

## SBML Model Report

# Model name: “Wolf2000 - Cellular interaction on glycolytic oscillations in yeast”



May 17, 2018

## 1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Matthew Grant Roberts<sup>1</sup> and Catherine Lloyd<sup>2</sup> at March 16<sup>th</sup> 2018 at 11:24 a. m. and last time modified at March 18<sup>th</sup> 2018 at 12:44 a. 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	3
species types	0	species	19
events	0	constraints	0
reactions	18	function definitions	5
global parameters	14	unit definitions	2
rules	6	initial assignments	0

## Model Notes

Wolf2000 - Cellular interaction on glycolytic oscillations in yeastA two-cell model of glycolysis.

This model is described in the article:[Effect of cellular interaction on glycolytic oscillations in yeast: a theoretical investigation](#). Wolf J, Heinrich R. Biochem. J. 2000 Jan; 345 Pt 2: 321-334  
Abstract:

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On the basis of a detailed model of yeast glycolysis, the effect of intercellular dynamics is analysed theoretically. The model includes the main steps of anaerobic glycolysis, and the production of ethanol and glycerol. Transmembrane diffusion of acetaldehyde is included, since it has been hypothesized that this substance mediates the interaction. Depending on the kinetic parameter, the single-cell model shows both stationary and oscillatory behaviour. This agrees with experimental data with respect to metabolite concentrations and phase shifts. The inclusion of intercellular coupling leads to a variety of dynamical modes, such as synchronous oscillations, and different kinds of asynchronous behavior. These oscillations can co-exist, leading to bi- and tri-rhythmicity. The corresponding parameter regions have been identified by a bifurcation analysis. The oscillatory dynamics of synchronized cell populations are investigated by calculating the phase responses to acetaldehyde pulses. Simulations are performed with respect to the synchronization of two subpopulations that are oscillating out of phase before mixing. The effect of the various process on synchronization is characterized quantitatively. While continuous exchange of acetaldehyde might synchronize the oscillations for appropriate sets of parameter values, the calculated synchronization time is longer than that observed experimentally. It is concluded either that addition to the transmembrane exchange of acetaldehyde, other processes may contribute to intercellular coupling, or that intracellular regulator feedback plays a role in the acceleration of the synchronization. for appropriate sets of parameter values, the calculated synchronization time is longer than that observed experimentally. It is concluded either that addition to the transmembrane exchange of acetaldehyde, other processes may contribute to intercellular coupling, or that intracellular regulator feedback plays a role in the acceleration of the synchronization.

This model is hosted on [BioModels Database](#) and identified by: [BIOMD0000000691](#).

To cite BioModels Database, please use: [Chelliah V et al. BioModels: ten-year anniversary. Nucl. Acids Res. 2015, 43\(Database issue\):D542-8.](#)

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## 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 volume

**Name** volume

**Definition** ml

### 2.2 Unit substance

**Name** substance

**Definition** mmol

### 2.3 Unit area

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

**Definition** m<sup>2</sup>

### 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 Compartments

This model contains three compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
Cell_1	Cell 1		3	1	litre	<input checked="" type="checkbox"/>	
Cell_2	Cell 2		3	1	litre	<input checked="" type="checkbox"/>	
Compartment	Compartment		3	1	litre	<input checked="" type="checkbox"/>	

