

SBML Model Report

Model name:
“Conant2007_WGD_glycolysis_2A3AB”



May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following three authors: Gavin Conant¹, Lukas Endler² and Kenneth Wolfe³ at August sixth 2008 at 10:23 a. m. and last time modified at May 16th 2012 at 2:25 p. m. Table 1 provides 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	25
events	0	constraints	0
reactions	19	function definitions	0
global parameters	11	unit definitions	8
rules	0	initial assignments	0

Model Notes

This a model from the article:

Increased glycolytic flux as an outcome of whole-genome duplication in yeast.

Conant GC, Wolfe KH Mol. Syst. Biol. [2007 ; Volume: 3 (Issue:)]: 129 [17667951](#) ,

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Abstract:

After whole-genome duplication (WGD), deletions return most loci to single copy. However, duplicate loci may survive through selection for increased dosage. Here, we show how the WGD increased copy number of some glycolytic genes could have conferred an almost immediate selective advantage to an ancestor of *Saccharomyces cerevisiae*, providing a rationale for the success of the WGD. We propose that the loss of other redundant genes throughout the genome resulted in incremental dosage increases for the surviving duplicated glycolytic genes. This increase gave post-WGD yeasts a growth advantage through rapid glucose fermentation; one of this lineage's many adaptations to glucose-rich environments. Our hypothesis is supported by data from enzyme kinetics and comparative genomics. Because changes in gene dosage follow directly from post-WGD deletions, dosage selection can confer an almost instantaneous benefit after WGD, unlike neofunctionalization or subfunctionalization, which require specific mutations. We also show theoretically that increased fermentative capacity is of greatest advantage when glucose resources are both large and dense, an observation potentially related to the appearance of angiosperms around the time of WGD.

The original model submitted by the authors was slightly altered and now comprises the models originally submitted as MODEL2426780967, MODEL2427021978, MODEL2427095802. It reproduces figures 2A,3A and 3B from the publication.

This model uses the glycolysis model from Pritchard and Kell (2002) with an additional parameter, **WGD_E**, to adjust for the differing enzyme concentrations before the whole genome duplication (WGD) and parameters **fV_xxx** that adjust the **Vmax** of the different reactions (xxx eg. HXT or PYK).

Figure 3A from the article can be reproduced by changing the value of the parameters **fV_xxx** to 0.9 individually, with xxx signifying the different enzymes (HXT, HXK ...)

Figure 3B from the publication can be reproduced by setting the parameter **WGD_E** to 0.75 and individually setting the parameters **fV_xxx** to 1.333.

To reproduce figure 2A from the article change the parameter **WGD_E** in the range between 0.65 and 1.0.

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To cite BioModels Database, please use: Li C, Donizelli M, Rodriguez N, Dharuri H, Endler L, Chelliah V, Li L, He E, Henry A, Stefan MI, Snoep JL, Hucka M, Le Novre N, Laibe C (2010) BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models. BMC Syst Biol., 4:92.

2 Unit Definitions

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

2.1 Unit `time`

Name minute

Definition 60 s

2.2 Unit `substance`

Name mmol

Definition mmol

2.3 Unit `mM`

Name mM

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

2.4 Unit `mmpmin`

Name mmolepermin

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

2.5 Unit `mMpmin`

Name mMpermin

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

2.6 Unit `pmin`

Name permin

Definition $(60 \text{ s})^{-1}$

2.7 Unit `lpmin`

Name permin

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

2.8 Unit `pmMpmin`

Name permMpermin

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

2.9 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition 1

2.10 Unit area

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

Definition m^2

2.11 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
cyto	cytoplasm		3	1	litre	<input checked="" type="checkbox"/>	

3.1 Compartment cyto

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

Name cytoplasm

4 Species

This model contains 25 species. The boundary condition of eight of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 7 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
GLCi	Fru2,6-P2	cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
ATP		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
G6P		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
ADP		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
F6P		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
F16bP		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
F26bP		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
AMP		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
DHAP		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
GAP		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
NAD		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
BPG		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
NADH		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
P3G		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
P2G		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
PEP		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
PYR		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
AcAld		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
GLCo		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
CO2		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
EtOH		cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
	Glycerol	cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
	Glycogen	cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
	Trehalose	cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
	Succinate	cyto	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>

5 Parameters

This model contains eleven global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
WGD_E	WGD enzyme conc change		1.0	dimensionless	<input checked="" type="checkbox"/>
fV_HXT			1.0	dimensionless	<input checked="" type="checkbox"/>
fV_HXK			1.0	dimensionless	<input checked="" type="checkbox"/>
fV_TDH			1.0	dimensionless	<input checked="" type="checkbox"/>
fV_ENO			1.0	dimensionless	<input checked="" type="checkbox"/>
fV_PFK			1.0	dimensionless	<input checked="" type="checkbox"/>
fV_FBA			1.0	dimensionless	<input checked="" type="checkbox"/>
fV_PYK			1.0	dimensionless	<input checked="" type="checkbox"/>
fV_PGK			1.0	dimensionless	<input checked="" type="checkbox"/>
fV_GPM			1.0	dimensionless	<input checked="" type="checkbox"/>
fV_PGI			1.0	dimensionless	<input checked="" type="checkbox"/>

