Suggested solutions TEP4170 Heat and combustion technology 25 May 2016
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1)

Introduce the Reynolds decomposition: $u_i = \overline{u}_i + u_i'$ (mean and fluctuation) into the given equation.

Average the equation.

Apply the rules for averaging (obtainable from the definition of averaging):

$$\overline{a+b} = \overline{a} + \overline{b} \ ; \ \overline{a'} = 0; \ \overline{\frac{\partial a}{\partial t}} = \frac{\partial \overline{a}}{\partial t} \ ; \ \overline{\overline{a} \cdot \overline{b}} = \overline{a} \cdot \overline{b} \ ; \ \overline{\overline{a} \cdot b} = \overline{a} \cdot \overline{b}$$

where a and b are variables (also products of variables).

$$\frac{\partial}{\partial t}(\overline{\rho \overline{u}_i} + \overline{\rho u_i'}) + \frac{\partial}{\partial x_j}(\overline{\rho \overline{u}_i \overline{u}_j} + \overline{\rho \overline{u}_i u_j'} + \overline{\rho u_i' \overline{u}_j} + \overline{\rho u_i' u_j'}) = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}(\overline{\tau_{ij}}) + \overline{\rho f_i}$$

Note: in principle, the density ρ can be decomposed. This is not required here. Density can be assumed constant, or (more precise) not to correlate with the velocity components.

The body-force acceleration f_i is usually constant (gravity).

The terms including the average of <u>one</u> fluctuating component will be zero, e.g. $\overline{\rho \overline{u}_i u_j'} = \rho \overline{u}_i \cdot \overline{u_j'} = 0$.

The other terms have to be kept. It is customary (but, strictly, not required) to move the two-fluctuation term to the RHS:

$$\frac{\partial}{\partial t}(\rho \overline{u}_i) + \frac{\partial}{\partial x_j}(\rho \overline{u}_i \overline{u}_j) = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}(\overline{\tau_{ij}} - \rho \overline{u_i' u_j'}) + \overline{\rho f_i}$$

Note 2: The pressure can be decomposed into mean and fluctuation. In this equation this is not necessary, since the pressure appears in the gradient as a term on its own. The average pressure appears when this term is treated according to the procedure.

The average behaviour is maintained, while much of the information of the instantaneous variation of the velocity and pressure (and density) is lost. Some effects of fluctuations on the mean flow are retained in the Reynolds stresses.

The Reynolds stresses originates from the convective term and expresses mean momentum transfer due to turbulent motions (fluctuating velocities). Seen from the mean flow, this is a diffusive effect (i.e. stresses when the matter is momentum). The effect is like enhancing the stresses of the flow.

2)

The Reynolds stresses are in general expressed from

$$-\rho \overline{u_i' u_j'} = \mu_t \left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} - \frac{2}{3}\frac{\partial \overline{u}_l}{\partial x_l}\delta_{ij} \right) - \frac{2}{3}\rho k \delta_{ij}, \text{ where } \mu_t = \rho C_\mu \frac{k^2}{\varepsilon}.$$

μ_t is the turbulence viscosity, k is the turbulence energy ; ε is the dissipation rate of turbulence energy (sink term of the k equation); C_μ is a modelling constant; δ_{ij} is =1 for $i = j$, =0 for $i \neq j$.

The Reynolds fluxes of species mass can be expressed from

$$-\rho \overline{Y_k' u_j'} = \rho D_t \frac{\partial \overline{Y}_k}{\partial x_j} = \frac{\mu_t}{\sigma_Y} \frac{\partial \overline{Y}_k}{\partial x_j},$$

where Y_k is the mass fraction of species k; D_t is the turbulence mass diffusivity; σ_Y is the turbulence Schmidt number (usually set as constant).

3)

Definitions: $u_1^+ = \dfrac{\overline{u}_1}{u_\tau}$; $u_\tau = \left(\tau_w / \rho\right)^{1/2}$; $x_2^+ = \dfrac{x_2 u_\tau}{\nu}$;

where $\overline{u}_1$ is the streamwise mean velocity of a boundary layer flow; x_2 is the coordinate normal to the wall; τ_w is the shear stress at the wall; ρ is the density of the fluid; ν is the kinematic viscosity of the fluid; u_τ is the shear velocity.

Near a wall, gradients parallel to the wall are much smaller than those normal to the wall, and velocities approaches zero, so that the mean momentum equation simplifies to

$0 = \dfrac{d}{dx_2}\left(\overline{\tau}_{12} - \rho\overline{u_1'u_2'}\right)$, or $\overline{\tau}_{12} - \rho\overline{u_1'u_2'} = \text{const}$. The constant has to equal the wall shear stress, τ_w .

