Suggested solutions TEP4170 Heat and combustion technology 30 May 2011

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1)

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, velocitites approaches zero, so that the mean momentum equation simplifies to

$$0 = \frac{\partial}{\partial x_2} \left(\overline{\tau}_{12} - \rho \overline{u_1' u_2'} \right), \text{ or } \overline{\tau}_{12} - \rho \overline{u_1' u_2'} = \text{const}$$

Very close to the wall, viscous stress dominates; thus $\overline{\tau}_{12} \gg \rho \overline{u_1' u_2'}$ and $\overline{\tau}_{12} = \rho \nu \dfrac{\partial \overline{u}_1}{\partial x_2} = \text{const}$

The constant has to equal the wall stress, τ_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 written $du_1^+ = dx_2^+$, and integrated: $u_1^+ = x_2^+ + C_w$. Since $\overline{u}_1(x_2 = 0) = 0$, the integration constant 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 $u_1^+ = \ln x_2^+ + C$, which is the second part of the given expression.

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

2)
The basic momentum equation can be written as

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}(\tau_{ij}) + \rho f_i$$

Introduce the Reynolds decomposition, $u_i = \overline{u}_i + u_i'$; assume that ρ is constant (or that it does not correlate with velocity):

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

Average the entire equation, that is, each term. Here $\overline{\overline{u}_i} = \overline{u}_i$; $\overline{u'_i} = 0$; $\overline{\overline{u}_i u'_j} = \overline{u}_i \cdot \overline{u'_j} = 0$, and we achieve the given equation (when the double-correlation term is moved over the the right-hand side).

The terms are (enumerated from left): 1) change of mean momentum with time; 2) transfer of mean momentum with mean flow; 3) mean pressure change in direction of the velocity component; 4) viscous transport/exchange of mean momentum; 5) transport/exchange of mean momentum due to turbulent motions; 6) influence of body forces (e.g. gravity).

The 5th term have to be modeled. The remaining terms are expressed from quantities already included in the problem.

3)

Steady state: $\dfrac{\partial}{\partial t}(\ ) = 0$; 2-dimensional: $\dfrac{\partial}{\partial x_3}(\ ) = 0$ and $\overline{u}_3 = 0$; Boundary layer (with x_2 normal to the wall): $\overline{u}_1 \gg \overline{u}_2$ and $\dfrac{\partial}{\partial x_1}(\ ) \ll \dfrac{\partial}{\partial x_2}(\ )$. Notice that the two convective terms for $\rho\overline{u}_1$ do not cancel. For a horizontal flow, the gravity is zero ($f_1 = 0$), but this is not general (since the flow can e.g. be vertical). The equation for the streamwise direction becomes

$$\frac{\partial}{\partial x_1}(\rho\overline{u}_1\overline{u}_1) + \frac{\partial}{\partial x_2}(\rho\overline{u}_1\overline{u}_2) = -\frac{\partial \overline{p}}{\partial x_1} + \frac{\partial}{\partial x_2}(\overline{\tau}_{12} - \rho\overline{u'_1 u'_2}) + \rho\overline{f}_1$$

(In the equation for the transverse direction, $\rho\overline{u}_2$, most terms cancels, and we are left with a relation between pressure and a normal turbulence stress. This was not expected developed in this problem.)

4)
The equation given in Problem 2 is a statistical or Reynolds-averaged equation. All turbulent motions are "filtered" away from the solution, and only the mean (averaged) motions are left. The effects of the turbulence have to be included through models for the Reynolds stresses.
In LES, only small-scale motions are "filtered", while large eddies are included in the solution. The small eddies are thought to be more more universal than the large; that is, less dependent on the external geometry of the flow. The effects of the small eddies have to be modeled.
When using Reynolds-averaged equations, the mean flow can (depending on the case) be considered non-transient and/or 2-dimensional. On the contrary, these approximations cannot be made with LES.

5)
For a global reaction, fuel + oxidizer $\rightarrow$ product, see sketch.

The burning velocity (flame speed) is the velocity of the unburned flow, $S_L = v_u$; the flame thickness is defined by the length δ where the temperature increase takes place; which is also the length where fuel is consumed and products are produced. The chemical timescale is the ratio of these, $\tau_c = \delta / S_L$ (Alternatively, the time scale can be defined in relation to the fuel reaction rate.)

For a multitude of (elementary) reactions, each reaction has its timescale and length scale. Some reactions occur only in a very thin zone; they are fast and consume species present only in a very

thin zone. These reactions have small time- and length scales. Other reactions occur over very long time and length.