6 Reactions

This model contains 19 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 5: Overview of all reactions

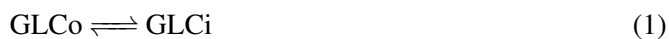
Nº	Id	Name	Reaction Equation	SBO
1	HXT	HXT	$\text{GLCo} \rightleftharpoons \text{GLCi}$	
2	H XK	H XK	$\text{GLCi} + \text{ATP} \rightleftharpoons \text{G6P} + \text{ADP}$	
3	PGI	PGI	$\text{G6P} \rightleftharpoons \text{F6P}$	
4	PFK	PFK	$\text{ATP} + \text{F6P} \xrightarrow{\text{AMP, F26bP}} \text{ADP} + \text{F16bP}$	
5	FBA	FBA	$\text{F16bP} \rightleftharpoons \text{DHAP} + \text{GAP}$	
6	TPI	TPI	$\text{DHAP} \rightleftharpoons \text{GAP}$	
7	TDH	TDH	$\text{GAP} + \text{NAD} \rightleftharpoons \text{BPG} + \text{NADH}$	
8	PGK	PGK	$\text{ADP} + \text{BPG} \rightleftharpoons \text{ATP} + \text{P3G}$	
9	GPM	GPM	$\text{P3G} \rightleftharpoons \text{P2G}$	
10	ENO	ENO	$\text{P2G} \rightleftharpoons \text{PEP}$	
11	PYK	PYK	$\text{ADP} + \text{PEP} \rightleftharpoons \text{ATP} + \text{PYR}$	
12	PDC	PDC	$\text{PYR} \longrightarrow \text{AcAld} + \text{CO}_2$	
13	ADH	ADH	$\text{NAD} + \text{EtOH} \rightleftharpoons \text{NADH} + \text{AcAld}$	
14	ATPase		$\text{ATP} \longrightarrow \text{ADP}$	
15	AK	adenylate kinase	$2 \text{ADP} \rightleftharpoons \text{ATP} + \text{AMP}$	
16	G3PDH	G3PDH	$\text{DHAP} + \text{NADH} \rightleftharpoons \text{NAD} + \text{Glycerol}$	
17	glycogen_branch	glycogenbranch	$\text{ATP} + \text{G6P} \longrightarrow \text{ADP} + \text{Glycogen}$	
18	trehalose_synth	trehalose_synthesis	$\text{ATP} + 2 \text{G6P} \longrightarrow \text{ADP} + \text{Trehalose}$	
19	succinate_syn	succinate_synthesis	$3 \text{NAD} + 2 \text{AcAld} \longrightarrow 3 \text{NADH} + \text{Succinate}$	

6.1 Reaction HXT

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

Name HXT

Reaction equation



Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
GLCo		

Product

Table 7: Properties of each product.

Id	Name	SBO
GLCi		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{V_{\max_1} \cdot fV_{\text{HXT}} \cdot \text{WGD.E.} \cdot ([\text{GLCo}] - [\text{GLCi}])}{K_{\text{glc_1}}} \quad (2)$$
$$1 + \frac{[\text{GLCo}] + [\text{GLCi}]}{K_{\text{glc_1}}} + \frac{K_{i_1} \cdot [\text{GLCo}] \cdot [\text{GLCi}]}{K_{\text{glc_1}}^2}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_1			97.240	mmol · (60 s) ⁻¹	✓
Kglc_1			1.192	l ⁻¹ · mmol	✓
Ki_1			0.910	dimensionless	✓

6.2 Reaction HXK

This is a reversible reaction of two reactants forming two products.

Name HXK

Reaction equation



Reactants

Table 9: Properties of each reactant.

Id	Name	SBO
GLCi		
ATP		

Products

Table 10: Properties of each product.

Id	Name	SBO
G6P		
ADP		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\text{vol}(\text{cyto}) \cdot \text{WGD_E} \cdot \text{fV_HXK} \cdot \text{Vmax_2} \cdot \left(\frac{[\text{GLCi}] \cdot [\text{ATP}]}{\text{Kglc_2} \cdot \text{Katp_2}} - \frac{[\text{G6P}] \cdot [\text{ADP}]}{\text{Kglc_2} \cdot \text{Katp_2} \cdot \text{Keq_2}} \right)}{\left(1 + \frac{[\text{GLCi}]}{\text{Kglc_2}} + \frac{[\text{G6P}]}{\text{Kg6p_2}} \right) \cdot \left(1 + \frac{[\text{ATP}]}{\text{Katp_2}} + \frac{[\text{ADP}]}{\text{Kadp_2}} \right)} \quad (4)$$

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_2			236.70	mmol · (60 s) ⁻¹ · l ⁻¹	✓
Kglc_2			0.08	l ⁻¹ · mmol	✓
Katp_2			0.15	l ⁻¹ · mmol	✓
Keq_2			2000.00	dimensionless	✓

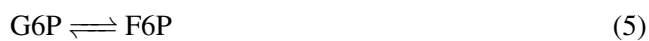
Id	Name	SBO	Value	Unit	Constant
Kg6p_2			30.00	$l^{-1} \cdot \text{mmol}$	<input checked="" type="checkbox"/>
Kadp_2			0.23	$l^{-1} \cdot \text{mmol}$	<input checked="" type="checkbox"/>

6.3 Reaction PGI

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

Name PGI

Reaction equation



Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
G6P		

Product

Table 13: Properties of each product.

