AME 60636
Examination 1
Prof. J. M. Powers
23 February 2022

1. Consider the irreversible reaction mechanism

$$\begin{aligned} 1: \mathrm{H_2} + \mathrm{O_2} &\rightarrow \mathrm{OH} + \mathrm{OH} \\ 2: \mathrm{H} + \mathrm{O_2} &\rightarrow \mathrm{OH} + \mathrm{O} \\ 3: \mathrm{C} + 2\mathrm{O} &\rightarrow \mathrm{CO_2} \\ 4: \mathrm{C} + \mathrm{H} &\rightarrow \mathrm{CH}. \end{aligned}$$

   (a) Identify the number of species N, reactions J, and elements L.

   (b) Find the $L \times N$ species-element matrix $\boldsymbol{\phi}$.

   (c) Find the $N \times J$ stoichiometric reaction matrix $\boldsymbol{\nu}$.

   (d) Demonstrate $\boldsymbol{\phi} \cdot \boldsymbol{\nu} = \mathbf{0}$.

   (e) For isothermal, isochoric kinetics, write an ordinary differential equation for the evolution of the concentration of H; define any necessary constants.

2. Find the most general stoichiometric balance for the reaction

$$\nu_1' \mathrm{H_2} + \nu_2' \mathrm{O_2} \leftrightharpoons \nu_3'' \mathrm{H_2O} + \nu_4'' \mathrm{H_2O_2}.$$

3. Species A and B have identical molecular masses and identical specific heats and undergo an irreversible reaction described by

$$A + A \rightarrow B + A.$$

   The reaction is *adiabatic* and *isochoric*. The fixed volume is V, and no mass enters or exits the volume. At $t = 0$, $T = T_o$, $\overline{\rho}_A = \overline{\rho}_{Ao}$, and $\overline{\rho}_B = 0$. The reaction has $\mathcal{E} = 0$ and $\beta = 0$. It has collision frequency factor a, constant $\overline{c}_v$, and is exothermic.

   (a) Write an appropriate simple ordinary differential equations for the change of $\overline{\rho}_A$ with respect to time.

   (b) Find the equilibrium concentration of A.

   (c) Find $\overline{\rho}_A(t)$ and $T(t)$.