SBML Model Report

Model name: "Wolf2000_Glycolytic_Oscillations"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by Harish Dharuri[1] at October sixth 2008 at 8:39 p. m. and last time modified at July fifth 2012 at 2:48 p. 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	1
species types	0	species	9
events	0	constraints	0
reactions	11	function definitions	0
global parameters	18	unit definitions	6
rules	0	initial assignments	0

Model Notes

Model reproduces the dynamics of ATP and NADH as depicted in Fig 4 of the paper. Model successfully tested on Jarnac and MathSBML.

[1]California Institute of Technology, hdharuri@cds.caltech.edu

In summary, you are entitled to use this encoded model in absolutely any manner you deem suitable, verbatim, or with modification, alone or embedded it in a larger context, redistribute it, commercially or not, in a restricted way or not.

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 nine unit definitions of which three are predefined by SBML and not mentioned in the model.

2.1 Unit `substance`

Name milli mole

Definition mmol

2.2 Unit `time`

Name min

Definition 60 s

2.3 Unit `mM`

Name mM

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

2.4 Unit `mM_min_1`

Name mM_min_1

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

2.5 Unit `min_1`

Name min_1

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

2.6 Unit mM_1_min_1

Name mM_1_min_1

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

2.7 Unit volume

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

Definition l

2.8 Unit area

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

Definition m^2

2.9 Unit length

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

Definition m

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

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

3.1 Compartment compartment

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

Name compartment

4 Species

This model contains nine species. 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
s1	Glucose	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
at	ATP	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
s2	F16P	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
s3	Triose_Gly3Phos_DHAP	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
na	NAD	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
s4	3PG	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
s5	Pyruvate	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
s6	Acetaldehyde	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
s6o	extracellular acetaldehyde	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 18 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k0	k0		50.0	mmol $\cdot$ 1^{-1} $\cdot$ $(60\ \mathrm{s})^{-1}$	☑
k1	k1		550.0	mmol^{-1} $\cdot$ 1 $\cdot$ $(60\ \mathrm{s})^{-1}$	☑
k2	k2		9.8	$(60\ \mathrm{s})^{-1}$	☑
k31	k31		323.8	mmol^{-1} $\cdot$ 1 $\cdot$ $(60\ \mathrm{s})^{-1}$	☑
k33	k33		57823.1	mmol^{-1} $\cdot$ 1 $\cdot$ $(60\ \mathrm{s})^{-1}$	☑
k32	k32		76411.1	mmol^{-1} $\cdot$ 1 $\cdot$ $(60\ \mathrm{s})^{-1}$	☑
k34	k34		23.7	mmol^{-1} $\cdot$ 1 $\cdot$ $(60\ \mathrm{s})^{-1}$	☑
k4	k4		80.0	mmol^{-1} $\cdot$ 1 $\cdot$ $(60\ \mathrm{s})^{-1}$	☑
k5	k5		9.7	$(60\ \mathrm{s})^{-1}$	☑
k6	k6		2000.0	mmol^{-1} $\cdot$ 1 $\cdot$ $(60\ \mathrm{s})^{-1}$	☑
k7	k7		28.0	$(60\ \mathrm{s})^{-1}$	☑
k8	k8		85.7	mmol^{-1} $\cdot$ 1 $\cdot$ $(60\ \mathrm{s})^{-1}$	☑
k9	k9		80.0	$(60\ \mathrm{s})^{-1}$	☑
k10	k10		375.0	$(60\ \mathrm{s})^{-1}$	☑
atot	atot		4.0	$\mathrm{mmol} \cdot 1^{-1}$	☑
ntot	ntot		1.0	$\mathrm{mmol} \cdot 1^{-1}$	☑
n	n		4.0	dimensionless	☑
ki	ki		1.0	$\mathrm{mmol} \cdot 1^{-1}$	☑

