SBML Model Report

Model name: "Galazzo1990-_FermentationPathwayKinetics"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following three authors: Jacky L Snoep[1], Harish Dharuri[2] and Lukas Endler[3] at August thirteenth 2006 at 7:32 p. m. and last time modified at April second 2014 at 0:54 a. m. Table 1 shows 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	2
species types	0	species	9
events	0	constraints	0
reactions	8	function definitions	0
global parameters	6	unit definitions	5
rules	2	initial assignments	0

Model Notes

This a model from the article:
Fermentation pathway kinetics and metabolic flux control in suspended and immobilized Saccharomyces cerevisiae

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Jorge L. Galazzo and James E. Bailey Enzyme and Microbial TechnologyVolume 12, Issue 3, 1990, Pages 162-172.
DOI:10.1016/0141-0229(90)90033-M
Abstract:
Measurements of rates of glucose uptake and of glycerol and ethanol formation combined with knowledge of the metabolic pathways involved in S. cerevisiae were employed to obtain in vivo rates of reaction catalysed by pathway enzymes for suspended and alginate-entrapped cells at pH 4.5 and 5.5. Intracellular concentrations of substrates and effectors for most key pathway enzymes were estimated from in vivo phosphorus-31 nuclear magnetic resonance measurements. These data show the validity in vivo of kinetic models previously proposed for phosphofructokinase and pyruvate kinase based on in vitro studies. Kinetic representations of hexokinase, glycogen synthetase, and glyceraldehyde 3-phosphate dehydrogenase, which incorporate major regulatory properties of these enzymes, are all consistent with the in vivo data. This detailed model of pathway kinetics and these data on intracellular metabolite concentrations allow evaluation of flux-control coefficients for all key enzymes involved in glucose catabolism under the four different cell environments examined. This analysis indicates that alginate entrapment increases the glucose uptake rate and shifts the step most influencing ethanol production from glucose uptake to phosphofructokinase. The rate of ATP utilization in these nongrowing cells strongly limits ethanol production at pH 5.5 but is relatively insignificant at pH 4.5.

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Biomodels Curation: The model reproduces Fig 2 of the paper. However, it appears that the figures are swapped, hence the plot for V/Vmax vs Glucose actually represnts V/Vmax vs ATP and the vice versa is true for the other figure. The rate of hexokinase reaction that is obtained upon simulation of the model is 17.24 mM/min, therefore V/Vmax has a value of 17.24/68.5=0.25. For steady state values of Glucose and ATP (0.038 and 1.213 mM respectively), the V/Vmax values correctly correspond to 0.25, if we were to assume that the figures are swapped.

BioModels Curation updated on 25th November 2010: Figure 3 of the reference publication has been reproduced and added as a curation figure for the model.

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 eight 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`

Name milliMolar

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

2.4 Unit `mM_per_minute`

Name mM per minute

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

2.5 Unit `min_inv`

Name minute_inverse

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

2.6 Unit `volume`

Notes Litre is the predefined SBML unit for `volume`.

Definition l

2.7 Unit area

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

Definition m^2

2.8 Unit length

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

Definition m

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
extracellular	Extracellular		3	1	litre	☑	
cytoplasm	Cytoplasm		3	1	litre	☑	extracellular

3.1 Compartment extracellular

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

Name Extracellular

3.2 Compartment cytoplasm

This is a three dimensional compartment with a constant size of one litre, which is surrounded by extracellular (Extracellular).

Name Cytoplasm

4 Species

This model contains nine species. The boundary condition of four of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 8 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`	Glucose inside the cell	`cytoplasm`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
`ATP`	ATP	`cytoplasm`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
`G6P`	Glucose 6-phosphate	`cytoplasm`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
`FDP`	Fructose 1,6-phosphate	`cytoplasm`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
`PEP`	Phosphoenol pyruvate	`cytoplasm`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
`Gly`	Glycerol	`cytoplasm`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☑
`EtOH`	Ethanol	`cytoplasm`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☑
`Carbo`	Glycogen and Trehalose	`cytoplasm`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☑
`Glco`	Glucose outside the cell	`extracellular`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☑

5 Parameters

This model contains six global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VappGly	VappGly		0.00	$\text{mmol} \cdot \text{l}^{-1} \cdot (60\ \text{s})^{-1}$	⊟
VratioVmax	VratioVmax_ATP		0.00	dimensionless	⊟
parameter_4	Trehalose and Glycogen formation_Vm3		14.31	$\text{mmol} \cdot \text{l}^{-1} \cdot (60\ \text{s})^{-1}$	☑
parameter_5	Trehalose and Glycogen formation_n3		8.25	dimensionless	☑
parameter_6	Trehalose and Glycogen formation_K3Gly		2.00	$\text{mmol} \cdot \text{l}^{-1}$	☑
parameter_7	Hexokinase_Vm2		68.50	$\text{mmol} \cdot \text{l}^{-1} \cdot (60\ \text{s})^{-1}$	☑

6 Rules

This is an overview of two rules.