Id	Name	SBO
F6P		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \frac{\text{vol}(\text{cyto}) \cdot V_{\text{max}_3} \cdot fV_PGI \cdot WGD_E \cdot \left(\frac{[G6P]}{K_{g6p_3}} - \frac{[F6P]}{K_{g6p_3} \cdot K_{eq_3}} \right)}{1 + \frac{[G6P]}{K_{g6p_3}} + \frac{[F6P]}{K_{f6p_3}}} \quad (6)$$

Table 14: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_3			1056.00	$\text{mmol} \cdot (60 \text{ s})^{-1} \cdot l^{-1}$	<input checked="" type="checkbox"/>

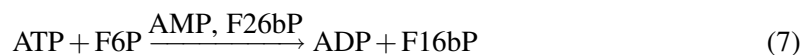
Id	Name	SBO	Value	Unit	Constant
Kg6p_3			1.40	$l^{-1} \cdot mmol$	<input checked="" type="checkbox"/>
Keq_3			0.29	dimensionless	<input checked="" type="checkbox"/>
Kf6p_3			0.30	$l^{-1} \cdot mmol$	<input checked="" type="checkbox"/>

6.4 Reaction PFK

This is an irreversible reaction of two reactants forming two products influenced by two modifiers.

Name PFK

Reaction equation



Reactants

Table 15: Properties of each reactant.

Id	Name	SBO
ATP		
F6P		

Modifiers

Table 16: Properties of each modifier.

Id	Name	SBO
AMP		
F26bP	Fru2,6-P2	

Products

Table 17: Properties of each product.

Id	Name	SBO
ADP		
F16bP		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{vol}(\text{cyto}) \cdot V_{\text{max_4}} \cdot fV_PFK \cdot WGD_E \quad (8)$$

$$\cdot \frac{gR_4 \cdot \frac{[F6P]}{Kf6p_4} \cdot \frac{[ATP]}{Katp_4} \cdot \left(1 + \frac{[F6P]}{Kf6p_4} + \frac{[ATP]}{Katp_4} + \frac{\frac{gR_4 \cdot [F6P]}{Kf6p_4} \cdot [ATP]}{Katp_4}\right)}{\left(1 + \frac{[F6P]}{Kf6p_4} + \frac{[ATP]}{Katp_4} + \frac{\frac{gR_4 \cdot [F6P]}{Kf6p_4} \cdot [ATP]}{Katp_4}\right)^2 + L0_4 \cdot \left(\frac{1 + \frac{Ciatp_4 \cdot [ATP]}{Kiatp_4}}{1 + \frac{[ATP]}{Kiatp_4}}\right)^2 \cdot \left(\frac{1 + \frac{Camp_4 \cdot [AMP]}{Kamp_4}}{1 + \frac{[AMP]}{Kamp_4}}\right)^2 \cdot \left(\frac{1 + \frac{Cf26_4 \cdot [F26bP]}{Kf26_4} + \frac{Cf16_4 \cdot [F16bP]}{Kf16_4}}{1 + \frac{[F26bP]}{Kf26_4} + \frac{[F16bP]}{Kf16_4}}\right)^2}$$

Table 18: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_4			110.000	mmol · (60 s) ⁻¹ · l ⁻¹	☑
gR_4			5.120	dimensionless	☑
Kf6p_4			0.100	l ⁻¹ · mmol	☑
Katp_4			0.710	l ⁻¹ · mmol	☑
L0_4			0.660	dimensionless	☑
Ciatp_4			100.000	dimensionless	☑
Kiatp_4			0.650	l ⁻¹ · mmol	☑
Camp_4			0.085	dimensionless	☑
Kamp_4			0.100	l ⁻¹ · mmol	☑
Cf26_4			0.017	dimensionless	☑
Kf26_4			6.82 · 10 ⁻⁴	l ⁻¹ · mmol	☑
Cf16_4			0.397	dimensionless	☑
Kf16_4			0.111	l ⁻¹ · mmol	☑
Catp_4			3.000	dimensionless	☑

6.5 Reaction FBA

This is a reversible reaction of one reactant forming two products.

Name FBA

Reaction equation



Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
F16bP		

Products

Table 20: Properties of each product.

Id	Name	SBO
DHAP		
GAP		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \frac{\text{vol}(\text{cyto}) \cdot V_{\text{max_5}} \cdot fV_{\text{FBA}} \cdot \text{WGD_E} \cdot \left(\frac{[\text{F16bP}]}{K_{\text{f16bp_5}}} - \frac{[\text{DHAP}] \cdot [\text{GAP}]}{K_{\text{f16bp_5}} \cdot K_{\text{eq_5}}} \right)}{1 + \frac{[\text{F16bP}]}{K_{\text{f16bp_5}}} + \frac{[\text{DHAP}]}{K_{\text{dhap_5}}} + \frac{[\text{GAP}]}{K_{\text{gap_5}}} + \frac{[\text{F16bP}] \cdot [\text{GAP}]}{K_{\text{f16bp_5}} \cdot K_{\text{igap_5}}} + \frac{[\text{DHAP}] \cdot [\text{GAP}]}{K_{\text{dhap_5}} \cdot K_{\text{gap_5}}}} \quad (10)$$

Table 21: Properties of each parameter.

