Suggested solutions TEP4170 Heat and combustion technology 4 June 2010

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1)

Called "exact" because it is developed from the Navier-Stokes equations, just by mathematical operations, witout adding any new modelling assumptions.

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

The equation for momentum reads

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

Insert the Reynolds decomposition, $u_i = \bar{u}_i + u'_i$, $u_j = \bar{u}_j + u'_j$

into the equation: $\frac{\partial}{\partial t}(\rho \bar{u}_i + \rho u'_i) + ... = ... \quad (2)$

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

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

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

Make use of the relation $d(u'^2_i) = 2u'_i \cdot du'_i$: $\frac{\partial}{\partial t}(\rho \tfrac{1}{2} u'^2_i) + ... = ...$

average this equation: $\frac{\partial}{\partial t}(\rho \tfrac{1}{2} \overline{u'^2_i}) + ... = ...$ which is the equation given in the problem

Interpretation of the terms (enumerated from the left):
(1): change (increase) with time, storage
(2): carried with the mean flow (mean convection)
(3): transported with molecular motions, molecular diffusion
(4): transported with turbulent motions, turbulence diffusion
(5): production of turbulence energy due to interaction between mean-flow gradients and turbulent motions; transfer of mechanical energy from mean motion to turbulent motions
(6): degradation of kinetic energy due to molecular motions (viscous forces), "dissipation"; transfer of energy from kinetic energy to thermal energy

2)

Based on the equation in Problem 1, term 4 and 5 modeled, term 6 found from a separate equation:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_j}(\rho k \bar{u}_j) = \frac{\partial}{\partial x_j}(\mu \frac{\partial k}{\partial x_j}) + \frac{\partial}{\partial x_j}(\frac{\mu_t}{\sigma_k}\frac{\partial k}{\partial x_j}) + \rho P_k - \rho \varepsilon$$

where

$$P_k = -\rho \overline{u'_i u'_j}\frac{\partial \bar{u}_i}{\partial x_j} = \mu_t(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i})\frac{\partial \bar{u}_i}{\partial x_j}$$

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_j}(\rho \varepsilon \bar{u}_j) = \frac{\partial}{\partial x_j}(\mu \frac{\partial \varepsilon}{\partial x_j}) + \frac{\partial}{\partial x_j}(\frac{\mu_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_j}) + \rho c_{\varepsilon 1}\frac{\varepsilon}{k}P_k - \rho c_{\varepsilon 2}\frac{\varepsilon}{k}\varepsilon$$

Here, $\sigma_k, \sigma_\varepsilon, c_{\varepsilon 1}, c_{\varepsilon 2}$ are model constants and μ_t is the (dynamic) turbulence viscosity.

3)
A wall function is an expression relating certain quantities (velocity, turbulence energy, turbulence stresses, dissipation, temperature, etc.) to the shear stress at the wall and the distance from the wall (and the heat and mass transfer from the wall, when relevant). The purpose is to provide a "bridge" between the wall and the outer part of the wall boundary layer by simple models and thereby avoid a very detailed resolution (=computationally demanding) of the wall shear layer.

A wall function for ε can be developed from a simplification of the k equation (Problems 1-2); assuming balance between production and dissipation and a one-gradient, 2-dimensional shear layer

$$-\rho \overline{u_1' u_2'} \frac{\partial \overline{u_1}}{\partial x_2} \approx \rho \varepsilon$$

On the the left-hand side, the turbulence shear stress can be approximated equal to the wall shear stress: $-\rho \overline{u_1' u_2'} \approx \tau_w \equiv \rho u_\tau^2$. The gradient is expressed by the approximation given in the "hint" (see problem), hence:

$$\varepsilon \approx u_\tau^2 \cdot \frac{u_\tau}{\kappa x_2} = \frac{u_\tau^3}{\kappa x_2} \quad \text{which can be used as a wall function.}$$

4)

In isotropic turbulence, the k equation reduces to $\dfrac{dk}{dt} = -\varepsilon$. Hence $\varepsilon(t) \sim t^{-(n+1)}$

A length scale can be expressed as $l = k^{3/2}/\varepsilon$, and hence $l(t) \sim t^{-3n/2+(n+1)} \sim t^{1-n/2}$

A Reynolds number can be expressed as $\text{Re}_T = k^2/(\upsilon \varepsilon)$, and hence $\text{Re}_T(t) \sim t^{-2n+(n+1)} \sim t^{-(n-1)}$

Since $1 < n < 1,5$, the exponent of the length scale will be positive and it will increase;
the exponent of the Reynolds number will be negative, and it will decrease.

