Metabolic Networks
Exercise 1

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Task 1

I built the model using cobrapy. The metabolites and reactions which I included are listed below. The last reactions without product are boundary reactions. These either pass metabolites into the system (e.g. carbon1 and carbon2) or pull them out of the system (e.g. biomass). These reactions also serve as constraints since I set the upper bound to the corresponding maximum transport rate.

Reactions

Tc1:carbon_1 --> A
Tc2:carbon_2 --> A
Tf:F_ext --> F
Th:H_ext --> H
To2:O2_ext --> O2
Td:D --> D_ext
Te:E --> E_ext
R_1:A + ATP --> B
R_2:B <=> 2.0 ATP + C + 2.0 NADH
R_3:B --> F
R_4:C --> G
R_5_a:G --> 0.8 C + 2.0 NADH
R_5_b:G --> 0.8 C + 2.0 NADH
R_6:C --> 2.0 ATP + 3.0 D
R_7:C + 4.0 NADH --> E
R_8:ATP + G + 2.0 NADH <=> H
R_res:NADH + O2 --> ATP
Growth:10.0 ATP + C + F + H --> biomass
EX_carbon_1:carbon_1 <=>
EX_carbon_2:carbon_2 <=>
EX_H_ext:H_ext <=>
EX_F_ext:F_ext <=>
EX_O2_ext:O2_ext <=>
DM_E_ext:E_ext -->
DM_D_ext:D_ext -->
DM_biomass:biomass -->

Metabolites
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carbon_1
A
carbon_2
F_ext
F
H_ext
H
O2_ext
O2
D
D_ext
E
E_ext
ATP
B
C
NADH
G
biomass

Task 2

I optimized the flow for the “Growth” reaction. The results are shown below.

IN FLUXES	OUT FLUXES	OBJECTIVES
O2_ext 15		Growth 3.64
carbon_1 10.5		
H_ext 5		
F_ext 3.64		
carbon_2 1.5		
None		

Task 3

The results of the FVA show that the transport reactions for carbon can vary but never drop to zero. The only reactions that have a minimum of zero are 3, 5a, 5b. Other than the carbon transport and 5a/5b there is no reaction that has any variability.

	minimum	maximum
Tc1	1.500000	1.050000e+01
Tc2	1.500000	1.050000e+01
Tf	3.636364	3.636364e+00
Th	5.000000	5.000000e+00
To2	15.000000	1.500000e+01
Td	12.000000	1.200000e+01
Te	4.928571	4.928571e+00
R_1	12.000000	1.200000e+01
R_2	12.000000	1.200000e+01
R_3	0.000000	4.884981e-15
R_4	2.629870	2.629870e+00
R_5_a	0.000000	3.993506e+00
R_5_b	0.000000	3.993506e+00
R_6	4.000000	4.000000e+00
R_7	4.928571	4.928571e+00
R_8	-1.363636	-1.363636e+00
R_res	15.000000	1.500000e+01
Growth	3.636364	3.636364e+00

Task 3

Below I listed the growth rate after a specific reaction is knocked out. Those that reduce the growth rate to zero are marked as essential. Other than the growth reaction itself there is no reaction that can reduce the growth rate to zero. The reactions that reduce the growth rate the most are reaction 1 and reaction 2. Reaction 5a and 5b can be knocked out without any reduction to the growth rate. If reaction 1 or 2 are blocked the metabolite H has to be used in reactions 5a or 5b to produce metabolite C, which then can be used to produce biomass. Due to the maximum transport rate of metabolite H the growth rate then decreases.

Tc1 blocked, new growth rate 3.5
Tc2 blocked, new growth rate 3.5
Tf blocked, new growth rate 3.076923
Th blocked, new growth rate 3.181818
To2 blocked, new growth rate 2.142857
Td blocked, new growth rate 2.909091
Te blocked, new growth rate 3.009091
R_1 blocked, new growth rate 1.883117
R_2 blocked, new growth rate 1.883117
R_3 blocked, new growth rate 3.636364
R_4 blocked, new growth rate 3.244681
R_5_a blocked, new growth rate 3.636364
R_5_b blocked, new growth rate 3.636364
R_6 blocked, new growth rate 2.909091
R_7 blocked, new growth rate 3.009091
R_8 blocked, new growth rate 3.5

R_res blocked, new growth rate 2.142857
Growth blocked, new growth rate 0.0 -------> ESSENTIAL