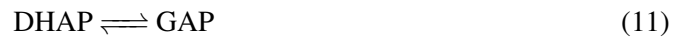
Id	Name	SBO	Value	Unit	Constant
Vmax_5			94.690	mmol · (60 s) ⁻¹ · l ⁻¹	✓
Kf16bp_5			0.300	l ⁻¹ · mmol	✓
Keq_5			0.069	l ⁻¹ · mmol	✓
Kdhap_5			2.000	l ⁻¹ · mmol	✓
Kgap_5			2.400	l ⁻¹ · mmol	✓
Kigap_5			10.000	l ⁻¹ · mmol	✓

6.6 Reaction TPI

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

Name TPI

Reaction equation



Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
	DHAP	

Product

Table 23: Properties of each product.

Id	Name	SBO
	GAP	

Kinetic Law

Derived unit $(60\text{ s})^{-1} \cdot \text{mmol}$

$$v_6 = \text{vol}(\text{cyto}) \cdot (k1_6 \cdot [\text{DHAP}] - k2_6 \cdot [\text{GAP}]) \quad (12)$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1_6			450000.000	$(60\text{ s})^{-1}$	<input checked="" type="checkbox"/>
k2_6			10^7	$(60\text{ s})^{-1}$	<input checked="" type="checkbox"/>

6.7 Reaction TDH

This is a reversible reaction of two reactants forming two products.

Name TDH

Reaction equation



Reactants

Table 25: Properties of each reactant.

Id	Name	SBO
	GAP	
	NAD	

Products

Table 26: Properties of each product.

Id	Name	SBO
	BPG	
	NADH	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \frac{\text{vol}(\text{cyto}) \cdot C_7 \cdot \left(\frac{V_{\text{maxf_7}} \cdot fV_{\text{TDH_WGD_E}} \cdot [\text{GAP}] \cdot [\text{NAD}]}{K_{\text{gap_7}} \cdot K_{\text{nad_7}}} - \frac{V_{\text{maxr_7}} \cdot fV_{\text{TDH_WGD_E}} \cdot [\text{BPG}] \cdot [\text{NADH}]}{K_{\text{bpg_7}} \cdot K_{\text{nadh_7}}} \right)}{\left(1 + \frac{[\text{GAP}]}{K_{\text{gap_7}}} + \frac{[\text{BPG}]}{K_{\text{bpg_7}}} \right) \cdot \left(1 + \frac{[\text{NAD}]}{K_{\text{nad_7}}} + \frac{[\text{NADH}]}{K_{\text{nadh_7}}} \right)} \quad (14)$$

Table 27: Properties of each parameter.

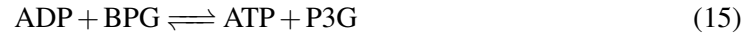
Id	Name	SBO	Value	Unit	Constant
C_7			1.000	dimensionless	✓
Vmaxf_7			1152.000	mmol · (60 s) ⁻¹ · l ⁻¹	✓
Kgap_7			0.210	l ⁻¹ · mmol	✓
Knad_7			0.090	l ⁻¹ · mmol	✓
Vmaxr_7			6719.000	mmol · (60 s) ⁻¹ · l ⁻¹	✓
Kbpg_7			0.010	l ⁻¹ · mmol	✓
Knadh_7			0.060	l ⁻¹ · mmol	✓

6.8 Reaction PGK

This is a reversible reaction of two reactants forming two products.

Name PGK

Reaction equation



Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
	ADP	
	BPG	

Products

Table 29: Properties of each product.

Id	Name	SBO
	ATP	
	P3G	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \frac{\text{vol}(\text{cyto}) \cdot \text{fV_PGK} \cdot V_{\text{max_8}} \cdot \text{WGD_E} \cdot \frac{\text{Keq_8} \cdot [\text{BPG}] \cdot [\text{ADP}] - [\text{P3G}] \cdot [\text{ATP}]}{\text{Kp3g_8} \cdot \text{Katp_8}}}{\left(1 + \frac{[\text{BPG}]}{\text{Kbpg_8}} + \frac{[\text{P3G}]}{\text{Kp3g_8}}\right) \cdot \left(1 + \frac{[\text{ADP}]}{\text{Kadp_8}} + \frac{[\text{ATP}]}{\text{Katp_8}}\right)} \quad (16)$$

Table 30: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_8			1288.000	mmol · (60 s) ⁻¹ · l ⁻¹	✓
Keq_8			3200.000	dimensionless	✓
Kp3g_8			0.530	l ⁻¹ · mmol	✓
Katp_8			0.300	l ⁻¹ · mmol	✓
Kbpg_8			0.003	l ⁻¹ · mmol	✓
Kadp_8			0.200	l ⁻¹ · mmol	✓

6.9 Reaction GPM

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

Name GPM

Reaction equation



Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
P3G		

Product

Table 32: Properties of each product.

