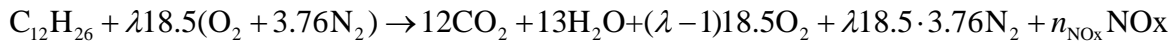


Suggested solutions TEP4170 Heat and combustion technology 15 May 2015  
by Ivar S. Ertesvåg. Revised 18 May 2016

1)

The global reaction balance can be written:



The amount of substance of fuel gas including H<sub>2</sub>O (“wet”) per kmol of fuel:

$$\frac{n_{\text{wet}}}{n_{\text{fuel}}} = 12 + 13 + 18.5(\lambda - 1) + 69.56\lambda = 6.5 + 88.06\lambda$$

Excluding the H<sub>2</sub>O (“dry”):  $\frac{n_{\text{dry}}}{n_{\text{fuel}}} = 12 + 18.5(\lambda - 1) + 69.56\lambda = -7.5 + 88.06\lambda$

The (actual) molar fraction of O<sub>2</sub>:  $\frac{n_{\text{O}_2}}{n_{\text{wet}}} = \frac{18.5(\lambda - 1)}{6.5 + 88.06\lambda} = 0.03$

$\rightarrow \lambda(18.5 - 0.03 \cdot 88.06) = 0.03 \cdot 6.5 + 18.5 \rightarrow \lambda = \frac{18.70}{15.86} = 1.18$  This is the actual air excess ratio,

which also gives  $\frac{n_{\text{wet}}}{n_{\text{fuel}}} = 110.3$

The regulations (“reference”) are specified for “dry”:  $\frac{n_{\text{O}_2,\text{ref}}}{n_{\text{dry,ref}}} = \frac{18.5(\lambda_{\text{ref}} - 1)}{-7.5 + 88.06\lambda_{\text{ref}}} = 0.15$

$\rightarrow \lambda_{\text{ref}}(18.5 - 0.15 \cdot 88.06) = 0.15 \cdot (-7.5) + 18.5 \rightarrow \lambda_{\text{ref}} = \frac{17.3}{5.29} = 3.28$

This is the reference air excess ratio, which gives  $\frac{n_{\text{dry,ref}}}{n_{\text{fuel}}} = 281.3$

The actual molar fraction of NOx is given as  $\frac{n_{\text{NOx}}}{n_{\text{wet}}} = 200 \text{ ppm} = 200 \cdot 10^{-6}$

The “reference” molar fraction of NOx becomes

$$\frac{n_{\text{NOx}}}{n_{\text{dry,ref}}} = \frac{n_{\text{NOx}}}{n_{\text{wet}}} \cdot \frac{n_{\text{wet}}}{n_{\text{dry,ref}}} = 200 \cdot 10^{-6} \frac{110.3}{281.3} = 78 \cdot 10^{-6} = \underline{78 \text{ ppm}}$$

2)

1 kmol C<sub>12</sub>H<sub>26</sub> (170.3 kg) gives 12 kmol CO<sub>2</sub> (12·44.0 kg) ;

that is,  $m_{\text{CO}_2} / m_{\text{fuel}} = (EI_{\text{CO}_2} =) 12 \cdot 44.0 \text{ kg} / 170.3 \text{ kg} = 3.1 \text{ kg CO}_2 / \text{kg fuel}$

1 kg fuel gives 44.1 MJ of thermal energy; with  $\eta = 0.25$ , the power will be  $0.25 \cdot 44.1 \text{ MJ/kg} = 11.03 \text{ MJ/kg}$ .

Mass specific emission (CO<sub>2</sub>):  $\frac{\dot{m}_{\text{CO}_2}}{\dot{W}} = \frac{3.1 \text{ kg}}{11.03 \text{ MJ}} = \underline{0.28 \text{ kg/MJ}}$

$$\text{For NO: } \frac{m_{\text{NO}}}{m_{\text{fuel}}} = \frac{n_{\text{NO}} M_{\text{NO}}}{n_{\text{fuel}} M_{\text{fuel}}} = \frac{M_{\text{NO}}}{M_{\text{fuel}}} \frac{n_{\text{NO}}}{n_{\text{wet}}} \frac{n_{\text{wet}}}{n_{\text{fuel}}} = \frac{30.0}{170.3} \cdot 200 \cdot 10^{-6} \cdot 110.3 \text{ kg/kg} = 3.9 \cdot 10^{-4} \text{ kg/kg}$$

Mass specific emission (NO):

$$\frac{\dot{m}_{\text{NO}}}{\dot{W}} = \frac{m_{\text{NO}}}{m_{\text{fuel}} \cdot h_{\text{LHV}} \cdot \eta} = \frac{3.9 \cdot 10^{-3} \text{ kg/kg}}{44.1 \text{ MJ/kg} \cdot 0.25} = 3.5 \cdot 10^{-4} \text{ kg/MJ} = \underline{0.35 \text{ g/MJ}}$$

