* CRNN with 3 neurons with each neuron modeling reactions in each region

* Reactions in each region represented by the ODE's given below

$\Rightarrow$ Region 1 :- [Not imp]

$\Rightarrow$ Region 2 $\left[LiC_1 \longrightarrow \text{products + heat} \right]$

$$\frac{d x_{LiC,1}}{dt} = - A_{LiC,1} \, x_{LiC,1}^{n_{LiC,1}} \, T^{b_{LiC,1}} \, \exp\left(\frac{-6_{LiC,1}}{KT}\right) \exp\left(\frac{-t s\epsilon_{1,1}}{t s\epsilon_{1,1}, \, ref}\right)$$

$$\frac{d\, t s\epsilon_{1,1}}{dt} = A_{LiC,1} \, x_{LiC,1}^{n_{LiC,1}} \, T^{b_{LiC,1}} \, \exp\left(\frac{-6_{LiC,1}}{KT}\right) \exp\left(\frac{-t s\epsilon_{1,1}}{t s\epsilon_{1,1}, \, ref}\right)$$

$\Rightarrow$ Region 3 $\left[\begin{array}{l} Li\text{-}EC \longrightarrow \text{products + heat} \\ LiC_2 \longrightarrow \text{product + heat} \end{array}\right]$

$$\frac{d x_{LiC,2}}{dt} = -A_{Li\text{-}EC} \, x_{Li\text{-}EC}^{n_{Li\text{-}EC}} \, T^{b_{Li\text{-}EC}} \exp\left[\frac{-E_{Li\text{-}EC}}{KT}\right] - A_{LiC,2} \, x_{LiC,2}^{n_{LiC,2}} \, T^{b_{LiC,2}} \exp\left(\frac{-6_{LiC,2}}{KT}\right) \exp\left(\frac{-t s\epsilon_{1,2}}{t s\epsilon_{1,2}, \, ref}\right)$$

$$\frac{d\, t s\epsilon_{1,2}}{dt} = -A_{LiC,2} \, x_{LiC,2}^{n_{LiC,2}} \, T^{b_{LiC,2}} \exp\left(\frac{-6_{LiC,2}}{KT}\right) \exp\left(\frac{-t s\epsilon_{1,2}}{t s\epsilon_{1,2}, \, ref}\right)$$

$\Rightarrow$ **Region 4** [Binder $\longrightarrow$ products + heat]

$$\frac{dx_B}{dt} = -A_B \, x_B \, \exp\left(\frac{-\varepsilon_B}{k_B T} \right)$$

Network architecture

x

(i) **Region 2**

$$\frac{dx_{Lic,1}}{dt} = -A_{Lic,1} \, x_{Lic,1}^{n_{Lic,1}} \, T^{b_{Lic,1}} \, \exp\left(\frac{-\varepsilon_{Lic,1}}{KT} \right) \exp\left(\frac{-t_{SE,1}}{t_{SE,1,ref}} \right)$$

$$\frac{d\,t_{SE,2,1}}{dt} = A_{Lic,1} \, x_{Lic,1}^{n_{Lic,1}} \, T^{b_{Lic,1}} \, \exp\left(\frac{-\varepsilon_{Lic,1}}{KT} \right) \exp\left(\frac{-t_{SE,1}}{t_{SE,1,ref}} \right)$$

