

Suggested solutions TEP4170 Heat and combustion technology 16 May 2017

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1)

Sketch: see textbook.

Main elements:

- the transverse motion from one position to another with (transverse) distance ℓ causes a streamwise

velocity difference $u' = \Delta u = \ell \frac{du}{dy}$,

- due to continuity, the transverse velocity disturbance will be of the same magnitude, $v' \sim u'$

- the transfer of momentum due to the motion (aka turbulence stress) is represented by these quantities,

$$\tau_{\text{turb}} = -\overline{\rho u'_1 u'_2} \sim \rho u' \cdot v' \sim \rho \ell \frac{d\bar{u}}{dy} \cdot \ell \frac{d\bar{u}}{dy} = \rho \ell^2 \left(\frac{d\bar{u}}{dy} \right)^2$$

- the sign of the stress has to be that of the gradient; and the constant of proportionality can be absorbed into the length scale. Hence (with the coordinate symbols used in the problem),

$$-\overline{\rho u'_1 u'_2} = \rho \ell^2 \left| \frac{d\bar{u}_1}{dx_2} \right| \cdot \frac{d\bar{u}_1}{dx_2}$$

- Expressed with a turbulence viscosity, the turbulence stress is $-\overline{\rho u'_1 u'_2} = \rho \nu_t \cdot \frac{d\bar{u}_1}{dx_2}$

Combining the latter two expressions, we get $\nu_t = \ell^2 \left| \frac{d\bar{u}_1}{dx_2} \right|$.

(Alternatively, include the density to form the dynamic turbulence viscosity $\mu_t = \rho \nu_t$)

2)

Definitions: $u_\tau = (\tau_w / \rho)^{1/2}$

where \bar{u}_1 is the streamwise mean velocity of a boundary layer flow; x_2 is the coordinate normal to the wall

($x_2 = 0$ at the wall); $u_\tau = (\tau_w / \rho)^{1/2}$ is the shear velocity; τ_w is the shear stress at the wall; ρ is the density of the fluid; κ is an empirical constant (von Kármán constant) for boundary layer flows.

Assume a simple boundary layer; flow along a plane wall, one dominating mean velocity gradient.

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

$$0 = \frac{d}{dx_2} (\bar{\tau}_{12} - \overline{\rho u'_1 u'_2}), \text{ or } \bar{\tau}_{12} - \overline{\rho u'_1 u'_2} = \text{const. The constant has to equal the wall shear stress, } \tau_w = \rho u_\tau^2.$$

In a part of this near-wall zone, the turbulence stress dominates. Hence, $-\overline{u'_1 u'_2} = \tau_w / \rho = u_\tau^2$

In this zone, assume balance between production and dissipation of turbulence energy: $\rho \varepsilon = -\overline{\rho u'_1 u'_2} \frac{d\bar{u}_1}{dx_2}$

Introduce the quantities for the shear stress and the gradient; $\varepsilon = u_\tau^2 \frac{u_\tau}{\kappa x_2} = \frac{u_\tau^3}{\kappa x_2}$ This is the wall function

for the dissipation rate.

The turbulence shear stress can be expressed from a turbulence viscosity: $-\overline{\rho u'_1 u'_2} = \rho \nu_t \cdot \frac{d\bar{u}_1}{dx_2}$

Introducing $\tau_w = \rho u_\tau^2$ for the stress and the given relation for the gradient gives $\overline{\rho u_\tau^2} = \rho v_t \cdot \frac{u_\tau}{\kappa x_2}$.

This can be rearranged to $v_t = \kappa u_\tau x_2$.

3)

The given relation is developed for the same zone as the one given in Problem 2; that is, the near wall zone of a wall boundary layer (although not the very thin layer just adjacent to the wall)

The heat flux directed from the wall can be expressed as $q_2 = -\rho C_p \left(\frac{\nu}{\sigma} + \frac{v_t}{\sigma_T} \right) \frac{d\bar{T}}{dx_2}$,

where σ and σ_T are the molecular and turbulence Prandtl numbers, respectively, and C_p is the specific heat capacity. These are assumed as constants in the near-wall layer. Furthermore, in this layer, the heat flux can be approximated to a constant, which has to be that at the wall; $q_2 = q_w$.