6.1 Rule VappGly

Rule VappGly is an assignment rule for parameter VappGly:

$$\text{VappGly} = \frac{\text{parameter\_4} \cdot [\text{G6P}]^{\text{parameter\_5}}}{\text{parameter\_6}^{\text{parameter\_5}} + [\text{G6P}]^{\text{parameter\_5}}} \tag{1}$$

6.2 Rule VratioVmax

Rule VratioVmax is an assignment rule for parameter VratioVmax:

$$\text{VratioVmax} = \frac{\text{Vhk}}{\text{vol}\,(\text{cytoplasm}) \cdot \text{parameter\_7}} \tag{2}$$

Derived unit dimensionless

7 Reactions

This model contains eight 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

№	Id	Name	Reaction Equation	SBO
1	`Vin`	Glucose in	$\text{Glco} \overset{\text{G6P}}{\rightleftharpoons} \text{Glci}$	
2	`Vhk`	Hexokinase	$\text{ATP} + \text{Glci} \rightleftharpoons \text{G6P}$	
3	`Vpol`	Trehalose and Glycogen formation	$\text{ATP} + \text{G6P} \rightleftharpoons \text{Carbo}$	
4	`Vpfk`	Phosphofructokinase	$\text{ATP} + \text{G6P} \rightleftharpoons \text{FDP}$	
5	`Vgapd`	GAPD	$\text{FDP} \rightleftharpoons 2\,\text{ATP} + 2\,\text{PEP}$	
6	`Vpk`	Pyruvate kinase	$\text{PEP} \overset{\text{FDP}}{\rightleftharpoons} \text{ATP} + \text{EtOH}$	
7	`Vgol`	Glycerol synthesis	$0 \cdot 5\,\text{FDP} \overset{\text{PEP, ATP}}{\rightleftharpoons} \text{Gly}$	
8	`Vatpase`	ATPase	$\text{ATP} \rightleftharpoons \emptyset$	

7.1 Reaction `Vin`

This is a reversible reaction of one reactant forming one product influenced by one modifier.

Name Glucose in

Reaction equation

$$\mathrm{Glco} \overset{\mathrm{G6P}}{\rightleftharpoons} \mathrm{Glci} \tag{3}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
`Glco`	Glucose outside the cell	

Modifier

Table 7: Properties of each modifier.

Id	Name	SBO
`G6P`	Glucose 6-phosphate	

Product

Table 8: Properties of each product.

Id	Name	SBO
`Glci`	Glucose inside the cell	

Kinetic Law

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

$$v_1 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot (\mathrm{Vm1} - \mathrm{Ki1G6P} \cdot [\mathrm{G6P}]) \tag{4}$$

Table 9: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm1			19.7	mmol · l^{-1} · $(60\ s)^{-1}$	☑
Ki1G6P			3.7	$(60\ s)^{-1}$	☑

7.2 Reaction Vhk

This is a reversible reaction of two reactants forming one product.

Name Hexokinase

Reaction equation

$$\mathrm{ATP} + \mathrm{Glci} \rightleftharpoons \mathrm{G6P} \tag{5}$$

Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
ATP	ATP	
Glci	Glucose inside the cell	

Product

Table 11: Properties of each product.

Id	Name	SBO
G6P	Glucose 6-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{Vm2}}{1 + \frac{\mathrm{Km2Glc}}{[\mathrm{Glci}]} + \frac{\mathrm{Km2ATP}}{[\mathrm{ATP}]} + \frac{\mathrm{Ks2Glc \cdot Km2ATP}}{[\mathrm{Glci}] \cdot [\mathrm{ATP}]}} \tag{6}$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm2			68.500	$\text{mmol} \cdot \text{l}^{-1} \cdot (60\ \text{s})^{-1}$	☑
Km2Glc			0.110	$\text{mmol} \cdot \text{l}^{-1}$	☑
Km2ATP			0.100	$\text{mmol} \cdot \text{l}^{-1}$	☑
Ks2Glc			0.006	$\text{mmol} \cdot \text{l}^{-1}$	☑

7.3 Reaction Vpol

This is a reversible reaction of two reactants forming one product.