6)
The relevant equations are the continuity, species conservation and energy conservation equations on one-dimensional, non-transient form. Here in the notation from Turns

Continuity: $\dfrac{d\dot{m}''}{dt} = 0$ or expressed with $\dot{m}'' = \rho v_x$

Species conservation: $\dot{m}'' \dfrac{dY_i}{dx} + \dfrac{d}{dx}\left(\rho Y_i v_{i,\text{diff}}\right) = \dot{\omega}_i M_i$ for $i = 1, 2, ..., N$ species

Energy conservation: $\dot{m}'' c_p \dfrac{dT}{dx} + \dfrac{d}{dx}\left(-k\dfrac{dT}{dx}\right) + \displaystyle\sum_{i=1}^{N}\rho Y_i v_{i,\text{diff}} c_{p,i}\dfrac{dT}{dx} = -\displaystyle\sum_{i=1}^{N} h_i \dot{\omega}_i M_i$

(notation and details can be different)

Quantities that have to be modeled (with the equations formulated as above): diffusion velocity $v_{i,\text{diff}}$ (e.g. by Ficks law) and reaction rate $\dot{\omega}_i$ (from Arrhenius expression). The expressions for $c_{p,i}(T)$ and $h_i(T)$, $k(T, Y_i)$ and the equation of state can also be regarded as models.

Boundary conditions: for $x = -\infty$: $T = T_u$; $Y_i = Y_{i,o}$; for $x = \infty$: $\dfrac{dT}{dx} = 0$; $\dfrac{dY_i}{dx} = 0$

7)
CO.1 is slow, initiating; does not contribute much to CO_2 formation, but important for initiating.
CO.2 is fast, chain branching (consume one radical, produce two). Speeds up the global reaction.
CO.3 is fast, chain propagating (consume one radical, produce one). Produce much CO2
CO.4 is chain branching, increase reaction
CO.2 and CO.4 supplies CO.3 with OH

If H_2 is present, the entire H_2-O-CO mechanism has to be considered (approx 20 elementary reactions).

8)
Reaction NO.2 is much faster than Reaction NO.1. N is mainly consumed as soon as it is available. This opens for assuming that N is in steady state, that is, the consumption and formation is in balance:

$\dfrac{d[N]}{dt} = k_1[O][N_2] - k_2[O_2][N] = 0$, where k_1 and k_2 are the rate constants for Reactions NO.1 and NO.2.

Hence, $[N]_{ss} = \dfrac{k_1[O][N_2]}{k_2[O_2]}$.
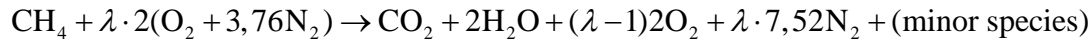
This can be used to express the change of other species, in the example here, NO:

$\dfrac{d[NO]}{dt} = k_1[O][N_2] + k_2[O_2][N] = k_1[O][N_2] + k_2[O_2]\dfrac{k_1[O][N_2]}{k_2[O_2]} = 2k_1[O][N_2]$

(This shows that Reaction NO.1 is rate determining for NO formation; although this is not asked for in this problem.)

9)

The global reaction balance can be written as

$$CH_4 + \lambda \cdot 2(O_2 + 3,76N_2) \rightarrow CO_2 + 2H_2O + (\lambda-1)2O_2 + \lambda \cdot 7,52N_2 + (\text{minor species})$$

where the amounts of minor species is assumed to be much smaller than the major species mentioned.

The amount of fuel can be approximated as $n_F = n_{CO_2} + n_{CO}$

The amount of product is $n_P = n_{CO_2} + n_{H_2O} + n_{O_2} + n_{N_2} = 1 + 2 + 2\lambda - 2 + 7,52 \cdot \lambda = 1 + 9,52 \cdot \lambda$
(minor species neglected)

The emission index for CO:

$$EI_{CO} = \frac{m_{CO}}{m_F} = \frac{n_{CO}M_{CO}}{n_F M_F} = \frac{n_{CO}M_{CO}}{(n_{CO_2} + n_{CO})M_F} = \frac{X_{CO}M_{CO}}{(X_{CO_2} + X_{CO})M_F} = \frac{100 \cdot 10^{-6} \cdot 28}{(0,036 + 0,0001) \cdot 16} = 4,86 \cdot 10^{-3}$$

