Suggested solutions TEP4170 Heat and combustion technology 18 May 2013 by Ivar S. Ertesvåg, with contributions from Khanh-Quang Tran (Problem 10). Revised 18 May 2016.

1)

Assumptions: constant density, non-fluctuating viscosity (or rather: no correlation between viscosity and velocity or pressure)

The equation for momentum reads

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}(\tau_{ij}) + \rho f_i \quad (1)$$

Introduce the Reynolds decomposition, $u_i = \overline{u_i} + u'_i$, $u_j = \overline{u_j} + u'_j$ into the equation:

$$\frac{\partial}{\partial t}(\rho \overline{u_i} + \rho u_i') + \dots = \dots \quad (2)$$

Assume constant density and average this equation (average each term): $\frac{\partial}{\partial t}(\rho \overline{u}_i) + \dots = \dots$ (3)

Subtract (3) from (2): $\frac{\partial}{\partial t}(\rho u'_i) + \dots = \dots$ (4)

Multiply (4) by $(u'_i): u'_i \frac{\partial}{\partial t} (\rho u'_i) + \dots = \dots$

Make use of the relation $d(u_i'^2) = 2u_i' \cdot du_i'$: $\frac{\partial}{\partial t} (\rho \frac{1}{2} u_i'^2) + \dots = \dots$

average this equation: $\frac{\partial}{\partial t} (\rho \frac{1}{2} \overline{u_i'^2}) + \dots = \dots$ Since $\frac{1}{2} \overline{u_i'^2} \equiv k$, this is the equation requested in the problem.

Terms No.1, 2, 3 and 5(enumerated from the left) in the equation given in the problem are retained as they are in the "exact" equation. (No. 5 contains the Reynolds stresses, which are modelled as part of the mean momentum eq.). Terms Nos. 4 and 6 are modelled. (No.6 found from a separate equation.)

2)

The ε equation is expressed in the same pattern as the k equation:

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \frac{\partial}{\partial x_j}(\rho\varepsilon\overline{u}_j) = \frac{\partial}{\partial x_j}\left(\mu\frac{\partial\varepsilon}{\partial x_j}\right) + \frac{\partial}{\partial x_j}\left((\frac{\mu_i}{\sigma_\varepsilon})\frac{\partial\varepsilon}{\partial x_j}\right) + \rho P_\varepsilon - \rho Q_\varepsilon$$

In the 4th term, the gradient model is used similar to that in the *k* equation, except with a different constant. In the 5th and 6th terms, the production and destruction of ε , are modeled proportional to the corresponding terms of the *k* equation:

$$\rho P_{\varepsilon} = C_{\varepsilon 1} \rho \frac{\varepsilon}{k} P_k$$
, where ρP_k is the 5th term of the *k* equation, and $\rho Q_{\varepsilon} = C_{\varepsilon 2} \rho \frac{\varepsilon}{k} \varepsilon$

The factor ε / k is introduced to give the right dimension, and C_{ε_1} and C_{ε_2} are model constants.

3)

In the following, the numbers are estimates, not exact. Other choices could also serve the purpose. A turbulence velocity can be estimated as $u' = 0.05 \cdot U = 0.5$ m/s, and a length scale as, say, $l' = 0.1 \cdot L = 0.1$ m

A Reynolds number of turbulence is then $\text{Re}_t = u'l' / v \approx (0.5 \cdot 0.1 / 10^{-5}) = 5000$, which is "large" and verifies that the flow is turbulent.

The turbulence energy can be estimated from $k \approx u'^2 = 0.25 \text{ m}^2/\text{s}^2$, and the dissipation rate from $\varepsilon \approx u'^3 / l' \approx 1.25 \text{ m}^2/\text{s}^3$ The Kolmogorov length scale then becomes $\eta = (v^3 / \varepsilon)^{1/4} \approx (10^{-15} / 1.25)^{0.25} \text{ m} = 0.17 \cdot 10^{-3} \text{ m}$

The quantity η/U can be seen as the time needed for a length η (representing small eddies) to flow past a point in the flow. If this point is, e.g., the location of a probe, the time interval between each sampling has to be shorter than η/U if the probe should be able to catch the small eddy.

4)

The maximum time step should be less than the least time scale of the case:

The Kolmogorov time scale can be estimated to $\tau = (\nu / \varepsilon)^{1/2} \approx (10^{-5} / 1.25)^{0.5}$ s = $2.8 \cdot 10^{-3}$ s

The mixing time scale (l'/u') will be larger than the Kolmogorov time scale

The convection time scale for the Kolmogorov length: $\eta / U = (0.17 \cdot 10^{-3} / 10) \text{ s} = 1.7 \cdot 10^{-3} \text{ s}$ A (least) reaction length scale can be estimated from the (least) reaction time scale; $\delta_r \sim (D \cdot \tau_c)^{1/2} \sim (v \cdot \tau_c)^{1/2} \approx (10^{-5} \cdot 10^{-6})^{1/2} \text{ m} \approx 3 \cdot 10^{-6} \text{ m}$

and the corresponding convection time scale: $\delta_r / U = (3 \cdot 10^{-6} / 10) \text{ s} = 3 \cdot 10^{-7} \text{ s}$

This (inaccurate) estimate indicates that the convection time scale for reaction lengths can be less than the least reaction time scale of 10^{-6} s, and is then the least time scale of the case and limits the time step of the numerical solution.

