Question 1

(a) Determine the products for the reaction

\[
C_{16}H_{34} + 20 (O_2 + 3.76 N_2) \rightarrow b CO_2 + c CO + d H_2O + e H_2 + f N_2
\]

at 2400 K in a diesel furnace, using the water-gas shift reaction

\[
CO + H_2O \leftrightarrow CO_2 + H_2.
\]

[14 marks]

For the reaction

\[
C_xH_y + a (O_2 + 3.76 N_2) \rightarrow b CO_2 + c CO + d H_2O + e H_2 + 3.76a N_2.
\]

\[
K_p = \exp\left(\frac{-\Delta G}{R_u T}\right) = \frac{b e}{c d}, \quad R_u = 8.3142 \text{ J/mole.K}
\]

\[
b = \frac{2a(K_p - 1) + x + y/2}{2(K_p - 1)} - \sqrt{\frac{2a(K_p - 1) + x + y/2}{2} - \frac{4K_p(K_p - 1)(2ax - x^2)}{2(K_p - 1)}}
\]

\[
g_f^0(CO_2,2400K) = -396.230 \text{ kJ/mole}, \quad g_f^0(H_2,2400K) = 0 \text{ kJ/mole},
\]

\[
g_f^0(CO,2400K) = -319.057 \text{ kJ/mole}, \quad g_f^0(H_2O,2400K) = -112.386 \text{ kJ/mole}
\]

(b) Consider the equilibrium reaction \(O_2 \leftrightarrow O + O\) in a closed vessel. Assume the vessel contains 1 mole of \(O_2\) when there is no disassociation. Determine the mole fractions of \(O_2\) and \(O\) in the vessel for \(T = 3000 \text{ K}, \ p = 2 \text{ atm}\). Comment on the effect of pressure on the extent of oxygen dissociation.

[11 marks]

\[
g_f^0(O_2,3000K) = 0 \text{ kJ/mole}, \quad g_f^0(O,3000K) = 54.554 \text{ kJ/mole}
\]
Question 2

Consider the following chain-reaction mechanism for the low pressure formation of water:

\[
\begin{align*}
H_2 + O_2 &\rightarrow OH + OH \\
OH + H_2 &\rightarrow H_2O + H \\
H + O_2 &\rightarrow OH + O \\
O + H_2 &\rightarrow OH + H \\
H + OH + M &\rightarrow H_2O + M
\end{align*}
\]

(a) Write out expressions for \( \frac{d[OH]}{dt} \), \( \frac{d[O]}{dt} \) and \( \frac{d[H]}{dt} \). \[6 \text{ marks}\]

(b) Assuming the concentrations of OH, O and H radicals are in equilibrium, and 
\( [H]_{eq} = \frac{k_2[H_2]}{k_4[M]} \), show that:

(i) \( [O]_{eq} = \frac{k_3[H]_{eq}[O_2]}{k_4[H_2]} = \frac{k_2k_3[O_2]}{k_4k_5[M]} \), \[4 \text{ marks}\]

(ii) \( [OH]_{eq} = \frac{k_1[O_2]}{k_2} + \frac{k_3[O_2]}{k_5[M]} \), \[8 \text{ marks}\]

(iii) \( \frac{d[H_2O]}{dt} = 2 \left( k_1 + \frac{k_2k_3}{k_4[M]} \right) [H_2][O_2] \). \[7 \text{ marks}\]
Question 3

(a) A simplified chemical explosion system involving linear termination is provided below.

\[ M \xrightarrow{k_1} R \quad \text{Chain initiating} \]
\[ R + M \xrightarrow{k_2} \alpha R + M \quad \text{Chain-branching} \]
\[ R + M \xrightarrow{k_3} P \]
\[ R \xrightarrow{k_4} M \]
\[ R \xrightarrow{k_5} \text{non-reactive species} \]

\( \{ \text{Chain terminating} \} \)

(i) Show that the solution for \([R](t)\) can be derived to be \([R](t) = \frac{k_1[M]}{\phi} (e^{\alpha t} - 1)\), where \(\phi = (\alpha - 1)k_2[M] - k_3[M] - (k_4 + k_5)\).

[8 marks]

(ii) Hence derive the pressure-temperature explosion limits.

[5 marks]

(b) The hydrogen-oxygen explosion curve is given in Figure Q3 below.

(i) Explain the chemistry underlying the first explosion limit, shown in Figure Q3 above, providing the relevant chemical reactions.

[8 marks]

(ii) Hence derive an expression for the pressure-temperature dependence of the first explosion limit.