Rearranging the expression, and using $v_t = \kappa u_\tau x_2$ (from Problem 2)

$$\frac{-\rho C_p}{q_w} dT = \frac{dx_2}{\nu \left(\frac{1}{\sigma} + \frac{\kappa}{\sigma_T} \frac{u_\tau x_2}{\nu} \right)}, \text{ or } \frac{-\rho C_p u_\tau}{q_w} dT = \frac{d \left(\frac{u_\tau x_2}{\nu} \right)}{\left(\frac{1}{\sigma} + \frac{\kappa}{\sigma_T} \frac{u_\tau x_2}{\nu} \right)}, \text{ or } \frac{-\rho C_p u_\tau}{q_w} dT = \frac{dx_2^+}{\left(\frac{1}{\sigma} + \frac{\kappa}{\sigma_T} x_2^+ \right)}$$

Integrating the left-hand side from the wall (temperature T_w at $x_2 = 0$) to a point in the layer (temperature

$$\bar{T} \text{ at } x_2), \text{ LHS} = \int_{T_w}^{\bar{T}} \frac{-\rho C_p u_\tau}{q_w} dT = \frac{-\rho C_p u_\tau}{q_w} (\bar{T} - T_w).$$

This equals the non-dimensional temperature, $T^+ = \text{LHS}$ (given in the problem).

Integration of the right-hand side have to be done in two steps. For the thin layer at the wall, molecular diffusion dominates, while in the next layer, the turbulence diffusion dominates. The boundary between these two zones is denoted $x_{2,d}$

$$\text{RHS} = \int_0^{x_{2,d}^+} \sigma dx_2^+ + \int_{x_{2,d}^+}^{x_2^+} \frac{\sigma_T}{\kappa} \frac{dx_2^+}{x_2^+} = \text{const}_1 + \frac{\sigma_T}{\kappa} \ln x_2^+ - \frac{\sigma_T}{\kappa} \ln x_{2,d}^+$$

Here, the last term is a constant, and the two constant terms can be merged into one constant, C_T ;

furthermore, the quantity $\kappa_T = \kappa / \sigma_T$ is introduced. Now, $\text{RHS} = \frac{1}{\kappa_T} \ln x_2^+ + C_T$

Setting the LHS and RHS together, we obtain the expression given in the problem.

4)

Multidimensional joint pdf:

- The state is a set of velocities and scalars $(u_1, u_2, u_3, \theta_1, \dots, \theta_n)$, i.e. a multidimensional vector.
- The state is realized with a (multi dimensional) distribution function F , and the corresponding pdf f .
- Any quantity, say G , can be described as a function of the state (the vector of variables)
- The mean value of this quantity is found as the integral of the quantity and the pdf over the realization of all variables.

The pdf is found from solving a “transport” equation for it. This equation contains terms for convection, body forces, pressure and reactions, viscous forces and molecular diffusion. Among these, the viscous and diffusive terms need modelling, while the reaction terms are closed and need no further modeling. (contrary to the corresponding terms e.g. in Reynolds averaged equations)

5)

The mixture fraction ξ is defined by $\xi = \frac{\varphi_{mix} - \varphi_2}{\varphi_1 - \varphi_2}$; or $\varphi_{mix} = \varphi_1 \xi + \varphi_2 (1 - \xi)$

where φ is a conserved scalar, φ_1 and φ_2 are its values at two different inflows (1) and (2), and φ_{mix} its value in the mixture.

A conserved scalar is a property with zero source (or sink) term.

The reaction balance is assumed as a single-step global reaction $1 \text{ kg fu} + r \text{ kg ox} \rightarrow (1+r) \text{ kg pr}$, which is fast and complete. r is the stoichiometric mass of air, here given as $r = 17,1 \text{ kg/kg}$.

the reaction rates (source terms) are related as $R_{fu} = \frac{1}{r} R_{ox} = \frac{1}{1+r} R_{prod}$

The combined term $R_{fu} - \frac{1}{r} R_{ox}$ becomes zero, and it is the source term of $\left(Y_{fu} - \frac{1}{r} Y_{ox} \right)$, which therefore is a conserved scalar.