### 3.1 Compartment Cell\_1

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

**Name** Cell 1

### 3.2 Compartment Cell\_2

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

**Name** Cell 2

### 3.3 Compartment Compartment

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

**Name** Compartment

## 4 Species

This model contains 19 species. The boundary condition of six of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 9 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__Cell_1_	S1	Cell_1	$\text{mmol} \cdot \text{ml}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
S1__Cell_2_	S1	Cell_2	$\text{mmol} \cdot \text{ml}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
S2__Cell_1_	S2	Cell_1	$\text{mmol} \cdot \text{ml}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
S2__Cell_2_	S2	Cell_2	$\text{mmol} \cdot \text{ml}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
S3__Cell_1_	S3	Cell_1	$\text{mmol} \cdot \text{ml}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
S3__Cell_2_	S3	Cell_2	$\text{mmol} \cdot \text{ml}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
S4__Cell_1_	S4	Cell_1	$\text{mmol} \cdot \text{ml}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
S4__Cell_2_	S4	Cell_2	$\text{mmol} \cdot \text{ml}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
N2__Cell_1_	N2	Cell_1	$\text{mmol} \cdot \text{ml}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
N2__Cell_2_	N2	Cell_2	$\text{mmol} \cdot \text{ml}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
A3__Cell_1_	A3	Cell_1	$\text{mmol} \cdot \text{ml}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
A3__Cell_2_	A3	Cell_2	$\text{mmol} \cdot \text{ml}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
S4_ex	S4_ex	Compartment	$\text{mmol} \cdot \text{ml}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
A	A	Compartment	$\text{mmol} \cdot \text{ml}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
N	N	Compartment	$\text{mmol} \cdot \text{ml}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
N1__Cell_1_	N1	Cell_1	$\text{mmol} \cdot \text{ml}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
N1__Cell_2_	N1	Cell_2	$\text{mmol} \cdot \text{ml}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
A2__Cell_1_	A2	Cell_1	$\text{mmol} \cdot \text{ml}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
A2__Cell_2_	A2	Cell_2	$\text{mmol} \cdot \text{ml}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>

## 5 Parameters

This model contains 14 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		100.00		<input checked="" type="checkbox"/>
K_I	K_I		0.52		<input checked="" type="checkbox"/>
q	q		4.00		<input checked="" type="checkbox"/>
k2	k2		6.00		<input checked="" type="checkbox"/>
k3	k3		16.00		<input checked="" type="checkbox"/>
k4	k4		100.00		<input checked="" type="checkbox"/>
k5	k5		1.28		<input checked="" type="checkbox"/>
k6	k6		12.00		<input checked="" type="checkbox"/>
k	k		1.50		<input checked="" type="checkbox"/>
J0	J0		3.00		<input checked="" type="checkbox"/>
J_cell_1	J_cell_1		1.30		<input type="checkbox"/>
j_cell_2	j_cell_2		0.00		<input type="checkbox"/>
kappa	kappa		13.00		<input checked="" type="checkbox"/>
phi	phi		0.10		<input checked="" type="checkbox"/>

## 6 Function definitions

This is an overview of five function definitions.

### 6.1 Function definition `Constant_flux_irreversible`

**Name** Constant flux (irreversible)

**Argument** v

**Mathematical Expression**

$$v \quad (1)$$

### 6.2 Function definition `function_for_v2`

**Name** function for v2

**Arguments** k2, S2, N1

**Mathematical Expression**

$$k2 \cdot S2 \cdot N1 \quad (2)$$

### 6.3 Function definition `function_for_d_dt_S4_ex`

**Name** function for d/dt(S4\_ex)

**Arguments** phi, J1, J2

**Mathematical Expression**

$$\frac{\text{phi}}{2} \cdot (J1 + J2) \quad (3)$$

### 6.4 Function definition `function_for_v1`

**Name** function for v1

**Arguments** k1, S1, A3, K\_I, q

**Mathematical Expression**

$$k1 \cdot S1 \cdot A3 \cdot \left(1 + \left(\frac{A3}{K_I}\right)^q\right)^1 \quad (4)$$

### 6.5 Function definition `function_for_v3`

**Name** function for v3

**Arguments** k3, S3, A2

**Mathematical Expression**

$$k3 \cdot S3 \cdot A2 \quad (5)$$

## 7 Rules

This is an overview of six rules.

### 7.1 Rule `j_cell_2`

Rule `j_cell_2` is an assignment rule for parameter `j_cell_2`:

$$j\_cell\_2 = \text{kappa} \cdot ([S4\_Cell\_2] - [S4\_ex]) \quad (6)$$

### 7.2 Rule `J_cell_1`

Rule `J_cell_1` is an assignment rule for parameter `J_cell_1`:

$$J\_cell\_1 = \text{kappa} \cdot ([S4\_Cell\_1] - [S4\_ex]) \quad (7)$$

### 7.3 Rule N1\_\_Cell\_2\_

Rule N1\_\_Cell\_2\_ is an assignment rule for species N1\_\_Cell\_2\_:

$$N1\_Cell\_2\_ = [N] - [N2\_Cell\_2\_]$$
(8)