The Reynolds number describes the intensity of turbulence. Isotropic turbulence, no turbulence energy is produced, only dissipated. Hence the turbulence is decaying/dying, and the Reynolds number will decrease.
The length scale can be understood as representing the turbulence eddies. With reduced kinetic energy, the inertial forces keeping the motion together is gradually lost, and the involved matter drifts apart; hence increasing length scale.

5)
a. the Reynolds shear stress: zero at both walls and at the center line; peak values close to walls. If a fixed (not rotating) coordinate is used from $-R$ to $+R$: anti-symmetric (symmetric but with opposite signs); linear about the centerline.
b. the Reynolds normal stress directed along the flow direction: zero at both walls, always positive (when non-zero), symmetric about center line, small but non-zero at centerline, peak close to the wall (more close and much sharper than for the shear stress)
c. the Reynolds normal stress directed normal to the wall: similar to the normal stress directed along the flow, except that the value is always smaller, the peak is smooth and farther from the wall than for the shear stress
d. the turbulence energy: similar to the normal stress directed along the flow

6)
A global/overall reaction is a balance between the species consumed and produced in the reaction. Intermediate species are not included and the actual combinations of reactants are not described. Example: Overall reaction for heptane and air, see Problem 9.
The global reaction is the sum of (or bookkeeping of) tens (for H2) hundreds/thousands (most other fuels) of elementary reactions. These describe the actual combinations of reactants (1, 2, in rare cases 3) and products, and intermediate species are included. Examples: see Problem 7.

The practical implication of reduced or simplified chemical kinetics is that computational efforts can be reduced (fewer species, fewer reactions) and that information is lost/left out.

7)
<u>chain reaction</u>: 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-propagating reaction</u>: an elementary reaction where a radical species reacts and a radical species is formed.
<u>chain-termination reaction</u>: an elementary reaction which consumes a radical species and forming only stable species

Radical species in the examples are O, OH, H and HO_2;
(CO.1) is chain-initiating; (CO.3), (CO.6) and (CO.7) are chain-propagating; none are chain terminating
Reactions (CO.2), (CO.4), and (CO.5) consume one radical species and produce two; these are called chain-branching. (In the context of the problem formulation, this can be regarded as chain propagating).

8)
Steps of soot formation and destruction in laminar diffusion (non-premixed) flames.
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.
4. Particle oxidation. – The particles oxidate in the oxidation zone. May burn completely, or some soot particles may escape.

Typical radial temperature profile and soot concentration profile in a vertical jet of non-premixed hydrocarbon laminar flames:
Steep peak of temperature in the outer part of the jet flow (reaction zone around stoichiometric contour); steep soot peak inside this zone, falling to a low value in the high-temperature zone and outside the jet.

9)
Two different types of turbulence combustion models are
Magnussen's "Eddy Dissipation" model and
models based on a prescribed probability density function (Norw: føreskriven sannsynstettleik), also called flamelet models.

Magnussen's model provide an expression for the mean reaction rate, which is the source term of the species mean mass fraction equation (Transport/PDE of the mean mass fractions). These equations are then solved.

The models based on a prescribed probability density function make use of a conserved scalar (mixture fraction for non-premixed flames) as a characteristic variable. Most other quantities are expressed as functions of this variable, and the mean values are obtained by integration over the pdf:

$$\bar{G} = \int_{-\infty}^{\infty} G(\xi)f(\xi)d\xi,$$ where G is the quantity of interest (T, Y_k, etc.), ξ is the characteristic

variable, and $f(\xi)$ is the pdf. When the characteristic variable is the mixture fraction, it is limited to the interval (0,1). The use of a characteristic variable relies on an assumption that this actually is relevant; usually justified by the flamelet assumptions (thin flames, low Re, high Da).

To determine the form of the pdf, transport equations for the mean and variance of the characteristic variable is solved. Other scalar transport equations are, however, not solved.

For both types of models, the mean momentum equations are solved and a turbulence model is used (usually including transport equations for turbulence quantities, e.g. turbulence energy and dissipation.