Id	Name	SBO
P2G		

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \frac{\text{vol}(\text{cyto}) \cdot V_{\text{max}_9} \cdot fV_{\text{GPM}} \cdot WGD_E \cdot \left(\frac{[\text{P3G}]}{K_{\text{p3g}_9}} - \frac{[\text{P2G}]}{K_{\text{p3g}_9} \cdot K_{\text{eq}_9}} \right)}{1 + \frac{[\text{P3G}]}{K_{\text{p3g}_9}} + \frac{[\text{P2G}]}{K_{\text{p2g}_9}}} \quad (18)$$

Table 33: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_9			2585.00	mmol · (60 s) ⁻¹ · l ⁻¹	✓
Kp3g_9			1.20	l ⁻¹ · mmol	✓
Keq_9			0.19	dimensionless	✓
Kp2g_9			0.08	l ⁻¹ · mmol	✓

6.10 Reaction ENO

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

Name ENO

Reaction equation



Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
P2G		

Product

Table 35: Properties of each product.

Id	Name	SBO
PEP		

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \frac{\text{vol}(\text{cyto}) \cdot V_{\text{max_10}} \cdot fV_{\text{ENO}} \cdot WGD_E \cdot \left(\frac{[\text{P2G}]}{K_{\text{p2g_10}}} - \frac{[\text{PEP}]}{K_{\text{p2g_10}} \cdot K_{\text{eq_10}}} \right)}{1 + \frac{[\text{P2G}]}{K_{\text{p2g_10}}} + \frac{[\text{PEP}]}{K_{\text{pep_10}}}} \quad (20)$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_10			201.60	mmol · (60 s) ⁻¹ · l ⁻¹	✓
Kp2g_10			0.04	l ⁻¹ · mmol	✓
Keq_10			6.70	dimensionless	✓
Kpep_10			0.50	l ⁻¹ · mmol	✓

6.11 Reaction PYK

This is a reversible reaction of two reactants forming two products.

Name PYK

Reaction equation



Reactants

Table 37: Properties of each reactant.

Id	Name	SBO
	ADP	
	PEP	

Products

Table 38: Properties of each product.

Id	Name	SBO
	ATP	
	PYR	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \frac{\text{vol}(\text{cyto}) \cdot V_{\text{max}_11} \cdot fV_{\text{PYK}} \cdot \text{WGD_E} \cdot \left(\frac{[\text{PEP}] \cdot [\text{ADP}]}{K_{\text{pep}_11} \cdot K_{\text{adp}_11}} - \frac{[\text{PYR}] \cdot [\text{ATP}]}{K_{\text{pep}_11} \cdot K_{\text{adp}_11} \cdot K_{\text{eq}_11}} \right)}{\left(1 + \frac{[\text{PEP}]}{K_{\text{pep}_11}} + \frac{[\text{PYR}]}{K_{\text{pyr}_11}} \right) \cdot \left(1 + \frac{[\text{ADP}]}{K_{\text{adp}_11}} + \frac{[\text{ATP}]}{K_{\text{atp}_11}} \right)} \quad (22)$$

Table 39: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_{max_11}			1000.00	$\text{mmol} \cdot (\text{60 s})^{-1} \cdot \text{l}^{-1}$	✓
K_{pep_11}			0.14	$\text{l}^{-1} \cdot \text{mmol}$	✓
K_{adp_11}			0.53	$\text{l}^{-1} \cdot \text{mmol}$	✓

Id	Name	SBO	Value	Unit	Constant
Keq_11			6500.00	dimensionless	<input checked="" type="checkbox"/>
Kpyr_11			21.00	$l^{-1} \cdot mmol$	<input checked="" type="checkbox"/>
Katp_11			1.50	$l^{-1} \cdot mmol$	<input checked="" type="checkbox"/>

6.12 Reaction PDC

This is an irreversible reaction of one reactant forming two products.

Name PDC

Reaction equation



Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
PYR		

Products

Table 41: Properties of each product.

Id	Name	SBO
AcAld		
CO2		

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \frac{\text{vol}(\text{cyto}) \cdot V_{\text{max}_12} \cdot WGD_E \cdot \left(\frac{[PYR]}{K_{\text{pyr}_12}} \right)^{nH_12}}{1 + \left(\frac{[PYR]}{K_{\text{pyr}_12}} \right)^{nH_12}} \quad (24)$$

Table 42: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_12			857.80	mmol · (60 s) ⁻¹ · l ⁻¹	<input checked="" type="checkbox"/>
Kpyr_12			4.33	l ⁻¹ · mmol	<input checked="" type="checkbox"/>
nH_12			1.90	dimensionless	<input checked="" type="checkbox"/>

6.13 Reaction ADH

This is a reversible reaction of two reactants forming two products.

Name ADH

Reaction equation



Reactants

Table 43: Properties of each reactant.

Id	Name	SBO
	NAD	
	EtOH	

Products

Table 44: Properties of each product.