[4 marks]
Question 4

(a) Flame stretch and aerodynamic strain affects the local laminar flame speed in curved, strained flames. The local stretched laminar flame speed is modified through the expression in the usual notation

\[ S_N = S_L \left(1 - \frac{L_M}{S_L} \frac{1}{A} \frac{dA}{dt}\right), \]

where \( S_N \) is the stretched laminar flame speed, \( S_L \) is the stretch-free laminar flame speed, \( L_M \) is the Markstein length, and \( \frac{1}{A} \frac{dA}{dt} \) is the normalised flame stretch rate.

(i) Show that the instantaneous flame stretch rate for a spherically expanding flame of radius \( r \) is

\[ \frac{1}{A} \frac{dA}{dt} = \frac{2}{r} \frac{dr}{dt}, \]

[4 marks]

(ii) By considering the mass rate of formation of burned gas behind a flame front, show that a spherically expanding flame propagates outward with a propagation speed of

\[ \frac{dr}{dt} = \frac{S_L}{\left(\frac{\rho_b}{\rho_u} + \frac{2L_M}{r}\right)}. \]

[8 marks]

(b) The rate of expansion of a spherically expanding flame can be related to the laminar flame speed through the relation

\[ \frac{dr}{dt} = \frac{S_L}{\left(\frac{\rho_b}{\rho_u} + \frac{2L_M}{r}\right)}. \]

Using the results obtained from the simplified laminar flame analysis, estimate the instantaneous rate of expansion of a spherically expanding, stoichiometric iso-octane-air flame of radius 10 mm, ignited in a low turbulence spark ignition engine (\( T_u = 650 \) K, \( p = 10 \) bar).

[13 marks]

Note: \( L_M = 1.6 \) mm,
\( S_L(\text{iso-octane-air}, \varphi = 1.0, T_u = 300 \) K, \( p = 1 \) bar) \( = 0.40 \) m/s.
\( T_b(\text{iso-octane-air}, \varphi = 1.0, T_u = 300 \) K, \( p = \text{constant pressure}) = 2325 \) K.
\( S_L \propto T_u^{0.375} T_b^{-n/2} p^{(n-2)/2} \exp(-15098K/T_u), n(\text{iso-octane-air}) = 1.4 \)
Relative atomic weight \( M(O) = 16, M(N) = 14, M(C) = 12, M(H) = 1. \)
Question 5

(a) Show that the quenching length \( d \) for a laminar flame can be derived to be

\[
d = \frac{\sqrt{8a\alpha}}{S_L} = \sqrt{2a\delta},
\]

where \( a \) is an appropriate length scaling factor, \( \alpha \) is the mean thermal diffusivity of the flame gases, \( S_L \) the laminar flame speed, and \( \delta \) is the laminar flame thickness. [8 marks]

(b) Using the laminar, isothermal jet model, estimate the flame height of a laminar ethylene (C\(_2\)H\(_4\)) jet flowing into ambient air (\( T = 298 \) K, \( p = 100 \) kPa), from a 0.5 cm diameter nozzle with an exit velocity of 15 cm/s. [7 marks]

\[
y_f(x,0) = \frac{0.375\rho_v v_e R^2}{\mu x}, \quad R_{air} = 287 \text{ J/kgK}, \quad R_{ethylene} = 297 \text{ J/kg.K},
\]

\[
\mu = 1.86 \times 10^{-5} \text{ kg/ms}.
\]

(c) Determine the flame height for a laminar jet of ethylene flowing into air subject to the conditions described in (a) above, with \( T_f = 2300 \) K, using Roper’s theoretical expression specified below. [5 marks]

\[
L_{f,th} = \frac{\dot{V}_f T_w}{4\pi D T_f \ln \left(1 + \left(\frac{n_r}{n_o}\right)_{S_i}\right)} \left(\frac{T_w}{T_f}\right)^{2/3}, \quad D = 1.584 \times 10^{-5} \text{ m}^2/\text{s}.
\]

(d) (i) By analogy with the definition of the laminar burning velocity, define the turbulent burning velocity \( v_t \) for a turbulent flame propagating through a turbulent, premixed fuel-air mixture. [3 marks]

(ii) Hence show that \( v_t = \frac{S_L A_{total}}{A} \). [2 marks]
**Question 6**

(a) Define the four dominant turbulence length-scales, and briefly explain the role each length-scale plays in turbulent flame propagation. **[10 marks]**

(b) In coal-fired power station, gaseous and particulate emissions need to be controlled. With the aid of Figure Q6 below:

(i) complete the schematic to include combustion gases flow, **[4 marks]**

(ii) indicate were in the process emission control mechanisms are applied, **[4 marks]**

(iii) explain the basis of each control mechanism. **[7 marks]**

![Figure Q6](image-url)