SBML Model Report

Model name: “Pfeiffer2001_ATP-ProducingPathways-_CooperationCompetition”

May 6, 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 Kieran Smallbone[2] at May twelveth 2011 at no o' clock in the morning. and last time modified at April 20th 2012 at 9:52 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	3
events	1	constraints	0
reactions	5	function definitions	0
global parameters	2	unit definitions	3
rules	0	initial assignments	0

Model Notes

This model is from the article:
Cooperation and Competition in the Evolution of ATP-Producing Pathways

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Thomas Pfeiffer, Stefan Schuster, Sebastian Bonhoeffer Science 2001 Apr; Volume:292 (Issue:5516); Page info:504-7 11283355 ,
Abstract:
Heterotrophic organisms generally face a trade-off between rate and yield of adenosine triphosphate (ATP) production. This trade-off may result in an evolutionary dilemma, because cells with a higher rate but lower yield of ATP production may gain a selective advantage when competing for shared energy resources. Using an analysis of model simulations and biochemical observations, we show that ATP production with a low rate and high yield can be viewed as a form of cooperative resource use and may evolve in spatially structured environments. Furthermore, we argue that the high ATP yield of respiration may have facilitated the evolutionary transition from unicellular to undifferentiated multicellular organisms.
Note:

This model reproduces the competition and invasion described in Supplemental Figure 2.

2 Unit Definitions

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

2.1 Unit `substance`

Definition dimensionless

2.2 Unit `time`

Definition dimensionless

2.3 Unit `volume`

Definition dimensionless

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
compartment			3	1	dimensionless	☑	

3.1 Compartment compartment

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

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
`S`	S	`compartment`	dimensionless $\cdot$ dimensionless^{-1}	$\boxminus$	$\boxminus$
`N1`	N1	`compartment`	dimensionless $\cdot$ dimensionless^{-1}	$\boxminus$	$\boxminus$
`N2`	N2	`compartment`	dimensionless $\cdot$ dimensionless^{-1}	$\boxminus$	$\boxminus$

5 Parameters

This model contains two global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v			10.0	dimensionless	☑
d			1.0	dimensionless	☑

6 Event

This is an overview of one event. Each event is initiated whenever its trigger condition switches from false to true. A delay function postpones the effects of an event to a later time point. At the time of execution, an event can assign values to species, parameters or compartments if these are not set to constant.

6.1 Event event_0

Trigger condition

$$\text{time} \geq 15 \tag{1}$$

Assignment

$$\text{N2} = 0.01 \tag{2}$$

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	`r1`	resource production	$\emptyset \rightleftharpoons \mathrm{S}$	0000393
2	`r2`	resource consumption and cell growth 1	$\mathrm{S} \rightleftharpoons 10\,\mathrm{N1}$	0000394
3	`r3`	resource consumption and cell growth 2	$\mathrm{S} \rightleftharpoons \mathrm{N2}$	0000394
4	`r4`	cell death 1	$\mathrm{N1} \rightleftharpoons \emptyset$	0000179
5	`r5`	cell death 2	$\mathrm{N2} \rightleftharpoons \emptyset$	0000179

7.1 Reaction r1

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

Name resource production

SBO:0000393 production

Reaction equation

$$\emptyset \rightleftharpoons \mathrm{S} \tag{3}$$

Product

Table 6: Properties of each product.

Id	Name	SBO
S	S	

Kinetic Law

Derived unit dimensionless

$$v_1 = \mathrm{v} \tag{4}$$

7.2 Reaction r2

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

Name resource consumption and cell growth 1

SBO:0000394 consumption

Reaction equation

$$\mathrm{S} \rightleftharpoons 10\,\mathrm{N1} \tag{5}$$

Reactant

Table 7: Properties of each reactant.

Id	Name	SBO
S	S	

Product

Table 8: Properties of each product.

Id	Name	SBO
N1	N1	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{[N1] \cdot [S]}{1 + [S]} \tag{6}$$

7.3 Reaction r3

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

Name resource consumption and cell growth 2

SBO:0000394 consumption

Reaction equation

$$S \rightleftharpoons N2 \tag{7}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
S	S	

Product

Table 10: Properties of each product.

Id	Name	SBO
N2	N2	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \frac{[\mathrm{N2}] \cdot 20 \cdot [\mathrm{S}]}{1 + [\mathrm{S}]} \tag{8}$$

7.4 Reaction `r4`

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

Name cell death 1

SBO:0000179 degradation

Reaction equation

$$\mathrm{N1} \rightleftharpoons \emptyset \tag{9}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
`N1`	N1	

Kinetic Law

Derived unit dimensionless^{-1}

$$v_4 = \mathrm{d} \cdot [\mathrm{N1}] \tag{10}$$

7.5 Reaction `r5`

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

Name cell death 2

SBO:0000179 degradation

Reaction equation

$$\mathrm{N2} \rightleftharpoons \emptyset \tag{11}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
N2	N2	

Kinetic Law

Derived unit $\text{dimensionless}^{-1}$

$$v_5 = \mathrm{d} \cdot [\mathrm{N2}] \tag{12}$$

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 S

Name S

Initial concentration $0.111111111111111\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in three reactions (as a reactant in r2, r3 and as a product in r1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S} = v_1 - v_2 - v_3 \tag{13}$$

8.2 Species N1

Name N1

Initial concentration $100\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in two reactions (as a reactant in r4 and as a product in r2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{N1} = 10\, v_2 - v_4 \tag{14}$$

8.3 Species N2

Name N2

Initial concentration $0\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

Involved in event event_0

This species takes part in two reactions (as a reactant in r5 and as a product in r3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{N2} = v_3 - v_5 \tag{15}$$

Furthermore, one event influences this species' rate of change.

A Glossary of Systems Biology Ontology Terms

SBO:0000179 **degradation:** Complete disappearance of a physical entity

SBO:0000393 **production:** Generation of a material or conceptual entity.

SBO:0000394 **consumption:** Decrease in amount of a material or conceptual entity.

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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