}{\partial x_k}\right)}_{\text{Termo de produção de tensão}} + \underbrace{\overline{p\left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i}\right)}}_{\text{Deformação por pressão}} - \underbrace{2\mu\overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_j'}{\partial x_k}}}_{\text{Dissipação}} + \underbrace{S}_{\text{Termo fonte}} \tag{8}$$

- Os termos de advecção, difusão molecular, produção de tensão não necessitam de modelagem, enquanto os termos de dissipação, difusão turbulenta e deformação por pressão são modelados.

Transport Equation for Turbulent Kinetic Energy

- The transport equation for the Turbulent Kinetic Energy is obtained by doing the contraction $i = j$ on the transport equation for the Reynolds Stress Tensor. Remember that doing the contraction $i = j$, we get the trace of the Reynolds Stress Tensor.

$$\underbrace{\frac{\partial}{\partial x_k}\left(\rho\overline{u_k}\,\overline{u_i'u_i'}\right)}_{\text{Advecção}} = \underbrace{\frac{\partial}{\partial x_k}\left[\mu\frac{\partial}{\partial x_k}\left(\overline{u_i'u_i'}\right)\right]}_{\text{Difusão molecular}} - \underbrace{\frac{\partial}{\partial x_k}\left[\rho\overline{u_i'u_i'u_k'} + \overline{p\left(\delta_{ki}u_i' + \delta_{ik}u_i'\right)}\right]}_{\text{Difusão turbulenta}}$$
$$-\underbrace{\rho\left(\overline{u_i'u_k'}\frac{\partial\overline{u_i}}{\partial x_k} + \overline{u_i'u_k'}\frac{\partial\overline{u_i}}{\partial x_k}\right)}_{\text{Termo de produção de tensão}} + \underbrace{\overline{p\left(\frac{\partial u_i'}{\partial x_i} + \frac{\partial u_i'}{\partial x_i}\right)}}_{\text{Deformação por pressão}} - \underbrace{2\mu\overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_i'}{\partial x_k}}}_{\text{Dissipação}} + \underbrace{S}_{\text{Termo fonte}} \tag{9}$$

Transport Equation for Turbulent Kinetic Energy

or in a short form (note that the pressure deformation term vanishes)

$$\underbrace{\frac{\partial}{\partial x_k}\left(\rho\overline{u_k}\,\overline{u_i' u_i'}\right)}_{\text{Advecção}} = \underbrace{\frac{\partial}{\partial x_k}\left[\mu\frac{\partial}{\partial x_k}\left(\overline{u_i' u_i'}\right)\right]}_{\text{Difusão molecular}} - \underbrace{\frac{\partial}{\partial x_k}\left[\rho\overline{u_i' u_i' u_k'} + 2\overline{p\left(\delta_{ki} u_i'\right)}\right]}_{\text{Difusão turbulenta}}$$
$$\underbrace{-2\rho\overline{u_i' u_k'}\frac{\partial\overline{u_i}}{\partial x_k}}_{\text{Termo de produção de tensão}} - 2\mu\underbrace{\overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_i'}{\partial x_k}}}_{\text{Dissipação}} + \underbrace{S}_{\text{Termo fonte}} \tag{10}$$

Transport Equation for Turbulent Kinetic Energy

dividing all the equation by 2, one obtains

$$\underbrace{\frac{\partial}{\partial x_k}\left(\rho \overline{u_k} k\right)}_{\text{Advecção}} = \underbrace{\frac{\partial}{\partial x_k}\left(\mu \frac{\partial k}{\partial x_k}\right)}_{\text{Difusão molecular}} - \underbrace{\frac{\partial}{\partial x_k}\left[\frac{1}{2}\rho \overline{u_i' u_i' u_k'} + \overline{p\left(\delta_{ki} u_i'\right)}\right]}_{\text{Difusão turbulenta}}$$
$$\underbrace{-\rho \overline{u_i' u_k'} \frac{\partial \overline{u_i}}{\partial x_k}}_{\text{Termo de produção de tensão}} \underbrace{- \mu \overline{\frac{\partial u_i'}{\partial x_k} \frac{\partial u_i'}{\partial x_k}}}_{\text{Dissipação}} + \underbrace{S}_{\text{Termo fonte}} \tag{11}$$

