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[1] and Catherine Lloyd[2] at March 16th 2018 at 11:24 a. m. and last time modified at March 18th 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 glycolyticoscillations 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.

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^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 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	☑	
`Cell_2`	Cell 2		3	1	litre	☑	
`Compartment`	Compartment		3	1	litre	☑	

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`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
`S1__Cell_2_`	S1	`Cell_2`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
`S2__Cell_1_`	S2	`Cell_1`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
`S2__Cell_2_`	S2	`Cell_2`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
`S3__Cell_1_`	S3	`Cell_1`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
`S3__Cell_2_`	S3	`Cell_2`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
`S4__Cell_1_`	S4	`Cell_1`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
`S4__Cell_2_`	S4	`Cell_2`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
`N2__Cell_1_`	N2	`Cell_1`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
`N2__Cell_2_`	N2	`Cell_2`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
`A3__Cell_1_`	A3	`Cell_1`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
`A3__Cell_2_`	A3	`Cell_2`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
`S4_ex`	S4_ex	`Compartment`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
`A`	A	`Compartment`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☑	☑
`N`	N	`Compartment`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☑	☑
`N1__Cell_1_`	N1	`Cell_1`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☑
`N1__Cell_2_`	N1	`Cell_2`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☑
`A2__Cell_1_`	A2	`Cell_1`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☑
`A2__Cell_2_`	A2	`Cell_2`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☑

5 Parameters

This model contains 14 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		100.00		☑
K_I	K_I		0.52		☑
q	q		4.00		☑
k2	k2		6.00		☑
k3	k3		16.00		☑
k4	k4		100.00		☑
k5	k5		1.28		☑
k6	k6		12.00		☑
k	k		1.50		☑
J0	J0		3.00		☑
J_cell_1	J_cell_1		1.30		☐
j_cell_2	j_cell_2		0.00		☐
kappa	kappa		13.00		☑
phi	phi		0.10		☑

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

$$v \tag{1}$$

6.2 Function definition function_for_v2

Name function for v2

Arguments k2, S2, N1

Mathematical Expression

$$k2 \cdot S2 \cdot N1 \tag{2}$$

6.3 Function definition function_for_d_dt_S4_ex

Name function for d/dt(S4_ex)

Arguments phi, J1, J2

Mathematical Expression

$$\frac{\mathrm{phi}}{2} \cdot (\mathrm{J1} + \mathrm{J2}) \tag{3}$$

6.4 Function definition function_for_v1

Name function for v1

Arguments k1, S1, A3, K_I, q

Mathematical Expression

$$\mathrm{k1} \cdot \mathrm{S1} \cdot \mathrm{A3} \cdot \left(1 + \left(\frac{\mathrm{A3}}{\mathrm{K\_I}}\right)^{\mathrm{q}}\right)^{1} \tag{4}$$

6.5 Function definition function_for_v3

Name function for v3

Arguments k3, S3, A2

Mathematical Expression

$$\mathrm{k3} \cdot \mathrm{S3} \cdot \mathrm{A2} \tag{5}$$

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:

$$\mathrm{j\_cell\_2} = \mathrm{kappa} \cdot ([\mathrm{S4\_\_Cell\_2\_}] - [\mathrm{S4\_ex}]) \tag{6}$$

7.2 Rule J_cell_1

Rule J_cell_1 is an assignment rule for parameter J_cell_1:

$$\mathrm{J\_cell\_1} = \mathrm{kappa} \cdot ([\mathrm{S4\_\_Cell\_1\_}] - [\mathrm{S4\_ex}]) \tag{7}$$

7.3 Rule `N1__Cell_2_`

Rule `N1__Cell_2_` is an assignment rule for species `N1__Cell_2_`:

$$\mathrm{N1\_\_Cell\_2\_} = [\mathrm{N}] - [\mathrm{N2\_\_Cell\_2\_}] \tag{8}$$

Derived unit $\mathrm{mmol} \cdot \mathrm{ml}^{-1}$

7.4 Rule `N1__Cell_1_`

Rule `N1__Cell_1_` is an assignment rule for species `N1__Cell_1_`:

$$\mathrm{N1\_\_Cell\_1\_} = [\mathrm{N}] - [\mathrm{N2\_\_Cell\_1\_}] \tag{9}$$

Derived unit $\mathrm{mmol} \cdot \mathrm{ml}^{-1}$

7.5 Rule `A2__Cell_1_`

Rule `A2__Cell_1_` is an assignment rule for species `A2__Cell_1_`:

$$\mathrm{A2\_\_Cell\_1\_} = [\mathrm{A}] - [\mathrm{A3\_\_Cell\_1\_}] \tag{10}$$