**Derived unit** mmol · ml<sup>-1</sup>

### 7.4 Rule N1\_\_Cell\_1\_

Rule N1\_\_Cell\_1\_ is an assignment rule for species N1\_\_Cell\_1\_:

$$N1\_Cell\_1\_ = [N] - [N2\_Cell\_1\_]$$
(9)

**Derived unit** mmol · ml<sup>-1</sup>

### 7.5 Rule A2\_\_Cell\_1\_

Rule A2\_\_Cell\_1\_ is an assignment rule for species A2\_\_Cell\_1\_:

$$A2\_Cell\_1\_ = [A] - [A3\_Cell\_1\_]$$
(10)

**Derived unit** mmol · ml<sup>-1</sup>

### 7.6 Rule A2\_\_Cell\_2\_

Rule A2\_\_Cell\_2\_ is an assignment rule for species A2\_\_Cell\_2\_:

$$A2\_Cell\_2\_ = [A] - [A3\_Cell\_2\_]$$
(11)

**Derived unit** mmol · ml<sup>-1</sup>



## 8 Reactions

This model contains 18 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

Nº	Id	Name	Reaction Equation	SBO
1	v1_cell1_1	v1_cell_1	$S1\_Cell\_1 + 2 A3\_Cell\_1 \longrightarrow 2 S2\_Cell\_1$	
2	v1_cell1_2	v1_cell_2	$S1\_Cell\_2 + 2 A3\_Cell\_2 \longrightarrow 2 S2\_Cell\_2$	
3	v2_cell1_1	v2_cell_1	$S2\_Cell\_1 + N1\_Cell\_1 \longrightarrow S3\_Cell\_1 + N2\_Cell\_1$	
4	v2_cell1_2	v2_cell_2	$S2\_Cell\_2 + N1\_Cell\_2 \longrightarrow S3\_Cell\_2 + N2\_Cell\_2$	
5	v3_cell1_1	v3_cell_1	$S3\_Cell\_1 + A2\_Cell\_1 \longrightarrow S4\_Cell\_1 + 2 A3\_Cell\_1$	
6	v3_cell1_2	v3_cell_2	$S3\_Cell\_2 + A2\_Cell\_2 \longrightarrow S4\_Cell\_2 + 2 A3\_Cell\_2$	
7	v4_cell1_1	v4_cell_1	$S4\_Cell\_1 + N2\_Cell\_1 \longrightarrow \emptyset$	
8	v4_cell1_2	v4_cell_2	$S4\_Cell\_2 + N2\_Cell\_2 \longrightarrow \emptyset$	
9	v5_cell1_1	v5_cell_1	$A3\_Cell\_1 \longrightarrow \emptyset$	
10	v5_cell1_2	v5_cell_2	$A3\_Cell\_2 \longrightarrow \emptyset$	
11	v6_cell1_1	v6_cell_1	$S2\_Cell\_1 + N2\_Cell\_1 \longrightarrow \emptyset$	
12	v6_cell1_2	v6_cell_2	$S2\_Cell\_2 + N2\_Cell\_2 \longrightarrow \emptyset$	
13	v7	v7	$S4\_ex \longrightarrow \emptyset$	
14	S1_cell1_1-glucose_influx	S1_cell_1 glucose influx	$\emptyset \longrightarrow S1\_Cell\_1$	
15	S1_cell1_2-glucose_influx	S1_cell_2 glucose influx	$\emptyset \longrightarrow S1\_Cell\_2$	

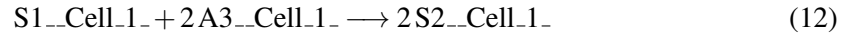
Nº	Id	Name	Reaction Equation	SBO
16	S4_cell_1- _export	S4_cell_1 export	$S4\_Cell\_1 \longrightarrow \emptyset$	
17	S4_cell_2- _export	S4_cell_2 export	$S4\_Cell\_2 \longrightarrow \emptyset$	
18	S4_ex_import	S4_ex import	$\emptyset \longrightarrow S4\_ex$	

### 8.1 Reaction v1\_cell\_1

This is an irreversible reaction of two reactants forming one product.

