SBML Model Report

Model name: “Messiha2013 - Pentose phosphate pathway model”

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: Vijayalakshmi Chelliah[1], Kieran Smallbone[2] and Kent Ed[3] at November nineth 2011 at noon. and last time modified at February 28th 2014 at 4:07 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	21
events	0	constraints	0
reactions	11	function definitions	0
global parameters	7	unit definitions	3
rules	2	initial assignments	0

Model Notes

Messiha2013 - Pentose phosphate pathway model

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This model describes the dynamic behaviour of the pentose phosphate pathway with the inclusion of various enzymes involved in the pathway. The model's predictions are compared with experimental observations of transient metabolite concentrations following a glucose pulse.

This model is described in the article:Enzyme characterisation and kinetic modelling of pentose phosphate pathway in yeast.Hanan L. Messiha, Edward Kent, Naglis Malys, Kathleen M. Carroll, Pedro Mendes, Kieran SmallbonePeerJ PrePrints 1:e146v2

Abstract:

We present the quantification and kinetic characterisation of the enzymes of the pentose phosphate pathway in Saccharomyces cerevisiae. The data are combined into a mathematical model that describes the dynamics of this system and allows for the predicting changes in metabolite concentrations and fluxes in response to perturbations. We use the model to study the response of yeast to a glucose pulse. We then combine the model with an existing glycolysis one to study the effect of oxidative stress on carbohydrate metabolism. The combination of these two models was made possible by the standardized enzyme kinetic experiments carried out in both studies. This work demonstrates the feasibility of constructing larger network models by merging smaller pathway models.

This model is hosted on BioModels Database and identifiedby: BIOMD0000000502 .

To cite BioModels Database, please use: BioModels Database: An enhanced, curated and annotated resourcefor published quantitative kinetic models .

2 Unit Definitions

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

2.1 Unit `substance`

Name mmol

Definition mmol

2.2 Unit `mM`

Name mM

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

2.3 Unit `per_s`

Name per s

Definition s^{-1}

2.4 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

2.5 Unit area

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

Definition m^2

2.6 Unit length

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

Definition m

2.7 Unit time

Notes Second is the predefined SBML unit for time.

Definition s

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
cell	cell	0000290	3	1	litre	☑	

3.1 Compartment cell

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

Name cell

SBO:0000290 physical compartment

4 Species

This model contains 21 species. The boundary condition of 13 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
E4P	E4P	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
G6L	G6L	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
NADPH	NADPH	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
P6G	P6G	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
R5P	R5P	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
Ru5P	Ru5P	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
S7P	S7P	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
X5P	X5P	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
NADP	NADP	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☑
G6P	G6P	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☑
F6P	F6P	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
GAP	GAP	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
GND1	GND1	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
GND2	GND2	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
NQM1	NQM1	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
RKI1	RKI1	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
RPE1	RPE1	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
SOL3	SOL3	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
TAL1	TAL1	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
TKL1	TKL1	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
ZWF1	ZWF1	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition

5 Parameters

This model contains seven global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sum_NADP			0.330	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
Kx5p_TAL			0.670	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
Ke4p_TAL			0.946	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
Kr5p_TAL			0.235	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
Kgap_TAL			0.100	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
Kf6p_TAL			1.100	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
Ks7p_TAL			0.150	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

6 Rules

This is an overview of two rules.

6.1 Rule G6P

Rule G6P is an assignment rule for species G6P:

$$\mathrm{G6P} = 0.9 + \begin{cases} \dfrac{44.1 \cdot \mathrm{t}}{48 + \mathrm{t} + 0.45 \cdot \mathrm{t}^2} & \text{if } \mathrm{t} \geq 0 \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

