SBML Model Report

Model name: "Bier2000_GlycolyticOscillation"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Vijayalakshmi Chelliah[1] and Martin Bier[2] at July 26$^{\text{th}}$ 2010 at 12:19 a. m. and last time modified at April eighth 2016 at 4:10 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	4
events	0	constraints	0
reactions	0	function definitions	0
global parameters	7	unit definitions	0
rules	6	initial assignments	0

Model Notes

This a model from the article:
How yeast cells synchronize their glycolytic oscillations: a perturbation analytic treatment
Bier M, Bakker BM, Westerhoff HV. Biophys. J2000 Mar;78(3):1087-93. 10692299,

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Abstract:
Of all the lifeforms that obtain their energy from glycolysis, yeast cells are among the most basic. Under certain conditions the concentrations of the glycolytic intermediates in yeast cells can oscillate. Individual yeast cells in a suspension can synchronize their oscillations to get in phase with each other. Although the glycolytic oscillations originate in the upper part of the glycolytic chain, the signaling agent in this synchronization appears to be acetaldehyde, a membrane-permeating metabolite at the bottom of the anaerobic part of the glycolytic chain. Here we address the issue of how a metabolite remote from the pacemaking origin of the oscillation may nevertheless control the synchronization. We present a quantitative model for glycolytic oscillations and their synchronization in terms of chemical kinetics. We show that, in essence, the common acetaldehyde concentration can be modeled as a small perturbation on the „pacemaker„ whose effect on the period of the oscillations of cells in the same suspension is indeed such that a synchronization develops.

2 Unit Definitions

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

2.1 Unit `substance`

Notes Mole is the predefined SBML unit for `substance`.

Definition mol

2.2 Unit `volume`

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

Definition l

2.3 Unit `area`

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

Definition m^2

2.4 Unit `length`

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

Definition m

2.5 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
`compartment`		0000290	3	1	litre	☑	

3.1 Compartment `compartment`

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

SBO:0000290 physical compartment

4 Species

This model contains four 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
G1	Glucose_1	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
T1	ATP_1	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
G2	Glucose_2	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
T2	ATP_2	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains seven global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_in			0.36		☑
k1			0.02		☑
kp			6.00		☑
km			13.00		☑
epsilon			0.01		☑
Tsum	Tsum		0.00		☐
Tdiff	Tdiff		0.00		☐

6 Rules

This is an overview of six rules.

6.1 Rule G1

Rule G1 is a rate rule for species G1:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G1} = \mathrm{V\_in} - \mathrm{k1} \cdot [\mathrm{G1}] \cdot [\mathrm{T1}] \tag{1}$$

6.2 Rule G2

Rule G2 is a rate rule for species G2:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G2} = \mathrm{V\_in} - \mathrm{k1} \cdot [\mathrm{G2}] \cdot [\mathrm{T2}] \tag{2}$$

6.3 Rule T1

Rule T1 is a rate rule for species T1:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{T1} = 2 \cdot \mathrm{k1} \cdot [\mathrm{T1}] \cdot [\mathrm{G1}] - \frac{\mathrm{kp} \cdot [\mathrm{T1}]}{\mathrm{km} + [\mathrm{T1}]} + \mathrm{epsilon} \cdot ([\mathrm{T2}] - [\mathrm{T1}]) \tag{3}$$

6.4 Rule T2

Rule T2 is a rate rule for species T2:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{T2} = 2 \cdot \mathrm{k1} \cdot [\mathrm{G2}] \cdot [\mathrm{T2}] - \frac{\mathrm{kp} \cdot [\mathrm{T2}]}{\mathrm{km} + [\mathrm{T2}]} - \mathrm{epsilon} \cdot ([\mathrm{T2}] - [\mathrm{T1}]) \tag{4}$$

6.5 Rule Tsum

Rule Tsum is an assignment rule for parameter Tsum:

$$\text{Tsum} = [\text{T2}] + [\text{T1}] \tag{5}$$

Derived unit $\text{mol} \cdot \text{l}^{-1}$

6.6 Rule Tdiff

Rule Tdiff is an assignment rule for parameter Tdiff:

$$\text{Tdiff} = [\text{T2}] - [\text{T1}] \tag{6}$$

Derived unit $\text{mol} \cdot \text{l}^{-1}$

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 G1

Name Glucose_1

SBO:0000247 simple chemical

Initial concentration $6.6 \text{ mol} \cdot \text{l}^{-1}$

Involved in rule G1

One rule which determines this species' quantity.

7.2 Species T1

Name ATP_1

SBO:0000247 simple chemical

Initial concentration $7.6 \text{ mol} \cdot \text{l}^{-1}$

Involved in rule T1

One rule which determines this species' quantity.

7.3 Species G2

Name Glucose_2

SBO:0000247 simple chemical

Initial concentration $10.3 \text{ mol} \cdot \text{l}^{-1}$

Involved in rule G2

One rule which determines this species' quantity.

7.4 Species T2

Name ATP_2

SBO:0000247 simple chemical

Initial concentration $0.41 \text{ mol} \cdot \text{l}^{-1}$

Involved in rule T2

One rule which determines this species' quantity.

A Glossary of Systems Biology Ontology Terms

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

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

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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