Suggested solutions TEP4170 Heat and combustion technology 15 Aug 2011 by Ivar S. Ertesvåg. Revised 11 May 2015.

1)

The sketch shows the flame height of a simple, non-premixed (diffusion) jet flame. The outflow (nozzle) velocity is gradually increased and the development of the flame is observed.

- In the first phase, the flame is laminar. Here the flame height increases with increasing velocity. This can be explained by the fact that more fuel needs a larger flame area to react since the flame is limited by the molecular diffusion. The only way to increase fuel consumption is to increase the flame.

-At a certain nozzle flow velocity, the flame becomes unstable and turbulent motion occurs. This happens when the ratio of inertia to viscous forces reaches a certain limit. The point of transition moves rapidly towards the nozzle at increasing nozzle velocity.

- In the last phase, a turbulent flame is fully developed. Here increased fuel follows more agitation (more turbulence) and leads to a larger flame area inside the flame.

2)

Mean-value (Reynolds-averaged, "RANS") modeling make use of a decomposition of the physical quantities into a mean and a fluctuating component, e.g. velocity: $u = \overline{u} + u'$.

When this is introduced into the basic equations (continuity, momentum, species mass, energy), and these equations are averaged, the Reynolds-averaged eguations are obtained. Since the averaged quantities show much less variation than the instantaneous equations, they can be solved with reasonable efforts for complex cases. The drawback is that new terms have appeared in the equations, which have to be modeled. In mean-value methods, all effects of turbulent motions are represented by the models.

Other methods:

*Large-eddy simulation: "filter" the small scales of turbulence, and model the effects of these, while the large-scale turbulent motions are resolved.

*Direct numerical simulation: all turbulent motions are resolved numerically, no model required (beyond constitutive models for molecular fluxes etc.).

*Transported joint probability density functions: Make use of the definition of average, and solve equations for the joint pdfs. In this case terms representing reactions reaction terms are closed, whereas molecular transport requires modeling.

3)

r is the stoichiometric (theoretical) amount of oxidizer on mass base; the mass of oxidizer used to burn one kg of fuel

r=6,47 for methanol with air.

$$R_{\text{ox}} = r \cdot R_{\text{fu}}$$
 and $R_{\text{prod}} = -(r+1) \cdot R_{\text{fu}}$

4)

A conserved scalar has zero source term.

The source term of the equation for the quantity $(Y_{fu} - \frac{1}{r}Y_{ox})$ will be $(R_{fu} - \frac{1}{r}R_{ox}) = R_{fu} - \frac{1}{r} \cdot r \cdot R_{fu} = 0$, that is, if the molecular diffusivities of fu and ox are the same and a simple one-step reaction (Problem 3) is assumed. When the source term is zero, the quantity is a conserved scalar.

Mixture fraction: $\xi = (\varphi - \varphi_2)/(\varphi_1 - \varphi_2)$, where φ is a conserved scalar and the subscripts 1 and 2 refer to two separate inflows.

The mixture fraction equation can be developed e.g. by combining two species mass fraction equations, cf. Problems 4 and 3:

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

Introducing the Reynolds decomposition, $u = \overline{u} + u'$ and $\xi = \overline{\xi} + \xi'$, and averaging each term gives

$$\frac{\partial(\rho\overline{\xi})}{\partial t} + \frac{\partial}{\partial x_{j}}(\rho\overline{\xi}\overline{u}_{j} + \rho\overline{\xi'u'}_{j}) = \frac{\partial}{\partial x_{j}}(\rho D\frac{\partial\overline{\xi}}{\partial x_{j}})$$

where the third term is often moved to the right-hand side.

6)

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: $k = \int_0^\infty E(\kappa) d\kappa$

The equilibrium range is the range of wave numbers from an approximate point somewhat larger than that of the maximum E value. In this range, the motions are not affected by the external dimensions and overall flow.