6.2 Rule NADP

Rule NADP is an assignment rule for species NADP:

$$\mathrm{NADP} = \mathrm{sum\_NADP} - [\mathrm{NADPH}] \tag{2}$$

Derived unit $\mathrm{mmol} \cdot \mathrm{l}^{-1}$

7 Reactions

This model contains eleven 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	GND	GND	$\mathrm{P6G} + \mathrm{NADP} \xrightarrow{\text{GND1, GND2, GND1, P6G, NADP, Ru5P, NADPH, GND2}} \mathrm{Ru5P} + \mathrm{NADPH}$	0000176
2	RKI	RKI	$\mathrm{Ru5P} \xrightleftharpoons{\text{RKI1, RKI1, Ru5P, R5P}} \mathrm{R5P}$	0000176
3	RPE	RPE	$\mathrm{Ru5P} \xrightleftharpoons{\text{RPE1, RPE1, Ru5P, X5P}} \mathrm{X5P}$	0000176
4	SOL	SOL	$\mathrm{G6L} \xrightarrow{\text{SOL3, SOL3, G6L, P6G}} \mathrm{P6G}$	0000176
5	TAL	TAL	$\mathrm{GAP} + \mathrm{S7P} \xrightleftharpoons{\text{TAL1, NQM1, TAL1, GAP, S7P, F6P, E4P, NQM1}} \mathrm{F6P} + \mathrm{E4P}$	0000176
6	TKL_E4P	TKL (E4P:F6P)	$\mathrm{X5P} + \mathrm{E4P} \xrightleftharpoons{\text{TKL1, R5P, S7P, TKL1, X5P, E4P, GAP, F6P, R5P, S7P}} \mathrm{GAP} + \mathrm{F6P}$	0000176
7	TKL_R5P	TKL (R5P:S7P)	$\mathrm{X5P} + \mathrm{R5P} \xrightleftharpoons{\text{TKL1, E4P, F6P, TKL1, X5P, R5P, GAP, S7P, E4P, F6P}} \mathrm{GAP} + \mathrm{S7P}$	0000176
8	ZWF	ZWF	$\mathrm{G6P} + \mathrm{NADP} \xrightarrow{\text{ZWF1, ZWF1, G6P, NADP, G6L, NADPH}} \mathrm{G6L} + \mathrm{NADPH}$	0000176
9	NADPH_oxidase	NADPH oxidase	$\mathrm{NADPH} \xrightarrow{\text{NADPH}} \mathrm{NADP}$	0000176
10	E4P_sink	E4P sink	$\mathrm{E4P} \xrightarrow{\text{E4P}} \emptyset$	0000176
11	R5P_sink	R5P sink	$\mathrm{R5P} \xrightarrow{\text{R5P}} \emptyset$	0000176

7.1 Reaction GND

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

Name GND

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{P6G} + \mathrm{NADP} \xrightarrow{\text{GND1, GND2, GND1, P6G, NADP, Ru5P, NADPH, GND2}} \mathrm{Ru5P} + \mathrm{NADPH} \tag{3}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
P6G	P6G	
NADP	NADP	

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
GND1	GND1	
GND2	GND2	
GND1	GND1	
P6G	P6G	
NADP	NADP	
Ru5P	Ru5P	
NADPH	NADPH	
GND2	GND2	

Products

Table 8: Properties of each product.

Id	Name	SBO
Ru5P	Ru5P	

Id	Name	SBO
NADPH	NADPH	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{cell}) \cdot \left(\frac{\frac{[\mathrm{GND1}] \cdot \mathrm{kcat\_GND1} \cdot [\mathrm{P6G}] \cdot [\mathrm{NADP}]}{\mathrm{Kp6g\_GND1} \cdot \mathrm{Knadp\_GND1}}}{\left(1 + \frac{[\mathrm{P6G}]}{\mathrm{Kp6g\_GND1}} + \frac{[\mathrm{Ru5P}]}{\mathrm{Kru5p\_GND1}}\right) \cdot \left(1 + \frac{[\mathrm{NADP}]}{\mathrm{Knadp\_GND1}} + \frac{[\mathrm{NADPH}]}{\mathrm{Knadph\_GND1}}\right)} + \frac{[\mathrm{GND2}] \cdot \mathrm{kcat\_GND2} \cdot [\mathrm{P6G}] \cdot [\mathrm{NADP}]}{\left(1 + \frac{[\mathrm{P6G}]}{\mathrm{Kp6g\_GND2}} + \frac{[\mathrm{Ru5P}]}{\mathrm{Kru5p\_GND2}}\right) \cdot \left(1 + \frac{[\mathrm{NADP}]}{\mathrm{Knadp\_GND2}} + \frac{[\mathrm{NADPH}]}{\mathrm{Knadph\_GND2}}\right)} \right) \tag{4}$$