Name Trehalose and Glycogen formation

Reaction equation

$$\text{ATP} + \text{G6P} \rightleftharpoons \text{Carbo} \tag{7}$$

Reactants

Table 13: Properties of each reactant.

Id	Name	SBO
ATP	ATP	
G6P	Glucose 6-phosphate	

Product

Table 14: Properties of each product.

Id	Name	SBO
Carbo	Glycogen and Trehalose	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \frac{\frac{\text{vol(cytoplasm)} \cdot 1.1 \cdot \text{Vm3} \cdot [\text{G6P}]^{n3}}{\text{K3Gly}^{n3} + [\text{G6P}]^{n3}}}{1 + \frac{\text{Km30}}{0.7} \cdot \left(1 + \frac{\text{Km3G6P}}{[\text{G6P}]}\right)} \tag{8}$$

Table 15: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm3			14.31	mmol · l^{-1} · $(60\ s)^{-1}$	☑
n3			8.25	dimensionless	☑
K3Gly			2.00	mmol · l^{-1}	☑
Km3O			1.00	mmol · l^{-1}	☑
Km3G6P			1.10	mmol · l^{-1}	☑

7.4 Reaction Vpfk

This is a reversible reaction of two reactants forming one product.

Name Phosphofructokinase

Reaction equation

$$\mathrm{ATP} + \mathrm{G6P} \rightleftharpoons \mathrm{FDP} \tag{9}$$

Reactants

Table 16: Properties of each reactant.

Id	Name	SBO
ATP	ATP	
G6P	Glucose 6-phosphate	

Product

Table 17: Properties of each product.

Id	Name	SBO
FDP	Fructose 1,6-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \frac{\frac{\text{vol(cytoplasm)}\cdot \text{Vm4}\cdot \text{g4R}\cdot 0.3\cdot [\text{G6P}]}{\text{K4F6P}}\cdot [\text{ATP}]\cdot\left(1+\frac{0.3\cdot[\text{G6P}]}{\text{K4F6P}}+\frac{[\text{ATP}]}{\text{K4ATP}}+\frac{\frac{\text{g4R}\cdot 0.3\cdot[\text{G6P}]}{\text{K4F6P}}\cdot[\text{ATP}]}{\text{K4ATP}}\right)}{\left(1+\frac{0.3\cdot[\text{G6P}]}{\text{K4F6P}}+\frac{[\text{ATP}]}{\text{K4ATP}}+\frac{\frac{\text{g4R}\cdot 0.3\cdot[\text{G6P}]}{\text{K4F6P}}\cdot[\text{ATP}]}{\text{K4ATP}}\right)^2+\text{L40}\cdot\left(\frac{1+\frac{\text{c4AMP}\cdot\left(3-[\text{ATP}]-0.5\cdot\left([\text{ATP}]+\left(12\cdot[\text{ATP}]-3\cdot[\text{ATP}]^2\right)^{0.5}\right)\right)}{\text{K4AMP}}}{1+\frac{3-[\text{ATP}]-0.5\cdot\left([\text{ATP}]+\left(12\cdot[\text{ATP}]-3\cdot[\text{ATP}]^2\right)^{0.5}\right)}{\text{K4AMP}}}\right)^2\cdot\left(1+\frac{\text{c4F6P}\cdot 0.3\cdot[\text{G}}{\text{K4F6P}}\right.} \tag{10}$$

Table 18: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm4			31.700	$\text{mmol}\cdot\text{l}^{-1}\cdot(60\ \text{s})^{-1}$	☑
g4R			10.000	dimensionless	☑
K4F6P			1.000	$\text{mmol}\cdot\text{l}^{-1}$	☑
K4ATP			0.060	$\text{mmol}\cdot\text{l}^{-1}$	☑
L40			3342.000	dimensionless	☑
c4AMP			0.019	dimensionless	☑
K4AMP			0.025	$\text{mmol}\cdot\text{l}^{-1}$	☑
c4F6P			$5\cdot10^{-4}$	dimensionless	☑
c4ATP			1.000	dimensionless	☑
gT			1.000	dimensionless	☑

7.5 Reaction Vgapd

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

Name GAPD

Reaction equation

$$\text{FDP} \rightleftharpoons 2\,\text{ATP} + 2\,\text{PEP} \tag{11}$$

Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
FDP	Fructose 1,6-phosphate	

Products

Table 20: Properties of each product.