Id	Name	SBO
	NADH	
	AcAld	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \frac{\text{vol}(\text{cyto}) \cdot V_{\text{max}_13} \cdot \text{WGD}_E \cdot \left(\frac{[\text{EtOH}] \cdot [\text{NAD}]}{\text{Ketoh}_13 \cdot \text{Kinad}_13} \right)}{1 + \frac{[\text{NAD}]}{\text{Kinad}_13} + \frac{[\text{EtOH}] \cdot \text{Knad}_13}{\text{Kinad}_13 \cdot \text{Ketoh}_13} + \frac{[\text{AcAld}] \cdot \text{Knadh}_13}{\text{Kinadh}_13 \cdot \text{Kacald}_13} + \frac{[\text{NADH}]}{\text{Kinadh}_13} + \frac{[\text{EtOH}] \cdot [\text{NAD}]}{\text{Kinad}_13 \cdot \text{Ketoh}_13} + \frac{[\text{NAD}] \cdot [\text{AcAld}] \cdot \text{Knadh}_13}{\text{Kinad}_13 \cdot \text{Kinadh}_13 \cdot \text{Kacald}_13} + \frac{[\text{EtOH}] \cdot [\text{NADH}]}{\text{Ketoh}_13 \cdot \text{Kinadh}_13}} \quad (26)$$

Table 45: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_13			209.500	$\text{mmol} \cdot (60 \text{ s})^{-1} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>
Ketoh_13			17.000	$\text{l}^{-1} \cdot \text{mmol}$	<input checked="" type="checkbox"/>
Kinad_13			0.920	$\text{l}^{-1} \cdot \text{mmol}$	<input checked="" type="checkbox"/>
Keq_13			$6.9 \cdot 10^{-5}$	dimensionless	<input checked="" type="checkbox"/>
Knad_13			0.170	$\text{l}^{-1} \cdot \text{mmol}$	<input checked="" type="checkbox"/>
Knadh_13			0.110	$\text{l}^{-1} \cdot \text{mmol}$	<input checked="" type="checkbox"/>
Kinadh_13			0.031	$\text{l}^{-1} \cdot \text{mmol}$	<input checked="" type="checkbox"/>
Kacald_13			1.110	$\text{l}^{-1} \cdot \text{mmol}$	<input checked="" type="checkbox"/>
Kiacald_13			1.100	$\text{l}^{-1} \cdot \text{mmol}$	<input checked="" type="checkbox"/>
Kietoh_13			90.000	$\text{l}^{-1} \cdot \text{mmol}$	<input checked="" type="checkbox"/>

6.14 Reaction ATPase

This is an irreversible reaction of one reactant forming one product.

Reaction equation



Reactant

Table 46: Properties of each reactant.

Id	Name	SBO
ATP		

Product

Table 47: Properties of each product.

Id	Name	SBO
ADP		

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \text{mmol}$

$$v_{14} = \text{vol}(\text{cyto}) \cdot \text{Katpase}_{14} \cdot [\text{ATP}] \quad (28)$$

Table 48: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Katpase_14			39.5	$(60\text{ s})^{-1}$	<input checked="" type="checkbox"/>

6.15 Reaction AK

This is a reversible reaction of one reactant forming two products.

Name adenylate kinase

Reaction equation



Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
	ADP	

Products

Table 50: Properties of each product.

Id	Name	SBO
	ATP	
	AMP	

Kinetic Law

Derived unit $(60\text{ s})^{-1} \cdot \text{mmol}$

$$v_{15} = \text{vol}(\text{cyto}) \cdot (k1_{15} \cdot [\text{ADP}] \cdot [\text{ADP}] - k2_{15} \cdot [\text{ATP}] \cdot [\text{AMP}]) \quad (30)$$

Table 51: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1_15			45.0	$\text{mmol}^{-1} \cdot (60\text{ s})^{-1} \cdot 1$	<input checked="" type="checkbox"/>

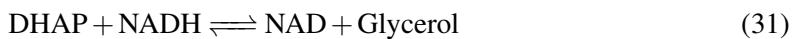
Id	Name	SBO	Value	Unit	Constant
k2_15			100.0	mmol ⁻¹ · (60 s) ⁻¹ · 1	<input checked="" type="checkbox"/>

6.16 Reaction G3PDH

This is a reversible reaction of two reactants forming two products.

Name G3PDH

Reaction equation



Reactants

Table 52: Properties of each reactant.

Id	Name	SBO
	DHAP	
	NADH	

Products

Table 53: Properties of each product.

Id	Name	SBO
	NAD	
	Glycerol	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \frac{\text{vol}(\text{cyto}) \cdot V_{\text{max}_16} \cdot \text{WGD}_E \cdot \left(\frac{[\text{DHAP}]}{K_{\text{dhap}_16}} \cdot \frac{[\text{NADH}]}{K_{\text{nadh}_16}} - \frac{[\text{Glycerol}]}{K_{\text{dhap}_16}} \cdot \frac{[\text{NAD}]}{K_{\text{nadh}_16}} \cdot \frac{1}{K_{\text{eq}_16}} \right)}{\left(1 + \frac{[\text{DHAP}]}{K_{\text{dhap}_16}} + \frac{[\text{Glycerol}]}{K_{\text{glycerol}_16}} \right) \cdot \left(1 + \frac{[\text{NADH}]}{K_{\text{nadh}_16}} + \frac{[\text{NAD}]}{K_{\text{nad}_16}} \right)} \quad (32)$$

Table 54: Properties of each parameter.