Table 9: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kcat_GND1			28.000	s^{-1}	☑
Kp6g_GND1			0.062	$mmol \cdot l^{-1}$	☑
Knadp_GND1			0.094	$mmol \cdot l^{-1}$	☑
Kru5p_GND1			0.100	$mmol \cdot l^{-1}$	☑
Knadph_GND1			0.055	$mmol \cdot l^{-1}$	☑
kcat_GND2			27.300	s^{-1}	☑
Kp6g_GND2			0.115	$mmol \cdot l^{-1}$	☑
Knadp_GND2			0.094	$mmol \cdot l^{-1}$	☑
Kru5p_GND2			0.100	$mmol \cdot l^{-1}$	☑
Knadph_GND2			0.055	$mmol \cdot l^{-1}$	☑

7.2 Reaction RKI

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

Name RKI

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{Ru5P} \overset{\mathrm{RKI1,\ RKI1,\ Ru5P,\ R5P}}{\rightleftharpoons} \mathrm{R5P} \tag{5}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
Ru5P	Ru5P	

Modifiers

Table 11: Properties of each modifier.

Id	Name	SBO
RKI1	RKI1	
RKI1	RKI1	
Ru5P	Ru5P	
R5P	R5P	

Product

Table 12: Properties of each product.

Id	Name	SBO
R5P	R5P	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\frac{\mathrm{vol(cell)} \cdot [\mathrm{RKI1}] \cdot \mathrm{kcat} \cdot \left([\mathrm{Ru5P}] - \frac{[\mathrm{R5P}]}{\mathrm{Keq}} \right)}{\mathrm{Kru5p}}}{1 + \frac{[\mathrm{Ru5P}]}{\mathrm{Kru5p}} + \frac{[\mathrm{R5P}]}{\mathrm{Kr5p}}} \tag{6}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kcat			335.00	s^{-1}	☑
Kru5p			2.47	$mmol \cdot l^{-1}$	☑
Kr5p			5.70	$mmol \cdot l^{-1}$	☑
Kiru5p			9.88	$mmol \cdot l^{-1}$	☑
Keq			4.00	dimensionless	☑

7.3 Reaction RPE

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

Name RPE

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{Ru5P} \xrightleftharpoons{\text{RPE1, RPE1, Ru5P, X5P}} \mathrm{X5P} \tag{7}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
Ru5P	Ru5P	

Modifiers

Table 15: Properties of each modifier.

Id	Name	SBO
RPE1	RPE1	
RPE1	RPE1	
Ru5P	Ru5P	
X5P	X5P	

Product

Table 16: Properties of each product.

Id	Name	SBO
X5P	X5P	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \frac{\frac{\mathrm{vol(cell)} \cdot [\mathrm{RPE1}] \cdot \mathrm{kcat} \cdot \left([\mathrm{Ru5P}] - \frac{[\mathrm{X5P}]}{\mathrm{Keq}} \right)}{\mathrm{Kru5p}}}{1 + \frac{[\mathrm{Ru5P}]}{\mathrm{Kru5p}} + \frac{[\mathrm{X5P}]}{\mathrm{Kx5p}}} \tag{8}$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kcat			4020.00	s^{-1}	☑
Kru5p			5.97	$mmol \cdot l^{-1}$	☑
Kx5p			7.70	$mmol \cdot l^{-1}$	☑
Keq			1.40	dimensionless	☑

7.4 Reaction SOL

This is an irreversible reaction of one reactant forming one product influenced by four modifiers.

Name SOL

SBO:0000176 biochemical reaction

Reaction equation

$$\text{G6L} \xrightarrow{\text{SOL3, SOL3, G6L, P6G}} \text{P6G} \tag{9}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
G6L	G6L	

Modifiers

Table 19: Properties of each modifier.

Id	Name	SBO
SOL3	SOL3	
SOL3	SOL3	
G6L	G6L	
P6G	P6G	

Product

Table 20: Properties of each product.

Id	Name	SBO
P6G	P6G	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \frac{\frac{\text{vol(cell)} \cdot [\text{SOL3}] \cdot \text{kcat} \cdot [\text{G6L}]}{\text{Kg6l}}}{1 + \frac{[\text{G6L}]}{\text{Kg6l}} + \frac{[\text{P6G}]}{\text{Kp6g}}} \tag{10}$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kcat			4.3	s^{-1}	☑
Kg6l			0.8	$mmol \cdot l^{-1}$	☑
Kp6g			0.5	$mmol \cdot l^{-1}$	☑

7.5 Reaction TAL

This is a reversible reaction of two reactants forming two products influenced by eight modifiers.

