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

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

⇒ Region 1 :- [Not imp]

⇒ Region 2 [$LiC_1 \longrightarrow$ products + heat]

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

$$\frac{dt_{SEI,1}}{dt} = A_{LiC,1} x_{LiC,1}^{n_{LiC,1}} T^{b_{LiC,1}} \exp\left(\frac{-E_{LiC,1}}{KT}\right) \exp\left(\frac{-t_{SEI,1}}{t_{SEI,1,ref}}\right)$$

⇒ Region 3 [LiC_2 + electrolyte $\longrightarrow$ products + heat ; $LiC_2 \longrightarrow$ product + heat]

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

LiC_2 + electrolyte ; LiC_2 + SEI breakdown

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

⇒ Region 4 [Binder ⟶ products + heat]

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

Network architecture

(i) Region 2

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

$$\frac{dt_{SEI,1}}{dt} = A_{LiC,1} x_{LiC,1}^{n_{LiC,1}} T^{b_{LiC,1}} \exp\left(\frac{-E_{LiC,1}}{KT}\right) \exp\left(\frac{-t_{SEI,1}}{t_{SEI,1,ref}}\right)$$

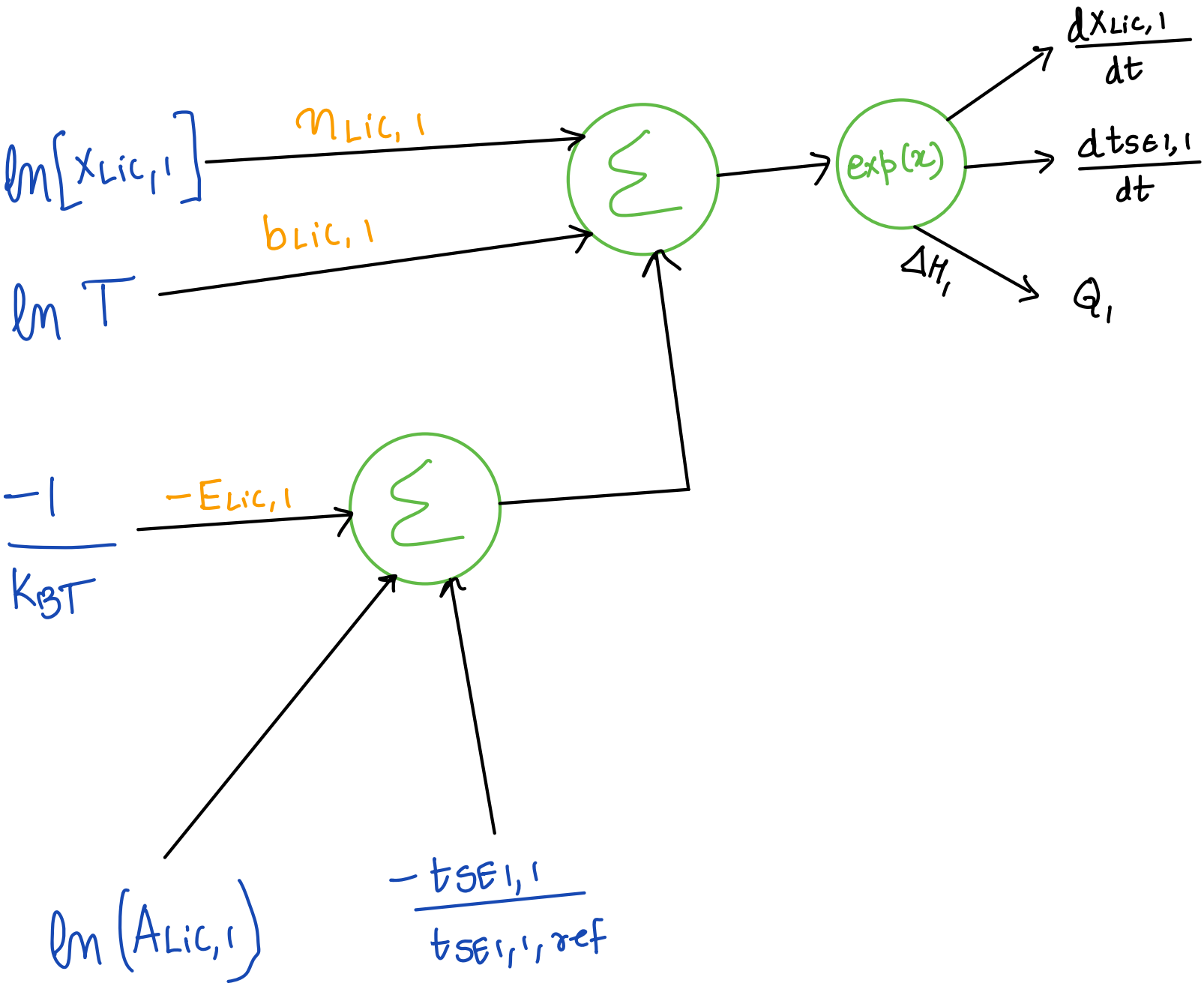
het

$$\eta_{LiC,1} = A_{LiC,1} x_{LiC,1}^{n_{LiC,1}} T^{b_{LiC,1}} \exp\left(\frac{-E_{LiC,1}}{KT}\right) \exp\left(\frac{-t_{SEI,1}}{t_{SEI,1,ref}}\right)$$