**Name** v1\_cell\_1

#### Reaction equation



#### Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
S1_Cell_1	S1	
A3_Cell_1	A3	

#### Product

Table 7: Properties of each product.

Id	Name	SBO
S2_Cell_1	S2	

#### Kinetic Law

**Derived unit** contains undeclared units

$$v_1 = \text{vol}(\text{Cell}_1) \cdot \text{function\_for\_v1}(k_1, [S1\_Cell\_1], [A3\_Cell\_1], K_I, q) \quad (13)$$

$$\text{function\_for\_v1}(k_1, S1, A3, K_I, q) = k_1 \cdot S1 \cdot A3 \cdot \left(1 + \left(\frac{A3}{K_I}\right)^q\right)^1 \quad (14)$$

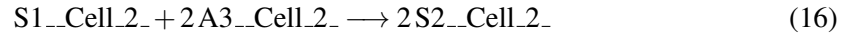
$$\text{function\_for\_v1}(k_1, S1, A3, K_I, q) = k_1 \cdot S1 \cdot A3 \cdot \left(1 + \left(\frac{A3}{K_I}\right)^q\right)^1 \quad (15)$$

### 8.2 Reaction v1\_cell\_2

This is an irreversible reaction of two reactants forming one product.

**Name** v1\_cell\_2

### Reaction equation



### Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
S1_Cell_2	S1	
A3_Cell_2	A3	

### Product

Table 9: Properties of each product.

Id	Name	SBO
S2_Cell_2	S2	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_2 = \text{vol}(\text{Cell}_2) \cdot \text{function\_for\_v1}(k_1, [S1\_Cell\_2], [A3\_Cell\_2], K_I, q) \quad (17)$$

$$\text{function\_for\_v1}(k_1, S1, A3, K_I, q) = k_1 \cdot S1 \cdot A3 \cdot \left(1 + \left(\frac{A3}{K_I}\right)^q\right)^{-1} \quad (18)$$

$$\text{function\_for\_v1}(k_1, S1, A3, K_I, q) = k_1 \cdot S1 \cdot A3 \cdot \left(1 + \left(\frac{A3}{K_I}\right)^q\right)^{-1} \quad (19)$$

### 8.3 Reaction v2\_cell\_1

This is an irreversible reaction of two reactants forming two products.

**Name** v2\_cell\_1

### Reaction equation



### Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
S2__Cell_1_	S2	
N1__Cell_1_	N1	

## Products

Table 11: Properties of each product.

Id	Name	SBO
S3__Cell_1_	S3	
N2__Cell_1_	N2	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_3 = \text{vol}(\text{Cell}_1) \cdot \text{function\_for\_v2}(k_2, [\text{S2\_Cell}_1], [\text{N1\_Cell}_1]) \quad (21)$$

$$\text{function\_for\_v2}(k_2, \text{S2}, \text{N1}) = k_2 \cdot \text{S2} \cdot \text{N1} \quad (22)$$

$$\text{function\_for\_v2}(k_2, \text{S2}, \text{N1}) = k_2 \cdot \text{S2} \cdot \text{N1} \quad (23)$$

## 8.4 Reaction v2\_cell\_2

This is an irreversible reaction of two reactants forming two products.

**Name** v2\_cell\_2

### Reaction equation



## Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
S2__Cell_2_	S2	
N1__Cell_2_	N1	

## Products

Table 13: Properties of each product.

Id	Name	SBO
S3__Cell_2_	S3	
N2__Cell_2_	N2	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_4 = \text{vol}(\text{Cell}_2) \cdot \text{function\_for\_v2}(k_2, [\text{S2\_Cell}_2], [\text{N1\_Cell}_2]) \quad (25)$$

$$\text{function\_for\_v2}(k_2, \text{S2}, \text{N1}) = k_2 \cdot \text{S2} \cdot \text{N1} \quad (26)$$

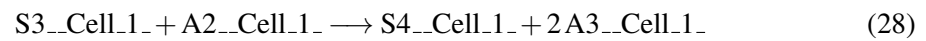
$$\text{function\_for\_v2}(k_2, \text{S2}, \text{N1}) = k_2 \cdot \text{S2} \cdot \text{N1} \quad (27)$$

## 8.5 Reaction v3\_cell\_1

This is an irreversible reaction of two reactants forming two products.

