Suggested solutions TEP4170 Heat and combustion technology 21 May 2012
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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.

"unimolar" , "bimolar" and "trimolar" refers to the number (1, 2 and 3m, respectively) of molecules that are the reactants in elementary reactions.

The reaction order is the number of moles of each reactant that takes part in a reaction. For elementary reactions, the reaction orders are always a positive integer. For global reaction the reaction order can have any (positive) rational number

2)
When each pair of reactions are in equilibrium, the equilibrium constants can be expressed as

$$K_1 = \frac{k_{1f}}{k_{1r}} = \frac{[\mathrm{OH}][\mathrm{O}]}{[\mathrm{H}][\mathrm{O_2}]}; \quad K_2 = \frac{k_{2f}}{k_{2r}} = \frac{[\mathrm{OH}][\mathrm{H}]}{[\mathrm{O}][\mathrm{H_2}]}; \quad K_3 = \frac{k_{3f}}{k_{3r}} = \frac{[\mathrm{H_2O}][\mathrm{H}]}{[\mathrm{OH}][\mathrm{H_2}]}$$

These three equations can be solved for the concentrations of the three radical species O, H and OH:

$$[\mathrm{O}] = K_1 K_3 \frac{[\mathrm{O_2}][\mathrm{H_2}]}{[\mathrm{H_2O}]} \text{ , } [\mathrm{H}] = \left(K_1 K_2 K_3^2 \frac{[\mathrm{O_2}][\mathrm{H_2}]^3}{[\mathrm{H_2O}]^2} \right)^{1/2} \text{ ,and } [\mathrm{OH}] = \left(K_1 K_2 [\mathrm{O_2}][\mathrm{H_2}] \right)^{1/2}$$

(For completeness, k_{1f} and k_{1r} can be introduced for K_1 etc.)

The reactions can be in (approximate) equilibrium when they are fast. This is more likely at higher temperatures.

3)
Isotropic turbulence is rotationally invariant; that is, any mean value is independent of the orientation of the framework/coordinate system of the observation. In practice, no spatial gradients of mean values.

In the k and ε equations, all terms with spatial gradients of mean quantities disappear, hence

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

The remaining source term of both equations are negative, hence both quantities will decrease.

Since there is no directional differences, the normal stresses are equal to each other: $\overline{u_1'^2} = \overline{u_2'^2} = \overline{u_3'^2} = \tfrac{2}{3}k$, and the shear stresses have to be zero $\overline{u_1'u_2'} = \overline{u_1'u_3'} = \overline{u_2'u_3'} = 0$

4)
Flammability limits:
Flammability limits are determined in a specially designed ("standardized") device. A premixed mixture of fuel, air and possibly inert species is contained in a tube and ignited from bottom. The mixtures in which

the flame can propagate are within the flame limits; “upper” limit for the richest mixture that can give a propagating flame, “lower” limit for the leanest mixture.
The physics of the limits is a balance between reaction heat release, heating of the unburned mixture to ignition (i.e. propagating flame) and heat loss to the surroundings. Hence, the flammability limits varies with the fuel, with the content of the mixture (fuel-oxidizer ratio and amount of inerts), with the preheating temperature and with the pressure, and it also depends on the geometry (apparatus).

The flammability limits are given as a molar percentage of the fuel in a mixture with air ate a specified temperature and pressure. Alternatively, any metric that precisely specifies the content of fuel in air (and intert) mixture can be used; for instance g/m^3 of fuel in air or kJ of LHV per m^3 of mixture.

5)
See textbook (Ertesvåg Figs. 10.3-10.4).
Horizontal axis: ratio of turbulence length scale to flame (chemical) length scale, (ℓ' / δ_L)
Vertical axis: ratio of turbulence velocity scale to flame (chemical) velocity scale, (u' / u_L)
Dahmköhler number = ratio of turbulence time scale to chemical time scale, $\mathrm{Da} = \theta / \tau_c$
Small-scale Dahmköhler number = ratio of Kolmogorov time scale to chemical time scale, $\mathrm{Da}_\mathrm{K} = \tau / \tau_c$
Turbulence number $\mathrm{Re}_{\ell'} = u'\ell' / \nu$

6)
See textbook (Ertesvåg Fig. 10.4).
Regimes: Laminar flames; wrinkled and stretched flamelets (small laminar flames); torn flamelets; thickened flames.
Wood stove: small length and velocity scales of turbulence, low intensity - wrinkled and stretched flamelets; possibley torn flamelets
Gas turbine: small length scales, large velocity scales, high intensity – stretched and torn flamelets
Large furnace: large length scales, medium to high velocity/intensity – thickened flames
Large fire: large length scales, medium to high velocity/intensity – thickened flames/torn flamelets

7)
Rearranging the given expression gives $\dfrac{d\overline{u}_1}{u_\tau} = d\left(\dfrac{\overline{u}_1}{u_\tau}\right) = \dfrac{1}{\kappa}\dfrac{dx_2}{x_2} = \dfrac{1}{\kappa}\dfrac{d(x_2 u_\tau / \nu)}{(x_2 u_\tau / \nu)}$

Integration gives $\dfrac{\overline{u}_1}{u_\tau} = \dfrac{1}{\kappa}\ln(\dfrac{x_2 u_\tau}{\nu}) + C$, where C is an integration constant.