3)

Definition, mixture fraction:  $\xi = \frac{\varphi - \varphi_2}{\varphi_1 - \varphi_2}$ , where  $\varphi$  is a conserved scalar and  $\varphi_1$  and  $\varphi_2$  are the values at the fuel and oxidizer inlets/inflows.

$$\text{The stoichiometric amount of air (mass based): } r = \left( \frac{m_{\text{air}}}{m_{\text{fuel}}} \right)_{\text{st}} = \frac{18.5(32 + 3.76 \cdot 28)}{170.3} = 14.9 \text{ kg/kg}$$

$$\text{The stoichiometric mixture fraction: } \xi_{\text{st}} = \left[ \frac{m_{\text{fuel}}}{m_{\text{fuel}} + m_{\text{air}}} \right]_{\text{st}} = \frac{1}{1 + (m_{\text{air}} / m_{\text{fuel}})_{\text{st}}} = \frac{1}{1 + r} = \underline{0.063}$$

$\varphi = Y_{\text{fu}} - \frac{1}{r} Y_{\text{air}}$  is a conserved scalar (has zero source term). For inlet 1 (fuel)  $\varphi_1 = Y_{\text{fu},1} = 1$ , and for inlet 2 (air)  $\varphi_2 = -\frac{1}{r} Y_{\text{air},2} = -r^{-1}$ .

$$\text{Hence, } \varphi = Y_{\text{fu}} - \frac{1}{r} Y_{\text{air}} = (\varphi_1 - \varphi_2)\xi + \varphi_2 = (1 + r^{-1})\xi - r^{-1}$$

For an infinitely fast and complete reaction, either fuel or oxygen is completely consumed. Hence, for a rich mixture ( $\xi_{\text{st}} \leq \xi \leq 1$ ),  $Y_{\text{air}} = 0$  and  $\varphi = Y_{\text{fu}} = (1 + r^{-1})\xi - r^{-1}$

For a lean mixture ( $0 \leq \xi \leq \xi_{\text{st}}$ ),  $Y_{\text{fuel}} = 0$  and  $\varphi = -\frac{1}{r} Y_{\text{air}} = (1 + r^{-1})\xi - r^{-1}$  or  $Y_{\text{air}} = 1 - (r + 1)\xi$

$$\text{For oxygen: } \frac{m_{\text{O}_2}}{m_{\text{air}}} = \frac{0.21 \cdot 32}{0.21 \cdot 32 + 0.79 \cdot 28} = 0.233 \text{ kg/kg}, \text{ and } Y_{\text{O}_2} = 0.233 \cdot Y_{\text{air}} = 0.233 \cdot (1 - (r + 1)\xi)$$

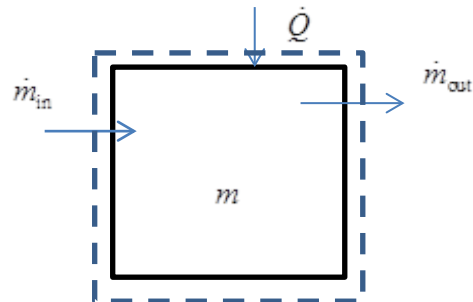
4)

Well stirred reactor or perfectly stirred reactor :

The reactor has one inlet and one outlet.

Assumptions/simplifications:

- No spatial gradients
- uniform and properties ( $T, p, \rho, Y_k$  etc.)
- steady flow, steady state



Mass balance:

$$\frac{dm_{\text{cv}}}{dt} = \dot{m}_{\text{in}} - \dot{m}_{\text{out}} = 0, \text{ that is } \dot{m}_{\text{in}} = \dot{m}_{\text{out}}$$

$$\text{Species mass balance: } 0 = \dot{m}_{\text{in}} Y_{k,\text{in}} - \dot{m}_{\text{out}} Y_{k,\text{out}} + \dot{m}_k'' \cdot V$$

$$\text{Energy balance: } 0 = \dot{m}_{\text{in}} h_{\text{in}} - \dot{m}_{\text{out}} h_{\text{out}} + \dot{Q}$$

Comment: In literature, the term WSR or PSR is also used without the steady flow, steady state assumption. In that case, the equations will have a non-zero transient term.

