

Suggested solutions TEP4170 Heat and combustion technology 5 June 2018

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1)

A global reaction is an overall balance of the mass/elements that take part in a reaction. It includes only the initial reactants and the final products, but not intermediate species. A global reaction is the sum of a large number of elementary reactions. An elementary reaction includes the species actually reacting with each other and the resulting product(s). Intermediate species take part as reactants and/or products in elementary reactions.

The reaction rate of a species A, reacting with species B can be expressed as

$$\frac{d[A]}{dt} = -k_G[A]^n[B]^m \quad \text{or} \quad R_A \sim [A]^n[B]^m \sim Y_A^n Y_B^m$$

Here, the parameters n and m are the reactions orders of species A and B, respectively.

For a reaction $A + B \xrightleftharpoons[k_r]{k_f} C + D$, the equilibrium constant can be expressed as $K_c = \frac{[C][D]}{[A][B]}$ and

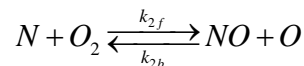
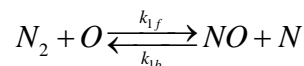
determined from enthalpy and entropy (or Gibbs energy) data for the involved species. Moreover, at equilibrium, the net reaction rate of each species will be zero, hence

$$\frac{d[A]}{dt} = -k_f[A][B] + k_r[C][D] = 0 \quad \text{and} \quad \frac{k_f}{k_r} = \frac{[C][D]}{[A][B]}, \quad \text{which equals the equilibrium constant.}$$

Hence, when k_f is known, the reverse coefficient can be determined as $k_r = \frac{k_f}{K_c}$.

2)

The Zeldovich mechanism



The first reaction is very slow compared to the second one.

Assumptions:

- the backward reactions are slow: Because the right-hand-side concentrations are much less than those at the left-hand side, $[NO] \ll [O_2] < [N_2]$
- N is in steady state: Because the first reaction is very slow compared second one, the consumption of N (in the 2nd reaction) adapts to the production (in the 1st reaction). Then N rapidly accumulates to a steady (and low) concentration.
- O in equilibrium with O₂: Because in high-temperature systems the NO formation reaction is typically much slower than other reactions involving O₂ and O. Thus O₂ and O will adapt to other, faster reactions and in the context of NO-formation, can be regarded in equilibrium with each other.

From the elementary reactions we can write

$$\frac{d[NO]}{dt} = k_{1f}[N_2][O] + k_{2f}[N][O_2]$$

$$\frac{d[\text{N}]}{dt} = k_{1f}[\text{N}_2][\text{O}] - k_{2f}[\text{N}][\text{O}_2]$$

where the reverse reactions are assumed negligible (i.e. much slower).

Assuming steady-state for N, ($d[\text{N}]/dt = 0$) gives

$$[\text{N}]_{ss} = \frac{k_{1f}[\text{N}_2][\text{O}]}{k_{2f}[\text{O}_2]}$$

Including this in the expression above,

$$\frac{d[\text{NO}]}{dt} = +k_{1f}[\text{N}_2][\text{O}] + k_{2f} \frac{k_{1f}[\text{N}_2][\text{O}]}{k_{2f}[\text{O}_2]}[\text{O}_2] = 2k_{1f}[\text{N}_2][\text{O}]$$

For the equilibrium between O and O₂, $\text{O}_2 \rightleftharpoons 2\text{O}$, the equilibrium constant $K_{c,O} = \frac{[\text{O}]^2}{[\text{O}_2]}$ can be

determined from thermodynamic data for O and O₂. Accordingly, $[\text{O}] = ([\text{O}_2]K_{c,O})^{1/2}$, and

$$\frac{d[\text{NO}]}{dt} = 2k_{1f}[\text{N}_2]([\text{O}_2]K_{c,O})^{1/2} = 2k_{1f}(K_{c,O})^{1/2}[\text{N}_2][\text{O}_2]^{1/2}$$

Here, the global rate coefficient $k_G = 2k_{1f}(K_{c,O})^{1/2}$ and the reaction orders $n=1$ and $m=\frac{1}{2}$ are identified.

Note that literature contains several formulations of the equilibrium constant, which are proportional to each other with factors that are combinations of reference pressure and gas constant (i.e. constants). Use of any of these is fully accepted.

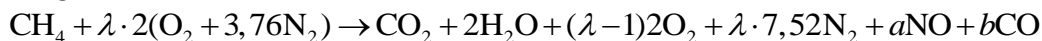
3)

The flame surface (stoichiometric contour) is the surface composed of the locations where the fuel/oxidizer ratio is stoichiometric, i.e. equivalence ratio $\Phi = 1$ or air-excess ratio $\lambda = 1$.

See Fig. 9.4 in the textbook (Turns, 3rd ed.). The soot will be located just inside the stoichiometric contour (maximum temperature).