If inlet (1) contains pure fuel ($Y_{fu,1} = 1, Y_{ox,1} = 0$) and inlet (2) is pure oxidizer (air) ($Y_{fu,2} = 0, Y_{ox,2} = 1$), the compound function can be expressed as

$$\left(Y_{fu} - \frac{1}{r} Y_{ox} \right) = \left(Y_{fu} - \frac{1}{r} Y_{ox} \right)_1 \xi + \left(Y_{fu} - \frac{1}{r} Y_{ox} \right)_2 (1 - \xi) = (1 - 0) \cdot \xi + \left(0 - \frac{1}{r} \cdot 1 \right) (1 - \xi) = \xi - \frac{1}{r} (1 - \xi)$$

At stoichiometric conditions, that is when $Y_{ox} = r Y_{fu}$, the mixture fraction is denoted $\xi = \xi_s$:

$$\left(Y_{fu} - \frac{1}{r} Y_{ox} \right) = 0 = \xi_s - \frac{1}{r} (1 - \xi_s) \quad \text{or} \quad \xi_s = \frac{1}{r + 1}$$

With the given, $r = 17,1 \text{ kg/kg}$ we obtain $\xi_s = 1 / (1 + 17,1) = 0,055$.

From the relations above is seen that $Y_{fu}(\xi)$ is linear. Furthermore, it goes from unity at inlet (1) (pure fuel) where $\xi = 1$ to zero at stoichiometric conditions ($\xi = \xi_s$). On the lean side, the fuel is consumed.

Hence, $\underline{Y_{fu}(\xi)} = \frac{\xi - \xi_s}{1 - \xi_s} \cdot 1 = \frac{\xi - 1 / (1 + r)}{1 - 1 / (1 + r)} = \frac{1}{r} ((1 + r)\xi - 1)$ for $\xi \geq \xi_s$, and $\underline{Y_{fu}(\xi)} = 0$ for $\xi \leq \xi_s$.

Similarly, the air (oxidizer) goes linearly from unity at inlet (2) ($\xi = 0$) to zero at $\xi = \xi_s$.

Hence, $Y_{air}(\xi) = 1 - \frac{\xi}{\xi_s} = 1 - (1 + r)\xi$ for $0 \leq \xi \leq \xi_s$, and $Y_{air}(\xi) = 0$ for $\xi_s \leq \xi \leq 1$.

Oxygen is a (given) fraction of the air, $\underline{Y_{O_2}(\xi)} = 0,233 Y_{air}(\xi)$.

Product is linear from $Y_{prod}(\xi = 0) = 0$ to $Y_{prod}(\xi_s) = 1$, and from there linear to $Y_{prod}(\xi = 1) = 0$.

Alternatively expressed, $Y_{prod}(\xi) = 1 - Y_{fu}(\xi) - Y_{air}(\xi)$

That is, $Y_{prod}(\xi) = 1 - 1 + (1 + r)\xi = (1 + r)\xi$ for $0 \leq \xi \leq \xi_s$, and

$$Y_{\text{prod}}(\xi) = 1 - \frac{1}{r}((1+r)\xi - 1) = \frac{1+r}{r}(1-\xi) \text{ for } \xi_s \leq \xi \leq 1.$$

For methane/air, the molar product is $\text{CO}_2 + 2\text{H}_2\text{O} + 7,52\text{N}_2$ per mole of methane;

Hence

$$\frac{m_{\text{CO}_2}}{m_{\text{prod}}} = \frac{44}{44 + 2 \cdot 18 + 7,52 \cdot 28} = 0,151 \quad \text{and} \quad Y_{\text{CO}_2}(\xi) = 0,151 Y_{\text{prod}}(\xi) \text{ with the } Y_{\text{prod}}(\xi) \text{ above.}$$

6)

$$\text{Mean mass fraction: } \bar{Y}_i = \int_0^1 Y_i(\xi) f(\xi) d\xi$$

$$\text{Mean temperature: } \bar{T} = \int_0^1 T(\xi) f(\xi) d\xi$$

$$\text{Variance of temperature: } \overline{T'^2} = \int_0^1 (T(\xi) - \bar{T})^2 f(\xi) d\xi$$

The probability density function (pdf) $f(\xi)$ have to be expressed (and expressible).

