Chemical Reactor

Leo Basov

December 2024

1 Introduction

The total energy of the system is given as

$$E_{tot} = E_{kin} + E_{rot} + E_{vib} \tag{1.1}$$

the individual components can be expressed as assuming a common kinetic temperature of the mixture

$$E_{kin} = \frac{3}{2} k_B T \sum_i N_i \tag{1.2}$$

$$E_{rot} = k_B \sum_i^{N_s} N_i \frac{\xi_i}{2} T_i \tag{1.3}$$

$$E_{vib} = k_B \sum_i^{N_s} \left(N_i \sum_m g_{i,m} \frac{\theta_{i,m}}{\exp(\theta_{i,m}/T_{i,m}) - 1} \right) \tag{1.4}$$

where the index i denotes the species and m the vibrational mode. We assume a constant volume thus we can work with per volume quantities and replace the particle number N with number density n. Assuming a thermalized rotational temperature we can write the per particle energy as

$$e_{kr,i} = \frac{3 + \xi_i}{2} k_B T \tag{1.5}$$

$$e_{v,i,m} = k_B g_{m,i} \frac{\theta_{i,m}}{\exp(\theta_{i,m}/T_{i,m}) - 1} \tag{1.6}$$

and therefore

$$\underbrace{E_{kin} + E_{rot}}_{E_{kr}} = \sum_i n_i e_{kr,i} = T k_B \sum_i n_i \frac{3 + \xi_i}{2} \tag{1.7}$$

$$E_{vib} = \sum_i \left(n_i \sum_m e_{v,i,m} \right) \tag{1.8}$$

We have

$$\frac{\partial E_{kr}}{\partial t} = \sum_i \left(\frac{\partial n_i}{\partial t} e_{kr,i} + n_i \frac{\partial e_{kr,i}}{\partial t} \right) + \Delta E_R \qquad (1.9)$$

$$\frac{\partial E_{vib}}{\partial t} = \sum_i \sum_m \left(\frac{\partial n_i}{\partial t} e_{v,i,m} + n_i \frac{\partial e_{v,i,m}}{\partial t} \right) \qquad (1.10)$$

$$\Delta E_R = \sum_r \nu_r \Delta e_r \qquad (1.11)$$

$$\frac{\partial n_i}{\partial t} = \sum_k n_i n_k r_{i,k}(T) \qquad (1.12)$$

$$\frac{\partial e_{kr,i}}{\partial t} = -\sum_m \frac{\partial e_{v,i,m}}{\partial t} \qquad (1.13)$$

$$\frac{\partial e_{v,i,m}}{\partial t} = \frac{e_{v,i,m}(T) - e_{v,i,m}(T_{i,m})}{\tau_{i,m}} \qquad (1.14)$$