Energy Process and Systems Engineering

Assignment 2

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Problem 1: Air Quantity – Mole Fractions (Mode: Molecules)

Given: Mole fractions of fuel components x_i; Molar weights MW_i

To determine: Minimum air demand $X_{air,min}$; Actual air demand $X_{air,in}$

Formulas:

1. **Mixture molar weight of fuel:**

$$MW_{fuel} = \sum_i \quad x_i MW_i \qquad (1)$$

2. **Mass fraction of fuel component:**

$$x_{mi} = \frac{x_i MW_i}{MW_{fuel}} \qquad (2)$$

3. **Stoichiometric air demand (moles of O_2):**

$$X_{O2,min} = \sum_j \quad \nu_{O2,j}\, n_j$$

where $\nu_{O2,j}$are stoichiometric coefficients of O_2 for each combustible component j.

4. **Total air demand (including excess air λ):**

$$X_{air,in} = \lambda\, X_{air,min} \qquad (3)$$

Problem 2: Air Quantity – Mass Fractions (Mode: Elements)

Given: Mass fractions of elements x_{mi}(C, H, S, …); Molar weights MW_i

To determine: Minimum air demand $W_{air,min}$; Actual air demand $W_{air,in}$

Formulas:

1. **Convert mass fractions to mole fractions:**

$$x_i = \frac{x_{mi}/MW_i}{\sum_i \quad x_{mi}/MW_i} \qquad (4)$$

2. **Stoichiometric air demand using elemental reactions:**

$$\begin{aligned} \mathrm{C} + O_2 &\rightarrow CO_2 \\ \mathrm{H} + \frac{1}{4}O_2 &\rightarrow \frac{1}{2}H_2O \\ \mathrm{S} + O_2 &\rightarrow SO_2 \end{aligned} \qquad (5)$$

3. **Total air demand including excess:**

$$W_{air,in} = \lambda\, W_{air,min} \qquad (6)$$

Problem 3: Exhaust Gas – Mole Fractions (Mode: Molecules)

Given: Input molar flow N_{in}; Mole fractions $x_{i,in}$; Stoichiometric matrix ν; Extent of reaction ξ_j

To determine: Output molar flow N_{out}; Mole fractions $x_{i,out}$

Formulas:

1. **Molar flow of each component exiting the system:**

$$N_{i,out} = x_{i,in}N_{in} + \sum_j \nu_{i,j}\xi_j \qquad (7)$$

2. **Total molar flow leaving system:**

$$N_{out} = \sum_i N_{i,out} \qquad (8)$$

3. **Exhaust gas mole fraction:**

$$x_{i,out} = \frac{N_{i,out}}{N_{out}} \qquad (9)$$

Problem 4: Exhaust Gas – Mass Fractions (Mode: Elements)

Given: Mass fractions x_{mi}; Stoichiometric matrix for elements; Extent of reaction ξ_j

To determine: Exhaust gas composition in mass fractions $x_{ex,out,mass}$

Formulas:

1. **Moles of elements reacting:**

$$n_i = \frac{x_{mi}}{MW_i} \qquad (10)$$

2. **Mass of exhaust components:**

$$m_{i,out} = n_i\, MW_i + \sum_j \quad \nu_{i,j}\xi_j\, MW_i \qquad (11)$$

3. **Mass fraction of exhaust component:**

$$x_{i,out,mass} = \frac{m_{i,out}}{\sum_i \quad m_{i,out}} \qquad (12)$$