The conditions for validity is that the mixture fraction is the characteristic variable from which the other quantities can be expressed. This is satisfied in the “flamelet” regime, where flame sheets are little or moderately affected by the turbulent motions.

7)

For a two-way reaction $\text{A} + \text{B} \rightleftharpoons \text{C} + \text{D}$ with forward and reverse coefficients $k_f(T)$ and

$$k_r(T), \text{ the reaction rate of one of the species, say A, is } \frac{d[\text{A}]}{dt} = k_f[\text{A}][\text{B}] - k_r[\text{C}][\text{D}]$$

$k_f(T)$ is given/known, while $k_r(T)$ has to be determined. Since both are functions of temperature (and not of composition or pressure), any relation for a certain set of conditions at a certain temperature will be valid for all other conditions, provided that the temperature is the same. One simply analyzable condition is equilibrium.

When the reaction is in equilibrium, the net reaction rate of A is zero; hence

$$0 = k_f[\text{A}][\text{B}] - k_r[\text{C}][\text{D}] \quad \text{or} \quad \frac{k_f}{k_r} = \frac{[\text{C}][\text{D}]}{[\text{A}][\text{B}]} \quad (\text{at equilibrium}). \quad \text{The right-hand side of this expression}$$

is recognized as the “equilibrium constant” for the reaction, which is a function of temperature

$$\text{only, hence } \frac{k_f}{k_r} = K_c(T) \quad \text{or} \quad k_r(T) = \frac{k_f(T)}{K_c(T)}.$$

Although the actual state is not in equilibrium, this relation is still valid.

The equilibrium constant is expressed from the change of Gibbs free energy of the reaction when the reactants and products of the particular reaction is exchanged at reference pressure (1 atm or 1 bar, depending on the data source) and the actual temperature T. That is, enthalpy and absolute entropy has to be known at temperature T and reference pressure for the participating species.

8)

$$\begin{aligned} \frac{d[\text{OH}]}{dt} = & k_{r1}[\text{H}][\text{O}_2] - k_{r1}[\text{OH}][\text{O}] \\ & + k_{r2}[\text{H}_2][\text{O}] - k_{r2}[\text{OH}][\text{H}] \\ & - k_{r3}[\text{OH}][\text{H}_2] + k_{r3}[\text{H}][\text{H}_2\text{O}] \\ & + 2k_{r4}[\text{H}_2\text{O}][\text{O}] - 2k_{r4}[\text{OH}]^2 \end{aligned}$$

9)

The simulation has to capture the range from biggest to smallest of length scales and time scales. The biggest length scales of each direction are the dimensions of the case: 0,4 m × 0,1 m × 0,1 m. The biggest time scale can be the through-flow timescale, 0,4 m/(10 m/s)=0,04 s, unless there is a longer timescale. Here, at least, the longest reaction time scale (given) is bigger.

The least length scale can be the Kolmogorov length or the (given) smallest reaction length scale. With the data given, the turbulence velocity scale can be estimated as $u' \approx 0,1 \cdot U = 1$ m/s

The large turbulence length scale can be estimated as $\ell' \approx L_y = 0,1$ m

From these, the dissipation rate can be estimated as $\varepsilon \approx u'^3 / \ell' \approx (1^3 / 0,1) \text{ m}^2 / \text{s}^3 = 10 \text{ m}^2 / \text{s}^3$

And the Kolmogorov length, $\eta = (\nu^3 / \varepsilon)^{1/4} \approx (10^{-5.3} / 10)^{1/4} \text{ m} = 10^{-4} \text{ m}$. This is bigger than the least reaction length scale.