Note that the Dissipação Term will be always positive

- Modeling of the unknown terms

Turbulent Transport (turbulent diffusion)

$$\underbrace{-\frac{\partial}{\partial x_k}\left[\frac{1}{2}\rho\overline{u_i' u_i' u_k'} + \overline{p\left(\delta_{ki} u_i'\right)}\right]}_{\text{Difusão turbulenta}} = \frac{\partial}{\partial x_k}\left[\frac{\mu_t}{\sigma_k}\frac{\partial k}{\partial x_k}\right] \tag{12}$$

- Modeling of the unknown terms

Production of k by the gradient of the mean velocity

$$\underbrace{-\rho\overline{u_i'u_k'}\frac{\partial\overline{u_i}}{\partial x_k}}_{\text{Produção de tensão}} = \left[\mu_t\left[\left(\frac{\partial\overline{u_i}}{\partial x_k}+\frac{\partial\overline{u_k}}{\partial x_i}\right)+\frac{2}{3}\delta_{ik}\left(\frac{\partial\overline{u_l}}{\partial x_l}\right)\right]-\frac{2}{3}\delta_{ik}\rho k\right]\frac{\partial\overline{u_i}}{\partial x_k} \tag{13}$$

considering that for the k equation if $i=k$ then

$$-\rho\overline{u_i'u_k'}\frac{\partial\overline{u_i}}{\partial x_k} = -\rho\overline{u_i'u_i'}\frac{\partial\overline{u_i}}{\partial x_i} = 0$$

and if $i\neq k, \delta_{ik}=0$

$$-\rho\overline{u_i'u_k'}\frac{\partial\overline{u_i}}{\partial x_k} = \left[\mu_t\left(\frac{\partial\overline{u_i}}{\partial x_k}+\frac{\partial\overline{u_k}}{\partial x_i}\right)\right]\frac{\partial\overline{u_i}}{\partial x_k}$$

- Modeling of the unknown terms

Rate of Dissipation of k

$$\underbrace{\mu \overline{\frac{\partial u_i'}{\partial x_k} \frac{\partial u_i'}{\partial x_k}}}_{\text{Dissipação}} = \varepsilon \tag{14}$$

The turbulent viscosity based on the turbulence kinetic energy k and its dissipation rate ε as

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \tag{15}$$

Equação de transporte da energia cinética turbulenta (k).

$$\frac{\partial \rho \overline{u}_j k}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + 2\mu_t \overline{S}_{ij}\overline{S}_{ij} - \varepsilon \tag{16}$$

Equação de transporte da taxa de dissipação (ε) de k

$$\frac{\partial \rho \overline{u}_j \varepsilon}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_j}\right) + C_{1\varepsilon}\frac{\varepsilon}{k} 2\mu_t \overline{S}_{ij}\overline{S}_{ij} - C_{2\varepsilon}\rho\frac{\varepsilon^2}{k}, \tag{17}$$

onde σ_k, σ_ε, $C_{1\varepsilon}$, $C_{2\varepsilon}$ são constantes de ajustes que neste modelo de turbulência têm os valores de $1,00$, $1,30$, $1,44$ e $1,92$.

Classical Turbulence Models - $k - \varepsilon$

$k - \varepsilon$ Prós-Contras:

Prós

- Very popular because of its simplicity and low computational costs
- It provides the turbulent time scale for both scales: the integral $\frac{k}{\varepsilon}$ and Kolmogorov $\sqrt{\frac{\nu}{\varepsilon}}$
- It provides the turbulent length scale for both scales: the integral $\frac{k^{3/2}}{\varepsilon}$ and Kolmogorov $\left(\frac{\nu^3}{\varepsilon}\right)^{1/4}$

Contra

- Exact balance equations for $k - \varepsilon$ can be derived but they need closure models with strong assumptions: high Reynolds Number, homogeneous and isotropic turbulence;
- Velocity fluctuations due to low frequency motions associated to intermittency and coherent structures are underestimated;
- the models needs correction for compressible flow

Classical Turbulence Models - Second Order Model (RSM)

O modelo das tensões de Reynolds compõe-se de equações que representam cada uma das componentes do tensor de Reynolds. O modelo é composto por equações de transporte das tensões de Reynolds, juntamente com uma equação para a taxa de dissipação da energia cinética turbulenta.