**Name** v3\_cell\_1

### Reaction equation



## Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
S3__Cell_1_	S3	
A2__Cell_1_	A2	

## Products

Table 15: Properties of each product.

Id	Name	SBO
S4__Cell_1_	S4	
A3__Cell_1_	A3	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_5 = \text{vol}(\text{Cell}_1) \cdot \text{function\_for\_v3}(k_3, [\text{S3\_Cell}_1], [\text{A2\_Cell}_1]) \quad (29)$$

$$\text{function\_for\_v3}(k_3, \text{S3}, \text{A2}) = k_3 \cdot \text{S3} \cdot \text{A2} \quad (30)$$

$$\text{function\_for\_v3}(k_3, \text{S3}, \text{A2}) = k_3 \cdot \text{S3} \cdot \text{A2} \quad (31)$$

## 8.6 Reaction v3\_cell\_2

This is an irreversible reaction of two reactants forming two products.

**Name** v3\_cell\_2

### Reaction equation



## Reactants

Table 16: Properties of each reactant.

Id	Name	SBO
S3__Cell_2_	S3	
A2__Cell_2_	A2	

## Products

Table 17: Properties of each product.

Id	Name	SBO
S4__Cell_2_	S4	
A3__Cell_2_	A3	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_6 = \text{vol}(\text{Cell}_2) \cdot \text{function\_for\_v3}(k_3, [\text{S3\_Cell}_2], [\text{A2\_Cell}_2]) \quad (33)$$

$$\text{function\_for\_v3}(k_3, \text{S3}, \text{A2}) = k_3 \cdot \text{S3} \cdot \text{A2} \quad (34)$$

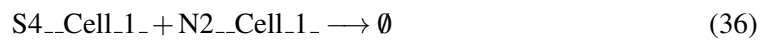
$$\text{function\_for\_v3}(k_3, \text{S3}, \text{A2}) = k_3 \cdot \text{S3} \cdot \text{A2} \quad (35)$$

## 8.7 Reaction v4\_cell\_1

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

**Name** v4\_cell\_1

### Reaction equation



## Reactants



Table 18: Properties of each reactant.

Id	Name	SBO
S4_Cell_1_	S4	
N2_Cell_1_	N2	

### Kinetic Law

**Derived unit** contains undeclared units

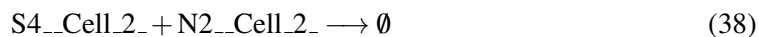
$$v_7 = \text{vol}(\text{Cell}_1) \cdot k_4 \cdot [\text{S4\_Cell}_1] \cdot [\text{N2\_Cell}_1] \quad (37)$$

### 8.8 Reaction v4\_cell\_2

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

**Name** v4\_cell\_2

### Reaction equation



### Reactants

Table 19: Properties of each reactant.

Id	Name	SBO
S4_Cell_2_	S4	
N2_Cell_2_	N2	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_8 = \text{vol}(\text{Cell}_2) \cdot k_4 \cdot [\text{S4\_Cell}_2] \cdot [\text{N2\_Cell}_2] \quad (39)$$

### 8.9 Reaction v5\_cell\_1

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

**Name** v5\_cell\_1

### Reaction equation



### Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
A3_Cell_1_	A3	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_9 = \text{vol}(\text{Cell\_1\_}) \cdot k_5 \cdot [\text{A3\_Cell\_1\_}] \quad (41)$$

### 8.10 Reaction v5\_cell\_2

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

**Name** v5\_cell\_2

### Reaction equation



### Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
A3_Cell_2_	A3	

### Kinetic Law

**Derived unit** contains undeclared units

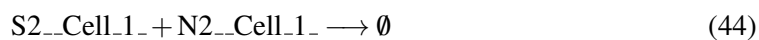
$$v_{10} = \text{vol}(\text{Cell\_2\_}) \cdot k_5 \cdot [\text{A3\_Cell\_2\_}] \quad (43)$$

### 8.11 Reaction v6\_cell\_1

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

**Name** v6\_cell\_1

### Reaction equation



### Reactants

Table 22: Properties of each reactant.

