Creating a Model

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INTRODUCTION

This tutorial explains the most basic functions provided by the COBRA Toolbox to create a model from scratch (i.e. define all relevant reactions and build a model from them).

MATERIALS

In this tutorial, two models are created a small toy model and a simple model of glycolysis. The latter is also used in the model manipulation tutorial.

PROCEDURE

1. Create a simple toy model

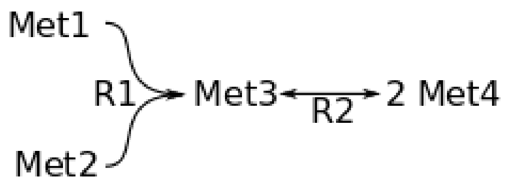
To create a new model, there is a simple function (createModel):

```
emptymodel = createModel()
```

Calling it as above, yields an empty model struct with all required fields defined. To add reactions or metabolites please have a look at the Tutorial for Model Manipulation.

There is also a possibility to immediately create a model with multiple reactions using createModel. To do so, a list of reaction identifiers, reaction names and reaction formulas has to be supplied.

Lets consider the following toy model:



The reactions are:

```
R1 = '1 Met1 + Met2 -> Met3'
R2 = 'Met3 <=> 2 Met4'
```

Reaction formulas are given as metabolites and their stoichiometric coefficient concatenated by +. Products and substrates are separated by a reversibility indicator, with -> indicating an irreversible reaction and <=> indicating a reversible reaction.

To be able to use createModel() to build this model, we also have to define the reaction Identifiers and the reaction names:

```
reactionIdentifiers = {'R1','R2'}
reactionNames = {'Reaction 1','Reaction 2'}
```

And we have to combine the reactions:

```
reactionFormulas = {R1,R2}
```

now we can call

```
model1 = createModel(reactionIdentifiers,reactionNames,reactionFormulas);
```

to create the model including the two reactions.

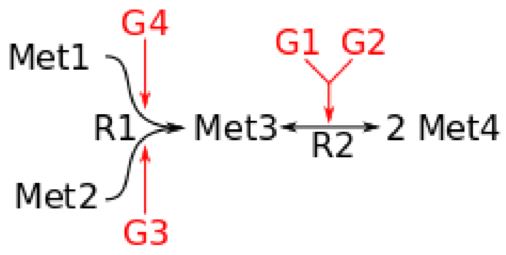
2. Explanation of options for the createModel function

createModel offers a couple of additional optional parameters. Those include:

- revFlagList - a double array of indications whether the reaction is reversible or not this will overwrite the indicator from the formula. (default 1 for reversible formulas, 0 for irreversible formulas)
- lowerBoundList - a double array indicating the lower bounds of the providing reactions (again, this will overwrite both revFlagList and the indication from the formula). E.g. if a revFlagList entry indicates a reversible reaction, but the lower bound is >0, the reaction will be considered as irreversible. (The default is to assume 0 for irreversible and 1000 for irreversible reactions)
- upperBoundList - a double array indicating the upper bounds of the reactions. (default 1000)
- subSystemList - a cell array indicating the subSystems of the reactions
- grRuleList - a cell array indicating the GPR rules for a formula (in textual format e.g. Gene1 and Gene2)
- geneNameList - a List of genes present in the grRuleList array
- systNameList - a List (of equal size as geneNameList), that is used to translate the genes from those used in the geneNameList to those used in this list.

3. Creating a model with Gene-Protein-Reaction Association (GPR) rules

Lets assume, our network has the following GPR associations:



i.e. A Complex of G1 and G2 catalyses R2 and either G3 or G4 catalyse R1. We further assume, that the flux maximum through R1 is 10 and 30 through R2

```
upperBounds = [10, 30];
grRuleR1 = 'G3 or G4';
grRuleR2 = 'G1 and G2';
grRuleList = {grRuleR1, grRuleR2};
```

The model creation call would then be:

```
model2 = createModel(reactionIdentifiers,reactionNames,reactionFormulas,...
                       'upperBoundList',upperBounds,'grRuleList',grRuleList);
```

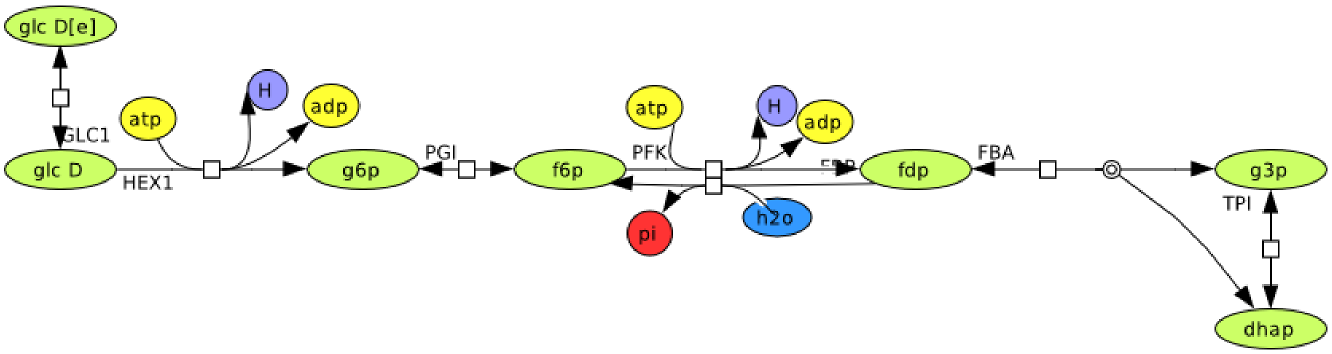
If we now compare the reactions, printing the GPR rules in both models

```
printRxnFormula(model1,'gprFlag',1);
printRxnFormula(model2,'gprFlag',1);
```

we see, that model 2 has assigned GPR rules, while model 1 does not have those.

4. Create a model of the upper part of glycolysis

We will now create a slightly more complex model (essentially, the upper part of the glycolysis) which will be used in other tutorials (e.g. ModelManipulation)



To create this model, we have to define the reactions:

```
ReactionFormulas = {'glc-D[e]  -> glc-D',...
    'glc-D + atp  -> H + adp + g6p',...
    'g6p  <=> f6p',...
    'atp + f6p  -> H + adp + fdp',...
    'fdp + h2o  -> f6p + pi',...
    'fdp  -> g3p + dhap',...
    'dhap  -> g3p'};
ReactionNames = {'GLCt1','HEX1','PGI','PFK','FBP','FBA','TPI'};
lowerbounds = [-20, 0, -20, 0, 0,-20,-20];
upperbounds = [20, 20, 20, 20, 20, 20, 20];
glycolysisModel = createModel(ReactionNames,ReactionNames,ReactionFormulas,...
                             'lowerBoundList',lowerbounds,'upperBoundList',upperbounds);
```