Derived unit $\mathrm{mmol} \cdot \mathrm{ml}^{-1}$

7.6 Rule `A2__Cell_2_`

Rule `A2__Cell_2_` is an assignment rule for species `A2__Cell_2_`:

$$\mathrm{A2\_\_Cell\_2\_} = [\mathrm{A}] - [\mathrm{A3\_\_Cell\_2\_}] \tag{11}$$

Derived unit $\mathrm{mmol} \cdot \mathrm{ml}^{-1}$

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

№	Id	Name	Reaction Equation	SBO
1	`v1_cell_1`	v1_cell_1	S1__Cell_1_ + 2 A3__Cell_1_ $\longrightarrow$ 2 S2__Cell_1_	
2	`v1_cell_2`	v1_cell_2	S1__Cell_2_ + 2 A3__Cell_2_ $\longrightarrow$ 2 S2__Cell_2_	
3	`v2_cell_1`	v2_cell_1	S2__Cell_1_ + N1__Cell_1_ $\longrightarrow$ S3__Cell_1_ + N2__Cell_1_	
4	`v2_cell_2`	v2_cell_2	S2__Cell_2_ + N1__Cell_2_ $\longrightarrow$ S3__Cell_2_ + N2__Cell_2_	
5	`v3_cell_1`	v3_cell_1	S3__Cell_1_ + A2__Cell_1_ $\longrightarrow$ S4__Cell_1_ + 2 A3__Cell_1_	
6	`v3_cell_2`	v3_cell_2	S3__Cell_2_ + A2__Cell_2_ $\longrightarrow$ S4__Cell_2_ + 2 A3__Cell_2_	
7	`v4_cell_1`	v4_cell_1	S4__Cell_1_ + N2__Cell_1_ $\longrightarrow \emptyset$	
8	`v4_cell_2`	v4_cell_2	S4__Cell_2_ + N2__Cell_2_ $\longrightarrow \emptyset$	
9	`v5_cell_1`	v5_cell_1	A3__Cell_1_ $\longrightarrow \emptyset$	
10	`v5_cell_2`	v5_cell_2	A3__Cell_2_ $\longrightarrow \emptyset$	
11	`v6_cell_1`	v6_cell_1	S2__Cell_1_ + N2__Cell_1_ $\longrightarrow \emptyset$	
12	`v6_cell_2`	v6_cell_2	S2__Cell_2_ + N2__Cell_2_ $\longrightarrow \emptyset$	
13	`v7`	v7	S4_ex $\longrightarrow \emptyset$	
14	`S1_cell_1-_glucose_influx`	S1_cell_1 glucose influx	$\emptyset \longrightarrow$ S1__Cell_1_	
15	`S1_cell_2-_glucose_influx`	S1_cell_2 glucose influx	$\emptyset \longrightarrow$ S1__Cell_2_	

№	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

$$\text{S1\_\_Cell\_1\_} + 2\,\text{A3\_\_Cell\_1\_} \longrightarrow 2\,\text{S2\_\_Cell\_1\_} \tag{12}$$

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

$$v_1 = \text{vol}\left(\text{Cell\_1}\right) \cdot \text{function\_for\_v1}\left(\text{k1}, [\text{S1\_\_Cell\_1\_}], [\text{A3\_\_Cell\_1\_}], \text{K\_I}, \text{q}\right) \tag{13}$$

$$\text{function\_for\_v1}\left(\text{k1}, \text{S1}, \text{A3}, \text{K\_I}, \text{q}\right) = \text{k1} \cdot \text{S1} \cdot \text{A3} \cdot \left(1 + \left(\frac{\text{A3}}{\text{K\_I}}\right)^{\text{q}}\right)^{1} \tag{14}$$

$$\text{function\_for\_v1}\left(\text{k1}, \text{S1}, \text{A3}, \text{K\_I}, \text{q}\right) = \text{k1} \cdot \text{S1} \cdot \text{A3} \cdot \left(1 + \left(\frac{\text{A3}}{\text{K\_I}}\right)^{\text{q}}\right)^{1} \tag{15}$$