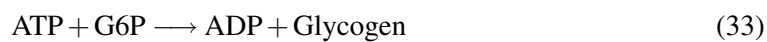
Id	Name	SBO	Value	Unit	Constant
Vmax_16			47.110	$\text{mmol} \cdot (\text{60 s})^{-1} \cdot \text{l}^{-1}$	✓
Kdhap_16			0.400	$\text{l}^{-1} \cdot \text{mmol}$	✓
Knadh_16			0.023	$\text{l}^{-1} \cdot \text{mmol}$	✓
Keq_16			4300.000	dimensionless	✓
Kglycerol_16			1.000	$\text{l}^{-1} \cdot \text{mmol}$	✓
Knad_16			0.930	$\text{l}^{-1} \cdot \text{mmol}$	✓

6.17 Reaction `glycogen_branch`

This is an irreversible reaction of two reactants forming two products.

Name `glycogenbranch`

Reaction equation



Reactants

Table 55: Properties of each reactant.

Id	Name	SBO
	ATP	
	G6P	

Products

Table 56: Properties of each product.

Id	Name	SBO
	ADP	
	Glycogen	

Kinetic Law

Derived unit $\text{mmol} \cdot (\text{60 s})^{-1}$

$$v_{17} = \text{vol}(\text{cyto}) \cdot \text{KGLYCOGEN_17} \quad (34)$$

Table 57: Properties of each parameter.

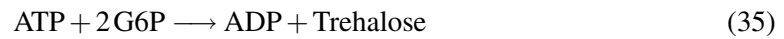
Id	Name	SBO	Value	Unit	Constant
KGlycogen_17			6.0	$\text{mmol} \cdot (\text{s})^{-1}$	<input checked="" type="checkbox"/>

6.18 Reaction `trehalose_synth`

This is an irreversible reaction of two reactants forming two products.

Name `trehalose_synthesis`

Reaction equation



Reactants

Table 58: Properties of each reactant.

Id	Name	SBO
	ATP	
	G6P	

Products

Table 59: Properties of each product.

Id	Name	SBO
	ADP	
	Trehalose	

Kinetic Law

Derived unit $\text{mmol} \cdot (\text{s})^{-1}$

$$v_{18} = \text{vol}(\text{cyto}) \cdot K_{\text{trehalose_18}} \quad (36)$$

Table 60: Properties of each parameter.

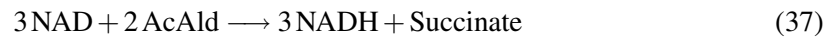
Id	Name	SBO	Value	Unit	Constant
Ktrehalose- _18			2.4	$\text{mmol} \cdot (\text{s})^{-1}$	<input checked="" type="checkbox"/>

6.19 Reaction `succinate_syn`

This is an irreversible reaction of two reactants forming two products.

Name `succinate_synthesis`

Reaction equation



Reactants

Table 61: Properties of each reactant.

Id	Name	SBO
	NAD	
	AcAld	

Products

Table 62: Properties of each product.

Id	Name	SBO
	NADH	
	Succinate	

Kinetic Law

Derived unit $(\text{s})^{-1} \cdot \text{mmol}$

$$v_{19} = \text{vol}(\text{cyto}) \cdot k_{19} \cdot [\text{AcAld}] \quad (38)$$

Table 63: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_19			21.4	$(60\text{ s})^{-1}$	<input checked="" type="checkbox"/>

7 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.

7.1 Species [GLCi](#)

Initial concentration $0.097652231064563\text{ mmol}\cdot\text{l}^{-1}$

This species takes part in two reactions (as a reactant in [HXX](#) and as a product in [HXT](#)).

$$\frac{d}{dt}\text{GLCi} = v_1 - v_2 \quad (39)$$

7.2 Species [ATP](#)

Initial concentration $2.52512746499271\text{ mmol}\cdot\text{l}^{-1}$

This species takes part in eight reactions (as a reactant in [HXX](#), [PFK](#), [ATPase](#), [glycogen_branch](#), [trehalose_synth](#) and as a product in [PGK](#), [PYK](#), [AK](#)).

$$\frac{d}{dt}\text{ATP} = v_8 + v_{11} + v_{15} - v_2 - v_4 - v_{14} - v_{17} - v_{18} \quad (40)$$

7.3 Species [G6P](#)

Initial concentration $2.67504014044787\text{ mmol}\cdot\text{l}^{-1}$

This species takes part in four reactions (as a reactant in [PGI](#), [glycogen_branch](#), [trehalose_synth](#) and as a product in [HXX](#)).

$$\frac{d}{dt}\text{G6P} = v_2 - v_3 - v_{17} - 2v_{18} \quad (41)$$

7.4 Species [ADP](#)

Initial concentration $1.28198768168719\text{ mmol}\cdot\text{l}^{-1}$

This species takes part in eight reactions (as a reactant in [PGK](#), [PYK](#), [AK](#) and as a product in [HXX](#), [PFK](#), [ATPase](#), [glycogen_branch](#), [trehalose_synth](#)).

$$\frac{d}{dt}\text{ADP} = v_2 + v_4 + v_{14} + v_{17} + v_{18} - v_8 - v_{11} - 2v_{15} \quad (42)$$

7.5 Species F6P

Initial concentration 0.624976405532373 mmol · l⁻¹

This species takes part in two reactions (as a reactant in [PFK](#) and as a product in [PGI](#)).