het

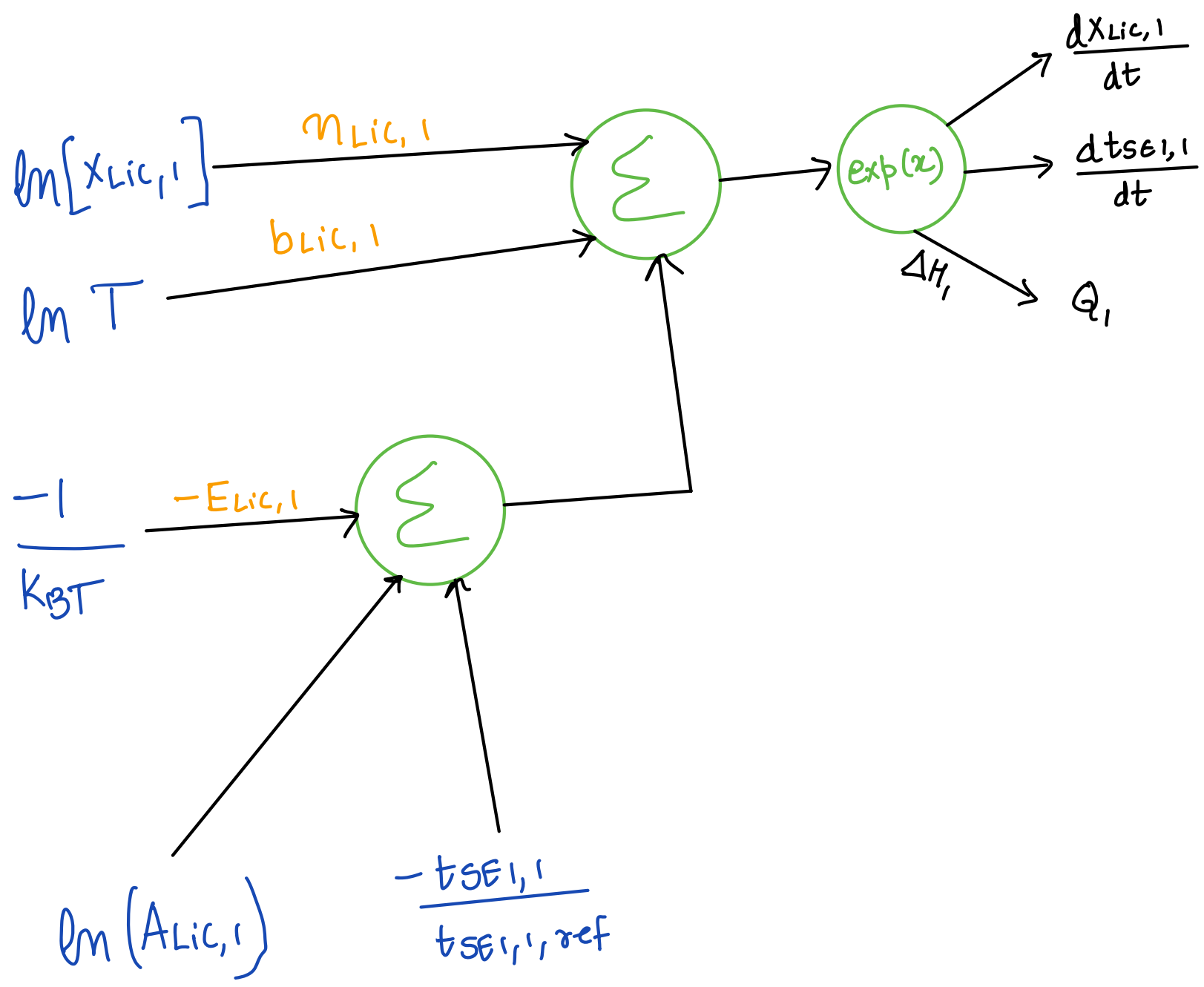$$n_{Lic,1} = A_{Lic,1} \, x_{Lic,1}^{n_{Lic,1}} \, T^{b_{Lic,1}} \, \exp\left(\frac{-\varepsilon_{Lic,1}}{KT} \right) \exp\left(\frac{-t_{SE,1}}{t_{SE,1,ref}} \right)$$

Taking $\ln$ on both sides

$$\ln\left(n_{Lic,1} \right) = \ln\left(A_{Lic,1} \right) + n_{Lic,1} \ln\left(x_{Lic,1} \right) + b_{Lic,1} \ln(T) + \ln\left(\exp\left(\frac{-\varepsilon_{Lic,1}}{KT} \right) \right) + \ln\left(\exp\left(\frac{-t_{SE,1}}{t_{SE,1,ref}} \right) \right)$$

$$\ln\left(a_{Lic,1}\right) = \ln\left(A_{Lic,1}\right) + n_{Lic,1} \ln\left(x_{Lic,1}\right) + b_{Lic,1} \ln\left(T\right) - \frac{E_{Lic,1}}{KT} - \frac{t_{SEI,1}}{t_{SEI,1\,ref}}$$

