

Model name: “Glycolysis ICSB Tutorial”



September 3, 2008

1 General Overview

This is a model in SBML Level 2 Version 1 format.

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

Element	Quantity	Element	Quantity
compartments	1	events	0
species	28	constraints	0
reactions	10	function definitions	10
global parameters	0	unit definitions	2
rules	0	initial assignments	0

Model Notes

This model has been created with the help of the SABIO-RK Database(<http://sabio.villa-bosch.de/SABIORK>)

2 Unit Definitions

This is an overview of seven unit definitions of which five are defined implicitly by SBML and not mentioned in the model.

2.1 Unit mMdivmin

Name mMdivmin

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

2.2 Unit mM

Name mM

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

2.3 Unit substance

Notes Mole is the default SBML built-in unit for substance.

Definition mol

2.4 Unit volume

Notes Liter is the default SBML built-in unit for volume.

Definition l

2.5 Unit area

Notes Square meter is the default SBML built-in unit for area.

Definition m²

2.6 Unit length

Notes Meter is the default SBML built-in unit for length.

Definition m

2.7 Unit time

Notes Second is the default SBML built-in 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
compartment_1	Cell		3	1	l	✓	

4 Species

This model contains 28 species.

Table 3: Properties of each species.

id	name	compartment	derived unit	constant	boundary condition
spc_1	alpha-D-Glucose	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
spc_2	ATP	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
spc_3	alpha-D-Glucose 6-phosphate	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
spc_4	ADP	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
enz_1	Hexokinase(Enzyme)	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
spc_5	Phosphoenolpyruvate	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
spc_6	Pyruvate	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
enz_2	Pyruvate kinase(Enzyme)	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
spc_7	2-Phospho-D-glycerate	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
spc_8	H2O	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
enz_3	Phosphopyruvate hydratase(Enzyme)	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
spc_9	Glycerate 3-phosphate	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
enz_4	Phosphoglycerate mutase(Enzyme)	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
spc_10	Glycerate 1,3-bisphosphate	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
enz_5	Phosphoglycerate kinase(Enzyme)	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
spc_11	NAD+	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
spc_12	D-Glyceraldehyde 3-phosphate	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
spc_13	Phosphate	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
spc_14	H+	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
spc_15	NADH	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
enz_6	Glyceraldehyde-3-phosphate dehydrogenase(Enzyme)	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
spc_16	Glycerone phosphate	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
enz_7	Triose-phosphate isomerase(Enzyme)	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
spc_17	beta-D-Fructose 1,6-bisphosphate	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×

id	name	compartment	derived unit	constant	boundary condition
enz_8	Fructose-bisphosphate aldolase(Enzyme)	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
spc_18	beta-D-Fructose 6-phosphate	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
enz_9	6-Phosphofructokinase(Enzyme)	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×
enz_10	Glucose-6-phosphate isomerase(Enzyme)	compart_1	$\text{mol} \cdot \text{l}^{-1}$	×	×

5 Function definitions

This is an overview of ten function definitions.

5.1 Function definition kl_0

Arguments Vf, P, Kms, Vr, Kmp, S

Mathematical Expression

$$\frac{\frac{Vf \cdot S}{Kms} - \frac{Vr \cdot P}{Kmp}}{1 + \frac{S}{Kms} + \frac{P}{Kmp}} \quad (1)$$

5.2 Function definition kl_1

Arguments S, Vr, P, Vf, Kmp, Kms

Mathematical Expression

$$\frac{\frac{Vf \cdot S}{Kms} - \frac{Vr \cdot P}{Kmp}}{1 + \frac{S}{Kms} + \frac{P}{Kmp}} \quad (2)$$

5.3 Function definition kl_2

Arguments Kmp, Vr, P, S, Kms, Vf

Mathematical Expression

$$\frac{\frac{Vf \cdot S}{Kms} - \frac{Vr \cdot P}{Kmp}}{1 + \frac{S}{Kms} + \frac{P}{Kmp}} \quad (3)$$

5.4 Function definition kl_3

Arguments Vr, Vf, Kms, Kmp, P, S

Mathematical Expression

$$\frac{\frac{Vf \cdot S}{Kms} - \frac{Vr \cdot P}{Kmp}}{1 + \frac{S}{Kms} + \frac{P}{Kmp}} \quad (4)$$

