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

a. For $\leftleftharpoons$ use code HW#3 with $V

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

b. Not balanced originally added in a

"$H_2O \rightarrow$ " - export rxn

"ATP $\rightarrow$ " $\rightarrow$ Exchange rxns

"$\rightarrow$ ADP"

This check is preformed in the same code for a. and the matrix whose columns for balanced compartmental rxns columns 1~7 are all 0, since sources and sink eqn's/rxns aren't elementally balanced as they describe sinks and sources, but overall all rows must be balance no matter what i.e each row must sum to 0 which they do in the balanced model.

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

- For V- boundaries they were calculated as substrate/metabolite

if only $\rightarrow \Rightarrow 0 \leq V_{\#} \leq k_{cat} E \left(\frac{a}{k_m + a}\right)$

k_{cat}, E: givens

$\left(\frac{a}{k_m + a}\right)$: calculated in excel file nChembio 2077-5313, 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;

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

or

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