170327 FBA och Fredrik Magnusson på JModelica forum

Explaining text.
In the file FBA1.mo we have the original model and run by fba1_test1.py
In the file FBA1.mop we have formulated the model as an optimisation problem run by fba1_test2.py Note in the plots we show mu and then the part of mu related to qGr and qEr respectively, and similarly for qO2.

The original model describes in a simplified way growth of yeast on a mixture of glucose and ethanol. As you see there is a “priority” of consuming glucose before ethanol. What optimisation problem is this the solution to? 😃

Well we can see this as a strategy that gives the maximal growth rate under the constraint of that the respiratory capacity is limited i.e.

Maximize: mu(qGr,qEr) = YGr*qGr + YEr*qEr
Under constraint: qO2(qGr,qEr) = kog*qGr + koe*qEr < qO2max

The solution to this is in the following way. The solution is for qGr and qEr on the constraint and gives a relation between qGr and qEr as

qEr = 1/koe*(qO2max-kog*qGr)

which gives

mu(qGr) = YEr/koe*qO2max + (YGr - YEr/koe*kog)*qGr

Since: YGr=3.5, YEr=1.32, kog=2.3, koe=1.6, qO2max = 0.00069, we have YGr-YEr/koe*kog>0
and therefore qGr maximal give the maximal growth and therefore:

qGr = min(qGr_pot, qO2max/kog)
qEr = min(qEr_pot, (qO2max-kog*qGr)/koe)

This is the optimal solution. In this case it was easy to derive an analytical solution of the problem to optimise mu. For more complicated models we rather would like to maximise mu on-line as a modelling step.

In FBA1.mop I have tried to formulate the optimisation problem, but I do not distinguish between potential and actual qGr and qEr and we loose some of the dynamics. But solution get reasonably similar.

Problem is that I cannot formulate in the criteria as objective = -mu which would be natural,
but have to take the round-about with the criteria as objectiveIntegrand = - VX

The key is perhaps to make the model to be optimised to include the distinction Between qEr_potential and qEr etc… and then using objective = -mu way work.
Not sure how to do it really. / Jan Peter