Id	Name	SBO
S2_Cell_1_	S2	
N2_Cell_1_	N2	

### Kinetic Law

**Derived unit** contains undeclared units

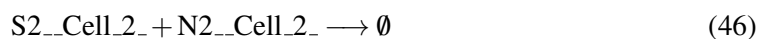
$$v_{11} = \text{vol}(\text{Cell}_1) \cdot k_6 \cdot [\text{S2\_Cell}_1] \cdot [\text{N2\_Cell}_1] \quad (45)$$

## 8.12 Reaction v6\_cell\_2

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

**Name** v6\_cell\_2

### Reaction equation



### Reactants

Table 23: Properties of each reactant.

Id	Name	SBO
S2_Cell_2_	S2	
N2_Cell_2_	N2	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{12} = \text{vol}(\text{Cell}_2) \cdot k_6 \cdot [\text{S2\_Cell}_2] \cdot [\text{N2\_Cell}_2] \quad (47)$$

### 8.13 Reaction $v_7$

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

**Name**  $v_7$

#### Reaction equation



#### Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
S4_ex	S4_ex	

#### Kinetic Law

**Derived unit** contains undeclared units

$$v_{13} = \text{vol}(\text{Compartment}) \cdot k \cdot [\text{S4\_ex}] \quad (49)$$

### 8.14 Reaction $\text{S1\_cell}_1\text{glucose\_influx}$

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

**Name**  $\text{S1\_cell}_1$  glucose influx

#### Reaction equation



#### Product

Table 25: Properties of each product.

Id	Name	SBO
S1_Cell_1	S1	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{14} = \text{vol}(\text{Cell\_1}) \cdot \text{Constant\_flux\_irreversible}(J0) \quad (51)$$

$$\text{Constant\_flux\_irreversible}(v) = v \quad (52)$$

$$\text{Constant\_flux\_irreversible}(v) = v \quad (53)$$

### 8.15 Reaction S1\_cell\_2\_glucose\_influx

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

**Name** S1\_cell\_2 glucose influx

### Reaction equation



### Product

Table 26: Properties of each product.

Id	Name	SBO
S1_Cell_2_	S1	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{15} = \text{vol}(\text{Cell\_2}) \cdot \text{Constant\_flux\_irreversible}(J0) \quad (55)$$

$$\text{Constant\_flux\_irreversible}(v) = v \quad (56)$$

$$\text{Constant\_flux\_irreversible}(v) = v \quad (57)$$

### 8.16 Reaction S4\_cell\_1\_export

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

**Name** S4\_cell\_1 export

### Reaction equation



### Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
S4_Cell_1_	S4	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{16} = \text{vol}(\text{Cell\_1}) \cdot \text{Constant\_flux\_irreversible}(\text{J\_cell\_1}) \quad (59)$$

$$\text{Constant\_flux\_irreversible}(v) = v \quad (60)$$

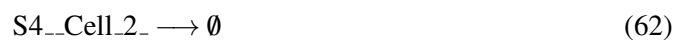
$$\text{Constant\_flux\_irreversible}(v) = v \quad (61)$$

## 8.17 Reaction S4\_cell\_2\_export

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

**Name** S4\_cell\_2 export

### Reaction equation



### Reactant

Table 28: Properties of each reactant.

Id	Name	SBO
S4_Cell_2_	S4	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{17} = \text{vol}(\text{Cell}_2) \cdot \text{Constant\_flux\_irreversible}(j\_cell\_2) \quad (63)$$

$$\text{Constant\_flux\_irreversible}(v) = v \quad (64)$$

$$\text{Constant\_flux\_irreversible}(v) = v \quad (65)$$

### 8.18 Reaction S4\_ex\_import

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

**Name** S4\_ex import

#### Reaction equation



#### Product

Table 29: Properties of each product.