$$\frac{d}{dt}F6P = v_3 - v_4 \quad (43)$$

7.6 Species F16bP

Initial concentration 6.22132076069411 mmol · l⁻¹

This species takes part in two reactions (as a reactant in [FBA](#) and as a product in [PFK](#)).

$$\frac{d}{dt}F16bP = v_4 - v_5 \quad (44)$$

7.7 Species F26bP

Name Fru2,6-P2

Initial concentration 0.02 mmol · l⁻¹

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

$$\frac{d}{dt}F26bP = 0 \quad (45)$$

7.8 Species AMP

Initial concentration 0.292884853320091 mmol · l⁻¹

This species takes part in two reactions (as a product in [AK](#) and as a modifier in [PFK](#)).

$$\frac{d}{dt}AMP = v_{15} \quad (46)$$

7.9 Species DHAP

Initial concentration 1.00415254899644 mmol · l⁻¹

This species takes part in three reactions (as a reactant in [TPI](#), [G3PDH](#) and as a product in [FBA](#)).

$$\frac{d}{dt}DHAP = v_5 - v_6 - v_{16} \quad (47)$$

7.10 Species GAP

Initial concentration 0.0451809175780963 mmol · l⁻¹

This species takes part in three reactions (as a reactant in [TDH](#) and as a product in [FBA](#), [TPI](#)).

$$\frac{d}{dt}\text{GAP} = v_5 + v_6 - v_7 \quad (48)$$

7.11 Species NAD

Initial concentration 1.50329030201531 mmol · l⁻¹

This species takes part in four reactions (as a reactant in [TDH](#), [ADH](#), [succinate_syn](#) and as a product in [G3PDH](#)).

$$\frac{d}{dt}\text{NAD} = v_{16} - v_7 - v_{13} - 3v_{19} \quad (49)$$

7.12 Species BPG

Initial concentration 7.36873499865602 · 10⁻⁴ mmol · l⁻¹

This species takes part in two reactions (as a reactant in [PGK](#) and as a product in [TDH](#)).

$$\frac{d}{dt}\text{BPG} = v_7 - v_8 \quad (50)$$

7.13 Species NADH

Initial concentration 0.0867096979846952 mmol · l⁻¹

This species takes part in four reactions (as a reactant in [G3PDH](#) and as a product in [TDH](#), [ADH](#), [succinate_syn](#)).

$$\frac{d}{dt}\text{NADH} = v_7 + v_{13} + 3v_{19} - v_{16} \quad (51)$$

7.14 Species P3G

Initial concentration 0.885688538360659 mmol · l⁻¹

This species takes part in two reactions (as a reactant in [GPM](#) and as a product in [PGK](#)).

$$\frac{d}{dt}\text{P3G} = v_8 - v_9 \quad (52)$$

7.15 Species P2G

Initial concentration 0.127695817386632 mmol · l⁻¹

This species takes part in two reactions (as a reactant in [ENO](#) and as a product in [GPM](#)).

$$\frac{d}{dt}P2G = v_9 - v_{10} \quad (53)$$

7.16 Species PEP

Initial concentration 0.0632352144936527 mmol · l⁻¹

This species takes part in two reactions (as a reactant in [PYK](#) and as a product in [ENO](#)).

$$\frac{d}{dt}PEP = v_{10} - v_{11} \quad (54)$$

7.17 Species PYR

Initial concentration 1.81531251192736 mmol · l⁻¹

This species takes part in two reactions (as a reactant in [PDC](#) and as a product in [PYK](#)).

$$\frac{d}{dt}PYR = v_{11} - v_{12} \quad (55)$$

7.18 Species AcAld

Initial concentration 0.178140579850657 mmol · l⁻¹

This species takes part in three reactions (as a reactant in [succinate_syn](#) and as a product in [PDC](#), [ADH](#)).

$$\frac{d}{dt}AcAld = v_{12} + v_{13} - 2v_{19} \quad (56)$$

7.19 Species GLCo

Initial concentration 50 mmol · l⁻¹

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

$$\frac{d}{dt}GLCo = 0 \quad (57)$$

7.20 Species CO₂

Initial concentration 1 mmol · l⁻¹

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

$$\frac{d}{dt}\text{CO}_2 = 0 \quad (58)$$

7.21 Species EtOH

Initial concentration 50 mmol · l⁻¹

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

$$\frac{d}{dt}\text{EtOH} = 0 \quad (59)$$

7.22 Species Glycerol

Initial concentration 0.15 mmol · l⁻¹

This species takes part in one reaction (as a product in [G3PDH](#)), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{Glycerol} = 0 \quad (60)$$

7.23 Species Glycogen

Initial concentration 0 mmol · l⁻¹

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

$$\frac{d}{dt}\text{Glycogen} = 0 \quad (61)$$

7.24 Species Trehalose

Initial concentration 0 mmol · l⁻¹

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

$$\frac{d}{dt}\text{Trehalose} = 0 \quad (62)$$

7.25 Species Succinate

Initial concentration 0 mmol · l⁻¹

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

$$\frac{d}{dt}\text{Succinate} = 0 \quad (63)$$

SBML2^ATeX 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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