Enyzmes

Macromolecular Composition

2 x protein P1 + 1 x protein P2 + 1 ion

Enzyme can be composed of macromolecules (protein, RNA, ...), ions and cofactors.

Efficiency

$k_{app} = C$

$k_{app} = a\mu + b$

$k_{app} = \frac{V_{max}[S]}{K_M + [S]}$

Apparent catalytic rate can be either a constant, linear function of the growth rate, or a Michaelis-Menten function of an external metabolite concentration.

$-k_{app_{i,\leftarrow}} E_i \leq \nu_i \leq k_{app_{i,\rightarrow}} E_i$

Flux through a reaction is limited by the efficiency and abundance of an enzyme.

Enzyme capacity constraint C_2

enzymes.xml (section 4)

Cellular processes

Molecular machines

Ribosome Secretion apparatus Chaperone

Structure and efficiency are defined in the same way as for an enzyme.

Process substrates

Proteins Processes

Each macromolecule can be assigned to a number of processes. New processes can easily be added to the model.

Translation

Secretion

Chaperoning

For a particular growth rate, abundance of the processing machinery needs to be sufficient to process all of its substrates:

$\mu P_T \leq k_T R$

$\mu P_S \leq k_S S$

$\mu P_C \leq k_C C$

Process capacity constraint C_2

processes.xml (section 5)

proteins.xml
rnas.xml
dna.xml
(section 3)

Cell growing at rate μ

Metabolic network

Byproducts

Precursors

Energy carriers

Ribosomes

Chaperones

Enzymes

Proteins

Metabolism

$S\nu = 0$

Stoichiometric matrix S is first extracted from the genome-scale metabolic model.

$S\nu - \mu\nu_P - \mu\nu_E + \mu\nu_B = 0$

Metabolism additionally needs to be able to produce sufficient **P**recursors and **E**nergy carriers, and to recycle the metabolic **B**yproducts of different cellular processes.

Mass conservation constraint C_1

metabolism.xml (section 2)

targets.xml (section 7)

Compartments

Each compartment has an upper limit on the amount of **M**acromolecules that it can accomodate.

Periplasm

Cytoplasm

For each compartment X:

$\sum_{i \in X} M_i \leq D_X(\mu)$

Compartment density constraint C_3

density.xml (section 6)

parameters.xml (section 8)