Id	Name	SBO
S4_ex	S4_ex	

#### Kinetic Law

**Derived unit** contains undeclared units

$$v_{18} = \text{vol}(\text{Compartment}) \cdot \text{function\_for\_d\_dt\_S4\_ex}(\text{phi}, J_{\text{cell}_1}, j_{\text{cell}_2}) \quad (67)$$

$$\text{function\_for\_d\_dt\_S4\_ex}(\text{phi}, J_1, J_2) = \frac{\text{phi}}{2} \cdot (J_1 + J_2) \quad (68)$$

$$\text{function\_for\_d\_dt\_S4\_ex}(\text{phi}, J_1, J_2) = \frac{\text{phi}}{2} \cdot (J_1 + J_2) \quad (69)$$

## 9 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.

### 9.1 Species `S1__Cell_1_`

**Name** S1

**Initial concentration** 5.8 mmol · ml<sup>-1</sup>

This species takes part in two reactions (as a reactant in `v1_cell_1` and as a product in `S1__cell_1_glucose_influx`).

$$\frac{d}{dt}S1\_Cell\_1\_ = v_{14} - v_1 \quad (70)$$

### 9.2 Species `S1__Cell_2_`

**Name** S1

**Initial concentration** 2.9 mmol · ml<sup>-1</sup>

This species takes part in two reactions (as a reactant in `v1_cell_2` and as a product in `S1__cell_2_glucose_influx`).

$$\frac{d}{dt}S1\_Cell\_2\_ = v_{15} - v_2 \quad (71)$$

### 9.3 Species `S2__Cell_1_`

**Name** S2

**Initial concentration** 0.9 mmol · ml<sup>-1</sup>

This species takes part in three reactions (as a reactant in `v2_cell_1`, `v6_cell_1` and as a product in `v1_cell_1`).

$$\frac{d}{dt}S2\_Cell\_1\_ = 2 v_1 - v_3 - v_{11} \quad (72)$$

### 9.4 Species `S2__Cell_2_`

**Name** S2

**Initial concentration** 0.45 mmol · ml<sup>-1</sup>

This species takes part in three reactions (as a reactant in `v2_cell_2`, `v6_cell_2` and as a product in `v1_cell_2`).

$$\frac{d}{dt}S2\_Cell\_2\_ = 2 v_2 - v_4 - v_{12} \quad (73)$$



### 9.5 Species S3\_\_Cell\_1\_

**Name** S3

**Initial concentration** 0.2 mmol · ml<sup>-1</sup>

This species takes part in two reactions (as a reactant in [v3\\_cell\\_1](#) and as a product in [v2\\_cell\\_1](#)).

$$\frac{d}{dt}S3\_Cell\_1\_ = v_3 - v_5 \quad (74)$$

### 9.6 Species S3\_\_Cell\_2\_

**Name** S3

**Initial concentration** 0.1 mmol · ml<sup>-1</sup>

This species takes part in two reactions (as a reactant in [v3\\_cell\\_2](#) and as a product in [v2\\_cell\\_2](#)).

$$\frac{d}{dt}S3\_Cell\_2\_ = v_4 - v_6 \quad (75)$$

### 9.7 Species S4\_\_Cell\_1\_

**Name** S4

**Initial concentration** 0.2 mmol · ml<sup>-1</sup>

This species takes part in three reactions (as a reactant in [v4\\_cell\\_1](#), [S4\\_cell\\_1\\_export](#) and as a product in [v3\\_cell\\_1](#)).

$$\frac{d}{dt}S4\_Cell\_1\_ = v_5 - v_7 - v_{16} \quad (76)$$

### 9.8 Species S4\_\_Cell\_2\_

**Name** S4

**Initial concentration** 0.1 mmol · ml<sup>-1</sup>

This species takes part in three reactions (as a reactant in [v4\\_cell\\_2](#), [S4\\_cell\\_2\\_export](#) and as a product in [v3\\_cell\\_2](#)).

$$\frac{d}{dt}S4\_Cell\_2\_ = v_6 - v_8 - v_{17} \quad (77)$$

### 9.9 Species N2\_\_Cell\_1\_

**Name** N2

**Initial concentration** 0.1 mmol · ml<sup>-1</sup>

This species takes part in three reactions (as a reactant in [v4\\_cell\\_1](#), [v6\\_cell\\_1](#) and as a product in [v2\\_cell\\_1](#)).