6 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	v1	v1	$s1 + 2\,at \rightleftharpoons s2$	
2	v2	v2	$s2 \rightleftharpoons 2\,s3$	
3	v3	v3	$s3 + na \rightleftharpoons s4 + at$	
4	v4	v4	$s4 \rightleftharpoons s5 + at$	
5	v5	v5	$s5 \rightleftharpoons s6$	
6	v7	v7	$at \rightleftharpoons \emptyset$	
7	v8	v8	$s3 \rightleftharpoons na$	
8	v9	v9	$s6o \rightleftharpoons \emptyset$	
9	v10	v10	$s6 \rightleftharpoons 0 \cdot 1\,s6o$	
10	v6	v6	$s6 \rightleftharpoons na$	
11	v0	v0	$\emptyset \rightleftharpoons s1$	

6.1 Reaction v1

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

Name v1

Reaction equation

$$\mathrm{s1} + 2\,\mathrm{at} \rightleftharpoons \mathrm{s2} \tag{1}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
s1	Glucose	
at	ATP	

Product

Table 7: Properties of each product.

Id	Name	SBO
s2	F16P	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{\mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k1} \cdot [\mathrm{s1}] \cdot [\mathrm{at}]}{1 + \left(\frac{[\mathrm{at}]}{\mathrm{ki}}\right)^{\mathrm{n}}} \tag{2}$$

6.2 Reaction v2

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

Name v2

Reaction equation

$$\mathrm{s2} \rightleftharpoons 2\,\mathrm{s3} \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
s2	F16P	

Product

Table 9: Properties of each product.

Id	Name	SBO
s3	Triose_Gly3Phos_DHAP	

Kinetic Law

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

$$v_2 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k2} \cdot [\mathrm{s2}] \tag{4}$$

6.3 Reaction v3

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

Name v3

Reaction equation

$$\mathrm{s3} + \mathrm{na} \rightleftharpoons \mathrm{s4} + \mathrm{at} \tag{5}$$

Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
s3	Triose_Gly3Phos_DHAP	
na	NAD	

Products

Table 11: Properties of each product.

Id	Name	SBO
s4	3PG	

Id	Name	SBO
at	ATP	

Kinetic Law

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

$$v_3 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{k31} \cdot \mathrm{k32} \cdot [\mathrm{s3}] \cdot [\mathrm{na}] \cdot (\mathrm{atot} - [\mathrm{at}]) - \mathrm{k33} \cdot \mathrm{k34} \cdot [\mathrm{s4}] \cdot [\mathrm{at}] \cdot (\mathrm{ntot} - [\mathrm{na}])}{\mathrm{k33} \cdot (\mathrm{ntot} - [\mathrm{na}]) + \mathrm{k32} \cdot (\mathrm{atot} - [\mathrm{at}])} \tag{6}$$

6.4 Reaction v4

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

Name v4

Reaction equation

$$\mathrm{s4} \rightleftharpoons \mathrm{s5} + \mathrm{at} \tag{7}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
s4	3PG	

Products

Table 13: Properties of each product.

Id	Name	SBO
s5	Pyruvate	
at	ATP	

Kinetic Law

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

$$v_4 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k4} \cdot [\mathrm{s4}] \cdot (\mathrm{atot} - [\mathrm{at}]) \tag{8}$$

6.5 Reaction v5

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

Name v5

Reaction equation

$$\mathrm{s5} \rightleftharpoons \mathrm{s6} \tag{9}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
s5	Pyruvate	

Product

Table 15: Properties of each product.

Id	Name	SBO
s6	Acetaldehyde	

Kinetic Law

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

$$v_5 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k5} \cdot [\mathrm{s5}] \tag{10}$$

6.6 Reaction v7

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

Name v7

Reaction equation

$$\mathrm{at} \rightleftharpoons \emptyset \tag{11}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
at	ATP	

Kinetic Law

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

$$v_6 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k7} \cdot [\mathrm{at}] \tag{12}$$

6.7 Reaction v8

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

Name v8

Reaction equation

$$\mathrm{s3} \rightleftharpoons \mathrm{na} \tag{13}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
s3	Triose_Gly3Phos_DHAP	

Product

Table 18: Properties of each product.