Very close to the wall, viscous stress dominates; thus $\overline{\tau}_{12} \gg (-\rho\overline{u_1'u_2'})$ and $\overline{\tau}_{12} = \rho\nu\dfrac{d\overline{u}_1}{dx_2} = \tau_w$

The expression can be rearranged to $d\overline{u}_1 = \dfrac{\tau_w}{\rho\nu}dx_2 = u_\tau^2\dfrac{dx_2}{\nu}$ or $d\left(\dfrac{\overline{u}_1}{u_\tau}\right) = d\left(\dfrac{u_\tau x_2}{\nu}\right)$, assuming that the

viscosity is constant. This can be written as $du_1^+ = dx_2^+$, and integrated: $u_1^+ = x_2^+ + C_w$.

Since $\overline{u}_1(x_2 = 0) = 0$, the integration constant C_w is zero, and we have obtained the first part of the given expression: $u_1^+ = x_2^+$

For somewhat larger values of x_2, experiments show that $\dfrac{d\overline{u}_1}{dx_2} = \dfrac{u_\tau}{\kappa x_2}$, where κ is a constant.

Rearranging this gives $\dfrac{d\overline{u}_1}{u_\tau} = d\left(\dfrac{\overline{u}_1}{u_\tau}\right) = \dfrac{1}{\kappa}\dfrac{dx_2}{x_2} = \dfrac{1}{\kappa}\dfrac{d(x_2 u_\tau/\nu)}{(x_2 u_\tau/\nu)}$ or $du_1^+ = \dfrac{1}{\kappa}\dfrac{dx_2^+}{x_2^+}$

Integrating this gives $u_1^+ = \dfrac{1}{\kappa}\ln x_2^+ + C$, which is the second part of the given expression.

κ and C are empirical constants

The practical use is as a wall-function boundary condition for velocity in CFD. Avoid very fine resolution near a wall.

4)
A conserved scalar is a property with zero source (or sink) term.
Examples: The elemental mass fractions; the enthalpy if all source terms can be neglected (radiation, pressure effects, body-force effects, viscous dissipation etc.); combinations of mass fractions that give zero

source: $\left(Y_{fu} - \dfrac{1}{r}Y_{ox}\right)$; $\left(Y_{fu} + \dfrac{1}{1+r}Y_{pr}\right)$ and $\left(Y_{ox} + \dfrac{r}{1+r}Y_{pr}\right)$, when the reaction balance is assumed as

$1\text{ kg fu} + r\text{ kg ox} \rightarrow (1+r)\text{ kg pr}$
In principle, the mixture fraction (below) is also a conserved scalar.

Mixture fraction, definition: $\xi = \dfrac{\varphi_{mix} - \varphi_2}{\varphi_1 - \varphi_2}$; where φ is a conserved scalar (other than the mixture fraction itself), φ_1 and φ_2 are its values at two different inflows, and φ_{mix} its value in the mixture.

The mixture fraction of a stoichiometric mixture of propane and air (21% O_2, 79 % N_2, molar):

Alternative I:

Use the conserved scalar $\varphi = \left(Y_{fu} - \dfrac{1}{r} Y_{ox} \right)$; inlet 1 is fuel: $\varphi_1 = Y_{fu,1} = 1$; Inlet 2 is air (oxidizer):

$\varphi_2 = -\dfrac{1}{r} Y_{ox,2} = -\dfrac{1}{r}$; stoichiometric mixture means $Y_{fu} = Y_{ox}/r$ and thus $\varphi_{mix} = 0$.

The stoichiometric amount of air (mass based): $r = \dfrac{m_{ox}}{m_{fu}} = \dfrac{5 \cdot \left(M_{O_2} + \frac{0.79}{0.21} M_{N_2} \right)}{M_{C_3H_8}} = \dfrac{5 \cdot \left(32 + \frac{0.79}{0.21} 28 \right)}{44} = 15.61$

Combined: $\xi_{st} = \dfrac{0 - \left(-r^{-1} \right)}{1 - \left(-r^{-1} \right)} = \dfrac{1}{1+r} = \dfrac{1}{1+15.61} = 0.0602$