4)

The global reaction balance can be written as



where the amounts of minor species (a and b) are assumed to be much smaller than the other (major) species (10 ppm is clearly "small" compared to the other mole fractions).

The amount of fuel can be found as $n_F = n_{\text{CO}_2} + n_{\text{CO}}$ (since CH₄, CO₂ and CO all contain one C atom, and any other C compounds are negligible)

The amount of product per mole of fuel is

$$n_P = n_{\text{CO}_2} + n_{\text{H}_2\text{O}} + n_{\text{O}_2} + n_{\text{N}_2} + n_{\text{CO}} + n_{\text{NO}} = 1 + 2 + 2\lambda - 2 + 7,52 \cdot \lambda + a + b \approx 1 + 9,52 \cdot \lambda$$

Using the mole fraction of $X_{O_2} = \frac{n_{O_2}}{n_p} = \frac{(\lambda - 1) \cdot 2}{1 + 9,52 \cdot \lambda}$ with the actual values of 0,127 gives $\lambda = 2,69$.

The emission index for NO:

$$EI_{NO} = \frac{m_{NO}}{m_F} = \frac{n_{NO} M_{NO}}{n_F M_F} = \frac{n_{NO} M_{NO}}{(n_{CO_2} + n_{CO}) M_F} = \frac{X_{NO} M_{NO}}{(X_{CO_2} + X_{CO}) M_F} = \frac{10 \cdot 10^{-6} \cdot 30}{(0,037 + 0,00001) \cdot 16} = 5,1 \cdot 10^{-4} \frac{kg}{kg}$$

Alternative:

$$EI_{NO} = \frac{m_{NO}}{m_F} = \frac{n_{NO} M_{NO}}{n_F M_F} = \frac{n_{NO}}{n_p} \frac{n_p M_{NO}}{n_F M_F} = X_{NO} \frac{n_p}{n_F} \frac{M_{NO}}{M_F} = 10 \cdot 10^{-6} \cdot (1 + 9,52 \cdot 2,69) \cdot \frac{30}{16} = 5,0 \cdot 10^{-4} \frac{kg}{kg}$$

(the difference is due to differences in truncation)

The reference value of $X_{O_2,15\%} = 0,150$ gives $\lambda = \lambda_{15\%} = 3,76$. This is the excess air that would give mole fractions that can be compared to the regulations. Since the amount of NO is the same, the mole fraction with the higher amount of air becomes

$$X_{NO,15\%} = \frac{n_{NO}}{n_{p,15\%}} = \frac{n_{NO}}{n_p} \frac{n_p}{n_{p,15\%}} = X_{NO} \frac{1 + 9,52 \cdot \lambda}{1 + 9,52 \cdot \lambda_{15\%}} = 10 \cdot 10^{-6} \frac{1 + 9,52 \cdot 2,69}{1 + 9,52 \cdot 3,76} = 7,2 \cdot 10^{-6} = 7,2 \text{ ppm}$$

Without the specification of O₂ concentration, adding air to the flue gas (diluting) will reduce the mole fraction of the pollutants. The recalculation to a reference content enable comparison with the regulations, comparison with other installations, and comparison with other time instances of the same installation (as the excess air, in practice, will show some variation).

5)

The Reynolds fluxes of a scalar φ can be expressed from

$$-\overline{\rho \varphi' u'_j} = \frac{\mu_t}{\sigma_\varphi} \frac{\partial \overline{\varphi}}{\partial x_j},$$

or in form of the turbulence diffusion term of the mean φ ,

$$D_{\varphi,t} = \frac{\partial}{\partial x_j} \left(-\overline{\rho \varphi' u'_j} \right) = \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_\varphi} \frac{\partial \overline{\varphi}}{\partial x_j} \right)$$

where φ is the relevant scalar, μ_t is the turbulence viscosity and σ_φ is the turbulence Prandtl-Schmidt number (usually set as constant, can be individual for different scalars).

The different scalars are transported by the same eddying motions of turbulence. Therefore, it is reasonable to assume that there is a great similarity in the turbulence fluxes. Deviations from this can to some extent be captured by using different values of the Prandtl-Schmidt numbers for different scalars.

6)

The (3-dimensional) energy spectrum is defined from the trace of the energy spectrum tensor

$$E(\kappa, t) = 2\pi\kappa^2 E_{ii}(\vec{\kappa}, t),$$

while the energy spectrum tensor $E_{ij}(\vec{\kappa}, t)$ is the Fourier transform of the two-point correlation,

$$R(\vec{r}, t) = \overline{u'_i(\vec{x}, t) u'_j(\vec{x} + \vec{r}, t)}.$$

Here, \vec{x} , is the location of the first point, $\vec{x} + \vec{r}$ is the location of the 2nd point, $\vec{\kappa}$ is the wave number vector, and $\kappa = |\vec{\kappa}|$ is the wave number

See sketch in Ertesvåg, Fig. 8.5

The curve shows the kinetic energy of turbulent motions as distributed over wave numbers (reciprocal of length scales).

