

Suggested solutions TEP4170 Heat and combustion technology 5 June 2009

by Ivar S. Ertesvåg, with contributions from Bjørn Lilleberg (Problem 6), Morten Grønli (10 and 12), and Nurun Nabi (9 and 11). Revised 14 May 2010.

Problem 1:

A conserved scalar is a quantity that has zero source term.

The transport equations (PDEs) for fuel and oxidizer mass can be expressed as

$$\frac{\partial}{\partial t}(\rho Y_{\text{fu}}) + \dots = \dots + R_{\text{fu}} \quad \text{and} \quad \frac{\partial}{\partial t}(\rho Y_{\text{ox}}) + \dots = \dots + R_{\text{ox}}$$

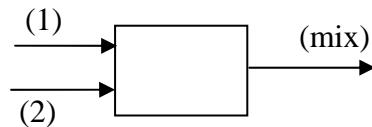
Dividing the latter equation by r , and subtracting it from the former, yields

$$\frac{\partial}{\partial t}(\rho(Y_{\text{fu}} - \frac{1}{r}Y_{\text{ox}})) + \dots = \dots + (R_{\text{fu}} - \frac{1}{r}R_{\text{ox}})$$

The stoichiometric (theoretical) amount of oxidant (aka. stoichiometric oxidizer-fuel ratio) is equal to the ratio of the source terms, $r = R_{\text{ox}} / R_{\text{fu}}$. Hence, the source term for $(Y_{\text{fu}} - \frac{1}{r}Y_{\text{ox}})$ is zero and it is a conserved scalar.

Problem 2

The mixture fraction is defined as $\xi = \frac{\varphi_{\text{mix}} - \varphi_2}{\varphi_1 - \varphi_2}$, where φ is a conserved scalar and subscripts mix, 1 and 2 refer, respectively, to mixture, inlet 1 and inlet 2 (cf. sketch).



Let (1)= methane, (2)= air; (3)=mix=stoichiometric mixture; $\varphi = Y_{\text{fu}} - \frac{1}{r}Y_{\text{ox}}$

mass:, $m_2 / m_1 = 17,16 \text{ kg/kg}$, $m_3 / m_1 = 18,16 \text{ kg/kg}$;

mass fractions: $Y_{\text{fu},1} = 1, Y_{\text{ox},1} = 0, Y_{\text{fu},2} = 0, Y_{\text{ox},2} = 0, Y_{\text{fu},2} = 1/18,16 = 0,055$,

$Y_{\text{fu},2} = 17,16/18,16 = 0,945$ (or $Y_{\text{fu},2} = 1 - Y_{\text{ox},2} = 0,945$)

$\varphi_1 = Y_{\text{fu},1} - \frac{1}{r}Y_{\text{ox},1} = 1$; $\varphi_2 = Y_{\text{fu},2} - \frac{1}{r}Y_{\text{ox},2} = -\frac{1}{r} = -(1/17,16) = -0,058$

$$\varphi_3 = Y_{\text{fu},3} - \frac{1}{r}Y_{\text{ox},3} = \left(\frac{1}{18,16} - \frac{1}{17,16} \cdot \frac{17,16}{18,16} \right) = 0$$

$$\xi_s = \frac{\varphi_3 - \varphi_2}{\varphi_1 - \varphi_2} = \frac{0 + 0,058}{1 + 0,058} = 0,055 \quad \text{or} \quad \xi_s = \frac{\varphi_3 - \varphi_2}{\varphi_1 - \varphi_2} = \frac{0 + 1/17,16}{1 + 1/17,16} = \frac{1}{17,16 + 1} = 0,055$$

Problem 3:

From Problem 2, we can use $(Y_{\text{fu}} - \frac{1}{r}Y_{\text{ox}}) = \xi \cdot (Y_{\text{fu}} - \frac{1}{r}Y_{\text{ox}})_1 + (1 - \xi) \cdot (Y_{\text{fu}} - \frac{1}{r}Y_{\text{ox}})_2 = \xi \cdot (1) + (1 - \xi) \cdot (-\frac{1}{r})$

For $\xi < \xi_s$, the mixture is lean and all the fuel is consumed (when the reaction is fast and complete):