5.5 Function definition kl_4

Arguments Vf, S, P, Kms, Kmp, Vr

Mathematical Expression

$$\frac{\frac{Vf \cdot S}{Kms} - \frac{Vr \cdot P}{Kmp}}{1 + \frac{S}{Kms} + \frac{P}{Kmp}} \quad (5)$$

5.6 Function definition `k1_5`

Arguments `Km`, `S`, `V`

Mathematical Expression

$$\frac{V \cdot S}{K_m + S} \quad (6)$$

5.7 Function definition `k1_6`

Arguments `V`, `Km`, `S`

Mathematical Expression

$$\frac{V \cdot S}{K_m + S} \quad (7)$$

5.8 Function definition `k1_7`

Arguments `Km`, `V`, `S`

Mathematical Expression

$$\frac{V \cdot S}{K_m + S} \quad (8)$$

5.9 Function definition `k1_8`

Arguments `Km`, `S`, `V`

Mathematical Expression

$$\frac{V \cdot S}{K_m + S} \quad (9)$$

5.10 Function definition `k1_9`

Arguments `S`, `Kms`, `Kmp`, `P`, `Vf`, `Vr`

Mathematical Expression

$$\frac{\frac{V_f \cdot S}{K_{ms}} - \frac{V_r \cdot P}{K_{mp}}}{1 + \frac{S}{K_{ms}} + \frac{P}{K_{mp}}} \quad (10)$$

6 Reactions

This model contains ten reactions.

6.1 Reaction `reac_0`

This is a reversible reaction.

Modifier `enz_1`

Reaction equation

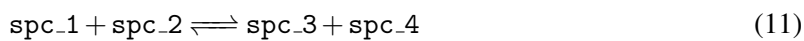


Table 4: Overview of participating species.

Reactants	Products	Modifiers
spc_1	spc_3	enz_1
spc_2	spc_4	

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot 0.999999999999998 \text{ mol} \cdot \text{l}^{-1}$

$$v_1 = k1_0(Vf, [\text{spc_3}], Kms_spc_1, Vr, Kmp_spc_3) \quad (12)$$

Table 5: Properties of each parameter.

id	name	SBO	value	unit	constant
Vf			33.000	mMdivmin	✓
Kms_spc_1			0.072	mM	✓
Vr			0.006	mMdivmin	✓
Kmp_spc_3			0.042	mM	✓

6.2 Reaction reac_1

This is a reversible reaction.

Modifier enz_2

Reaction equation

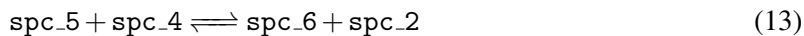


Table 6: Overview of participating species.

Reactants	Products	Modifiers
spc_5	spc_6	enz_2
spc_4	spc_2	

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot 0.999999999999998 \text{ mol} \cdot \text{l}^{-1}$

$$v_2 = k1_1([\text{spc_5}], Vr, [\text{spc_6}], Vf, Kmp_spc_6) \quad (14)$$

Table 7: Properties of each parameter.

id	name	SBO	value	unit	constant
Vr			0.63	mMdivmin	✓
Vf			566.00	mMdivmin	✓
Kmp_spc_6			10.00	mM	✓
Kms_spc_5			0.11	mM	✓

6.3 Reaction reac_2

This is a reversible reaction.

Modifier enz_3

Reaction equation



Table 8: Overview of participating species.

Reactants	Products	Modifiers
spc_7	spc_5 spc_8	enz_3

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot 0.9999999999999998 \text{ mol} \cdot \text{l}^{-1}$

$$v_3 = k1_2(Kmp_spc_5, Vr, [\text{spc}_5], [\text{spc}_7], Kms_spc_7) \quad (16)$$

Table 9: Properties of each parameter.

id	name	SBO	value	unit	constant
Kmp_spc_5			0.089	mM	✓
Vr			120.000	mMdivmin	✓
Kms_spc_7			0.045	mM	✓
Vf			111.000	mMdivmin	✓

6.4 Reaction reac_3

This is a reversible reaction.

Modifier enz_4

Reaction equation



Table 10: Overview of participating species.

Reactants	Products	Modifiers
spc_9	spc_7	enz_4

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot 0.9999999999999998 \text{ mol} \cdot \text{l}^{-1}$

$$v_4 = k1_3(Vr, Vf, Kms_spc_9, Kmp_spc_7, [\text{spc_7}]) \quad (18)$$

Table 11: Properties of each parameter.

id	name	SBO	value	unit	constant
Vr			2880.000	mMdivmin	✓
Vf			674.000	mMdivmin	✓
Kms_spc_9			0.145	mM	✓
Kmp_spc_7			0.139	mM	✓

6.5 Reaction reac_4

This is a reversible reaction.

