Combustion in Air-breathing Aero Engines Assignment No. 1

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This assignment contains 8 multiple choice questions with 4 possible answers to each. Only one of the choice is correct and so select the choice that best answers the question. Correct choice rewards you with 1 point for each question. Wrong answers will reward you with 0 points (no negative marking). The questionnaire contains both numerical and concept-based questions. All the best!!!

Q1: Equivalence ratio can be defined as:

(a) $\frac{(F/O)_{st}}{(F/O)}$ (b) $\frac{(O/F)_{st}}{(O/F)}$ (c) $\frac{(F/O)}{(F/O)_{st}}$

(d) $\frac{(O/F)}{(O/F)}_{st}$

Select the correct choice:

- 1. a. only
- 2. c. only
- 3. b. & c.
- 4. a. & d.

Ans: Both b. and c. are same. The correct choice is 3.

Q2: At chemical equilibrium

- 1. Entropy is maximum; Gibbs free energy is maximum
- 2. Entropy is maximum; Gibbs free energy is minimum
- 3. Entropy is minimum; Gibbs free energy is maximum
- 4. Entropy is minimum; Gibbs free energy is minimum

Ans: The correct choice is 2.

Q3: The following is an assertion and reasoning question. Select the correct choice from the situations given in the table 1.

Assertion: For hydrocarbons undergoing combustion, as pressure increases adiabatic flame temperature peaks near stoichiometry.

Reason: Pressure tends to reduce the extent of dissociation of CO_2 and H_2O based on the Le-Chatelier principle

Ans: Dissociation of CO_2 and H_2O can be given by:

Choice	Assertion	Reason	Remark
1.	True	True	Explanation is correct
2.	True	True	Explanation is incorrect
3.	False	True	
4.	False	False	

Table 1

$$\begin{array}{c} \mathrm{CO}_2 \rightleftharpoons \mathrm{CO} + \mathrm{O} \\ \mathrm{H}_2 \mathrm{O} \rightleftharpoons \mathrm{OH} + \mathrm{O} \end{array}$$

As the number of moles increase when the CO_2 and H_2O dissociate, an increase in pressure will shift the equilibrium towards lesser number of moles, in accordance with the Le-Chatelier principle. This suppresses the dissociation of CO_2 and H_2O . The energy, released on combustion of hydrocarbons, which was used in dissociation reactions earlier is now available in the system and is manifested in the form of temperature rise.

Since, the assertion and the reason, both are true and the reason explains the assertion, the correct choice is 1.

Q4: Determine the adiabatic flame temperature (in SI units) for constant-pressure combustion of a stoichiometric propane-air mixture assuming the reactants at 298K and pressure of 1atm. Assume no dissociation of the products and evaluate the constant specific heats of the products at a) 298K and b) 1200K. Select the option from below that closely matches with your solution. Following data can be used.

	$ \begin{array}{ c c } \Delta h_f^o \mbox{ at } T = 298 \mbox{K and } P = 1 \mbox{atm} \\ (\mbox{kJ/kmol}) \end{array} $	c_P at $T = 298 \text{K} \text{ (kJ/kmol-K)}$	c_P at $T = 1200$ K (kJ/kmol-K)
C_3H_8	-103,847	35.64	78.84
O_2	0	29.32	35.59
N_2	0	29.07	33.71
CO_2	-393,546	37.20	56.21
H_2O	-241,845	33.45	43.87

Table 2

- 1. a. 2388K b. 2879K
- 2. a. 2581K b. 2090K

3. a. 2090K b. 2581K

4. a. 2879K b. 2388K

Ans: At stoichiometry and assuming no dissociation, the propane-air reaction can be written as:

$$\mathrm{C_3H_8} + 5\,(\mathrm{O_2} + 3\,\cdot76\,\mathrm{N_2}) \longrightarrow 3\,\mathrm{CO_2} + 4\,\mathrm{H_2O} + 18\,\cdot8\,\mathrm{N_2}$$

Adiabatic flame temperature T_{ad} at constant pressure is found by equating the enthalpy of the reactant mixture at initial conditions with the enthalpy of the product mixture at T_{ad}

$$H_R(T_i, P) = H_P(T_{ad}, P) \tag{1}$$

Mixture enthalpy is evaluated as:

$$H_{mix} = \sum_{i=1}^{N} N_i h_i \tag{2}$$

where, $h_i(T) = \Delta h_f^o + \int_{T_{ref}}^T c_{P,i} dT$ and N is the no. of moles Evaluating, H_R using Eqn. 2

$$H_R = N_{C_3H_8}h_{C_3H_8} + N_{O_2}h_{O_2} + N_{N_2}h_{N_2}$$

= 1(-103847) + 5(0) + 18.8(0)
= -103847

Similarly, we evaluate H_P using Eqn. 2. For c_P , the questions considers evaluating them at T = 298K and at T = 1200K. Here, we show the calculations for T = 298K. For other case the calculation is similar with suitable substitution of values.