$Y_{fu} = 0$ and $(Y_{fu} - \frac{1}{r}Y_{ox}) = (-\frac{1}{r}Y_{ox}) = \xi + (1 - \xi) \cdot (-\frac{1}{r})$, or $Y_{ox} = -r\xi + (1 - \xi) = 1 - \xi(1 + r)$

For $\xi > \xi_s$, the mixture is rich and all the air is consumed: $Y_{ox} = 0$, and

$(Y_{fu} - \frac{1}{r}Y_{ox}) = (Y_{fu} - 0) = Y_{fu} = \xi + (1 - \xi) \cdot (-\frac{1}{r}) = \frac{1}{r}(\xi(1 + r) - 1)$

For $\xi = \xi_s$, both fuel and air is consumed, $Y_{fu} = 0, Y_{ox} = 0$

Together these expressions constitute the functions $Y_{fu} = Y_{fu}(\xi)$ and $Y_{ox} = Y_{ox}(\xi)$.

Problem 4:

The equation for the mixture fraction reads

$$\frac{\partial}{\partial t}(\rho\xi) + \frac{\partial}{\partial x_j}(\rho u_j \xi) = \frac{\partial}{\partial x_j}(\rho D \frac{\partial \xi}{\partial x_j}) \quad (1)$$

Insert the Reynolds decomposition, $\xi = \bar{\xi} + \xi'$ into the equation: $\frac{\partial}{\partial t}(\rho\bar{\xi} + \rho\xi') + \dots = \dots$ (2)

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

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

Multiply (4) by $(2\xi')$: $2\xi' \frac{\partial}{\partial t}(\rho\xi') + \dots = \dots$

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

average this equation: $\frac{\partial}{\partial t}(\rho\overline{\xi'^2}) + \dots = \dots$ 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 $\overline{\xi'^2}$ due to interaction between mean-flow gradients and turbulent motions

(6): degradation of $\overline{\xi'^2}$ (smoothing of differences) due to molecular motions, "scalar dissipation"

Problem 5:

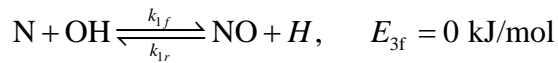
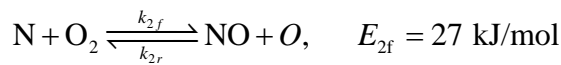
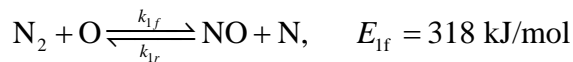
The general gradient model can be used in the form $-\rho\overline{u'_j \xi'} = \Gamma_\xi \frac{\partial \bar{\xi}}{\partial x_j} = \frac{\mu_t}{\sigma_\xi} \cdot \frac{\partial \bar{\xi}}{\partial x_j}$ in the 5th term,

and in the form $-\rho\overline{u'_j \xi'^2} = \Gamma_\xi \frac{\partial \overline{\xi'^2}}{\partial x_j} = \frac{\mu_t}{\sigma_\xi} \cdot \frac{\partial \overline{\xi'^2}}{\partial x_j}$ in the 4th term.

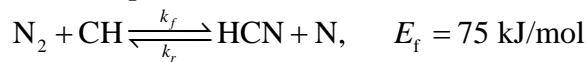
Problem 6:

The 3 most important mechanisms for NO formation from N_2 in air,

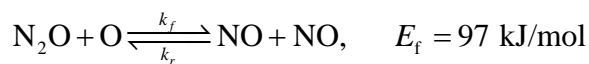
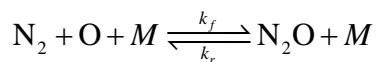
Thermal NO formation mechanism:



The Prompt NO formation (Fennimore) mechanism:



The N₂O mechanism:



Influence of temperature:

Temperature influences NO formation directly through the temperature dependence of the reaction constants. A large (positive) activation energy in a reaction constant makes the exponential term in the reaction constant increasingly temperature sensitive. Comparing only the activation energies for the above mentioned NO formation mechanisms thermal NO formation is clearly most temperature sensitive due to the high activation energy of the first (initiating) reaction. This reaction therefore also becomes rate-limiting. Prompt NO formation is much less temperature sensitive when only considering the activation energy of the initiating reaction. The same is the case for the NO producing reaction in the N₂O mechanism. However, great care should be taken when analysing the relative importance of NO formation mechanisms as a function of temperature, since several other parameters than the activation energy are involved. Some of these parameters are indirectly temperature dependent, e.g. radical concentrations.