$$
\begin{aligned}
&\underbrace{\frac{\partial}{\partial x_k}\left(\rho \overline{u_k}\,\overline{u_i' u_j'}\right)}_{\text{Advecção}} \\
&= \underbrace{\frac{\partial}{\partial x_k}\left[\mu \frac{\partial}{\partial x_k}\left(\overline{u_i' u_j'}\right)\right]}_{\text{Difusão molecular}} - \underbrace{\frac{\partial}{\partial x_k}\left[\rho \overline{u_i' u_j' u_k'} + \overline{p'\left(\delta_{kj} u_i' + \delta_{ik} u_j'\right)}\right]}_{\text{Difusão turbulenta}} \\
&- \underbrace{\rho\left(\overline{u_i' u_k'}\frac{\partial \overline{u_j}}{\partial x_k} + \overline{u_j' u_k'}\frac{\partial \overline{u_i}}{\partial x_k}\right)}_{\text{Termo de produção de tensão}} - \underbrace{\rho\beta\left(g_i \overline{u_j'\theta} + g_j \overline{u_i'\theta}\right)}_{\text{Produção de empuxo (\textit{buoyancy})}} + \underbrace{\overline{p'\left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i}\right)}}_{\text{Deformação por pressão}} \\
&- \underbrace{2\mu \overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_j'}{\partial x_k}}}_{\text{Dissipação}} - \underbrace{2\rho\Omega_k\left(\overline{u_j' u_m'}\varepsilon_{ikm} + \overline{u_i' u_m'}\varepsilon_{jkm}\right)}_{\text{Produção por rotação do sistema}} + \underbrace{S}_{\text{Termo fonte}}
\end{aligned}
\tag{18}
$$

- Os termos de advecção, difusão molecular, produção de tensão e produção por rotação do sistema não necessitam de modelagem, enquanto os termos de dissipação, difusão turbulenta, produção de empuxo e deformação por pressão são modelados.
- O modelo das tensões de Reynolds requer a imposição de condições de contorno para cada componente do tensor de Reynolds e para a taxa de dissipação turbulenta. Como esses valores raramente são conhecidos, a sua estimativa é uma desvantagem de se utilizar esse tipo de modelo.

- Deformação por pressão

$$\underbrace{\overline{p'\left(\frac{\partial u'_i}{\partial x_j}+\frac{\partial u'_j}{\partial x_i}\right)}}_{\text{Deformação por pressão}} = - C_1\rho\varepsilon\left(\frac{\overline{u'_i u'_j}}{k}-\frac{2}{3}\delta_{ij}\right)+C_2\delta_{ij}\rho\overline{u'_m u'_n}\frac{\partial\overline{u}_m}{\partial x_n}$$

$$- C_3\rho P_{ij}+C_4\rho k\left(\frac{\partial\overline{u}_i}{\partial x_j}+\frac{\partial\overline{u}_j}{\partial x_i}\right)-\frac{2}{3}C_4 k\frac{\partial\overline{u}_k}{\partial x_k}\delta_{ij}$$

$$-\left(\frac{3}{2}C_2+C_3\right)\left(\rho\overline{u'_m u'_j}\frac{\partial\overline{u}_m}{\partial x_i}+\rho\overline{u'_m u'_i}\frac{\partial\overline{u}_m}{\partial x_j}\right) \quad (19)$$

Sendo $C_1 = 3,0$; $C_2 = -0,44$; $C_3 = 0,46$; $C_4 = 0,23$

Favre Averaging

- In reactive flows (combustion) the density fluctuates. If one uses the Reynolds averaging procedure, one has for the Continuity Equation

$$\frac{\partial}{\partial x_i}\overline{\rho}\overline{u_i} = -\frac{\partial}{\partial x_i}\overline{\rho' u_i'} \tag{20}$$

and for the Momentum Equation

$$\begin{aligned}\frac{\partial \overline{\rho}\overline{u_i}\,\overline{u_j}}{\partial x_j} = &-\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}\left(\mu\frac{\partial \overline{u_k}}{\partial x_k}\right)\right] \\ &- \frac{\partial}{\partial x_j}\left[\overline{\rho}\overline{u_i' u_j'} + \overline{\rho' u_i'}\,\overline{u_j} + \overline{\rho' u_j'}\,\overline{u_i} + \overline{\rho' u_i' u_j'}\right],\end{aligned} \tag{21}$$

