Suggested solutions TEP4170 Heat and combustion technology 7 June 2019

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1)

The basic equation (given):

$$\frac{\partial}{\partial t}(\rho Y_k)+\frac{\partial}{\partial x_j}(\rho Y_k u_j)=\frac{\partial}{\partial x_j}\left(\rho D\frac{\partial Y_k}{\partial x_j}\right)+R_k$$

Note: In the exam, due to a typo, the ρ was left out from ρD in the 2nd RHS term. Then it has to be interpreted into D (i.e. similar to dynamic viscosity vs. kinematic viscosity). This does not affect the answer.

Introduce the Reynolds decomposition, $u_i=\overline{u}_i+u_i'\,;Y_k=\overline{Y}_k+Y_k'$.

$$\frac{\partial}{\partial t}(\rho(\overline{Y}_k+Y_k'))+\frac{\partial}{\partial x_j}(\rho(\overline{Y}_k\overline{u}_j+\overline{Y}_k u_j'+Y_k'\overline{u}_j+Y_k'u_j'))=\frac{\partial}{\partial x_j}\left(\rho D\frac{\partial}{\partial x_j}(\overline{Y}_k+Y_k')\right)+R_k$$

Assume (cf. problem) that density ρ and diffusivity D do not fluctuate.

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

$$\frac{\partial}{\partial t}(\rho\overline{Y}_k)+\frac{\partial}{\partial x_j}(\rho\overline{Y}_k\overline{u}_j)=\frac{\partial}{\partial x_j}\left(D\frac{\partial\overline{Y}_k}{\partial x_j}-\rho\overline{Y_k'u_j'}\right)+\overline{R}_k$$

The terms are (enumerated from left): 1) change of mean species mass with time; 2) transfer of mean species mass with mean flow; 3) transport/exchange of mean species mass by molecular diffusion; 4) transport/exchange of mean species mass due to turbulent motions; 5) mean species mass reaction (production) rate.

New quantities are:

$\overline{Y}_k$ and $\overline{u}_j$ are the mean values of Y_k and u_j, i.e. mean species mass fraction of species k and mean velocity in x_j direction. $-\rho\overline{Y_k'u_j'}$ are the fluxes of mean species mass in x_j direction due to turbulent motions. $\overline{R}_k$ is the mean of the volumetric reaction (production) rate of species k.

2)

A conserved scalar is a quantity with zero source term.

For a global reaction $1\text{ kg fu}+r\text{ kg ox}\rightarrow(1+r)\text{ kg prod}$, where r is the stoichiometric mass of oxidizer for the fuel, the relations between the reaction rates are $R_{\text{ox}}=rR_{\text{fu}}$ and $R_{\text{prod}}=-(1+r)R_{\text{fu}}$. The reaction rates are the source terms for $\rho Y_{\rm ox}$, $\rho Y_{\rm fu}$ and $\rho Y_{\rm prod}$. Accordingly, the quantities $\rho(rY_{\rm fu} - Y_{\rm ox})$, $\rho((1+r)Y_{\rm fu} + Y_{\rm prod})$ and $\rho((1+r)Y_{ox} + rY_{\rm prod})$ have source terms , respectively, $rR_{\rm fu} - R_{\rm ox} = 0$, $(1+r)R_{\rm fu} + R_{\rm prod} = 0$ and $(1+r)R_{\rm ox} + rR_{\rm prod} = 0$.

This means that the three quantities (or variants divided by r or $1+r$) are conserved scalars with the indicated simplifications.

Other examples:

The elemental mass is conserved. Thus the elemental mass fractions are conserved scalars. (That is, with the assumptions normally made in combustion engineering: no relativity considered.)

Mass fractions of inert species (e.g. Ar and in some cases N_2) have zero sources. Therefore, these are conserved scalars.

With some simplifications (no radiation, weak pressure gradients, negligible viscous dissipation, negligible effects of body forces) the total enthalpy (formation+thermal+kinetic) has zero (or negligible) source term, and is hence, a conserved scalar.

The mixture fraction ξ is defined by $\xi = \dfrac{\varphi_{mix} - \varphi_2}{\varphi_1 - \varphi_2}$; 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.