Influence of pressure:

The reaction constant of a true elemental reaction is not pressure dependent, but the reaction rate is influenced by pressure through changing reactant concentrations, which speed up the reaction rate for increasing pressure. Looking at the NO formation mechanisms, the reaction constants in the thermal NO and prompt NO formation reactions are not pressure dependent, while the reaction constant in the initiating reaction in the N₂O mechanism is, since it is a third body reaction needing a “collision between three molecules” to form two molecules. This is not a true elemental reaction, but a series of reactions, where the reaction constant in the overall reaction becomes pressure dependent. In addition this reaction will be heavily influenced by pressure through its relative influence on reactant and product concentrations.

Influence of residence time:

Residence time influences NO formation heavily for the thermal NO formation mechanism, since the reaction rate in general is low due to its heavy temperature dependence, i.e. slow reactions need a longer residence time to reach equilibrium.

Influence of flame type:

The flame type influences the relative importance of the NO formation mechanisms. Basically the flame type influences the temperature levels where NO is formed (non-premixed flame, premixed

flame, lean flames, staged flames, etc.) through changes in residence time at high temperatures and radical concentrations. Hence, only considering the activation energy or the temperature dependence of the reaction constant is in many cases a great simplification. Also the availability of key radicals such as O, OH and CH are very much important, often resulting in a considerable degree of temperature dependence also for the prompt NO mechanism.

Problem 7:

Propane, mass: $m_{\text{prop}} = 0,464 \text{ kg}$, molar mass: $M_{\text{prop}} = 44 \text{ kg/kmol}$; amount: $n_{\text{prop}} = 0,0105 \text{ kmol}$

Overall (global) reaction: $\text{C}_3\text{H}_8 + \frac{1}{\Phi} (5)\text{O}_2 + \frac{79}{21}\text{N}_2 \rightarrow 3\text{CO}_2 + 4\text{H}_2\text{O} + \dots$

Volume of the room: $V = 3,66 \cdot 4,27 \cdot 2,44 \text{ m}^3 = 38,13 \text{ m}^3$, temperature $T=293 \text{ K}$ (20 °C),
pressure: $p= 1 \text{ atm} = 1,01 \text{ bar}=101 \text{ kPa}$ ($\text{kPa}=\text{kN/m}^2=\text{kJ/m}^3$)

Amount of air: $n_{\text{air}} = \frac{pV}{R_u T} = \frac{101 \cdot 38,13}{8,314 \cdot 293} \text{ kmol}=1,58 \text{ kmol}$

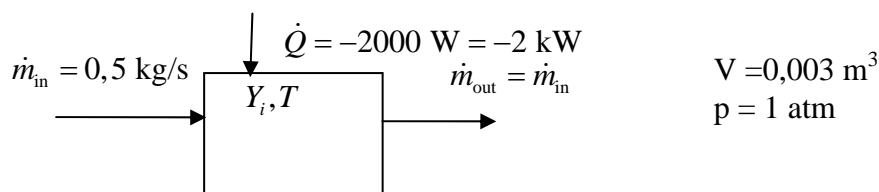
Air-fuel ratio:

actual: $\frac{n_{\text{air}}}{n_{\text{prop}}} = \overline{\text{AF}} = \frac{1,58}{0,0105} = 150,5$; stoichiometric: $\left(\frac{n_{\text{air}}}{n_{\text{prop}}} \right)_{\text{st}} = \overline{\text{AF}}_{\text{st}} = 5 \cdot (1 + 3,76) = 23,8$

$\Phi = \frac{1}{\lambda} = \frac{\overline{\text{AF}}_{\text{st}}}{\overline{\text{AF}}} = \frac{23,8}{150,5} = 0,158$ Therefore, as $\Phi < \Phi_{\text{min}}$ ($=0,51$), the mixture is not flammable

Discussion: During the process there can be larger and smaller volumes with a flammable mixture, i.e. local Φ that is within the limits.

