PSet #3, Daniel Markiewitz ChemE 5440 3/9/2019

a. For $\underline{\underline{S}}$ use code HW#3 with $V

$$\$V = \begin{cases} \text{Balance.JL} & \text{for balanced } \underline{\underline{S}} \\ \text{out Balance.JL} & \text{for unbalanced } \underline{\underline{S}} \end{cases}$$

b. Not balanced originally added in a

"$H_2O \rightarrow$" - export rxn

"ATP $\Leftrightarrow$ ADP" - Exchange rxn or coupled rxn need to provide energy for other rxns.

This check is preformed in the same code for a. and the matrix that is the $\underline{\underline{0}}$ when balanced elementally is called ebs,

C. Optimal value is contained in opt_value, produced by code HW #3 FBA.jl, used balanced $\underline{\underline{S}}$ here, Also used given assumptions in Pset #3,

- For V- boundaries they were calculated as

if only $\rightarrow$ $\Rightarrow$ $0 \leq V_{\#} \leq \underbrace{k_{cat}\, E}_{\text{givens}} \left(\frac{a}{k_m + a}\right)$ ← substrate/metabolite

calculated in excel file 2077-5310 nChembio and matched

The usual definition of k_m

if $\rightleftharpoons$ $\Rightarrow$ $-k_{cat} E \left(\frac{a}{k_m + a}\right) \leq V_{\#} \leq k_{cat} E \left(\frac{a}{k_m + a}\right)$

if not an exchange flux else it is;

$$0 \leq V_{\#} \leq 10 \frac{\text{mmol}}{\text{gDW} \cdot \text{hr}} \quad \text{if} \rightarrow$$

or

$$-10 \frac{\text{mmol}}{\text{gDW} \cdot \text{hr}} \leq V_{\#} \leq 10 \frac{\text{mmol}}{\text{gDW} \cdot \text{hr}} \quad \text{if} \leftrightharpoons$$