(ii) Region 3

* 2 reaction groups $\left[\begin{array}{l}\to \text{Li-EC reaction } (\mathcal{R}_{Li-EC}) \\ \to \text{SEI decomposition } (\mathcal{R}_{SEI}) \\ \quad (+ \text{ thickness reduction})\end{array}\right.$

* Both reaction group consumes LiC_2

* $\dfrac{dx_{LiC_2}}{dt} = -\mathcal{R}_{Li-EC} - \mathcal{R}_{SEI}$

* Each reaction modeled using a separate neuron

$$\mathcal{R}_{Li-EC} = A_{Li-EC} \, x_{LiC_2}^{n_{Li-EC}} \, T^{b_{Li-EC}} \exp\left[\frac{-E_{Li-EC}}{KT}\right]$$

$$\mathcal{R}_{SEI} = A_{LiC,2} \, x_{LiC,2}^{n_{LiC,2}} \, T^{b_{LiC,2}} \exp\left(\frac{-E_{LiC,2}}{KT}\right) \exp\left(\frac{-t_{SEI,2}}{t_{SEI,2,ref}}\right)$$

Coupled ODE

x $\underline{\hspace{3cm}}$ x

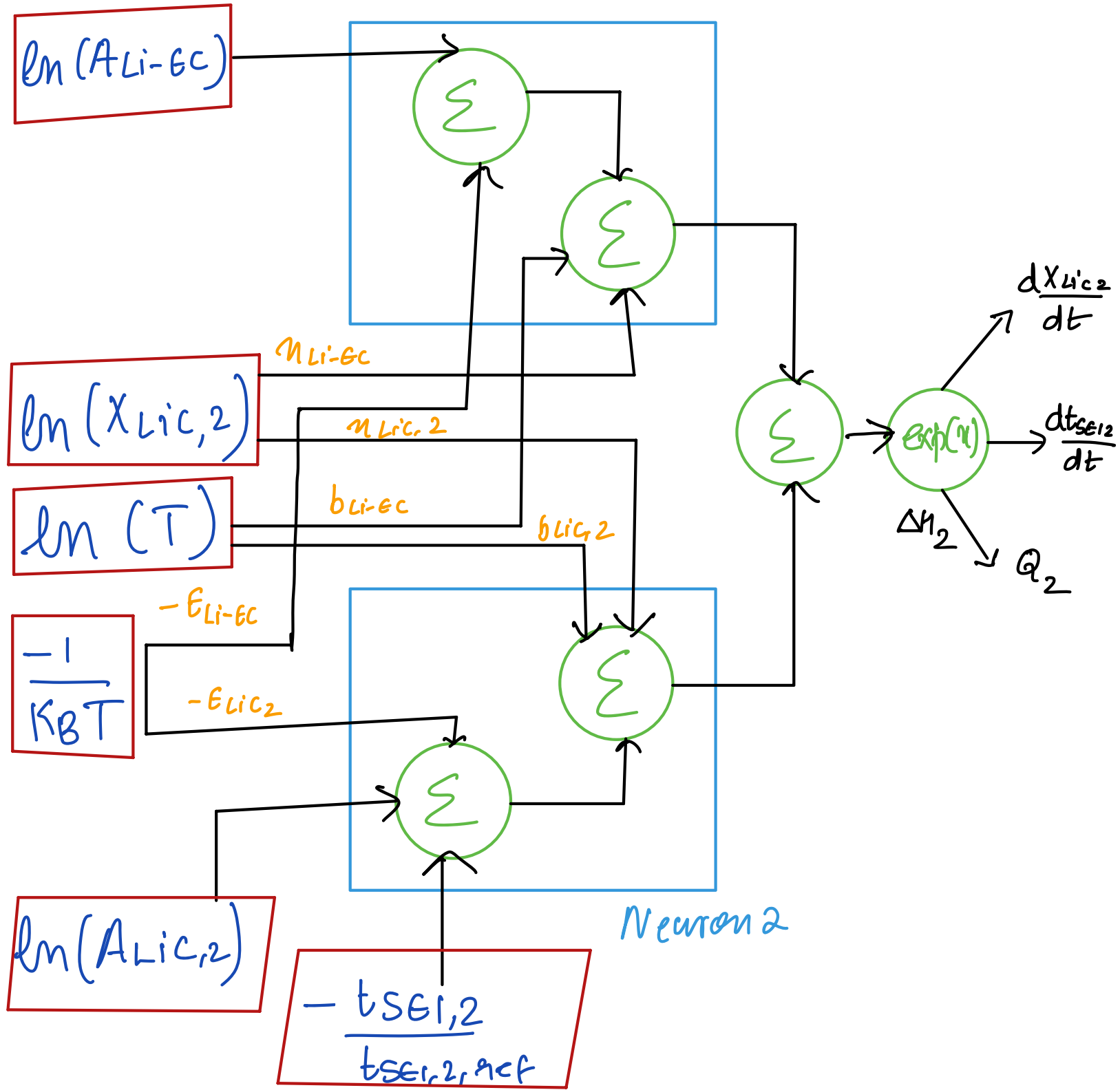$$\frac{dx_{LiC,2}}{dt} = -A_{Li-EC} \, x_{LiC}^{n_{Li-EC}} \, T^{b_{Li-EC}} \exp\left[\frac{-E_{Li-EC}}{KT}\right] - A_{LiC,2} \, x_{LiC,2}^{n_{LiC,2}} \, T^{b_{LiC,2}} \exp\left(\frac{-E_{LiC,2}}{KT}\right) \exp\left(\frac{-t_{SEI,2}}{t_{SEI,2,ref}}\right)$$