- In order to avoid modelling the new unknown correlations, we use the Favre-Averaging Procedure

Favre Averaging

The mass-weighted average is defined by

$$\widetilde{\phi} \equiv \frac{\overline{\rho\phi}}{\overline{\rho}} \tag{22}$$

Any quantity ϕ can be split into mean and fluctuating component as

$$\phi \equiv \widetilde{\phi} + \phi'' \tag{23}$$

with $\widetilde{\phi''} = 0$ and $\overline{\rho\phi''} = 0$. Multiplying eq. (23) by ρ

$$\rho\phi \equiv \rho\widetilde{\phi} + \rho\phi'' \tag{24}$$

and applying the averaging operator yields

$$\overline{\rho\phi} \equiv \overline{\rho\widetilde{\phi}} + \overline{\rho\phi''} \tag{25}$$

Favre Averaging

with eq.(22) for the LHS one obtains

$$\overline{\rho}\widetilde{\phi} \equiv \overline{\rho}\widetilde{\phi} + \overline{\rho\phi''} \tag{26}$$

so that

$$\overline{\rho\phi''} = 0 \tag{27}$$

rewriting eq.(27) considering $\rho = \overline{\rho} + \rho'$

$$\begin{aligned} \overline{\rho\phi''} &= \overline{(\overline{\rho} + \rho')\phi''} = 0 \\ &= \overline{\overline{\rho}\phi''} + \overline{\rho'\phi''} = 0 \end{aligned} \tag{28}$$

$$\overline{\overline{\rho}\phi''} = -\overline{\rho'\phi''} \tag{29}$$

$$\overline{\phi''} = -\frac{\overline{\rho'\phi''}}{\overline{\rho}} \tag{30}$$

Favre Averaging and Reynolds Averaging

$$\phi = \widetilde{\phi} + \phi'' = \overline{\phi} + \phi' \tag{31}$$

multiplying by ρ and taking the average

$$\overline{\rho\widetilde{\phi} + \rho\phi''} = \overline{\rho\overline{\phi} + \rho\phi'} \tag{32}$$

$$\overline{\rho}\widetilde{\phi} + \underbrace{\overline{\rho\phi''}}_{0} = \overline{\rho}\overline{\phi} + \overline{\rho\phi'} \tag{33}$$

$$\overline{\rho}\widetilde{\phi} = \overline{\rho}\overline{\phi} + \overline{(\overline{\rho} + \rho')\phi'} \tag{34}$$

$$\overline{\rho}\widetilde{\phi} = \overline{\rho}\overline{\phi} + \overline{\overline{\rho}\phi'} + \overline{\rho'\phi'} \tag{35}$$

$$\overline{\rho}\widetilde{\phi} = \overline{\rho}\overline{\phi} + \underbrace{\overline{\rho}\overline{\phi'}}_{0} + \overline{\rho'\phi'} \tag{36}$$

so that the difference between Favre and Reynolds averages is

$$\widetilde{\phi} - \overline{\phi} = \frac{\overline{\rho'\phi'}}{\overline{\rho}} \tag{37}$$

Favre Averaging Transport Equations

- Continuity Equation

$$\frac{\partial}{\partial x_i}(\rho u_i) = 0 \quad \rightarrow \quad \frac{\partial}{\partial x_i}\left[(\overline{\rho} + \rho')\widetilde{u_i} + \rho u_i''\right] = 0 \tag{38}$$

taking the average

$$\frac{\partial}{\partial x_i}\left[\overline{(\overline{\rho} + \rho')\widetilde{u_i} + \rho u_i''}\right] = 0 \quad \rightarrow \quad \frac{\partial}{\partial x_i}\left[\overline{(\overline{\rho}\widetilde{u_i})} + \underbrace{\overline{\rho'\,\widetilde{u_i}}}_{=0} + \underbrace{\overline{\rho u_i''}}_{=0}\right] = 0 \tag{39}$$