Alternative II:
Use the knowledge that the mixture fraction is the ratio of the mass from fuel inlet to the total mass (fuel+air). Thus, for stoichiometric conditions: $\xi_{st} = 1/(1+r)$, with further calculations as in Alternative I.
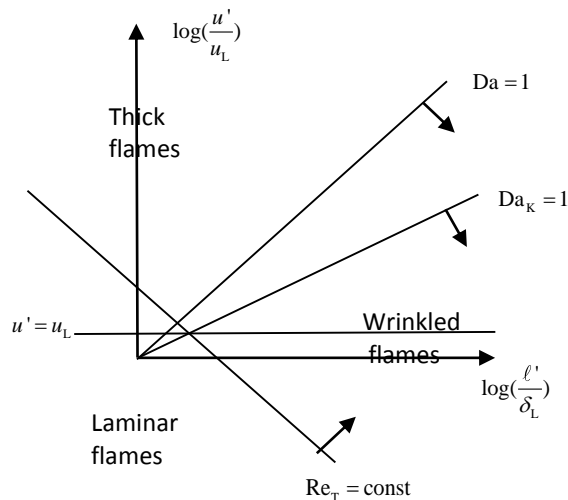
5)
$$\frac{d[OH]}{dt} = 2k_{f2}[O][H_2O] - 2k_{r2}[OH]^2 - k_{f3}[CO][OH] + k_{r3}[CO_2][H] + k_{f4}[H][O_2] - k_{r4}[OH][O]$$

In Reaction 1forward, the reactants are stable species. All the other reactions (including Reaction 1 reverse) involve a radical as reactant, which is very reactive and these reactions are likely to be "fast". Thus Reaction 1forward can be suspected to be slower.

6)
Borghi diagram, premixed flames

u': turbulence velocity ($\sim k^{1/2}$)
ℓ': turbulence length scale
u_L: laminar flame speed
δ_L: laminar flame thickness
$Da = \theta/\tau_c$: Damköhler number
$Da_K = \tau/\tau_c$: Damköhler number
$\tau_c = \delta_L/u_L$: chemical timescale
$\theta = k/\varepsilon \sim \ell'/u'$: "large" turbulence timescale
τ : Kolmogorov timescale
$Re_T = k^2/(\nu\varepsilon) \sim u'\ell'/\nu$: turbulence Reynolds number

7)
Main parts of EDC and purposes:
- The cascade model: Provide a link between the "fine structures" (small scales), where reactions occur, and the large scales, which are represented by a
turbulence model. It express characteristic quantities of the fine structures in terms of quantities obtained by the turbulence model.
- The reactor model: Provide the reaction rates for fine structures and the mean reaction rates.

EDC provides the source term for the averaged species mass balances. For CFD (here restricted to solutions of averaged basic equations, aka. RANS), the following is needed in addition:
- Turbulence model (provide the Reynolds stresses and a turbulence time scale; if relevant, a turbulence viscosity)
- A model for turbulence diffusion of scalars(the Reynolds fluxes of scalars)
- Radiation model (if radiation heat transfer is important)
- Constitutive laws (Fourier's law, Fick's law, Newton's viscous stress relation) and thermal properties (conductivity, diffusivity, viscosity)
- Relations between enthalpy (and/or specific heat) and temperature.
- A chemical mechanism (can be simple or complex).

8)
The expression is based on the reactor model of EDC.

Put up the mass balance for a species: $\dot{M}_{\text{in}} Y_k^o - \dot{M}_{\text{out}} Y_k^* = -R_k^* \dfrac{M_{\text{FS}}}{\rho^*}$

Assume that the reactor is steady state, $\dot{M}_{\text{in}} = \dot{M}_{\text{out}} = \dot{M}$

Introduce $\dot{m}^* = \dot{M}/M_{\text{FS}}$, and rearrange to $-R_k^* = \rho^* \dot{m}^* \left(Y_k^o - Y_k^* \right)$

$\gamma^* = M_{\text{FS}} / M_{\text{tot}}$ is the ratio of mass in fine structures to the total mass.

Assume that all reactions take place in the "fine structures"; since R_k is reactions per volume

(=mass/density) and time, this means $\bar{R}_k = \left(R_k^* \dfrac{M_{\text{FS}}}{\rho^*} \right) \left(\dfrac{M_{\text{tot}}}{\bar{\rho}} \right)^{-1} = \dfrac{\bar{\rho}}{\rho^*} \gamma^* R_k^*$

This is the case if all the fine structure reacts. Since this may not be the case, the reactions can take place in

a certain fraction χ of the fine structures, hence $\bar{R}_k = \dfrac{\bar{\rho}}{\rho^*} \gamma^* \chi R_k^*$. With the expression for R_k^* introduced,
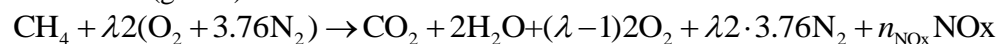
this gives $\bar{R}_k = \bar{\rho} \dot{m}^* \gamma^* \chi \left(Y_k^o - Y_k^* \right)$

Using the symbol $\dot{m} = \gamma^* \dot{m}^*$ and the mass-fractions relation given in the problem, the requested relation is

obtained: $\bar{R}_k = -\dfrac{\bar{\rho} \dot{m} \chi}{1 - \gamma^* \chi} (\tilde{Y}_k - Y_k^*)$

9)
The overall (global) reaction balance can be written as:
$$CH_4 + \lambda 2(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + (\lambda-1)2O_2 + \lambda 2 \cdot 3.76N_2 + n_{\text{NOx}} NOx$$

The amount of NOx is very small, thus the assumption $n_{\text{NOx}} \ll 1$ can simplify some calculations.