Taking ln on both sides

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

$$\ln(\eta_{LIC,1}) = \ln(A_{LIC,1}) + n_{LIC,1}\ln(x_{LIC,1}) + b_{LIC,1}\ln(T) - \frac{E_{LIC,1}}{KT} - \frac{tse_{1,1}}{tse_{1,1,ref}}$$



(ii) Region 3

* 2 reaction groups → LiC_2 + electrolyte ($\eta_{Li\text{-}EC}$)
* 2 reaction groups → SEI decomposition (η_{SEI}) (+ thickness reduction)

* Both reaction group consumes LiC_2

* $\frac{dx_{LiC_2}}{dt} = -\eta_{Li\text{-}EC} - \eta_{SEI}$

* Each reaction modeled using a separate neuron

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

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

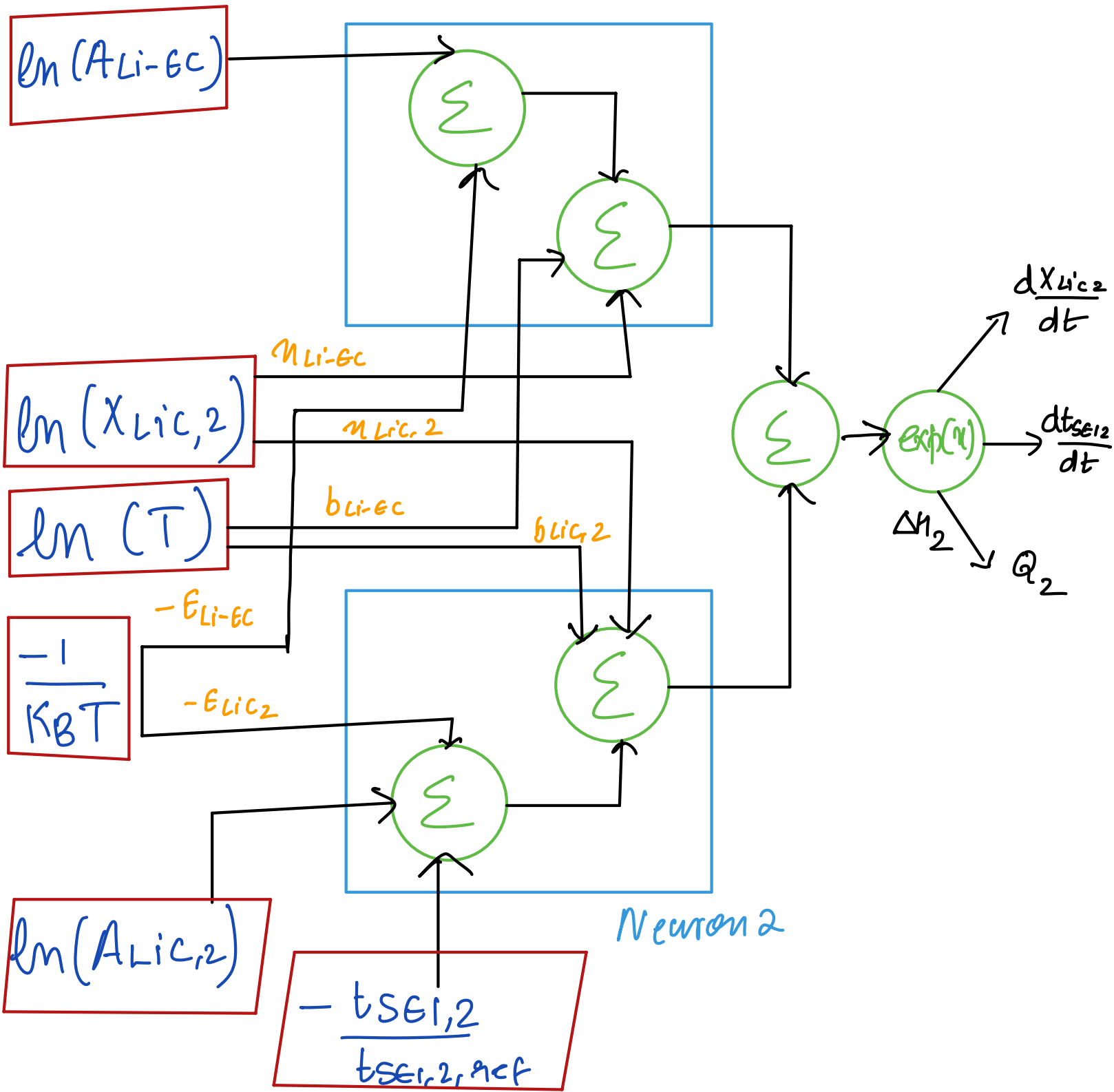
Coupled ODE

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

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

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

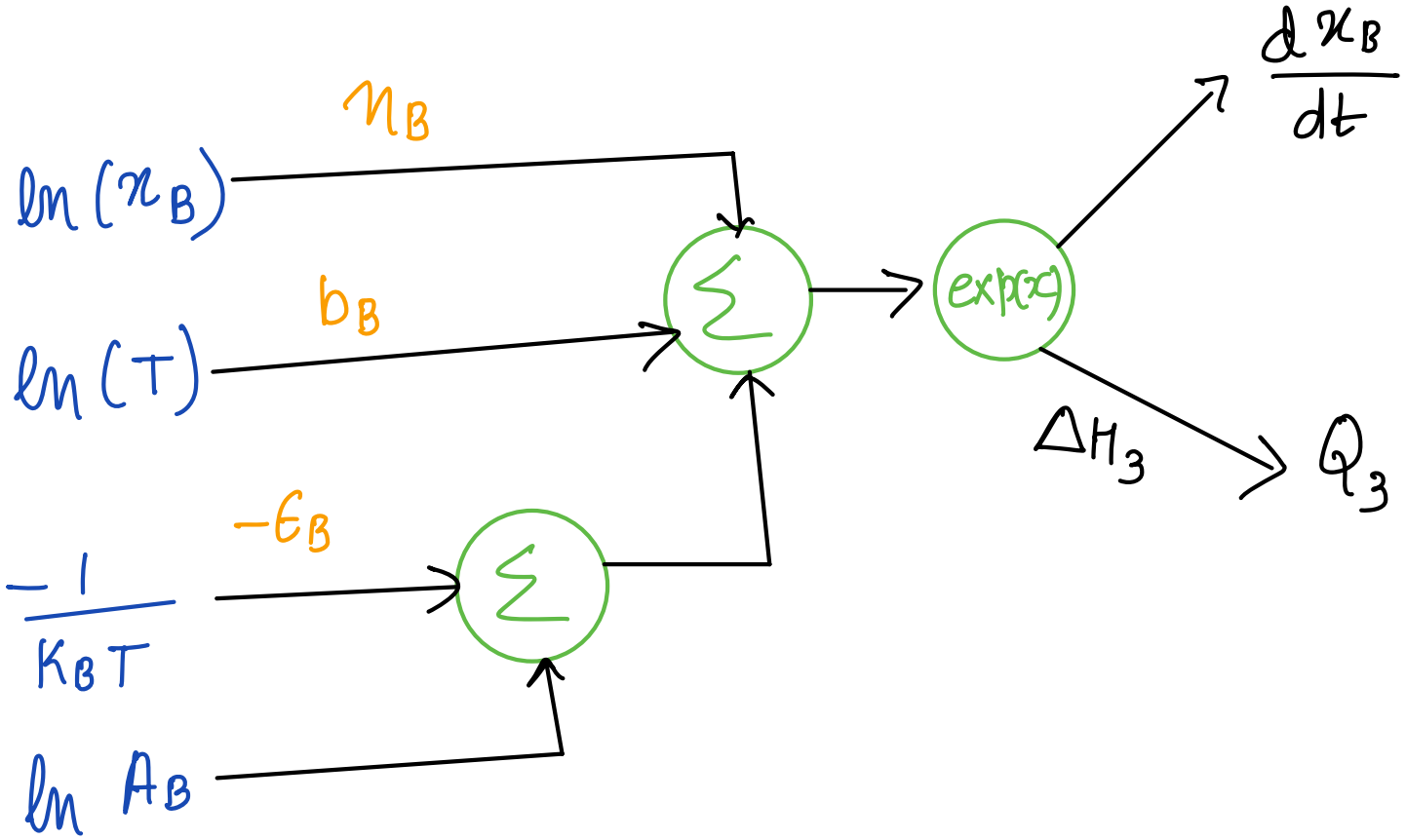
Neuron. 1



(iii) Region 4

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

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



Complete CRNN