Alternatively, the definitions $u_1^+ = \dfrac{\overline{u}_1}{u_\tau}$; $u_\tau = \left(\tau_\mathrm{w} / \rho\right)^{1/2}$; $x_2^+ = \dfrac{x_2 u_\tau}{\nu}$ can be introduced, the expression rearranged to $du_1^+ = \dfrac{1}{\kappa}\dfrac{dx_2^+}{x_2^+}$ and integrated to $u_1^+ = \dfrac{1}{\kappa}\ln x_2^+ + C$.

This relation is valid in a region of the boundary layer where equilibrium between production and dissipation of turbulence energy is assumed, that is, $P_k = \varepsilon$ or $-\overline{u_1' u_2'}\dfrac{\partial \overline{u}_1}{\partial x_2} = \varepsilon$.

Moreover, in the same region it is assumed that the turbulence shear stress is approximately constant and equal to the wall shear stress, $-\overline{u_1' u_2'} = \left(\tau_\mathrm{w} / \rho\right) = u_\tau^2$

Combining these expressions $-\overline{u_1'u_2'}\frac{\partial \overline{u}_1}{\partial x_2} = u_\tau^2 \frac{u_\tau}{\kappa x_2}$ or $\varepsilon = u_\tau^3 / (\kappa x_2)$, which can be used as a "wall function" for the dissipation rate ε.

8)
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, $u = \overline{u}_i + u_i'$ and $\xi = \overline{\xi} + \xi'$; assume that ρ is constant (or that it does not correlate with velocity and the mixture fraction):

$$\frac{\partial}{\partial t}(\rho(\overline{\xi} + \xi')) + \frac{\partial}{\partial x_j}(\rho(\overline{\xi}\overline{u}_j + \overline{\xi}u_j' + \xi'\overline{u}_j + \overline{\xi'u_j'})) = \frac{\partial}{\partial x_j}(D(\frac{\partial \overline{\xi}}{\partial x_j} + \frac{\partial \xi'}{\partial x_j}))$$

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

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

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

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

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

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

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

9)
The flow velocity averaged over the cross-section (bulk velocity) is $u_b = 0{,}1/(0{,}1)^2$ m/s = 10 m/s
The duct-flow Reynolds number is $\mathrm{Re}_D = u_b D/\nu = 10 \cdot 0{,}1/(1{,}5 \cdot 10^{-5}) = 6{,}7 \cdot 10^4$. This is well above the "critical" Reynolds number value, which indicate transition from laminar to turbulent flow.
The turbulence intensity can be assumed to 5%, that is a turbulence velocity scale approximated to 0,05 times the bulk velocity: $u' \approx 0{,}05 \cdot u_b = 0{,}5$ m/s.
The turbulence energy is estimated to the square of this: $k \approx u'^2 \approx 0{,}25\ \mathrm{m^2/s^2}$
The turbulence length scale can be estimated to the duct width (or a fraction of it): $\ell' \approx D = 0{,}1$ m
The dissipation rate of turbulence energy is estimated from
$\varepsilon \approx u'^3 / \ell' \approx (0{,}5\ \mathrm{m/s})^3 / (0{,}1\ \mathrm{m}) = 1{,}25\ \mathrm{m^2/s^3}$

With these results, the Kolmogorov length scale becomes
$\eta = (\nu^3 / \varepsilon)^{1/4} = (1,5\cdot 10^{-5})^{3/4} / (1,25)^{1/4}$ m = $2.3\cdot 10^{-4}$ m
The turbulence Reynolds number $\mathrm{Re}_\mathrm{t} = u'\ell'/\nu \approx 0,5\cdot 0,1/(1,5\cdot 10^{-5}) = 3\cdot 10^3$

10)
Heating at constant temperature in inert atmosphere:

- Moisture evaporation (decreasing mass, then stable)
- Volatiles evaporation (decreasing mass, then stable)

Add air after a certain time

- Fixed-carbon burn out (decreasing mass)
- Ash remaining (stable mass)