The amount of substance of flue gas including H_2O ("wet") per kmol of fuel (neglecting NOx):

$$\frac{n_{\text{wet}}}{n_{\text{fuel}}} = 1 + 2 + 2(\lambda - 1) + 7.52\lambda = 1 + 9.52\lambda$$

The (actual) molar fraction of O_2 (wet): $\dfrac{n_{O_2}}{n_{\text{wet}}} = \dfrac{2(\lambda - 1)}{1 + 9.52\lambda} = 0.13$

$\rightarrow \lambda(2 - 0.13 \cdot 9.52) = 2 + 0.13 \rightarrow \lambda = 2.79$

This is the actual air excess ratio, which also gives $\dfrac{n_{\text{wet}}}{n_{\text{fuel}}} = 27.56$

Excluding the H_2O ("dry"): $\dfrac{n_{\text{dry}}}{n_{\text{fuel}}} = 1 + 2(\lambda - 1) + 7.52\lambda = -1 + 9.52\lambda = -1 + 9.52 \cdot 2.79 = 25.56$

Alternatively: $\dfrac{n_{\text{dry}}}{n_{\text{fuel}}} = \dfrac{n_{\text{wet}} - n_{\text{H}_2\text{O}}}{n_{\text{fuel}}} = 27.56 - 2 = 25.56$

The content (molar fraction or volume fraction) of NOx at dry conditions

$$\frac{n_{\text{NOx}}}{n_{\text{dry}}} = \frac{n_{\text{NOx}}}{n_{\text{wet}}} \cdot \frac{n_{\text{wet}}}{n_{\text{dry}}} = 20 \cdot 10^{-6} \frac{27.56}{25.56} = 21.6 \cdot 10^{-6} = \underline{21.6 \text{ ppm}}$$

The regulations ("reference") are specified for $\dfrac{n_{O_2,\text{ref}}}{n_{\text{wet,ref}}} = \dfrac{2(\lambda_{\text{ref}} - 1)}{1 + 9.52\lambda_{\text{ref}}} = 0.15$

$\rightarrow \lambda_{\text{ref}}(2 - 0.15 \cdot 9.52) = 2 + 0.15 \rightarrow \lambda_{\text{ref}} = 3.76$

This is the reference air excess ratio, which gives $\dfrac{n_{\text{wet,ref}}}{n_{\text{fuel}}} = 1 + 9.52 \cdot 3.76 = 36.80$

The corrected or "reference" molar fraction of NOx becomes

$$\left(X_{\text{NOx}}\right)_{\text{dry}} = \frac{n_{\text{NOx}}}{n_{\text{wet,ref}}} = \frac{n_{\text{NOx}}}{n_{\text{wet}}} \cdot \frac{n_{\text{wet}}}{n_{\text{wet,ref}}} = 20 \cdot 10^{-6} \frac{27.56}{36.80} = 15.0 \cdot 10^{-6} = \underline{15.0 \text{ ppm}}$$

The emission index: $\text{EI}_{\text{NO}} = \dfrac{m_{\text{NO}}}{m_{\text{fu}}} = \dfrac{n_{\text{NO}} M_{\text{NO}}}{n_{\text{fuel}} M_{\text{fuel}}} = \dfrac{n_{\text{NO}}}{n_{\text{wet}}} \dfrac{n_{\text{wet}} M_{\text{NO}}}{n_{\text{fuel}} M_{\text{fuel}}} = 20 \cdot 10^{-6} \cdot 27.56 \dfrac{30}{16} = 1.03 \cdot 10^{-3} \dfrac{\text{kg}}{\text{kg}}$

Mass of NO per fuel lower heating value:

$$\frac{m_{\text{NO}}}{H_{\text{fuel}}} = \frac{m_{\text{NO}}}{m_{\text{fuel}} h_{\text{LHV}}} = \text{EI}_{\text{NO}} \frac{1}{h_{\text{LHV}}} = 1.03 \cdot 10^{-3} \frac{\text{kg}}{\text{kg}} \frac{\text{kg}}{50 \text{ MJ}} = 20.6 \cdot 10^{-6} \frac{\text{kg}}{\text{MJ}}$$

10)
Exhaust gas recirculation
- Reduce oxygen content (mole fraction)
- Increase specific heating capacity c_p of flue gas – lower temperature (less thermal NOx)
- May reduce fuel concentration (less Fennimore/prompt NOx)
- May reduce temperature fluctuations, i.e. peak temperatures