Name TAL

SBO:0000176 biochemical reaction

Reaction equation

$$\text{GAP} + \text{S7P} \xrightleftharpoons{\text{TAL1, NQM1, TAL1, GAP, S7P, F6P, E4P, NQM1}} \text{F6P} + \text{E4P} \tag{11}$$

Reactants

Table 22: Properties of each reactant.

Id	Name	SBO
GAP	GAP	
S7P	S7P	

Modifiers

Table 23: Properties of each modifier.

Id	Name	SBO
TAL1	TAL1	
NQM1	NQM1	
TAL1	TAL1	
GAP	GAP	
S7P	S7P	
F6P	F6P	
E4P	E4P	
NQM1	NQM1	

Products

Table 24: Properties of each product.

Id	Name	SBO
F6P	F6P	
E4P	E4P	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{cell}) \cdot \left(\frac{\frac{[\mathrm{TAL1}] \cdot \mathrm{kcat\_TAL1} \cdot \left([\mathrm{GAP}] \cdot [\mathrm{S7P}] - \frac{[\mathrm{F6P}] \cdot [\mathrm{E4P}]}{\mathrm{Keq}} \right)}{\mathrm{Kgap\_TAL1} \cdot \mathrm{Ks7p\_TAL1}}}{\left(1 + \frac{[\mathrm{GAP}]}{\mathrm{Kgap\_TAL1}} + \frac{[\mathrm{F6P}]}{\mathrm{Kf6p\_TAL1}} \right) \cdot \left(1 + \frac{[\mathrm{S7P}]}{\mathrm{Ks7p\_TAL1}} + \frac{[\mathrm{E4P}]}{\mathrm{Ke4p\_TAL1}} \right)} + \frac{\frac{[\mathrm{NQM1}] \cdot \mathrm{kcat\_NQM1} \cdot \left([\mathrm{GAP}] \cdot [\mathrm{S7P}] - \frac{[\mathrm{F6P}] \cdot [\mathrm{E4P}]}{\mathrm{Keq}} \right)}{\mathrm{Kgap\_NQM1} \cdot \mathrm{Ks7p\_NQM1}}}{\left(1 + \frac{[\mathrm{GAP}]}{\mathrm{Kgap\_NQM1}} + \frac{[\mathrm{F6P}]}{\mathrm{Kf6p\_NQM1}} \right) \cdot \left(1 + \frac{[\mathrm{S7P}]}{\mathrm{Ks7p\_NQM1}} + \frac{[\mathrm{E4P}]}{\mathrm{Ke4p\_NQM1}} \right)} \right) \tag{12}$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kcat_TAL1			0.694	s^{-1}	☑
Kgap_TAL1			0.272	$mmol \cdot l^{-1}$	☑
Ks7p_TAL1			0.786	$mmol \cdot l^{-1}$	☑
Kf6p_TAL1			1.440	$mmol \cdot l^{-1}$	☑
Ke4p_TAL1			0.362	$mmol \cdot l^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
kcat_NQM1			0.694	s^{-1}	☑
Kgap_NQM1			0.272	$mmol \cdot l^{-1}$	☑
Ks7p_NQM1			0.786	$mmol \cdot l^{-1}$	☑
Kf6p_NQM1			1.040	$mmol \cdot l^{-1}$	☑
Ke4p_NQM1			0.305	$mmol \cdot l^{-1}$	☑
Keq			1.050	dimensionless	☑

7.6 Reaction TKL_E4P

This is a reversible reaction of two reactants forming two products influenced by ten modifiers.

Name TKL (E4P:F6P)

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{X5P} + \mathrm{E4P} \xrightleftharpoons{\text{TKL1, R5P, S7P, TKL1, X5P, E4P, GAP, F6P, R5P, S7P}} \mathrm{GAP} + \mathrm{F6P} \qquad (13)$$

Reactants

Table 26: Properties of each reactant.

Id	Name	SBO
X5P	X5P	
E4P	E4P	

Modifiers

Table 27: Properties of each modifier.