Id	Name	SBO
ATP	ATP	
PEP	Phosphoenol pyruvate	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \frac{\text{vol}\,(\text{cytoplasm}) \cdot \text{Vm5}}{1 + \frac{\text{K5G3P}}{0.01 \cdot [\text{FDP}]} + \left(\frac{\text{K5NAD}}{\text{NAD}} + \frac{\text{K5G3P} \cdot \text{K5NAD}}{\text{NAD} \cdot 0.01 \cdot [\text{FDP}]} + \frac{\text{K5G3P} \cdot \text{K5NAD} \cdot \text{NADH}}{\text{NAD} \cdot 0.01 \cdot [\text{FDP}] \cdot \text{K5NADH}}\right) \cdot \left(1 + \frac{0.5 \cdot \left([\text{ATP}] + (12 \cdot [\text{ATP}] - 3 \cdot [\text{ATP}]^2)^{0.5}\right)}{\text{K5ADP}} + \frac{3 - [\text{ATP}]}{}\right.} \quad (12)$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm5			49.900	$\text{mmol} \cdot 1^{-1} \cdot (60\ \text{s})^{-1}$	☑
K5G3P			0.003	$\text{mmol} \cdot 1^{-1}$	☑
K5NAD			0.180	dimensionless	☑
NAD			1.919	$\text{mmol} \cdot 1^{-1}$	☑
NADH			0.081	$\text{mmol} \cdot 1^{-1}$	☑
K5NADH			$3 \cdot 10^{-4}$	$\text{mmol} \cdot 1^{-1}$	☑
K5ADP			1.500	$\text{mmol} \cdot 1^{-1}$	☑
K5AMP			1.100	$\text{mmol} \cdot 1^{-1}$	☑
K5ATP			2.500	$\text{mmol} \cdot 1^{-1}$	☑

7.6 Reaction Vpk

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

Name Pyruvate kinase

Reaction equation

$$\text{PEP} \overset{\text{FDP}}{\rightleftharpoons} \text{ATP} + \text{EtOH} \quad (13)$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
PEP	Phosphoenol pyruvate	

Modifier

Table 23: Properties of each modifier.

Id	Name	SBO
FDP	Fructose 1,6-phosphate	

Products

Table 24: Properties of each product.

Id	Name	SBO
ATP	ATP	
EtOH	Ethanol	

Kinetic Law

Derived unit contains undeclared units

$$v_6 \tag{14}$$

$$= \frac{\mathrm{vol}\left(\mathrm{cytoplasm}\right) \cdot \mathrm{Vm6} \cdot \frac{\frac{[\mathrm{PEP}]}{\mathrm{K6PEP}} \cdot 0.5 \cdot \left([\mathrm{ATP}] + \left(12 \cdot [\mathrm{ATP}] - 3 \cdot [\mathrm{ATP}]^2\right)^{0.5}\right)}{\mathrm{K6ADP}} \cdot \left(\mathrm{g6R} \cdot \left(1 + \frac{[\mathrm{PEP}]}{\mathrm{K6PEP}} + \frac{0.5 \cdot \left([\mathrm{ATP}] + \left(12 \cdot [\mathrm{ATP}] - 3 \cdot [\mathrm{ATP}]^2\right)^{0.5}\right)}{\mathrm{K6ADP}} \right. \right.}{\left(1 + \frac{9.55 \cdot 10^{-9}}{\mathrm{h6}}\right) \cdot \left(\left(1 + \frac{[\mathrm{PEP}]}{\mathrm{K6PEP}} + \frac{0.5 \cdot \left([\mathrm{ATP}] + (12 \cdot [\mathrm{ATP}] - 3 \cdot [\mathrm{ATP}]^2)^{0.5}\right)}{\mathrm{K6ADP}} + \right.\right.}$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm6			3440.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
K6PEP			0.008	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K6ADP			5.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
g6R			0.100	dimensionless	☑
q6			1.000	dimensionless	☑
L60			164.084	dimensionless	☑
c6FDP			0.010	dimensionless	☑
K6FDP			0.200	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
g6T			1.000	dimensionless	☑
c6PEP			$1.58793 \cdot 10^{-4}$	dimensionless	☑
c6ADP			1.000	dimensionless	☑
h6			$1.14815 \cdot 10^{-7}$	dimensionless	☑

7.7 Reaction Vgol

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name Glycerol synthesis

Reaction equation

$$0{\cdot}5\,\mathrm{FDP} \overset{\mathrm{PEP,\ ATP}}{\rightleftharpoons} \mathrm{Gly} \tag{15}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
FDP	Fructose 1,6-phosphate	

Modifiers

Table 27: Properties of each modifier.