The oxygen mole fraction is $X_{O_2} = \frac{n_{O_2}}{n_P} = \frac{(\lambda-1) \cdot 2}{1 + 9,52 \cdot \lambda}$; the actual value of 0,130 gives $\lambda = 2,80$

The reference value of $X_{O_2,15\%} = 0,150$ gives $\lambda = \lambda_{15\%} = 3,77$. This is the excess air that would give mole fractions that can be compared to the regulations. Since the amount of CO is the same, the mole fraction with the higher amount of air becomes

$$X_{CO,15\%} = \frac{n_{CO}}{n_{P,15\%}} = \frac{n_{CO}}{n_P} \frac{n_P}{n_{P,15\%}} = X_{CO} \frac{1 + 9,52 \cdot \lambda}{1 + 9,52 \cdot \lambda_{15\%}} = 100 \cdot 10^{-6} \frac{1 + 9,52 \cdot 2,80}{1 + 9,52 \cdot 3,77} = 75 \cdot 10^{-6} = 75 \text{ ppm}$$

10)

See sketch in Turns (fig. 14.7).
Solid surface | CO/CO$_2$ zone | flame sheet | O$_2$/CO$_2$ zone - free air

Solid carbon reacts with CO$_2$ on the surface: $C + CO_2 \rightarrow 2CO$

CO diffuses towards flame sheet where it reacts with oxygen: $CO + \frac{1}{2}O_2 \rightarrow CO_2$

CO$_2$ diffuses inward to surface and outward to free air; O$_2$ diffuses from free air to the flame sheet

One-film model: reaction $C + O_2 \rightarrow CO_2$ at the surface; no flame sheet and no CO considered.

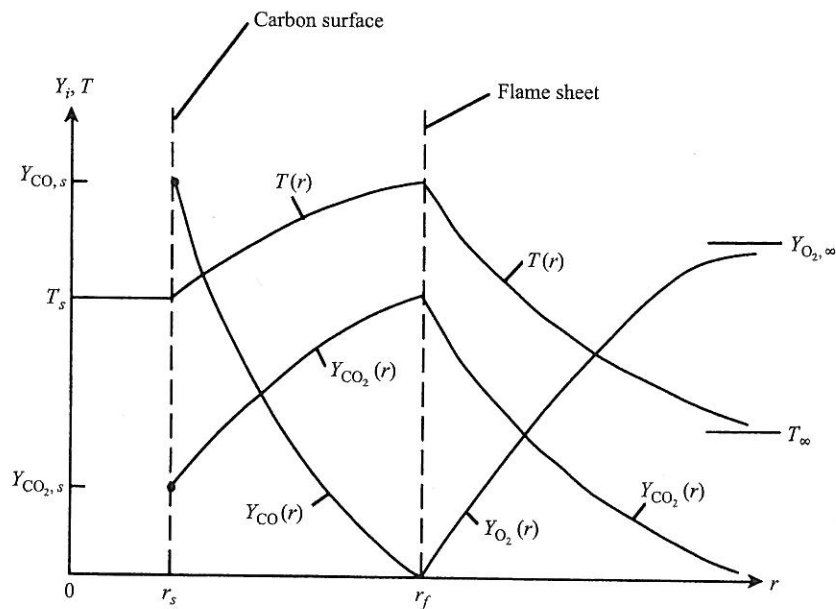skisse til nr. 5
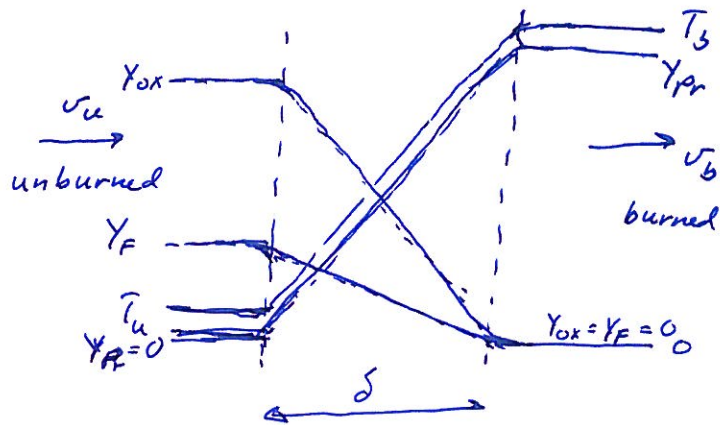
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Figure 14.7 Species mass fractions and temperature profiles for a two-film model of a burning spherical carbon particle.