Modifier enz_5

Reaction equation

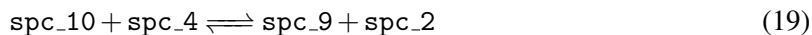


Table 12: Overview of participating species.

Reactants	Products	Modifiers
spc_10	spc_9	enz_5
spc_4	spc_2	

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot 0.9999999999999998 \text{ mol} \cdot \text{l}^{-1}$

$$v_5 = k1_4(Vf, [\text{spc_10}], [\text{spc_9}], Kms_spc_10, Kmp_spc_9) \quad (20)$$

Table 13: Properties of each parameter.

id	name	SBO	value	unit	constant
Vf			15060.000	mMdivmin	✓
Kms_spc_10			0.021	mM	✓
Kmp_spc_9			0.510	mM	✓
Vr			959.000	mMdivmin	✓

6.6 Reaction reac_5

This is a reversible reaction.

Modifier enz_6

Reaction equation

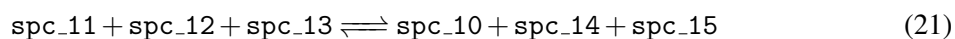


Table 14: Overview of participating species.

Reactants	Products	Modifiers
spc_11	spc_10	enz_6
spc_12	spc_14	
spc_13	spc_15	

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot 0.9999999999999998 \text{ mol} \cdot \text{l}^{-1}$

$$v_6 = k1_5(Km_spc_12, [\text{spc_12}]) \quad (22)$$

Table 15: Properties of each parameter.

id	name	SBO	value	unit	constant
Km_spc_12			0.042	mM	✓
V			321.000	mMdivmin	✓

6.7 Reaction reac_6

This is a reversible reaction.

Modifier enz_7

Reaction equation



Table 16: Overview of participating species.

Reactants	Products	Modifiers
spc_16	spc_12	enz_7

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot 0.9999999999999998 \text{ mol} \cdot \text{l}^{-1}$

$$v_7 = k1_6(V, Km_spc_16) \quad (24)$$

Table 17: Properties of each parameter.

id	name	SBO	value	unit	constant
V			356.00	mMdivmin	✓
Km_spc_16			1.53	mM	✓

6.8 Reaction reac_7

This is a reversible reaction.

Modifier enz_8

Reaction equation



Table 18: Overview of participating species.

Reactants	Products	Modifiers
spc_17	spc_16 spc_12	enz_8

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot 0.9999999999999998 \text{ mol} \cdot \text{l}^{-1}$

$$v_8 = k1_7(Km_spc_17, V) \quad (26)$$

Table 19: Properties of each parameter.

id	name	SBO	value	unit	constant
Km_spc_17			0.038	mM	✓
V			59.500	mMdivmin	✓

6.9 Reaction reac_8

This is a reversible reaction.

Modifier enz_9

Reaction equation



Table 20: Overview of participating species.

Reactants	Products	Modifiers
spc_2	spc_17	enz_9
spc_18	spc_4	

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot 0.9999999999999998 \text{ mol} \cdot \text{l}^{-1}$

$$v_9 = k1_8(Km_spc_18, [\text{spc_18}]) \quad (28)$$

Table 21: Properties of each parameter.

id	name	SBO	value	unit	constant
Km_spc_18			0.224	mM	✓
V			79.700	mMdivmin	✓

6.10 Reaction reac_9

This is a reversible reaction.

Modifier enz_10

Reaction equation



Table 22: Overview of participating species.

Reactants	Products	Modifiers
spc_3	spc_18	enz_10

Kinetic Law

Derived unit $(60\text{ s})^{-1} \cdot 0.9999999999999998\text{ mol} \cdot \text{l}^{-1}$

$$v_{10} = k1_9([spc_3], Kms_spc_3, Kmp_spc_18, [spc_18], Vf) \quad (30)$$

Table 23: Properties of each parameter.

id	name	SBO	value	unit	constant
Kms_spc_3			0.425	mM	✓
Kmp_spc_18			0.175	mM	✓
Vf			604.000	mMdivmin	✓
Vr			576.000	mMdivmin	✓

7 Rate Equations

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

Identifiers for kinetic equations, which are highlighted in gray, cannot be evaluated to a substance unit and may therefore be problematic for SBML interpreters, which are unable to perform unit conversion. 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.