3)

The reaction balance is assumed as in Problem 2, with methane as fuel, air as oxidized and $r = 17{,}1$ kg/kg. Here, “product” includes the N_2 associated with the O_2 consumed in the reaction

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

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

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

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

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

From the relations above is seen that $Y_{\rm fu}(\xi)$ 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, $\underline{Y_{\rm fu}(\xi)} = \dfrac{\xi - \xi_s}{1-\xi_s}\cdot 1 = \dfrac{\xi - 1/(1+r)}{1-1/(1+r)} = \dfrac{1}{r}((1+r)\xi - 1)$ for $\xi \geq \xi_s$, and $\underline{Y_{\rm fu}(\xi)} = 0$ 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, $Y_{\rm air}(\xi) = 1 - \dfrac{\xi}{\xi_s} = 1 - (1+r)\xi$ for $0 \leq \xi \leq \xi_s$, and $Y_{\rm air}(\xi) = 0$ for $\xi_s \leq \xi \leq 1$.

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

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

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

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

Strictly, the problem did not ask for mass fractions of individual species (other than fuel).

Oxygen and nitrogen are (given) fractions of the air, $\underline{Y_{\text{O}_2}(\xi)} = 0,233 Y_{\text{air}}(\xi)$; $\underline{Y_{N_2}(\xi)} = 0,767 Y_{\text{air}}(\xi)$

Similarly, the product consists of CO_2, H_2O and N_2 and their mass fractions can be expressed from the product mass fraction.

4)

Models using a prescribed probability density function (pdf).

The pdf is expressed in terms of a characteristic variable. For non-premixed flames, usually the mixture fraction. When relevant quantities (species mass fractions, temperature, etc.) are expressed as functions of the mixture fraction, these functions can be integrated with the pdf over the sample space (from 0 to 1 for the mixture fraction) to obtain the mean values.

The pdf has to parameters, which are determined by solving modeled "transport" equations of two quantities, usually (for non-premixed flames) the mean and variance of the mixture fraction.

A condition for this type of model is that the mixture fraction is a representative variable. This can be true for flames in the flamelet regime; i.e. thin flame sheets not to much broken by turbulent eddies. That is, when the chemical time scale is smaller than the Kolmogorov time scale.

5)

$\overline{R}_{\text{fu}} = A\rho\frac{\varepsilon}{k}\overline{Y}_{\text{min}} = A\rho\frac{\varepsilon}{k}\min\left\{\overline{Y}_{\text{fu}}, \frac{1}{r}\overline{Y}_{\text{ox}}, \frac{B}{1+r}\overline{Y}_{\text{prod}}\right\}$; and then $\overline{R}_{ox} = r\overline{R}_{\text{fu}}$, $\overline{R}_{\text{prod}} = -(1+r)\overline{R}_{\text{fu}}$

A and *B* are model constants, and r is the stoichiometric mass-based oxidizer requirement of the fuel.

The mean mass fractions $\overline{Y}_{\text{fu}}$ and $\overline{Y}_{\text{ox}}$ are determined from the transport equations (cf. Problem 1). The mean product mass fraction can also be found from an equation, but more simply from the relation $\overline{Y}_{\text{prod}} = 1 - \overline{Y}_{\text{fu}} - \overline{Y}_{\text{ox}}$.

The turbulence energy k and its dissipation rate ε are found from some turbulence model (with equations).

This model is limited to reactions that can be represented by one or more fast, global, irreversible (one-way) reactions. (If there are more reactions, a priority has to be defined for the access to the limited supply of oxidizer.)

6)

This is for the inner part of the boundary layer of a flow close to a wall, except the very most close to the wall layer.

$\bar{u}_1$ 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); $u_\tau = \left(\tau_\mathrm{w} / \rho\right)^{1/2}$ 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.

In this zone the turbulence transfer, including turbulence stress dominates over molecular transfer, inlcuing viscous stresses. Moreover, the shear stress is assumed approximately constant. Hence, $-\overline{u_1'u_2'} = \tau_\mathrm{w} / \rho = u_\tau^2$.

In this zone, assume balance between production and dissipation of turbulence energy: $\rho\varepsilon = -\rho\overline{u_1'u_2'}\dfrac{d\bar{u}_1}{dx_2}$

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

The turbulence shear stress can be expressed from a turbulence viscosity: $-\rho\overline{u_1'u_2'} = \rho\nu_\mathrm{t} \cdot \dfrac{d\bar{u}_1}{dx_2}$

Introducing $\tau_\mathrm{w} = \rho u_\tau^2$ for the stress and the given relation for the gradient gives $\rho u_\tau^2 = \rho\nu_\mathrm{t} \cdot \dfrac{u_\tau}{\kappa x_2}$.