The Continuity Equation reads then

$$\frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u_i}) = 0 \tag{40}$$

which is the same structure of the Reynolds Averaged Continuity Equation

Favre Averaging Transport Equations

- Linear Momentum Equation

$$\frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}\left(\mu\frac{\partial u_k}{\partial x_k}\right)\right] + \rho g_i, \quad (41)$$

applying the Favre decomposition for the velocities

$$\frac{\partial}{\partial x_j}\left(\rho\widetilde{u}_i\widetilde{u}_j + \rho\widetilde{u}_i u_j'' + \rho u_i''\widetilde{u}_j + \rho u_i'' u_j''\right) = \rho g_i - \frac{\partial}{\partial x_i}(\overline{p} + p')$$
$$+\frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial}{\partial x_j}(\widetilde{u}_i + u_i'') + \frac{\partial}{\partial x_i}(\widetilde{u}_j + u_j'')\right) - \frac{2}{3}\delta_{ij}\left(\mu\frac{\partial}{\partial x_k}(\widetilde{u}_k + u_k'')\right)\right] \quad (42)$$

Favre Averaging Transport Equations

applying the averaging operator

$$\frac{\partial}{\partial x_j}\left(\underbrace{\overline{\rho\widetilde{u}_i\widetilde{u}_j}}_{\overline{\rho}\widetilde{u}_i\widetilde{u}_j}+\underbrace{\overline{\rho\widetilde{u}_i u_j''}}_{A}+\underbrace{\overline{\rho u_i''\widetilde{u}_j}}_{B}+\underbrace{\overline{\rho u_i'' u_j''}}_{\overline{\rho u_i'' u_j''}}\right)=\overline{\rho}g_i-\frac{\partial}{\partial x_i}(\underbrace{\overline{\overline{p}}}_{\overline{p}}+\underbrace{\overline{p'}}_{=0})$$
$$+\frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial}{\partial x_j}(\underbrace{\overline{\widetilde{u}_i}}_{\widetilde{u}_i}+\underbrace{\overline{u_i''}}_{=0})+\frac{\partial}{\partial x_i}(\underbrace{\overline{\widetilde{u}_j}}_{\widetilde{u}_j}+\underbrace{\overline{u_j''}}_{=0})\right)\right]$$
$$-\frac{\partial}{\partial x_j}\left[\frac{2}{3}\delta_{ij}\left(\mu\frac{\partial}{\partial x_k}(\underbrace{\overline{\widetilde{u}_k}}_{\widetilde{u}_k}+\underbrace{\overline{u_k''}}_{=0})\right)\right] \quad (43)$$

$$A\rightarrow\widetilde{u}_i\overline{\rho u_j''}=0\ \ ;\ \ B\rightarrow\widetilde{u}_j\overline{\rho u_i''}=0$$

Favre Averaging Transport Equations

rewriting

$$\frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{u}_i\widetilde{u}_j + \overline{\rho u_i'' u_j''}\right) = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\left(\frac{\partial \widetilde{u}_i}{\partial x_j} + \frac{\partial \widetilde{u}_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}\frac{\partial \widetilde{u}_k}{\partial x_k}\right)\right] + \overline{\rho}g_i, \tag{44}$$

or

$$\frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{u}_i\widetilde{u}_j\right) = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\left(\frac{\partial \widetilde{u}_i}{\partial x_j} + \frac{\partial \widetilde{u}_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}\frac{\partial \widetilde{u}_k}{\partial x_k}\right) - \overline{\rho u_i'' u_j''}\right] + \overline{\rho}g_i, \tag{45}$$

It should be noted that the structure of this equation is the same as the RANS for constant ρ. No new correlation involving the density fluctuation arose.

Favre Averaging for the Reynolds Stress Tensor

The same procedure applied to the RANS equations can be used to write the Favre transport equation for the Reynolds Stress Tensor. After some manipulation one obtains

