SBML Model Report

Model name: "Ataullahkhanov1996_Adenylate"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Harish Dharuri[1] at April twelveth 2006 at 10:04 p. m. and last time modified at July fifth 2012 at 2:43 p. m. Table 1 gives 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	3
events	0	constraints	0
reactions	5	function definitions	0
global parameters	10	unit definitions	2
rules	2	initial assignments	0

Model Notes

The model reproduces ion and adenylate pool concentration corresponding to line 2 of Fig 3 of the publication. This model was tested successfully on Jarnac

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

2.1 Unit `substance`

Name millimole (default)

Definition mmol

2.2 Unit `time`

Name hour (default)

Definition 3600 s

2.3 Unit `volume`

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

Definition l

2.4 Unit `area`

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

Definition m^2

2.5 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
`cell`	Erythrocyte		3	1	litre	☑	

3.1 Compartment `cell`

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

Name Erythrocyte

4 Species

This model contains three species. 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
I	Ions	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
E	Energy pool	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
A	Adenylate pool	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains ten global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
T	ATP		1.000		⊟
M	AMP		0.010		⊟
P	Membrane permeability		0.121		☑
J	Extracellular ion concentration		100.000		☑
W2	Ion pump activity		0.200		☑
W3	Glycolytic activity		13.480		☑
U	de novo AMP synthesis		0.020		☑
W	AMP degradation		0.010		☑
n	Dependence of AMP degradation on ATP		1.200		☑
k	Dependence of AMP degradation on AMP		−1.000		☑

6 Rules

This is an overview of two rules.

6.1 Rule T

Rule T is an assignment rule for parameter T:

$$\mathrm{T} = \frac{[\mathrm{A}] + 3 \cdot [\mathrm{E}] - \left(6 \cdot [\mathrm{A}] \cdot [\mathrm{E}] - 3 \cdot [\mathrm{E}]^2 + [\mathrm{A}]^2\right)^{0.5}}{6} \tag{1}$$

6.2 Rule M

Rule M is an assignment rule for parameter M:

$$\mathrm{M} = \frac{7 \cdot [\mathrm{A}] - 3 \cdot [\mathrm{E}] - \left(6 \cdot [\mathrm{A}] \cdot [\mathrm{E}] - 3 \cdot [\mathrm{E}]^2 + [\mathrm{A}]^2\right)^{0.5}}{6} \tag{2}$$

7 Reactions

This model contains five 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	U1	Passive ion influx	$\emptyset \longrightarrow \mathrm{I}$	
2	U2	ATP consumption by ion pump	$3\,\mathrm{I} + \mathrm{E} \longrightarrow \emptyset$	
3	U3	ATP from glycolysis	$\emptyset \longrightarrow \mathrm{E}$	
4	U6_plus_3U7	AMP synthesis de novo	$\mathrm{E} \longrightarrow \emptyset$	
5	U6_plus_U7_minus_U8	Adenylate pool	$\emptyset \longrightarrow \mathrm{A}$	

7.1 Reaction U1

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

Name Passive ion influx

Reaction equation

$$\emptyset \longrightarrow \mathrm{I} \tag{3}$$

Product

Table 6: Properties of each product.

Id	Name	SBO
I	Ions	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{P} \cdot \mathrm{J} \tag{4}$$

7.2 Reaction U2

This is an irreversible reaction of two reactants forming no product.

Name ATP consumption by ion pump

Reaction equation

$$3\,\mathrm{I} + \mathrm{E} \longrightarrow \emptyset \tag{5}$$

Reactants

Table 7: Properties of each reactant.

Id	Name	SBO
I	Ions	
E	Energy pool	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{W2} \cdot [\mathrm{I}] \cdot \mathrm{T} \tag{6}$$

7.3 Reaction U3

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

Name ATP from glycolysis

Reaction equation

$$\emptyset \longrightarrow \mathrm{E} \tag{7}$$

Product

Table 8: Properties of each product.

Id	Name	SBO
E	Energy pool	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{W3} \cdot \mathrm{T}^{0.52} \cdot \mathrm{M}^{0.41} \tag{8}$$

7.4 Reaction U6_plus_3U7

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

Name AMP synthesis de novo

Reaction equation

$$\mathrm{E} \longrightarrow \emptyset \tag{9}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
E	Energy pool	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{cell}) \cdot 2 \cdot \mathrm{U} \tag{10}$$

7.5 Reaction U6_plus_U7_minus_U8

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

Name Adenylate pool

Reaction equation

$$\emptyset \longrightarrow \mathrm{A} \tag{11}$$

Product

Table 10: Properties of each product.

Id	Name	SBO
A	Adenylate pool	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{U} \cdot \left(1 - \mathrm{W} \cdot \mathrm{T}^{\mathrm{n}} \cdot \mathrm{M}^{\mathrm{k}}\right) \tag{12}$$

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 I

Name Ions

Initial concentration $10\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in U2 and as a product in U1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{I} = v_1 - 3\,v_2 \tag{13}$$

8.2 Species E

Name Energy pool

Initial concentration $2.1\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in U2, U6_plus_3U7 and as a product in U3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E} = v_3 - v_2 - v_4 \tag{14}$$

8.3 Species A

Name Adenylate pool

Initial concentration $1.11\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in one reaction (as a product in U6_plus_U7_minus_U8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A} = v_5 \tag{15}$$

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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