This can be rearranged to $\nu_\mathrm{t} = \kappa u_\tau x_2$.

In a k -ε model, the turbulence viscosity can be expressed $\nu_\mathrm{t} = C_\mu k^2 / \varepsilon$. Introducing the expressions for ε and ν_t above, provides $u_\tau^4 = C_\mu k^2$ or $k = u_\tau^2 / \sqrt{C_\mu}$.

7)

The given relation is developed for the same zone as the one given in Problem 6; 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 $q_2 = -\rho C_p \left(\dfrac{\nu}{\sigma} + \dfrac{\nu_\mathrm{t}}{\sigma_T}\right)\dfrac{d\bar{T}}{dx_2}$,

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; $q_2 = q_\mathrm{w}$.

Rearranging the expression, and using $\nu_\mathrm{t} = \kappa u_\tau x_2$ (from Problem 6)

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

Integrating the left-hand side from the wall (temperature T_w at $x_2 = 0$) to a point in the layer (temperature $\bar{T}$ at x_2), $\text{LHS} = \int_{T_w}^{\bar{T}} \frac{-\rho C_p u_\tau}{q_\text{w}} dT = \frac{-\rho C_p u_\tau}{q_\text{w}} (\bar{T} - T_\text{w})$.

This equals the non-dimensional temperature, $T^+ = \text{LHS}$.

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 $x_{2,\text{d}}$

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

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 $T^+ = \frac{1}{\kappa_T} \ln x_2^+ + C_T$

8)

Reaction orders, 1f: 1st order; 1r, 2f and 2r: 2nd order

Reaction (production) rates from the reactions given (consumption rates are the negative of these)

$$\frac{d[\text{O}_3]}{dt} = -k_{1f}[\text{O}_3] + k_{1r}[\text{O}][\text{O}_2] - k_{2f}[\text{O}][\text{O}_3] + k_{2r}[\text{O}_2]^2$$

$$\frac{d[\text{O}_2]}{dt} = k_{1f}[\text{O}_3] - k_{1r}[\text{O}][\text{O}_2] + 2k_{2f}[\text{O}][\text{O}_3] - 2k_{2r}[\text{O}_2]^2$$

$$\frac{d[\text{O}]}{dt} = k_{1f}[\text{O}_3] - k_{1r}[\text{O}][\text{O}_2] - k_{2f}[\text{O}][\text{O}_3] + k_{2r}[\text{O}_2]^2$$

Radicals, here monatomic O, are far more reactive than the more stable compounds O_2 and O_3. (Indeed, O_3 is less stable than O_2, however, relatively stable in comparison with O). O can be assumed to be consumed as soon as it is formed.

Assuming steady-state for O ($d[\text{O}]/dt = 0$), gives from the expression above

$$[\text{O}]_{ss} = \frac{k_{1f}[\text{O}_3] + k_{2r}[\text{O}_2]^2}{k_{1r}[\text{O}_2] + k_{2f}[\text{O}_3]}$$

9)

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

$$\text{C}_8\text{H}_{18} + 12{,}5(\text{O}_2 + 3.76\text{N}_2) \rightarrow 8(1-a)\text{CO}_2 + 8a\text{CO} + 9\text{H}_2\text{O} + \tfrac{1}{2}8a\text{O}_2 + 12{,}5 \cdot 3.76\text{N}_2$$

The amount of flue gas ("wet", i.e. with H2O included in the mixture when other species are specified) is $\frac{n_\text{fg}}{n_\text{fuel}} = 8 - 8a + 8a + 9 + 4a + 47 = 64 + 4a$, while the amount of CO is $\frac{n_\text{CO}}{n_\text{fuel}} = 8a$.