$$\frac{d}{dt}N2\_Cell\_1\_ = v_3 - v_7 - v_{11} \quad (78)$$

### 9.10 Species N2\_\_Cell\_2\_

**Name** N2

**Initial concentration** 0.05 mmol · ml<sup>-1</sup>

This species takes part in three reactions (as a reactant in [v4\\_cell\\_2](#), [v6\\_cell\\_2](#) and as a product in [v2\\_cell\\_2](#)).

$$\frac{d}{dt}N2\_Cell\_2\_ = v_4 - v_8 - v_{12} \quad (79)$$

### 9.11 Species A3\_\_Cell\_1\_

**Name** A3

**Initial concentration** 3.2 mmol · ml<sup>-1</sup>

This species takes part in three reactions (as a reactant in [v1\\_cell\\_1](#), [v5\\_cell\\_1](#) and as a product in [v3\\_cell\\_1](#)).

$$\frac{d}{dt}A3\_Cell\_1\_ = 2 v_5 - 2 v_1 - v_9 \quad (80)$$

### 9.12 Species A3\_\_Cell\_2\_

**Name** A3

**Initial concentration** 0.2 mmol · ml<sup>-1</sup>

This species takes part in three reactions (as a reactant in [v1\\_cell\\_2](#), [v5\\_cell\\_2](#) and as a product in [v3\\_cell\\_2](#)).

$$\frac{d}{dt}A3\_Cell\_2\_ = 2 v_6 - 2 v_2 - v_{10} \quad (81)$$

### 9.13 Species [S4\\_ex](#)

**Name** S4\_ex

**Initial concentration** 0.1 mmol · ml<sup>-1</sup>

This species takes part in two reactions (as a reactant in [v7](#) and as a product in [S4\\_ex\\_import](#)).

$$\frac{d}{dt}S4\_ex = v_{18} - v_{13} \quad (82)$$

### 9.14 Species [A](#)

**Name** A

**Initial concentration** 4 mmol · ml<sup>-1</sup>

$$\frac{d}{dt}A = 0 \quad (83)$$

### 9.15 Species [N](#)

**Name** N

**Initial concentration** 1 mmol · ml<sup>-1</sup>

$$\frac{d}{dt}N = 0 \quad (84)$$

### 9.16 Species [N1\\_\\_Cell\\_1\\_](#)

**Name** N1

**Initial concentration** 0.9 mmol · ml<sup>-1</sup>

**Involved in rule** [N1\\_\\_Cell\\_1\\_](#)

This species takes part in one reaction (as a reactant in [v2\\_cell\\_1](#)). Not this but one rule determines the species' quantity because this species is on the boundary of the reaction system.

### 9.17 Species [N1\\_\\_Cell\\_2\\_](#)

**Name** N1

**Initial concentration** 0.95 mmol · ml<sup>-1</sup>

**Involved in rule** [N1\\_\\_Cell\\_2\\_](#)

This species takes part in one reaction (as a reactant in [v2\\_cell\\_2](#)). Not this but one rule determines the species' quantity because this species is on the boundary of the reaction system.

### 9.18 Species A2\_\_Cell\_1\_

**Name** A2

**Initial concentration**  $0.8 \text{ mmol} \cdot \text{ml}^{-1}$

**Involved in rule** A2\_\_Cell\_1\_

This species takes part in one reaction (as a reactant in v3\_cell\_1). Not this but one rule determines the species' quantity because this species is on the boundary of the reaction system.

### 9.19 Species A2\_\_Cell\_2\_

**Name** A2

**Initial concentration**  $3.8 \text{ mmol} \cdot \text{ml}^{-1}$

**Involved in rule** A2\_\_Cell\_2\_

This species takes part in one reaction (as a reactant in v3\_cell\_2). Not this but one rule determines the species' quantity because this species is on the boundary of the reaction system.

SBML2<sup>AT</sup>EX was developed by Andreas Dräger<sup>a</sup>, Hannes Planatscher<sup>a</sup>, Dieudonné M Wouamba<sup>a</sup>, Adrian Schröder<sup>a</sup>, Michael Hucka<sup>b</sup>, Lukas Endler<sup>c</sup>, Martin Golebiewski<sup>d</sup> and Andreas Zell<sup>a</sup>. Please see <http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX> for more information.

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