Id	Name	SBO
TKL1	TKL1	
R5P	R5P	
S7P	S7P	
TKL1	TKL1	
X5P	X5P	
E4P	E4P	
GAP	GAP	
F6P	F6P	
R5P	R5P	

Id	Name	SBO
S7P	S7P	

Products

Table 28: Properties of each product.

Id	Name	SBO
GAP	GAP	
F6P	F6P	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \frac{\frac{\text{vol(cell)} \cdot [\text{TKL1}] \cdot \text{kcat} \cdot \left([\text{X5P}] \cdot [\text{E4P}] - \frac{[\text{GAP}] \cdot [\text{F6P}]}{\text{Keq}} \right)}{\text{Kx5p\_TAL} \cdot \text{Ke4p\_TAL}}}{\left(1 + \frac{[\text{X5P}]}{\text{Kx5p\_TAL}} + \frac{[\text{GAP}]}{\text{Kgap\_TAL}} \right) \cdot \left(1 + \frac{[\text{E4P}]}{\text{Ke4p\_TAL}} + \frac{[\text{F6P}]}{\text{Kf6p\_TAL}} + \frac{[\text{R5P}]}{\text{Kr5p\_TAL}} + \frac{[\text{S7P}]}{\text{Ks7p\_TAL}} \right)} \quad (14)$$

Table 29: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kcat			47.1	s^{-1}	☑
Keq			10.0	dimensionless	☑

7.7 Reaction TKL_R5P

This is a reversible reaction of two reactants forming two products influenced by ten modifiers.

Name TKL (R5P:S7P)

SBO:0000176 biochemical reaction

Reaction equation

$$\text{X5P} + \text{R5P} \xrightleftharpoons{\text{TKL1, E4P, F6P, TKL1, X5P, R5P, GAP, S7P, E4P, F6P}} \text{GAP} + \text{S7P} \quad (15)$$

Reactants

Table 30: Properties of each reactant.

Id	Name	SBO
X5P	X5P	
R5P	R5P	

Modifiers

Table 31: Properties of each modifier.

Id	Name	SBO
TKL1	TKL1	
E4P	E4P	
F6P	F6P	
TKL1	TKL1	
X5P	X5P	
R5P	R5P	
GAP	GAP	
S7P	S7P	
E4P	E4P	
F6P	F6P	

Products

Table 32: Properties of each product.

Id	Name	SBO
GAP	GAP	
S7P	S7P	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \frac{\frac{\mathrm{vol(cell)} \cdot [\mathrm{TKL1}] \cdot \mathrm{kcat} \cdot \left([\mathrm{X5P}] \cdot [\mathrm{R5P}] - \frac{[\mathrm{GAP}] \cdot [\mathrm{S7P}]}{\mathrm{Keq}} \right)}{\mathrm{Kx5p\_TAL} \cdot \mathrm{Kr5p\_TAL}}}{\left(1 + \frac{[\mathrm{X5P}]}{\mathrm{Kx5p\_TAL}} + \frac{[\mathrm{GAP}]}{\mathrm{Kgap\_TAL}}\right) \cdot \left(1 + \frac{[\mathrm{E4P}]}{\mathrm{Ke4p\_TAL}} + \frac{[\mathrm{F6P}]}{\mathrm{Kf6p\_TAL}} + \frac{[\mathrm{R5P}]}{\mathrm{Kr5p\_TAL}} + \frac{[\mathrm{S7P}]}{\mathrm{Ks7p\_TAL}}\right)} \quad (16)$$

Table 33: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kcat			40.5	s^{-1}	☑
Keq			1.2	dimensionless	☑

7.8 Reaction ZWF

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

Name ZWF

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{G6P} + \mathrm{NADP} \xrightarrow{\text{ZWF1, ZWF1, G6P, NADP, G6L, NADPH}} \mathrm{G6L} + \mathrm{NADPH} \tag{17}$$

Reactants

Table 34: Properties of each reactant.

Id	Name	SBO
G6P	G6P	
NADP	NADP	

Modifiers

Table 35: Properties of each modifier.

Id	Name	SBO
ZWF1	ZWF1	
ZWF1	ZWF1	
G6P	G6P	
NADP	NADP	
G6L	G6L	
NADPH	NADPH	

Products

Table 36: Properties of each product.