Turbulence energy: $k = \int_0^\infty E(\kappa) d\kappa$ This is the area under the E curve.

When the turbulence Reynolds number is reduced, the turbulence energy is reduced (lesser area under the E curve). Moreover, the extent of the spectrum is reduced (lesser ratio of “large” to “small” eddies/length scales, and the characteristic “large” length scale (the length scale of the peak) becomes larger (or the wave number of the peak becomes smaller).

Hence, the peak of the spectrum will move towards left and the spectrum will shrink. See Fig. 8.6 in the textbook (Ertesvåg).

7)

The equation for the instantaneous mixture fraction can be written as

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

(Notice that there is no source term)

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

$$\frac{\partial}{\partial t}(\rho(\bar{\xi} + \xi')) + \frac{\partial}{\partial x_j}(\rho(\bar{\xi}\bar{u}_j + \bar{\xi}u'_j + \xi'\bar{u}_j + \xi'u'_j)) = \frac{\partial}{\partial x_j} \left(D \left(\frac{\partial \bar{\xi}}{\partial x_j} + \frac{\partial \xi'}{\partial x_j} \right) \right)$$

Average the entire equation, that is, each term. Here, $\bar{u}_i = \bar{u}_i$; $\bar{u}'_i = 0$; $\bar{u}_i u'_j = \bar{u}_i \cdot \bar{u}'_j = 0$ etc., and we achieve

$$\frac{\partial}{\partial t}(\rho\bar{\xi}) + \frac{\partial}{\partial x_j}(\rho\bar{\xi}\bar{u}_j) = \frac{\partial}{\partial x_j} \left(D \frac{\partial \bar{\xi}}{\partial x_j} - \rho\overline{\xi'u'_j} \right)$$

Subtracting this from the instantaneous equation gives an equation for the fluctuating mixture fraction:

$$\left(\frac{\partial}{\partial t}(\rho\xi) + \dots = \dots \right) - \left(\frac{\partial}{\partial t}(\rho\bar{\xi}) + \dots = \dots \right) = \left(\frac{\partial}{\partial t}(\rho\xi') + \dots = \dots \right)$$

Multiply this with $2\xi'$ and include this factor into the derivation:

$$2\xi' \cdot \left(\frac{\partial}{\partial t}(\rho\xi') + \dots = \dots \right) = \left(\frac{\partial}{\partial t}(\rho\xi'^2) + \dots = \dots \right)$$

When the last equation is averaged (term by term), the equation given in the problem is obtained.

8)

The mean and variance of the mixture fraction can be expressed as

$$\bar{\xi} = \int_0^1 \xi f(\xi) d\xi = \int_0^1 \xi \frac{\xi^{a-1}(1-\xi)^{b-1}}{B(a,b)} d\xi$$

$$\overline{\xi'^2} = \int_0^1 (\xi - \bar{\xi})^2 f(\xi) d\xi = \int_0^1 (\xi - \bar{\xi})^2 \frac{\xi^{a-1}(1-\xi)^{b-1}}{B(a,b)} d\xi$$

When the local $\bar{\xi}$ and $\overline{\xi'^2}$ are known (resolved from their transport equations), the local values of the parameters a and b can be calculated from the two expressions.

To obtain the mean and variance of temperature, a relation $T(\xi)$ have to be known (from simple approximation, experiments, detailed simulations, etc.). When this is available, the following can be expressed:

$$\bar{T} = \int_0^1 T(\xi) f(\xi) d\xi$$

$$\overline{T'^2} = \int_0^1 (T(\xi) - \bar{T})^2 f(\xi) d\xi$$

9)

EDC cascade model, see textbook

Sketch with u, L, ω, w, q at various levels from mean flow to fine structure.

Expressions for w, q at the different levels $w_n \sim u_n^2 \frac{u_n}{L_n} \sim u_n^2 \omega_n$; $q_n \sim \nu \omega_n^2$

Expressions for *dissipation rate*: $\varepsilon = \frac{4}{3} q^* = \frac{4}{3} w^*$ and $\varepsilon \approx w''$

Relations for u^*, L^* , functions of ε and ν .

The purpose is to link the "fine structures" (small eddies), where the reactions occur, to the large eddies and mean flow, which are determined from a turbulence model.

10)

EDC reactor model, see textbook.

Sketch, surroundings values, reactor values:

Species mass balance, fine-structure reaction rate, R_k^*

Mean reaction rate, \bar{R}_k , by weighting between reactor and surroundings,

The link to the cascade model is the use of quantities emerging from it; $\dot{m}^* = 1/\tau^*, \gamma^*, \gamma_\lambda$