Problem 8:



$h_{\text{f, fu}}^{\circ} = -2000 \text{ kJ/kg}$; $h_{\text{f, pr}}^{\circ} = -4000 \text{ kJ/kg}$; $h_{\text{f, ox}}^{\circ} = 0$; all species: $M_i = 29 \text{ kg/kmol}$; $c_p = 1,1 \text{ kJ/(kg K)}$

Given inlet: $Y_{\text{fu, in}} = 0,2$; $Y_{\text{ox, in}} = 0,8$; for a well-stirred reactor: $Y_{i, \text{out}} = Y_i$; $T_{\text{out}} = T$

Given for outlet: $Y_{\text{fu, out}} = 0,001$; $Y_{\text{ox, out}} = 0,003$

Species mass balance (steady state): $0 = \dot{m}_{i, \text{in}} - \dot{m}_{i, \text{out}} + R_i \cdot V$

For the fuel: $0 = (Y_{\text{fu, in}} - Y_{\text{fu, out}}) \dot{m}_{\text{in}} + R_{\text{fu}} \cdot V$

$(-R_{\text{fu}} \cdot V) = (0,2 - 0,001) \cdot 0,5 \text{ kg/s} = 0,0995 \text{ kg/s} = -\Delta \dot{m}_{\text{fu}}$

$-\Delta \dot{n}_{\text{fu}} = 0,0995 / 29 \text{ kmol/s} = 3,43 \cdot 10^{-3} \text{ kmol/s}$

$$(-R_{\text{air}} \cdot V) = (Y_{\text{air,in}} - Y_{\text{air,out}}) \dot{m}_{\text{in}} = (0,8 - 0,003) \cdot 0,5 \text{ kg/s} = 0,3985 \text{ kg/s} = -\Delta \dot{m}_{\text{air}}$$

$$\Delta \dot{m}_{\text{prod}} = -(\Delta \dot{m}_{\text{air}} + \Delta \dot{m}_{\text{fu}}) = 0,498 \text{ kg/s}$$

$$\text{Energy balance: } 0 = \dot{H}_{\text{in}} - \dot{H}_{\text{out}} + \dot{Q} = (-\Delta \dot{m}_{\text{fu}}) h_{\text{f, fu}}^{\circ} - \Delta \dot{m}_{\text{prod}} h_{\text{f, pr}}^{\circ} - \dot{m}_{\text{in}} c_p (T_{\text{out}} - T_{\text{ref}}) + \dot{Q}$$

$$T_{\text{out}} - T_{\text{ref}} = \frac{(0,0995 \cdot (-2000) - 0,498 \cdot (-4000) - 2,0) \text{ kJ/s}}{0,5 \text{ kg/s} \cdot 1,1 \text{ kJ/(kg K)}} = 3256 \text{ K};$$

$$T_{\text{out}} = 298 \text{ K} + 3256 \text{ K} = 3554 \text{ K}$$

$$\text{Reactor mass: } m = \frac{pV}{R_u T} = \frac{101 \text{ kPa} \cdot 0,003 \text{ m}^3}{(8,314/29) \text{ kJ/(kg K)} \cdot 3554 \text{ K}} = 3,0 \cdot 10^{-4} \text{ kg}$$

$$\text{Residence time: } \tau = m / \dot{m}_{\text{in}} = (3,0 \cdot 10^{-4} \text{ kg}) / (0,5 \text{ kg/s}) = 5,9 \cdot 10^{-4} \text{ s}$$

Problem 9

Mainly oxides of nitrogen, carbon monoxide, carbon dioxide, total unburned hydrocarbon, soot and oxides of sulfur.

Exhaust gas recirculation (EGR): A certain percentage of exhaust gas is recirculated to the engine is known as EGR. The purpose of EGR is to reduce NOx emission. When a certain portion of exhaust gas is recirculated to the cylinder, the amount of fresh air will be reduced, and as a result percentage of excess oxygen is reduced; eventually NOx is reduced. On the other hand, EGR reduced the combustion temperature. Reduction of temperature means reduction of NOx. As NOx formation is mainly responsible for temperature and oxygen concentration.