5)

See sketch at the attached (last) page

6)

In the inertial subrange, all statistical quantities of the turbulence, including the 3D energy spectrum E are independent of the external geometry, mean flow and the largest eddies, and also of the viscous forces and smallest scales. The remaining dependency for this range is then the size of the eddies and the transfer of turbulence energy from larger eddies and further to smaller eddies.

The size is represented by the wave number κ and the energy transfer is represented by the dissipation rate ε .

By dimensional analysis: $[E] = L^3 / T^2 = [\varepsilon^a \kappa^b] = (L^2 / T^3)^a \cdot (L^{-1})^b = L^{2a-b} / T^{3a}$ This gives a = 2/3 and b = -5/3. With a constant of proportionality, the relation becomes $E = C_{\kappa} \cdot \varepsilon^{2/3} \cdot \kappa^{-5/3}$ 7) See sketch at the attached (last) page.

The flow is steady state (which means that the propagation speed of the flame equals the speed of the upstream (unburnt) flow. This is the flame speed, u_L .

The flame thickness δ_L can be defined as from the temperature increase, related to the temperature difference between the far upstream (unburnt) and the far downstream (burnt). The distance from a point where the temperature has increased, say, 2% of the total increase to the point where it has increased, say, 98% of the total increase.

The time scale is the ratio $\tau_c = \delta_L / u_L$

For a non-premixed flame, the velocity and length cannot be readily visualized. However, both for premixed and non-premixed flames, the time scale can be expressed from the (global) reaction rate, $\tau_c \sim R_{\rm fu}^{-1}$, and the velocity and length can be expressed from the time scale and the diffusivity: $u_L \sim (D/\tau_c)^{1/2}$ and $\delta_L \sim (\tau_c D)^{1/2}$

8)

The case is 1-dimensional and steady state (time-independent); thus the basic equations will be simplified:

Continuity: $\frac{d}{dx}(\rho v_x) = 0$, or $\rho v_x = \dot{m}'' = \text{ constant}$

Momentum equation: $\frac{dp}{dx} = 0$ or p = constant

Species mass balance: $\frac{d}{dx}(\rho v_x Y_i) + \frac{d}{dx}(\rho v_{i,diff} Y_i) = \dot{\omega}_i M_i$, for species i = 1, 2, ..., NThe first term can be reformulated with the continuity equation. In the 2nd term, the diffusion can be modelled with Fick's law, and for the last term, the symbols \dot{m}_i^m or R_i are also used;

$$\rho v_x \frac{dY_i}{dx} + \frac{d}{dx} (-\rho D_i \frac{dY_i}{dx}) = \dot{m}'$$

The energy balance:
$$\rho v_x c_p \frac{dT}{dx} + \frac{d}{dx}(-k\frac{dT}{dx}) + \sum \rho v_{i,\text{diff}} Y_i c_{p,i} \frac{dT}{dx} = S_T$$

Here, the energy balance is expressed as a temperature equation. In the 2^{nd} term, Fourier's law is introduced, and in the 3^{rd} term, Fick's law can be introduced. In the source term, the main contributions are the thermal heat release due to reactions and heat exchange due to radiation.

Equation of state (ideal gas): $p = \rho RT$

Relations for specific heat, conductivity and diffusivity have to be expressed as functions of temperature (and pressure, when relevant).

The reaction rates have to be expressed from a chemical mechanism.

Boundary conditions: This depends on the simplifications. The minimum conditions are:

Far upstream (
$$x = -\infty$$
): $T = T_u$,; $Y_i = Y_{i,0}$ (=0 for most *i*). Far downstream ($x = +\infty$): $\frac{dT}{dx} = \frac{dY_i}{dx} = 0$

If all simplifications of the textbook (Turns) are introduced (one-step complete reaction, shape of temperature profile, diffusivities, etc.), solution of the species mass balances can be avoided and therefore,

also the boundary conditions on the mass fractions. In this case, the <u>additional</u> conditions are required for the temperature:

Far upstream (
$$x = -\infty$$
): $\frac{dT}{dx} = 0$. Far downstream ($x = +\infty$): $T = T_b$

9)

The Bunsen burner is sketched in Fig. 8.3 in Turns (see last, attached page).

When a steady state flame is established and the volumetric flow rate is known, the velocity of the unburnt mixture in the tube, v_{μ} can be calculated. Alternatively, v_{μ} can be measured in the tube.

The angle α can be measured, and the flame speed will be the component of the unburnt velocity normal to the flame, $v_{u,n}$.

By geometrical considerations, this is expressed as $u_L (= S_L) = v_u \sin \alpha$

10)

The two-step analysis needed to develop an expression between conversion time and radius include:

- 1. Examine a typical partially reacted particle, writing the flux relationships for this condition, assuming the core is stationary
- 2. Apply the relationships for all value of r_c , in other words, integrate r_c between R and O

The assumption that the core is stationary is needed because both reactant A and the boundary of the unreacted core move inward toward the center of the particle. But for G/S systems, like coal combustion in air, the shrinkage of the unreacted core is slower than the flow rate of A toward the unreacted core by a factor of about 1000, which is roughly the ratio of densities of solid and gas. Because of this consideration it is reasonable to assume that the unreacted core is stationary.