Thus, the spatial resolution has to be less than the smallest reaction length scale: $\Delta x < \delta_{r,\min} = 10^{-5} \text{ m}$

The large turbulence mixing time scale, $\theta = k / \varepsilon \approx u'^2 / \varepsilon \approx 1^2 / 10 \text{ s} = 0,1 \text{ s}$

The Kolmogorov time scale, $\tau = (\nu / \varepsilon)^{1/2} \approx (10^{-5} / 10)^{1/2} \text{ s} = 10^{-3} \text{ s}$

The convective time of the Kolmogorov length scale, $\tau_U = \eta / U \approx (10^{-4} / 10) \text{ s} = 10^{-5} \text{ s}$

The convective time of the least reaction length scale, $\tau_{U,\delta_{r,\min}} = \delta_{r,\min} / U \approx (10^{-5} / 10) \text{ s} = 10^{-6} \text{ s}$

Thus, the latter will be the least time scale and the time resolution: $\Delta t < \tau_{U,\delta_{r,\min}} \approx 10^{-6} \text{ s}$

The longest time scales will be the turbulence mixing time and the longest reaction time, which are of the same magnitude: $\theta \approx \tau_{r,\max}$

The number of time steps will be $N_t > \theta / \Delta t > 0,1 \text{ s} / 10^{-6} \text{ s} = 10^5$

The number of cells (or nodes) in the transverse directions will be

$N_z = N_y > L_y / \Delta x > 0,1 \text{ m} / 10^{-5} \text{ m} = 10^4$, while 4 times more in the streamwise direction.

Hence $N_p = N_x \cdot N_y \cdot N_z > 4 \cdot 10^{12}$

10)

The overall (global) reaction balance can be written as:



Apparently, the amount of CO is small compared to CO₂ and O₂, so that $a \ll 1$.

(This approximation is not necessary, but simplifies the calculations. It has to be checked afterwards.)

“dry” flue gas is without accounting the water vapor;

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

$$X_{\text{O}_2, \text{dry}} = \frac{n_{\text{O}_2}}{n_{\text{dry}}} = \frac{2(\lambda - 1) + \frac{1}{2}a}{9.52\lambda - 1 + \frac{1}{2}a} \approx \frac{2(\lambda - 1)}{9.52\lambda - 1};$$

This value is given as 0,13; Hence the actual excess air ratio is $\lambda \approx 2,45$, and $\frac{n_{\text{dry}}}{n_{\text{fuel}}} \approx 9.52\lambda - 1 \approx 22,32$

$$\text{Furthermore, } X_{\text{CO}, \text{dry}} = 25 \cdot 10^{-6} = \frac{n_{\text{CO}}}{n_{\text{dry}}} = \frac{a}{9.52\lambda - 1 + \frac{1}{2}a} \approx \frac{a}{9.52\lambda - 1} \approx \frac{a}{22,32}$$

Hence, $a = 5,6 \cdot 10^{-4}$. (Then we see that the assumption $a \ll 1$ was appropriate.)

$$\text{Now, we can calculate } \frac{m_{\text{CO}}}{m_{\text{fuel}}} = \frac{n_{\text{CO}}}{n_{\text{fuel}}} \frac{M_{\text{CO}}}{M_{\text{fuel}}} = a \frac{M_{\text{CO}}}{M_{\text{fuel}}} = 5,6 \cdot 10^{-4} \frac{28}{16} = \underline{\underline{0,98 \cdot 10^{-3} \text{ kg/kg}}}$$

The reference conditions for the regulations was at 15% O₂, dry.

$$X_{\text{O}_2, \text{dry}}^{\text{ref}} = 0,15 = \frac{n_{\text{O}_2, \text{ref}}}{n_{\text{ref}}} \approx \frac{2(\lambda_{\text{ref}} - 1)}{9.52\lambda_{\text{ref}} - 1}, \text{ which gives } \lambda_{\text{ref}} \approx 2,45 \text{ and}$$

$$\frac{n_{\text{ref}}}{n_{\text{fuel}}} \approx 9.52\lambda_{\text{ref}} - 1 \approx 29,75$$

$$X_{\text{CO}, \text{dry}}^{\text{ref}} = \frac{n_{\text{CO}}}{n_{\text{ref}}} = \frac{n_{\text{CO}}}{n_{\text{dry}}} \frac{n_{\text{dry}}}{n_{\text{ref}}} = 25 \cdot 10^{-6} \cdot \frac{22,32}{29,75} = \underline{\underline{18,8 \cdot 10^{-6} = 18,8 \text{ ppm}}}$$