The mole fraction of CO in the flue gas $X_{\mathrm{CO}} = \dfrac{n_{\mathrm{CO}}}{n_{\mathrm{fg}}} = \dfrac{8a}{64+4a} = \dfrac{2a}{16+a} = 0,035$; Solving this: $a = 0,29$

Amount of emitted CO: $\dfrac{n_{\mathrm{CO}}}{n_{\mathrm{fuel}}} = 8a = 2,3\ \mathrm{mol/mol}$

Emission index: $\mathrm{EI}_{\mathrm{CO}} = \dfrac{m_{\mathrm{CO}}}{m_{\mathrm{fu}}} = \dfrac{n_{\mathrm{CO}} M_{\mathrm{CO}}}{n_{\mathrm{fu}} M_{\mathrm{fu}}} = 2,32 \cdot \dfrac{28\ \mathrm{kg/kmol}}{114\ \mathrm{kg/kmol}} = 0,57\ \mathrm{kg/kg}$

Fraction of heating value: $\dfrac{H_{\mathrm{LHV,CO}}}{H_{\mathrm{LHV,fuel}}} = \dfrac{n_{\mathrm{CO}} h_{\mathrm{LHV,CO}}}{n_{\mathrm{fuel}} h_{\mathrm{LHV,fuel}}} = 2,32 \cdot \dfrac{283\ \mathrm{kJ/mol}}{5075\ \mathrm{kg/mol}} = 0.13 = 13\%$

Comment: modern cars have catalytic converters, and emit much less CO. However, that is from the tailpipe. The CO content in the flue gas leaving the engine has approximately the value above. The remaining chemical energy is converted to thermal energy in the catalytic converter.

10)

The fuel mass balance and energy balance for the reactor in steady state can be expressed as, respectively,

$$R_{\mathrm{fu}} = -\frac{1}{\tau *}\left(Y_{\mathrm{fu}}^{o} - Y_{\mathrm{fu}}^{*}\right) \text{ and } c_p (T^* - T^o) = \left(Y_{fu}^{o} - Y_{fu}^{*}\right) h_{LHV} ,$$

where c_p is the specific heat (average for the relevant temperatures) and h_{LHV} is the lower heating value of the fuel.

The reaction rate can also be expressed from composition and temperature $(-R_{fu}) \sim Y_{\mathrm{fu}}^{*\,m} Y_{\mathrm{ox}}^{*\,n} \exp(-E/(R_u T^*))$, where *m* and *n* are reaction orders, E activation energy and R_u the universal gas constant.

For the discussion, it can be convenient to define a "degree of reaction" $Y = \dfrac{Y_{\mathrm{fu}}^{o} - Y_{\mathrm{fu}}^{*}}{Y_{\mathrm{fu}}^{o}}$, which is the fraction of inflow mass that is consumed in the reactor.

The energy balance gives a linear $Y - T^*$ relation, $Y = \dfrac{Y_{\mathrm{fu}}^{o} - Y_{\mathrm{fu}}^{*}}{Y_{\mathrm{fu}}^{o}} = \dfrac{c_p}{Y_{\mathrm{fu}}^{o} h_{LHV}} (T^* - T^o)$

The mass balance gives: $Y = \dfrac{Y_{\mathrm{fu}}^{o} - Y_{\mathrm{fu}}^{*}}{Y_{\mathrm{fu}}^{o}} = \dfrac{\tau *}{Y_{\mathrm{fu}}^{o}} (-R_{\mathrm{fu}}) \sim \dfrac{\tau *}{Y_{\mathrm{fu}}^{o}} Y_{\mathrm{fu}}^{*\,m} Y_{\mathrm{ox}}^{*\,n} \exp(-E/(R_u T^*))$

At low conversion (high availability of fuel and oxidizer) this forms an exponential relation. When the conversion approaches completion, the lack of reactants limits the reaction towards the asymptote $Y = 1$

Hence, an S-shaped curve will be seen.

Both curves will start in $(Y, T^*) = (0, T^o)$. Possible conditions requires both relations to be satisfied; hence $(Y = 0, T^* = T^o)$ is a trivial solution to the system of the two equations. The S-shaped curve describing the mass balance may cross the linear energy balance in two points, touch it in one point, or not in any other point. In the latter case only the trivial solution remains, which means extinction.

With two solutions (in adition to the trivial no-reaction solution), the upper one will be stable, while the lower will be unstable. This can be seen by perturbing the solution.

Reducing the temperature at the lower solution will reduce the reaction rate, which will reduce the heat release, which will reduce the temperature, and so on to no reaction. Alternatively, increasing the temperature will increase the reaction rate, increase the heat release, increase the temperature and so on to the other solution:

Reducing the temperature at the upper solution will reduce the reaction rate, make more fuel available (notice that reactant availability is a limiting factor at the high conversion ratio), which increases the reaction rate (back the solution). Increasing the temperature will increase reaction rate, make the reactants even more scares, which decreases the reaction rate (back to the solution). Thus, it is stable.