7.1 Species spc_1

Name alpha-D-Glucose

$$\frac{dspc_1}{dt} = -v_1 \quad (31)$$

7.2 Species spc_2

Name ATP

$$\frac{dspc_2}{dt} = v_2 + v_5 - v_1 - v_9 \quad (32)$$

7.3 Species `spc_3`

Name alpha-D-Glucose 6-phosphate

$$\frac{d\text{spc_3}}{dt} = v_1 - v_{10} \quad (33)$$

7.4 Species `spc_4`

Name ADP

$$\frac{d\text{spc_4}}{dt} = v_1 + v_9 - v_2 - v_5 \quad (34)$$

7.5 Species `enz_1`

Name Hexokinase(Enzyme)

$$\frac{d\text{enz_1}}{dt} = 0 \quad (35)$$

7.6 Species `spc_5`

Name Phosphoenolpyruvate

$$\frac{d\text{spc_5}}{dt} = v_3 - v_2 \quad (36)$$

7.7 Species `spc_6`

Name Pyruvate

$$\frac{d\text{spc_6}}{dt} = v_2 \quad (37)$$

7.8 Species `enz_2`

Name Pyruvate kinase(Enzyme)

$$\frac{d\text{enz_2}}{dt} = 0 \quad (38)$$

7.9 Species `spc_7`

Name 2-Phospho-D-glycerate

$$\frac{d\text{spc_7}}{dt} = v_4 - v_3 \quad (39)$$

7.10 Species `spc_8`

Name H2O

$$\frac{dspc_8}{dt} = v_3 \quad (40)$$

7.11 Species `enz_3`

Name Phosphopyruvate hydratase(Enzyme)

$$\frac{denz_3}{dt} = 0 \quad (41)$$

7.12 Species `spc_9`

Name Glycerate 3-phosphate

$$\frac{dspc_9}{dt} = v_5 - v_4 \quad (42)$$

7.13 Species `enz_4`

Name Phosphoglycerate mutase(Enzyme)

$$\frac{denz_4}{dt} = 0 \quad (43)$$

7.14 Species `spc_10`

Name Glycerate 1,3-bisphosphate

$$\frac{dspc_10}{dt} = v_6 - v_5 \quad (44)$$

7.15 Species `enz_5`

Name Phosphoglycerate kinase(Enzyme)

$$\frac{denz_5}{dt} = 0 \quad (45)$$

7.16 Species `spc_11`

Name NAD+

$$\frac{dspc_11}{dt} = -v_6 \quad (46)$$

7.17 Species `spc_12`

Name D-Glyceraldehyde 3-phosphate

$$\frac{dspc_12}{dt} = v_7 + v_8 - v_6 \quad (47)$$

7.18 Species `spc_13`

Name Phosphate

$$\frac{dspc_13}{dt} = -v_6 \quad (48)$$

7.19 Species `spc_14`

Name H+

$$\frac{dspc_14}{dt} = v_6 \quad (49)$$

7.20 Species `spc_15`

Name NADH

$$\frac{dspc_15}{dt} = v_6 \quad (50)$$

7.21 Species `enz_6`

Name Glyceraldehyde-3-phosphate dehydrogenase(Enzyme)

$$\frac{denz_6}{dt} = 0 \quad (51)$$

7.22 Species `spc_16`

Name Glycerone phosphate

$$\frac{dspc_16}{dt} = v_8 - v_7 \quad (52)$$

7.23 Species `enz_7`

Name Triose-phosphate isomerase(Enzyme)

$$\frac{denz_7}{dt} = 0 \quad (53)$$

7.24 Species `spc_17`

Name beta-D-Fructose 1,6-bisphosphate

$$\frac{dspc_17}{dt} = v_9 - v_8 \quad (54)$$

7.25 Species `enz_8`

Name Fructose-bisphosphate aldolase(Enzyme)

$$\frac{denz_8}{dt} = 0 \quad (55)$$

7.26 Species `spc_18`

Name beta-D-Fructose 6-phosphate

$$\frac{dspc_18}{dt} = v_{10} - v_9 \quad (56)$$

7.27 Species `enz_9`

Name 6-Phosphofructokinase(Enzyme)

$$\frac{denz_9}{dt} = 0 \quad (57)$$

7.28 Species `enz_10`

Name Glucose-6-phosphate isomerase(Enzyme)

$$\frac{denz_10}{dt} = 0 \quad (58)$$