$$\begin{split} H_P &= N_{CO_2} h_{CO_2} + N_{H_2O} h_{H_2O} + N_{N_2} h_{N_2} \\ &= 3(-393546 + 37.20 \left(T_{ad} - 298\right)) + 4(-241845 + 33.45 \left(T_{ad} - 298\right)) + 18.8(29.07 \left(T_{ad} - 298\right)) \\ &= -2148018 + 791.92 \left(T_{ad} - 298\right) \end{split}$$

Using Eqn. 1, we get $T_{ad} = 2879$ K. Similarly for c_P evaluated at T = 1200K, we get $T_{ad} = 2388$ K. Therefore, the correct answer is 4.

Q5: Consider the following chain reaction mechanism for the high-temperature formation of nitric oxide, i.e., the Zeldovich mechanism:

$$O + N_2 \xrightarrow{k_1} NO + N$$

 $N + O_2 \xrightarrow{k_2} NO + O$

When the following reaction is added to the above two reactions, the NO formation mechanism is called the extended Zeldovich mechanism:

$$N + OH \xrightarrow{k_3} NO + H$$

Select the expression from below that best expresses the steady-state N-atom concentration, neglecting reverse reactions.

1.
$$[N] = \frac{k_1[O][N_2]}{k_2[O_2] + k_3[OH]}$$

2. $[N] = \frac{k_2[O_2] + k_3[OH]}{k_1[O][N_2]}$

$$k_1[O][N_0]$$

3.
$$[N] = \frac{n_1[O_1[N_2]}{k_2[O_2]}$$

4.
$$[N] = \frac{k_2[O_2]}{k_1[O][N_2]}$$

Ans: The rate of change of concentration of N can be expressed as:

$$\frac{d[N]}{dt} = k_1[O][N_2] - k_2[N][O_2] - k_3[N][OH]$$

For the steady-state approximation to hold $\frac{d[N]}{dt} \approx 0$. Hence, steady-state concentration of N-atom will be

$$[N] = \frac{k_1[O][N_2]}{k_2[O_2] + k_3[OH]}$$

Therefore, the correct choice is 1.

Q6: For question 5 calculate the formation rate for NO, neglecting reverse reactions.

1.
$$\frac{d[NO]}{dt} = k_1[O][N_2]$$

2. $\frac{d[NO]}{dt} = 2k_1[O][N_2]$
3. $\frac{d[NO]}{dt} = k_2[O][N_2]$
4. $\frac{d[NO]}{dt} = 2k_1[O][N_2]$

Ans: The rate expression for rate of formation of NO is as follows:

$$\frac{d[NO]}{dt} = k_1[O][N_2] + k_2[O_2][N] + k_3[OH][N]$$
$$= k_1[O][N_2] + (k_2[O_2] + k_3[OH])[N]$$

substituting the expression for [N] obtained previously, we get

$$\frac{d[NO]}{dt} = 2k_1[O][N_2]$$

Therefore, the correct choice is 2.

Q7: In a global, single-step mechanism for butane combustion, the reaction order with respect to butane is 0.15 and with respect to oxygen is 1.6. The rate coefficient can be expressed in Arrhenius form: the pre-exponential factor is $4.16 \times 10^9 [(\text{kmol/m}^3)^{-0.75}/\text{s}]$ and the activation energy is 125,000 kJ/kmol. R_u is the universal gas constant. Which expression from below best matches with rate of destruction of butane:

$$1. \quad \frac{d[C_4H_{10}]}{dt} = 125000 exp\left(\frac{-4.16 \times 10^9}{R_u T}\right) [C_4H_{10}]^{0.15} [O_2]^{1.6}$$

$$2. \quad \frac{d[C_4H_{10}]}{dt} = 4.16 \times 10^9 exp\left(\frac{125000}{R_u T}\right) [C_4H_{10}]^{1.6} [O_2]^{0.15}$$

$$3. \quad \frac{d[C_4H_{10}]}{dt} = 4.16 \times 10^9 exp\left(-\frac{125000}{R_u T}\right) [C_4H_{10}]^{0.15} [O_2]^{1.6}$$

$$4. \quad \frac{d[C_4H_{10}]}{dt} = 125000 exp\left(\frac{4.16 \times 10^9}{R_u T}\right) [C_4H_{10}]^{0.15} [O_2]^{1.6}$$

Ans: The correct choice is 3.

Q8: Which of the following is not true:

- (a) For elementary reactions, reaction orders will always be integers
- (b) For global reactions, reaction orders are not necessarily integers
- (c) Collision theory provide no means to determine the activation energy

Select the correct choice:

- 1. a.
- 2. a. & b.
- 3. a., b. & c.
- 4. none of the above

Ans: Since all of the above statements are true, therefore the correct choice is 4.