5)

$$\frac{d[\text{O}]}{dt} = -2k_{f1}[\text{O}]^2[\text{M}] + 2k_{r1}[\text{O}_2][\text{M}] - k_{f2}[\text{O}][\text{H}][\text{M}] + k_{r2}[\text{OH}][\text{M}] + k_{f3}[\text{O}_2][\text{CO}] - k_{r3}[\text{O}][\text{CO}_2]$$

6)

At equilibrium, the forward and reverse reactions balance and give no net reaction rate: Thus

$$0 = -k_{f1}[\text{O}]^2[\text{M}] + k_{r1}[\text{O}_2][\text{M}] \quad \text{or} \quad \frac{k_{f1}}{k_{r1}} = \frac{[\text{O}_2][\text{M}]}{[\text{O}]^2[\text{M}]}$$

The right-hand side of the latter expression is also equal to the equilibrium constant  $K_{c1}$  of this

$$\text{reaction. Hence, } k_{r1} = \frac{k_{f1}}{K_{c1}} = k_{f1} \frac{[\text{O}]^2}{[\text{O}_2]}$$

7)

The first three terms include quantities that are already part of our model (including  $k$  that became part of it when we introduced the  $k$  equation). These terms can be retained.

The fifth term includes the Reynolds stresses. These are found in the momentum equations and already modeled since we are using a turbulence viscosity. The term has to be modelled, but the model is already introduced. The fourth and sixth term include correlations that are unknown and not already modeled.

$$\text{a,b) } IV = \frac{\partial}{\partial x_j} \left( \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_j} \right); \quad V = \mu_t \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \frac{\partial \bar{u}_i}{\partial x_j} - \frac{2}{3} (\rho k + \mu_t \frac{\partial \bar{u}_i}{\partial x_i}) \frac{\partial \bar{u}_i}{\partial x_i};$$

$$\text{a) } VI = \rho C_D k^{3/2} / L \quad \text{b) } VI = \rho \varepsilon$$

(For constant density,  $\partial u_i / \partial x_i = 0$ , and the last part of term  $V$  cancels.)

Here  $\sigma_k$  (Prandtl-Schmidt number for  $k$ ) and  $C_D$  are model constants;  $L$  is a length (“mixing length”) that has to be specified for each flow configuration. In a), the length scale is the same that has to be specified for the turbulence-viscosity expression,  $\mu_t = C_\mu \rho \sqrt{k} / L$ , where one of the constants  $C_D$  and  $C_\mu$  is independent.

8)

Isotropic turbulence is rotationally invariant. No statistical quantities should change when the coordinate system is rotated.

$$\frac{dk}{dt} = -\varepsilon \quad \text{and} \quad \frac{d\varepsilon}{dt} = -c_{\varepsilon 2} \frac{\varepsilon^2}{k}$$

$$\overline{u'_i u'_j} = \frac{2}{3} k \quad \text{for } i = j \quad \text{and} \quad \overline{u'_i u'_j} = 0 \quad \text{for } i \neq j; \quad \text{or} \quad \overline{u'_1 u'_1} = \overline{u'_2 u'_2} = \overline{u'_3 u'_3} = \frac{2}{3} k \quad \text{and} \quad \overline{u'_1 u'_2} = \overline{u'_1 u'_3} = \overline{u'_2 u'_3} = 0$$

9)  
Graph:

The areas under the  $E$  and  $D$  curves, respectively, equal  $k$  and  $\varepsilon$  :

$$\int_0^{\infty} E(\kappa) d\kappa = k \quad \text{and} \quad \int_0^{\infty} D(\kappa) d\kappa = \varepsilon$$

10)

The dissipative range is the part of the energy spectrum which is

- independent of mean motion, large eddies and external geometry
- dependent on viscous forces
- dependent on the transfer of kinetic energy from larger to smaller eddies; this transfer equals the dissipation rate of kinetic energy,  $\varepsilon$  (which is the transfer to thermal energy by viscous forces)
- In addition, any scale (size of eddies) depends on its own size (length scale, wavenumber)

Hence, the scales of the dissipative range must be functions of the kinematic viscosity  $\nu$  and the dissipation rate,  $\varepsilon$ . The length scale:  $\eta = \eta(\nu, \varepsilon)$ .

Dimensional analysis gives:  $\eta = \nu^a \varepsilon^b$  where  $[\eta] = L$ ,  $[\nu] = L^2 / T$ ,  $[\varepsilon] = L^2 / T^3$  ( $L$ =length,  $T$ =time)

Thus,  $1 = 2a + 2b$  for length and  $0 = a + 3b$  for time, or  $b = -1/4$  and  $a = 3/4$

That is,  $\eta = \nu^{3/4} \varepsilon^{-1/4} = (\nu^3 / \varepsilon)^{1/4}$ .

For the velocity scale:  $v = v(\nu, \varepsilon) = \nu^a \varepsilon^b$  and  $[v] = L / T$ ;  $1 = 2a + 2b$  and  $1 = a + 3b$ ,  
or  $b = 1/4$  and  $a = 1/4$ . That is,  $v = (\nu \varepsilon)^{1/4}$ .

Time scale:  $\tau = \eta / v = \nu^{3/4-1/4} \varepsilon^{-1/4-1/4} = (\nu / \varepsilon)^{1/2}$ . Dimensional analysis can also be used.