10)
Balanced reaction:
$C_7H_{16} + 1.4 \cdot 11 \cdot (O_2 + 3.76\ N_2) \rightarrow 7\ CO_2 + 8\ H_2O + 0.4 \cdot 11\ O_2 + 1.4 \cdot 11 \cdot 3.76\ N_2$
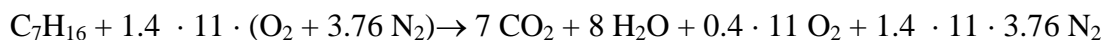
$X_{CO2}(dry) = 7/(7 + 4.4 + 1.4 \cdot 11 \cdot 3.76) = 7/\ 69.3 = 0.101$

a.
$EI_{NO} = m_{NO}/m_F = (n_{NO}\cdot M_{NO})/(n_F\cdot M_F) = (n_{NO}\cdot M_{NO})/(n_{CO2}\cdot M_F) \cdot (n_{CO2}/n_F)=$
$=(X_{NO}/X_{CO2}) \cdot (x \cdot M_{NO}/M_F) = (200\cdot10^{-6}\ /\ 0.101) \cdot 7 \cdot (30.01/100.21)$ kg/kg
$= 0.00415$ kg/kg $= \underline{4.15\ g/kg}$

b.
$(MSE)_{NO} = m_{NO}/W = m_{NO}/(m_F \cdot \eta \cdot h_{LHV}) = EI_{NO}/(\eta \cdot h_{LHV}) = 4.15$ g/kg $/(0.40 \cdot 44,5$ MJ/kg$)$
$= 0,233$ g/MJ $= 0,233$ g/MJ $\cdot 3.6$ MJ/kWh $= 0,84$ g/kWh
or:
Fuel energy input, $H_F = W/\eta = 90$ kW/0.4 $= 225$ kW $= 0.225$ MJ/s
Mass flow fuel, $m_F = 0.225$ MJ/s $/ 44.5$ MJ/kg $=0.00506$ kg/s $= 18.2$ kg/h
$(MSE)_{NO} = m_F \cdot EI_{NO}/W = 18.2$ kg/h $\cdot (4.15$ g/kg$) / (90$ kW$) = \underline{0.84\ g/kWh}$

c. $(MSE)_{NO} = m_{NO}/H_F = m_{NO}/(m_F \cdot h_{LHV}) = EI_{NO}/h_{LHV} = (4.15$ g/kg$) / (44.5$ MJ/kg$) = \underline{0.093\ g/MJ}$

d. The purpose of expressing the emissions as mass specific or energy specific values is to be able to compare the emissions from different application (e.g. gas turbines, diesel engines, gas burners etc.), and at different operational conditions (different excess air ratios, different brake thermal efficiencies etc.).

11)

- Drying, at around 100 ºC
- Devolatilization or pyrolysis, at around 350 ºC, and volatiles combustion (flame, homogeneous reaction)
- Char combustion (heterogeneous reaction)

There are three simplified film models for carbon combustion: one-film, two-film, and continuous-film models. In the one-film models, there is no flame in the gas phase and the maximum temperature occurs at the carbon surface. In the two-film models, a flame sheet lies at some distance from the surface, where the CO produced at the surface reacts with incoming oxygen. In the continuous-film models, a flame zone is distributed within the boundary layer, rather than occurring in a sheet.

12)

Here we have a shrinking particle with only 2 possible resistances, film diffusion control and reaction control. Since it is assumed that film diffusion control plays no role, we are left with reaction control alone. So we solve the problem for this case, using τ formula for small particles (Stokes regime),

$$\tau = \frac{\rho_B R_0}{b \cdot k'' \cdot C_{Ag}}$$

where $\rho_B = (2.2 \text{ g/cm}^3)/(12 \text{ g/mol}) = 0.183 \text{ mol/cm}^3$

$C_{Ag} = (1 \text{ mol})/(224,000 \text{ cm}^3) \cdot 273 \text{ K} / 1173 \text{ K} \cdot 0.08 = 0.183 \text{ mol/cm}^3 = 8.30 \times 10^{-7} \text{ mol/cm}^3$

and $b = 1$ for the reaction $C + O_2 \rightarrow CO_2$

Replacing these quantities in the τ expression gives
$\tau = (0.183 \cdot 0.5) / (1 \cdot 20 \cdot 8.3 \cdot 10^{-7}) \text{ s} = 5510 \text{ s} = 1.53 \text{ h}$

Answer: The time needed for complete combustion of the given graphite particle is 1.53 hours