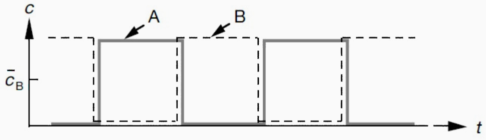
$$
\begin{aligned}
&\underbrace{\frac{\partial}{\partial x_k}\left(\widetilde{u}_k \overline{\rho u_i'' u_j''}\right)}_{\text{Advecção}} \\
&= \underbrace{-\frac{\partial}{\partial x_k}\left[\overline{\rho u_i'' u_j'' u_k''} + \overline{p'\left(\delta_{kj} u_i'' + \delta_{ik} u_j''\right)}\right]}_{\text{Difusão turbulenta}} + \underbrace{\frac{\partial}{\partial x_k}\left[\nu \frac{\partial}{\partial x_k}\left(\overline{\rho u_i'' u_j''}\right)\right]}_{\text{Difusão molecular}} \\
&- \underbrace{\left(\overline{\rho u_i'' u_k''}\frac{\partial \widetilde{u}_j}{\partial x_k} + \overline{\rho u_j'' u_k''}\frac{\partial \widetilde{u}_i}{\partial x_k}\right)}_{\text{Termo de produção de turbulencia}} + \underbrace{\overline{p'\left(\frac{\partial u_i''}{\partial x_j} + \frac{\partial u_j''}{\partial x_i}\right)}}_{\text{Deformação por pressão}} - \underbrace{2\mu \overline{\frac{\partial u_i''}{\partial x_k}\frac{\partial u_j''}{\partial x_k}}}_{\text{Dissipação}}
\end{aligned}
\tag{46}
$$

Favre Averaging for the Reynolds Stress Tensor

The unknown terms: Turbulent Diffusion, Pressure-Strain Correlation and Dissipation are modelled as already presented for the RANS formulation with constant ρ.

The mean (of filtered) Reaction Rate

Consider a hypothetical time behavior of the concentrations of species A and B inside a reactor



The instantaneous reaction rate is

$$\dot{\omega}_i = -k_R c_A c_B = 0 \tag{47}$$

and the mean (or filtered) reaction rate is $\overline{\dot{\omega}}_i = 0$.

The mean (of filtered) Reaction Rate

If one attempts to calculate the mean reaction rate replacing the average of the product of the concentrations by the product of the average concentrations it yields

$$\overline{\dot{\omega}_i} = -k_R \overline{c_A c_B} = -k_R \left(\overline{c_A} . \overline{c_B} + \overline{c_A' c_B'} \right) \neq k_R \left(\overline{c_A} . \overline{c_B} \right) \tag{48}$$

The mean (of filtered) Reaction Rate

Como a taxa de reação é não linear, modelar os termos $\dot{\omega}_k$ não é simplesmente expressá-lo como uma função das quantidades filtradas $\widetilde{Y}_F$, $\widetilde{Y}_O$ e $\widetilde{T}$. Por meio de uma expansão em série de Taylor, obtem-se

$$\widetilde{\dot{\omega}}_F = -A\bar{\rho}^2\,\widetilde{T}^{\alpha}\,\widetilde{Y}_F\,\widetilde{Y}_O \exp\left(\frac{-T_a}{\widetilde{T}}\right)\left[1 + \frac{Y_O''}{\widetilde{Y}_O} + \frac{Y_F''}{\widetilde{Y}_F} + \frac{Y_F''\,Y_O''}{\widetilde{Y}_O\,\widetilde{Y}_F} + \right.$$
$$(P_1 + Q_1)\left(\frac{T''}{\widetilde{T}} + \frac{Y_F''\,T''}{\widetilde{T}\,\widetilde{Y}_F} + \frac{T''\,Y_O''}{\widetilde{Y}_O\,\widetilde{T}} + \frac{T''\,Y_F''\,Y_O''}{\widetilde{T}\,\widetilde{Y}_F\,\widetilde{Y}_O}\right)$$
$$\left. +(P_2 + P_1Q_1 + Q_2)\left(\frac{T''^2}{\widetilde{T}^2} + \frac{Y_F''\,T''^2}{\widetilde{T}^2\,\widetilde{Y}_F} + \frac{T''^2\,Y_O''}{\widetilde{Y}_O\,\widetilde{T}^2} + \frac{T''^2\,Y_F''\,Y_O''}{\widetilde{T}^2\,\widetilde{Y}_F\,\widetilde{Y}_O}\right) + \ldots\right] \tag{49}$$

The mean (of filtered) Reaction Rate

Após filtrar a temperatura, $T = \widetilde{T} + T^{''}$, dada uma função $f(T)$ tem-se que $f(T) = f(\widetilde{T} + T^{''})$. Expandindo $f(T)$ em série de Taylor obtem-se

$$f(T) = f(\widetilde{T} + T^{''}) = f(\widetilde{T}) + T^{''} f_{\widetilde{T}}(\widetilde{T}) + \frac{T^{''2}}{2} f_{\widetilde{T}\widetilde{T}}(\widetilde{T}) + O(T^{''3}), \quad (50)$$