Id	Name	SBO
PEP	Phosphoenol pyruvate	
ATP	ATP	

Product

Table 28: Properties of each product.

Id	Name	SBO
Gly	Glycerol	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \frac{\mathrm{Vm7} \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\frac{[\mathrm{PEP}]}{\mathrm{K6PEP}} \cdot 0.5 \cdot \left([\mathrm{ATP}] + \left(12 \cdot [\mathrm{ATP}] - 3 \cdot [\mathrm{ATP}]^2\right)^{0.5}\right)}{\mathrm{K6ADP}} \cdot \left(\mathrm{g6R} \cdot \left(1 + \frac{[\mathrm{PEP}]}{\mathrm{K6PEP}} + \frac{0.5 \cdot \left([\mathrm{ATP}] + \left(12 \cdot [\mathrm{ATP}] - 3 \cdot [\mathrm{ATP}]^2\right)^{0.5}\right)}{\mathrm{K6ADP}}\right.\right.}{\left(1 + \frac{9.55 \cdot 10^{-9}}{\mathrm{h6}}\right) \cdot \left(\left(1 + \frac{[\mathrm{PEP}]}{\mathrm{K6PEP}} + \frac{0.5 \cdot \left([\mathrm{ATP}] + (12 \cdot [\mathrm{ATP}] - 3 \cdot [\mathrm{ATP}]^2)^{0.5}\right)}{\mathrm{K6ADP}} + \right.\right.} \tag{16}$$

Table 29: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm7			203.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
K6PEP			0.008	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K6ADP			5.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
g6R			0.100	dimensionless	☑
q6			1.000	dimensionless	☑
L60			164.084	dimensionless	☑
c6FDP			0.010	dimensionless	☑
K6FDP			0.200	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
g6T			1.000	dimensionless	☑
c6PEP			$1.58793 \cdot 10^{-4}$	dimensionless	☑
c6ADP			1.000	dimensionless	☑
h6			$1.14815 \cdot 10^{-7}$	dimensionless	☑

7.8 Reaction Vatpase

This is a reversible reaction of one reactant forming no product.

Name ATPase

Reaction equation

$$\mathrm{ATP} \rightleftharpoons \emptyset \tag{17}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
ATP	ATP	

Kinetic Law

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

$$v_8 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{Vm8} \cdot [\mathrm{ATP}] \tag{18}$$

Table 31: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm8			25.1	$(60\ \mathrm{s})^{-1}$	☑

8 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.

Identifiers for kinetic laws highlighted in gray cannot be verified to evaluate to units of SBML `substance` per `time`. As a result, some SBML interpreters may not be able to verify the consistency of the units on quantities in the model. Please check if

- parameters without an unit definition are involved or
- volume correction is necessary because the `hasOnlySubstanceUnits` flag may be set to `false` and `spacialDimensions`> 0 for certain species.

8.1 Species Glci

Name Glucose inside the cell

Initial concentration $0.0345\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in Vhk and as a product in Vin).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glci} = v_1 - v_2 \tag{19}$$

8.2 Species ATP

Name ATP

Initial concentration $1.19\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in seven reactions (as a reactant in Vhk, Vpol, Vpfk, Vatpase and as a product in Vgapd, Vpk and as a modifier in Vgol).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ATP} = 2\,v_5 + v_6 - v_2 - v_3 - v_4 - v_8 \tag{20}$$

8.3 Species G6P

Name Glucose 6-phosphate

Initial concentration $1.011\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in Vpol, Vpfk and as a product in Vhk and as a modifier in Vin).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G6P} = v_2 - v_3 - v_4 \tag{21}$$

8.4 Species FDP

Name Fructose 1,6-phosphate

Initial concentration $9.144\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in Vgapd, Vgol and as a product in Vpfk and as a modifier in Vpk).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{FDP} = v_4 - v_5 - 0.5\,v_7 \tag{22}$$

8.5 Species PEP

Name Phosphoenol pyruvate

Initial concentration $0.0095\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in Vpk and as a product in Vgapd and as a modifier in Vgol).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PEP} = 2\,v_5 - v_6 \tag{23}$$

8.6 Species Gly

Name Glycerol

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gly} = 0 \tag{24}$$

8.7 Species EtOH

Name Ethanol

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{EtOH} = 0 \tag{25}$$

8.8 Species Carbo

Name Glycogen and Trehalose

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Carbo} = 0 \tag{26}$$

8.9 Species Glco

Name Glucose outside the cell

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glco} = 0 \tag{27}$$

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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