Instruction

First step is to build a COBRA model from the SBML file by:

model = ReadCBModel (select Supplemental_Data7.xml)

Declaring the biomass function as objective function:

model=changeObjective(model,'R351',1)

To obtain the presented results shown in Figure 2, the following constraints have to be set to the metabolic model:

The photon influx is varied from 0 (non photothropic growth conditions) to 7 photons g^{-1} DW^{-1}. This is accomplished by setting the upper and lower reaction bounds of reaction 'R203' to the specific value:

model = changeRxnBounds(model, 'R203',0,'b')

...

model = changeRxnBounds(model, 'R203',7,'b')

In this scenario the hydrogencarbonate uptake is constrained from 0 to 0.45 mmol g^{-1} DW^{-1}:

model = changeRxnBounds(model, 'R344',0,'b')

...

model = changeRxnBounds(model, 'R344',0.45,'b')

The cellular ATP consumption is fixed to 0.27 mmol g^{-1} DW^{-1}:

model = changeRxnBounds(model, 'R205',0.27,'b')

and urea uptake is prohibited that only nitrate serves as the sole nitrogen source:

model = changeRxnBounds(model, 'R372',0,'b')

For the given flux distribution shown in Figure 3, which reflects maximal phototrophic growth yield, the photon influx has to be set to 1308.9:

model = changeRxnBounds(model, 'R203',1308.9,'b')

the cellular ATP consumption is fixed to 50.49:

model = changeRxnBounds(model, 'R205',50.49,'b')

and the urea uptake is set to 0:

model = changeRxnBounds(model, 'R372',0,'b').

Under this specification a relative comparision of all fluxes to the synthesis of RuBP (100%) is possible.

To simulate growth under the utilization of glycogen (shown in Figure 4), first the metabolite C00369 (glycogen) must be declared as an external species and the degradation of C00369 must be constraint:

The flux through two of three glycogen degrading reactions 'R27' and 'R28' is set to 0 mmol g^{-1} DW^{-1}

model = changeRxnBounds(model, 'R27',0,'b')

model = changeRxnBounds(model, 'R28',0,'b')

and the flux through the remaining reaction 'R26' is varied from $0 - 0.035$ mmol g^{-1} DW^{-1}:

model = changeRxnBounds(model, 'R26',0,'b')

...

model = changeRxnBounds(model, 'R26',0.035,'b')

The photon influx as well as the ATP consumption and the urea uptake are specified in the same way like in the scenario from Figure 2

model = changeRxnBounds(model, 'R203',0,'b')

...

model = changeRxnBounds(model, 'R203',7,'b')

model = changeRxnBounds(model, 'R205',0.27,'b')

model = changeRxnBounds(model, 'R372',0,'b')

The hydrogencarbonate uptake remains unconstrained.