Id	Name	SBO
na	NAD	

Kinetic Law

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

$$v_7 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k8} \cdot [\mathrm{s3}] \cdot (\mathrm{ntot} - [\mathrm{na}]) \tag{14}$$

6.8 Reaction v9

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

Name v9

Reaction equation

$$\mathrm{s6o} \rightleftharpoons \emptyset \tag{15}$$

Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
s6o	extracellular acetaldehyde	

Kinetic Law

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

$$v_8 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k9} \cdot [\mathrm{s6o}] \tag{16}$$

6.9 Reaction v10

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

Name v10

Reaction equation

$$\mathrm{s6} \rightleftharpoons 0{\cdot}1\,\mathrm{s6o} \tag{17}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
s6	Acetaldehyde	

Product

Table 21: Properties of each product.

Id	Name	SBO
s6o	extracellular acetaldehyde	

Kinetic Law

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

$$v_9 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k10} \cdot ([\mathrm{s6}] - [\mathrm{s6o}]) \tag{18}$$

6.10 Reaction v6

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

Name v6

Reaction equation

$$\mathrm{s6} \rightleftharpoons \mathrm{na} \tag{19}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
s6	Acetaldehyde	

Product

Table 23: Properties of each product.

Id	Name	SBO
na	NAD	

Kinetic Law

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

$$v_{10} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k6} \cdot [\mathrm{s6}] \cdot (\mathrm{ntot} - [\mathrm{na}]) \tag{20}$$

6.11 Reaction v0

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

Name v0

Reaction equation

$$\emptyset \rightleftharpoons \mathrm{s1} \tag{21}$$

Product

Table 24: Properties of each product.

Id	Name	SBO
s1	Glucose	

Kinetic Law

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

$$v_{11} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k0} \tag{22}$$

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 s1

Name Glucose

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

This species takes part in two reactions (as a reactant in v1 and as a product in v0).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s1} = v_{11} - v_1 \tag{23}$$

7.2 Species at

Name ATP

Initial concentration $2\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in v1, v7 and as a product in v3, v4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{at} = v_3 + v_4 - 2v_1 - v_6 \tag{24}$$

7.3 Species s2

Name F16P

Initial concentration $5\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in v2 and as a product in v1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s2} = v_1 - v_2 \tag{25}$$

7.4 Species s3

Name Triose_Gly3Phos_DHAP

Initial concentration $0.6\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in v3, v8 and as a product in v2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s3} = 2v_2 - v_3 - v_7 \tag{26}$$

7.5 Species na

Name NAD

Initial concentration $0.6\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in v3 and as a product in v8, v6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{na} = v_7 + v_{10} - v_3 \tag{27}$$

7.6 Species s4

Name 3PG

Initial concentration $0.7\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in v4 and as a product in v3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s4} = v_3 - v_4 \tag{28}$$

7.7 Species s5

Name Pyruvate

Initial concentration $8\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in v5 and as a product in v4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s5} = v_4 - v_5 \tag{29}$$

7.8 Species s6

Name Acetaldehyde

Initial concentration $0.08\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in v10, v6 and as a product in v5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s6} = v_5 - v_9 - v_{10} \tag{30}$$

7.9 Species s6o

Name extracellular acetaldehyde

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

This species takes part in two reactions (as a reactant in v9 and as a product in v10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s6o} = 0.1v_9 - v_8 \tag{31}$$

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.

[a]Center for Bioinformatics Tübingen (ZBIT), Germany
[b]California Institute of Technology, Beckman Institute BNMC, Pasadena, United States
[c]European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom
[d]EML Research gGmbH, Heidelberg, Germany