Id	Name	SBO
G6L	G6L	
NADPH	NADPH	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \frac{\frac{\text{vol(cell)} \cdot [\text{ZWF1}] \cdot \text{kcat} \cdot [\text{G6P}] \cdot [\text{NADP}]}{\text{Kg6p} \cdot \text{Knadp}}}{\left(1 + \frac{[\text{G6P}]}{\text{Kg6p}} + \frac{[\text{G6L}]}{\text{Kg6l}}\right) \cdot \left(1 + \frac{[\text{NADP}]}{\text{Knadp}} + \frac{[\text{NADPH}]}{\text{Knadph}}\right)} \tag{18}$$

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kcat			189.000	s^{-1}	☑
Kg6p			0.042	$mmol \cdot l^{-1}$	☑
Knadp			0.045	$mmol \cdot l^{-1}$	☑
Kg6l			0.010	$mmol \cdot l^{-1}$	☑
Knadph			0.017	$mmol \cdot l^{-1}$	☑

7.9 Reaction NADPH_oxidase

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

Name NADPH oxidase

SBO:0000176 biochemical reaction

Reaction equation

$$\text{NADPH} \xrightarrow{\text{NADPH}} \text{NADP} \tag{19}$$

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
NADPH	NADPH	

Modifier

Table 39: Properties of each modifier.

Id	Name	SBO
NADPH	NADPH	

Product

Table 40: Properties of each product.

Id	Name	SBO
NADP	NADP	

Kinetic Law

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

$$v_9 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k} \cdot [\mathrm{NADPH}] \tag{20}$$

Table 41: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k			1.0	s^{-1}	☑

7.10 Reaction E4P_sink

This is an irreversible reaction of one reactant forming no product influenced by one modifier.

Name E4P sink

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{E4P} \xrightarrow{\mathrm{E4P}} \emptyset \tag{21}$$

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
E4P	E4P	

Modifier

Table 43: Properties of each modifier.

Id	Name	SBO
E4P	E4P	

Kinetic Law

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

$$v_{10} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k} \cdot [\mathrm{E4P}] \tag{22}$$

Table 44: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k			1.0	s^{-1}	☑

7.11 Reaction R5P_sink

This is an irreversible reaction of one reactant forming no product influenced by one modifier.

Name R5P sink

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{R5P} \xrightarrow{\mathrm{R5P}} \emptyset \tag{23}$$

Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
R5P	R5P	

Modifier

Table 46: Properties of each modifier.

Id	Name	SBO
R5P	R5P	

Kinetic Law

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

$$v_{11} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k} \cdot [\mathrm{R5P}] \tag{24}$$

Table 47: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k			1.0	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 E4P

Name E4P

SBO:0000247 simple chemical

Initial concentration $0.029\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in TKL_E4P, E4P_sink and as a product in TAL and as a modifier in TAL, TKL_E4P, TKL_R5P, TKL_R5P, E4P_sink).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E4P} = v_5 - v_6 - v_{10} \tag{25}$$

8.2 Species G6L

Name G6L

SBO:0000247 simple chemical

Initial concentration $0.1\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in SOL and as a product in ZWF and as a modifier in SOL, ZWF).

$$\frac{\text{d}}{\text{d}t}\text{G6L} = v_8 - v_4 \tag{26}$$

8.3 Species NADPH

Name NADPH

SBO:0000247 simple chemical

Initial concentration $0.16\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in NADPH_oxidase and as a product in GND, ZWF and as a modifier in GND, ZWF, NADPH_oxidase).

$$\frac{\text{d}}{\text{d}t}\text{NADPH} = v_1 + v_8 - v_9 \tag{27}$$

8.4 Species P6G

Name P6G

SBO:0000247 simple chemical

Initial concentration $0.25\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in GND and as a product in SOL and as a modifier in GND, SOL).

$$\frac{\text{d}}{\text{d}t}\text{P6G} = v_4 - v_1 \tag{28}$$

8.5 Species R5P

Name R5P

SBO:0000247 simple chemical

Initial concentration $0.118\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in eight reactions (as a reactant in TKL_R5P, R5P_sink and as a product in RKI and as a modifier in RKI, TKL_E4P, TKL_E4P, TKL_R5P, R5P_sink).