The inertial subrange is the lower part of the equilibrium range; this range is also independent of visous forces. Hence, statistical quantities (such as the energy spectrum) in this range depends only on the transferred energy (approximated by the dissipation rate, ε) and the size of the scales (eddies), which can be expressed by the wave number. Thus $E = f(\varepsilon, \kappa) = C_{\kappa} \cdot \varepsilon^{\alpha} \cdot \kappa^{\beta}$, where the exponents are constants. A dimensional analysis gives $\alpha = 2/3$ and $\beta = -5/3$, hence "Kolmogorov's 5/3-law".

7)

Kolmogorov assumed that small-scale turbulent motions are independent of the large-scale motions. With this local lack of dependency, all directions should be equally probable, and hence, these motions should be isotropic ("iso": even, equal, "tropos": turn).

The Kolmogorov microscales are scales of velocity, length and time for the dissipative range, that is the smaller scales of turbulence. They are obtained by assuming equilibrium between inertia and viscous forces, and determined from dimensional analysis assuming dependence only on dissipation rate and viscosity: $v = v(\varepsilon, \upsilon) = (\upsilon \varepsilon)^{1/4}$, $\eta = \eta(\varepsilon, \upsilon) = (\upsilon^3 / \varepsilon)^{1/4}$ and $\tau = \eta / v = (\upsilon / \varepsilon)^{1/2}$.

8)

In non-premixed (diffusion) flames soot is formed on the fuel-rich side of the flame sheet. The main steps are

- 1. Formation of precursor species. PAH thought to be important intermediates. Chemical kinetics plays an important role. Subject to research
- 2. Beginning particle formation (Particle inception). Formation of small particles from large molecules that grows and coagulate (solidify)
- 3. Surface growth and agglomeration. The small initial particles gain mass from the fuel and by agglomeration with other particles.

5)

4. Particle oxidation. – The particles oxidate in the oxidation zone. May burn completely, or some soot particles may escape.

Soot has the largest concentration on the fuel rich side of the peak temperature; it is falling to a low value in the high-temperature zone and have a low (or zero) value on the oxygen-rich side.

In premixed flames soot can occur when the mixture is rich; depending on the temperature.

9)

Chain reactions involve the production of a radical species, which reacts to produce another radical species, and so on until formation of only stable species.

<u>chain-initiation reaction</u>: an elementary reaction forming one or more radical species from only stable species

<u>chain-branching reaction</u>: an elementary reaction forming more radical species than it consumes (usually consuming one and producing two)

chain-propagating reaction: an elementary reaction where a radical species reacts and a radical species is formed.

chain-termination reaction: an elementary reaction which consumes a radical species and forming only stable species

10)

1kg moist fuel gives w kg water (w=0,15) and (1-w=0,85) kg dry matter ("dm").

This contains

0,85.0,49 kg of C, which is converted to 0,85.0,49.44/12 kg CO₂ = 1.527 kg CO₂, which is emitted. This consumes (1,527-0,85.0,49)kg =1,111 kg of oxygen.

0,85.0,06 kg of H, which is converted to 0,85.0,06.18/2 kg $H_2O = 0,459$ kg H_2O , which is emitted together with the 0,15 kg of moisture, giving a total of 0,609 kg H_2O

This consumes $(0,459-0,85\cdot0,06)$ kg =0,408 kg of oxygen.

 $0,85 \cdot 0,44$ kg of O =0,374 kg oxygen, which enters the reaction of C and H.

The net oxygen requirement from the air is then (1,111+0,609-0,374) kg=1,346 kg oxygen (as O₂).

The surplus O₂ is $(\lambda - 1) \cdot 1,346$ kg = $0,1 \cdot 1,346$ kg=0,135 kg, which is emitted with the reaction products.

The effective heating value is the heating value of the dry matter minus the heat required to evaporate the water:

 $h_{\text{eff}} = (1 - w) \cdot h_{\text{dm}} + w \cdot (-h_{\text{fg}}) = 0,85 \cdot 19 \text{ MJ/kg} - 0,15 \cdot 2,47 \text{ MJ/kg} = 15,8 \text{ MJ/kg}$