The mean (of filtered) Reaction Rate

Assim, os termos T^α e $\exp(-T_a/T)$ após a filtragem são substituidos, respectivamente por

$$T^\alpha = \widetilde{T}^\alpha \left(1 + \sum_{n=1}^{\infty} Q_n \frac{T''^n}{\widetilde{T}^n}\right) = \widetilde{T}^\alpha \left(1 + \alpha \frac{T''}{\widetilde{T}} + \frac{\alpha(\alpha-1)}{2}\frac{T''^2}{\widetilde{T}^2} + O(T''^3)\right),$$

$$\begin{aligned}\exp\left(\frac{-T_a}{T}\right) &= \exp\left(\frac{-T_a}{\widetilde{T}}\right)\left(1 + \sum_{n=1}^{\infty} P_n \frac{T''^n}{\widetilde{T}^n}\right)\\ &= \exp\left(\frac{-T_a}{\widetilde{T}}\right)\left[1 + \frac{T_a}{\widetilde{T}}\frac{T''}{\widetilde{T}} + \left(\frac{T_a^2}{\widetilde{T}^4} - 2\frac{T_a}{\widetilde{T}^3}\right)\frac{T''^2}{2} + O(T''^3)\right),\end{aligned}$$

onde Q_n e P_n são dados pelas expressões

$$Q_n = \frac{1}{n!}\prod_{k=1}^{n}(\alpha - k - n) \quad \text{e} \quad P_n = \sum_{k=1}^{n} \frac{(n-1)!}{(n-k)![(k-1)!]^2 k}\left(\frac{T_a}{\widetilde{T}}\right)^n.$$

The mean (of filtered) Reaction Rate

So, the replacement of instantaneous values by its mean value, is valid only if

$$\frac{T_a.T^{''}}{\widetilde{T}^2} << 1 \tag{51}$$

Typical values of the activation temperature, $T_a = 15000$, $\widetilde{T} = 1500$ would limit the temperature fluctuation

$$\frac{15000.T^{''}}{1500^2} = 1 \tag{52}$$

on $T^{''} = 150$ or 10% of the mean value. In technical combustion process, fluctuations about 70% are observed.

Therefore a statistical description of the turbulence is required. Here we use the Presumed $\beta - PDF$ approach.

Favre decomposition

Carring out the Favre-decomposition for the mass fraction of specie k and modeling the unkown terms, one has

$$\frac{\partial \bar{\rho}\widetilde{Y_k}}{\partial t} + \frac{\partial \bar{\rho}\widetilde{Y_k}\widetilde{u_j}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D_k \frac{\partial \widetilde{Y_k}}{\partial x_j}\right) + \widetilde{\dot{\omega}_k}, \tag{53}$$

and for the mixture fraction

$$\frac{\partial \bar{\rho}\widetilde{f}}{\partial t} + \frac{\partial \bar{\rho}\widetilde{f}\widetilde{u_j}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D_t \frac{\partial \widetilde{f}}{\partial x_j}\right); \tag{54}$$

Favre decomposition

A transport equation for the Favre averaged variance of the mixture fraction can be obtained as

$$\frac{\partial \overline{\rho}\widetilde{f''^2}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}_i \widetilde{f''^2}}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\rho D_t \frac{\partial \widetilde{f''^2}}{\partial x_j}\right) = C_{g,1}\overline{\rho} D_{Eff} \left|\frac{\partial \widetilde{f}}{\partial x_i}\right|^2 C_{g,2}\overline{\rho}\frac{\varepsilon}{k}\widetilde{f''^2} \quad (55)$$

where D_{Eff} is the effective coeficient of difusivity, including the turbulence effect. $C_{g,1} = 2.8$ e $C_{g,2} = 2$.

The Favre averaged absolute enthalpy equation reads

$$\frac{\partial \bar{\rho}\widetilde{h}}{\partial t} + \frac{\partial \bar{\rho}\widetilde{h}\widetilde{u}_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_t}\frac{\partial \widetilde{h}}{\partial x_j}\right), \quad (56)$$