Emission index for species i is the ratio of the mass of species i to the mass of fuel burned
 $EI_i = \text{mass of species } i / \text{mass of fuel burned}$

Mass specific emission = mass flow rate of pollutant/brake power output

Given that

$$X_i = 367 \text{ ppm} = 367 \cdot 10^{-6}; X_{\text{CO}} = 0.0012; X_{\text{CO}_2} = 0.1247; x = 8;$$

Molar mass of $i = \text{C}_6\text{H}_{14}$: $6 \cdot 12 + 14 = 86 \text{ g/mol}$; Fuel: C_8H_{18} (octane): $8 \cdot 12 + 18 = 114 \text{ g/mol}$

$$EI_i = \left(\frac{X_i}{X_{\text{CO}} + X_{\text{CO}_2}} \right) \left(\frac{x M_i}{M_F} \right)$$

$$EIC6H14 = (367 \cdot 10^{-6}) / (0.1247 + 0.0012) \cdot (8 \cdot 86) / (114) = 0.0176 \text{ kg/kg} = 17.6 \text{ g/kg}$$

Considering unburned hydrocarbon

$$EI_i = \left(\frac{X_i}{X_{\text{CO}} + X_{\text{CO}_2} + X_{\text{C}_6\text{H}_{14}}} \right) \left(\frac{x M_i}{M_F} \right)$$

$$EIC6H14 = (367 \cdot 10^{-6}) / (0.1247 + 0.0012 + 367 \cdot 10^{-6}) \cdot (8 \cdot 86) / (114) = 0.0173 \text{ kg/kg} = 17.3 \text{ g/kg}$$

Problem 11

Gasoline combustion is a homogeneous combustion, while diesel combustion is a heterogeneous combustion. (Additional difference: Gasoline combustion is mainly occurred with a source of ignition known as spark plug, while the diesel combustion is occurred with heat of compression, in gasoline combustion air and fuel mixture is compressed and a spark is occurred just before or the end of compression while in diesel combustion only air is compressed and fuel is injected into the compressed air).

Figure for rate of heat release (ROHR) diagram for diesel combustion
(Not included here – see reading material when relevant)

Ignition delay is defined as the delay between start of fuel injection to start of ignition.

Conventional fuels for IC engines are gasoline and diesel. Researchers are trying to reduce the harmful pollutants in different ways. Among them, modification of combustion chamber design, changing of conventional fuel like diesel and gasoline and exhaust after treatment are the main methods of reducing harmful pollutants or emissions. Gasoline and diesel are fossil fuels and they are depleting tremendously day by day, therefore, the researchers are considering for alternative fuels. From the exhaust emissions' point of view, researchers found much lower exhaust emissions with alternative fuels compared to those of conventional gasoline and diesel fuels.

The alternative fuels are biodiesel, oxygenated fuels such as methanol, ethanol, DMM (dimethoxy methane), DGM (diethylene glycol dimethyl ether), DME (dimethyl ether), gas to liquid fuel, liquefied petroleum gas (LPG), compressed natural gas (CNG), FT (Fischer Tropsch) fuel etc.

Brake power (BP) = $2\pi \times \text{Torque} \times \text{rpm}$

Torque (T) = $\text{BP} / (2\pi \times \text{rpm}) = (4 \times 1000 \times 60) / (2 \times 3.14 \times 1500) = 25.47 \text{ Nm}$

Also, Brake power (BP) =

Brake mean effective pressure \times stroke \times area \times rpm \times no. of cylinder = $PlaNk$

$$P = \frac{\text{BP}}{laNk} = \frac{4 \cdot 1000 \cdot 60}{0.11 \cdot \pi / 4 \cdot 0.08^2 \cdot 1500 / 2 \cdot 1} = 578745.2 \text{ N/m}^2 = 5.78 \text{ bar} = 0.578 \text{ MPa}$$

Problems 10 and 12: see separate file