SBML Model Report

Model name: "Cronwright2002_Glycerol_Synthesis"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Jacky L Snoep[1] and Harish Dharuri[2] at November sixth 2006 at 2:32 a. m. and last time modified at May 16th 2012 at 10:18 a. m. Table 1 gives an overview of the quantities of all components of this model.

Table 1: Number of components in this model, which are described in the following sections.

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	3
events	0	constraints	0
reactions	2	function definitions	0
global parameters	0	unit definitions	4
rules	0	initial assignments	0

Model Notes

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SBML level 2 code generated for the JWS Online project by Jacky Snoep using PySCeS
Run this model online at http://jjj.biochem.sun.ac.za
To cite JWS Online please refer to: Olivier, B.G. and Snoep, J.L. (2004) Web-based modelling using JWS Online , Bioinformatics, 20:2143-2144

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Biomodels Curation The model reproduces the flux value of „Gpp p„ (rate of Glycerol synthesis) as depicted in Fig 3 of the paper. The model reproduces the flux for early exponential phase , however it can be used to reproduce the values for other phases by plugging in appropriate values for maximal rates as given in Table 1 and metabolite concentrations as given in Table 2 of the paper. The model was succesfully reproduced using Jarnac.

2 Unit Definitions

This is an overview of seven unit definitions of which three are predefined by SBML and not mentioned in the model.

2.1 Unit `substance`

Name millimole

Definition mmol

2.2 Unit `time`

Name minute

Definition 60 s

2.3 Unit `mM_per_minute`

Name mM_per_minute

Definition $\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$

2.4 Unit `mM`

Name mM

Definition $\mathrm{mmol} \cdot \mathrm{l}^{-1}$

2.5 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

2.6 Unit area

Notes Square metre is the predefined SBML unit for area since SBML Level 2 Version 1.

Definition m^2

2.7 Unit length

Notes Metre is the predefined SBML unit for length since SBML Level 2 Version 1.

Definition m

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
compartment	Cytoplasm		3	1	litre	☑	

3.1 Compartment compartment

This is a three dimensional compartment with a constant size of one litre.

Name Cytoplasm

4 Species

This model contains three species. The boundary condition of two of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 6 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
G3P	Glycerol 3-phosphate	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Gly	Glycerol	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
DHAP	DHAP	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑

5 Reactions

This model contains two reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 4: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	Gpd_p	Glycerol 3-phosphate dehydrogenase	DHAP $\rightleftharpoons$ G3P	
2	Gpp_p	Glycerol 3-phosphatase	G3P $\rightleftharpoons$ Gly	

5.1 Reaction Gpd_p

This is a reversible reaction of one reactant forming one product.

Name Glycerol 3-phosphate dehydrogenase

Reaction equation

$$\mathrm{DHAP} \rightleftharpoons \mathrm{G3P} \tag{1}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
DHAP	DHAP	

Product

Table 6: Properties of each product.

Id	Name	SBO
G3P	Glycerol 3-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{\frac{\mathrm{vol(compartment)} \cdot \mathrm{Vf1}}{\mathrm{K1nadh} \cdot \mathrm{K1dhap}} \cdot \left(\mathrm{NADH} \cdot [\mathrm{DHAP}] - \frac{\mathrm{NAD} \cdot [\mathrm{G3P}]}{\mathrm{Keq1}}\right)}{\left(1 + \frac{\mathrm{F16BP}}{\mathrm{K1f16bp}} + \frac{\mathrm{ATP}}{\mathrm{K1atp}} + \frac{\mathrm{ADP}}{\mathrm{K1adp}}\right) \cdot \left(1 + \frac{\mathrm{NADH}}{\mathrm{K1nadh}} + \frac{\mathrm{NAD}}{\mathrm{K1nad}}\right) \cdot \left(1 + \frac{[\mathrm{DHAP}]}{\mathrm{K1dhap}} + \frac{[\mathrm{G3P}]}{\mathrm{K1g3p}}\right)} \tag{2}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vf1			47.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
K1nadh			0.023	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K1dhap			0.540	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
NADH			1.870	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
NAD			1.450	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
Keq1			10000.000	dimensionless	☑

Id	Name	SBO	Value	Unit	Constant
F16BP			6.010	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
K1f16bp			4.800	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
ATP			2.370	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
K1atp			0.730	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
ADP			2.170	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
K1adp			2.000	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
K1nad			0.930	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
K1g3p			1.200	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑

5.2 Reaction Gpp_p

This is a reversible reaction of one reactant forming one product.

Name Glycerol 3-phosphatase

Reaction equation

$$\mathrm{G3P} \rightleftharpoons \mathrm{Gly} \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
G3P	Glycerol 3-phosphate	

Product

Table 9: Properties of each product.

Id	Name	SBO
Gly	Glycerol	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\frac{\mathrm{vol(compartment)}\cdot \mathrm{V2}\cdot[\mathrm{G3P}]}{\mathrm{K2g3p}}}{\left(1+\frac{[\mathrm{G3P}]}{\mathrm{K2g3p}}\right)\cdot\left(1+\frac{\mathrm{Phi}}{\mathrm{K2phi}}\right)} \tag{4}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V2			53.0	$\text{mmol} \cdot \text{l}^{-1} \cdot (60\ \text{s})^{-1}$	☑
K2g3p			3.5	$\text{mmol} \cdot \text{l}^{-1}$	☑
Phi			1.0	$\text{mmol} \cdot \text{l}^{-1}$	☑
K2phi			1.0	$\text{mmol} \cdot \text{l}^{-1}$	☑

6 Derived Rate Equations

When interpreted as an ordinary differential equation framework, this model implies the following set of equations for the rates of change of each species.

6.1 Species G3P

Name Glycerol 3-phosphate

Initial concentration $0\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in Gpp_p and as a product in Gpd_p).

$$\frac{\text{d}}{\text{d}t}\text{G3P} = v_1 - v_2 \tag{5}$$

6.2 Species Gly

Name Glycerol

Initial concentration $15.1\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in Gpp_p), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\text{d}}{\text{d}t}\text{Gly} = 0 \tag{6}$$

6.3 Species DHAP

Name DHAP

Initial concentration $0.59\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a reactant in Gpd_p), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\text{d}}{\text{d}t}\text{DHAP} = 0 \tag{7}$$

SBML2LaTeX was developed by Andreas Dräger[a], Hannes Planatscher[a], Dieudonné M Wouamba[a], Adrian Schröder[a], Michael Hucka[b], Lukas Endler[c], Martin Golebiewski[d] and Andreas Zell[a]. Please see http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX for more information.

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