$$\frac{\text{d}}{\text{d}t}\text{R5P} = v_2 - v_7 - v_{11} \tag{29}$$

8.6 Species Ru5P

Name Ru5P

SBO:0000247 simple chemical

Initial concentration $0.033\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in RKI, RPE and as a product in GND and as a modifier in GND, RKI, RPE).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ru5P} = v_1 - v_2 - v_3 \tag{30}$$

8.7 Species S7P

Name S7P

SBO:0000247 simple chemical

Initial concentration $0.082\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in TAL and as a product in TKL_R5P and as a modifier in TAL, TKL_E4P, TKL_E4P, TKL_R5P).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S7P} = v_7 - v_5 \tag{31}$$

8.8 Species X5P

Name X5P

SBO:0000247 simple chemical

Initial concentration $0.041\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in TKL_E4P, TKL_R5P and as a product in RPE and as a modifier in RPE, TKL_E4P, TKL_R5P).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X5P} = v_3 - v_6 - v_7 \tag{32}$$

8.9 Species NADP

Name NADP

SBO:0000247 simple chemical

Initial concentration $0.17\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

Involved in rule NADP

This species takes part in five reactions (as a reactant in GND, ZWF and as a product in NADPH-_oxidase and as a modifier in GND, ZWF). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

8.10 Species G6P

Name G6P

SBO:0000247 simple chemical

Initial concentration $0.9\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

Involved in rule G6P

This species takes part in two reactions (as a reactant in ZWF and as a modifier in ZWF). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

8.11 Species F6P

Name F6P

SBO:0000247 simple chemical

Initial concentration $0.325\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a product in TAL, TKL_E4P and as a modifier in TAL, TKL_E4P, TKL_R5P, TKL_R5P), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{F6P} = 0 \tag{33}$$

8.12 Species GAP

Name GAP

SBO:0000247 simple chemical

Initial concentration $0.067\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in TAL and as a product in TKL_E4P, TKL_R5P and as a modifier in TAL, TKL_E4P, TKL_R5P), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GAP} = 0 \tag{34}$$

8.13 Species GND1

Name GND1

SBO:0000252 polypeptide chain

Initial concentration $0.013\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a modifier in GND, GND), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GND1} = 0 \tag{35}$$

8.14 Species GND2

Name GND2

SBO:0000252 polypeptide chain

Initial concentration $0.0030\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a modifier in GND, GND), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GND2} = 0 \tag{36}$$

8.15 Species NQM1

Name NQM1

SBO:0000252 polypeptide chain

Initial concentration $0.02\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a modifier in TAL, TAL), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NQM1} = 0 \tag{37}$$

8.16 Species RKI1

Name RKI1

SBO:0000252 polypeptide chain

Initial concentration $0.05\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a modifier in RKI, RKI), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{RKI1} = 0 \tag{38}$$

8.17 Species RPE1

Name RPE1

SBO:0000252 polypeptide chain

Initial concentration $0.03\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a modifier in RPE, RPE), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{RPE1} = 0 \tag{39}$$

8.18 Species SOL3

Name SOL3

SBO:0000252 polypeptide chain

Initial concentration $0.0296\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a modifier in SOL, SOL), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{SOL3} = 0 \tag{40}$$

8.19 Species TAL1

Name TAL1

SBO:0000252 polypeptide chain

Initial concentration $0.144\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a modifier in TAL, TAL), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{TAL1} = 0 \tag{41}$$

8.20 Species TKL1

Name TKL1

SBO:0000252 polypeptide chain

Initial concentration $0.455\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a modifier in TKL_E4P, TKL_E4P, TKL_R5P, TKL_R5P), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{TKL1} = 0 \tag{42}$$

8.21 Species ZWF1

Name ZWF1

SBO:0000252 polypeptide chain

Initial concentration $0.02\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a modifier in ZWF, ZWF), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ZWF1} = 0 \tag{43}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000176 biochemical reaction: An event involving one or more chemical entities that modifies the electrochemical structure of at least one of the participants.

SBO:0000247 simple chemical: Simple, non-repetitive chemical entity

SBO:0000252 polypeptide chain: Naturally occurring macromolecule formed by the repetition of amino-acid residues linked by peptidic bonds. A polypeptide chain is synthesized by the ribosome. CHEBI:1654

SBO:0000290 physical compartment: Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions

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