$$\frac{dt_{SEI,2}}{dt} = -A_{LiC,2} \, x_{LiC,2}^{n_{LiC,2}} \, T^{b_{LiC,2}} \exp\left(\frac{-E_{LiC,2}}{KT}\right) \exp\left(\frac{-t_{SEI,2}}{t_{SEI,2,ref}}\right)$$

$$\eta_3 = \underbrace{-A_{Li\text{-}EC}\, x_{Li\text{-}EC}^{\,n_{Li\text{-}EC}}\, T^{\,b_{Li\text{-}EC}}\, \exp\left[\frac{-E_{Li\text{-}EC}}{KT}\right]}_{\eta_{Li\text{-}EC}} \underbrace{-A_{Lic,2}\, x_{Lic,2}^{\,n_{Lic,2}}\, T^{\,b_{Lic,2}}\, \exp\left(\frac{-E_{Lic,2}}{KT}\right)\exp\left(\frac{-t_{SEI,2}}{t_{SEI,2,ref}}\right)}_{\eta_{SEI}}$$

Neuron. 1

$\ln(A_{Li\text{-}EC})$

$\sum$

$\sum$

$\ln(X_{Lic,2})$

$n_{Li\text{-}EC}$

$n_{Lic,2}$

$\ln(T)$

$b_{Li\text{-}EC}$

$b_{Lic,2}$

$-E_{Li\text{-}EC}$

$\dfrac{-1}{K_B T}$

$-E_{Lic_2}$

$\sum$

$\sum$

$\exp(x)$

$\dfrac{dX_{Lic_2}}{dt}$

$\dfrac{dt_{SEI_2}}{dt}$

$\Delta \eta_2$

Q_2

$\ln(A_{Lic,2})$

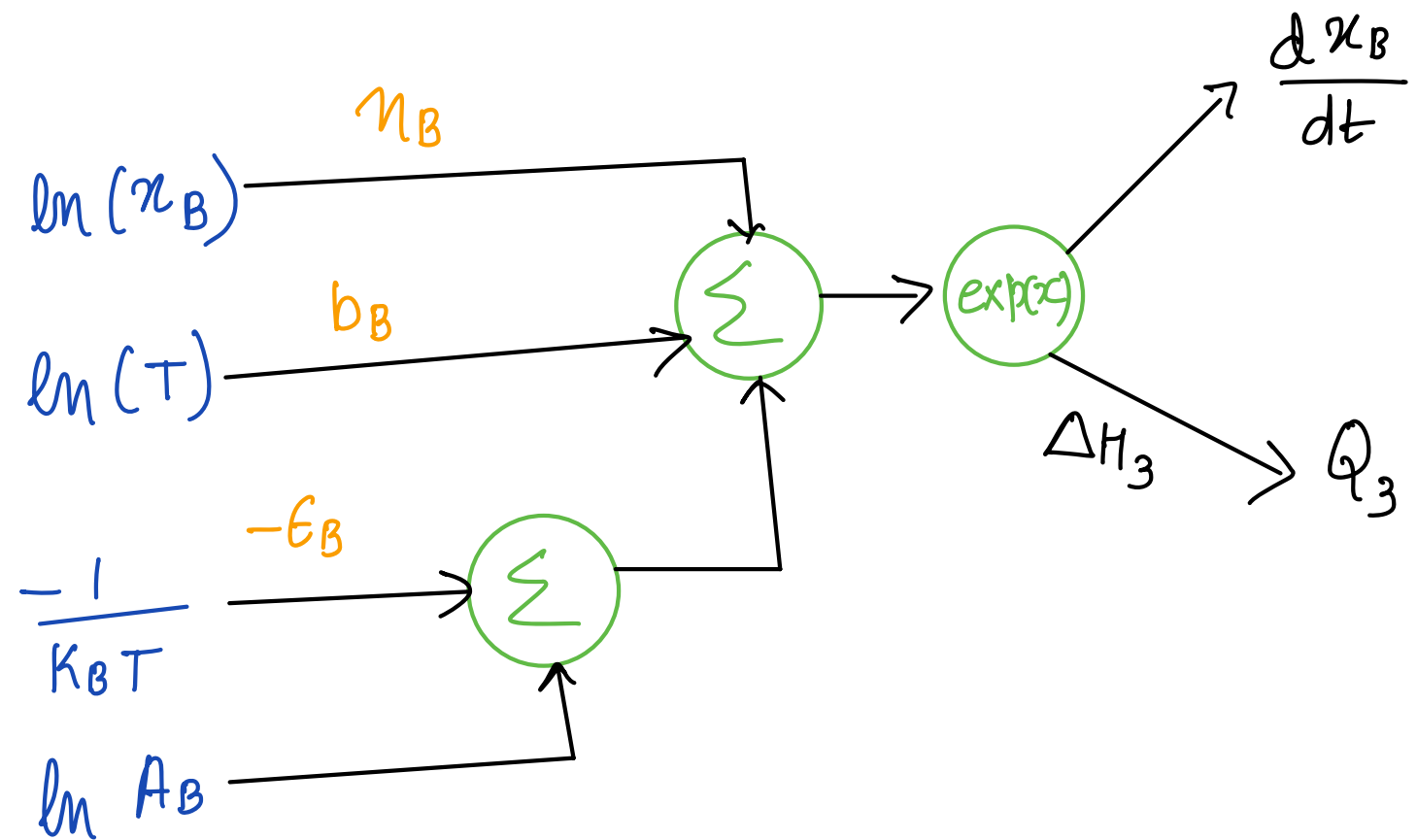$-\dfrac{t_{SEI,2}}{t_{SEI,2,ref}}$

Neuron 2

(iii) Region 4

$$\frac{dx_B}{dt} = -A_B \, x_B^{n_B} \, T^{b_B} \, \exp\left(\frac{-\varepsilon_B}{K_B T}\right)$$

$x_B \Rightarrow$ dimensionless concn of binder & other rxn products from previous reactions.

Complete CRNN