8.2 Reaction `v1_cell_2`

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

Name v1_cell_2

Reaction equation

$$\mathrm{S1\_\_Cell\_2\_} + 2\,\mathrm{A3\_\_Cell\_2\_} \longrightarrow 2\,\mathrm{S2\_\_Cell\_2\_} \tag{16}$$

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

$$v_2 = \mathrm{vol}\left(\mathrm{Cell\_2}\right) \cdot \mathrm{function\_for\_v1}\left(\mathrm{k1}, [\mathrm{S1\_\_Cell\_2\_}], [\mathrm{A3\_\_Cell\_2\_}], \mathrm{K\_I}, \mathrm{q}\right) \tag{17}$$

$$\mathrm{function\_for\_v1}\left(\mathrm{k1}, \mathrm{S1}, \mathrm{A3}, \mathrm{K\_I}, \mathrm{q}\right) = \mathrm{k1} \cdot \mathrm{S1} \cdot \mathrm{A3} \cdot \left(1 + \left(\frac{\mathrm{A3}}{\mathrm{K\_I}}\right)^{\mathrm{q}}\right)^{1} \tag{18}$$

$$\mathrm{function\_for\_v1}\left(\mathrm{k1}, \mathrm{S1}, \mathrm{A3}, \mathrm{K\_I}, \mathrm{q}\right) = \mathrm{k1} \cdot \mathrm{S1} \cdot \mathrm{A3} \cdot \left(1 + \left(\frac{\mathrm{A3}}{\mathrm{K\_I}}\right)^{\mathrm{q}}\right)^{1} \tag{19}$$

8.3 Reaction `v2_cell_1`

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

Name v2_cell_1

Reaction equation

$$\mathrm{S2\_\_Cell\_1\_} + \mathrm{N1\_\_Cell\_1\_} \longrightarrow \mathrm{S3\_\_Cell\_1\_} + \mathrm{N2\_\_Cell\_1\_} \tag{20}$$

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

$$v_3 = \mathrm{vol}\left(\mathrm{Cell\_1}\right) \cdot \mathrm{function\_for\_v2}\left(\mathrm{k2}, [\mathrm{S2\_\_Cell\_1\_}], [\mathrm{N1\_\_Cell\_1\_}]\right) \tag{21}$$

$$\mathrm{function\_for\_v2}\left(\mathrm{k2}, \mathrm{S2}, \mathrm{N1}\right) = \mathrm{k2} \cdot \mathrm{S2} \cdot \mathrm{N1} \tag{22}$$

$$\mathrm{function\_for\_v2}\left(\mathrm{k2}, \mathrm{S2}, \mathrm{N1}\right) = \mathrm{k2} \cdot \mathrm{S2} \cdot \mathrm{N1} \tag{23}$$

8.4 Reaction v2_cell_2

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

Name v2_cell_2

Reaction equation

$$\mathrm{S2\_\_Cell\_2\_} + \mathrm{N1\_\_Cell\_2\_} \longrightarrow \mathrm{S3\_\_Cell\_2\_} + \mathrm{N2\_\_Cell\_2\_} \tag{24}$$

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

$$v_4 = \mathrm{vol}\left(\mathrm{Cell\_2}\right) \cdot \mathrm{function\_for\_v2}\left(\mathrm{k2}, [\mathrm{S2\_\_Cell\_2\_}], [\mathrm{N1\_\_Cell\_2\_}]\right) \tag{25}$$

$$\mathrm{function\_for\_v2}\left(\mathrm{k2}, \mathrm{S2}, \mathrm{N1}\right) = \mathrm{k2} \cdot \mathrm{S2} \cdot \mathrm{N1} \tag{26}$$

$$\mathrm{function\_for\_v2}\left(\mathrm{k2}, \mathrm{S2}, \mathrm{N1}\right) = \mathrm{k2} \cdot \mathrm{S2} \cdot \mathrm{N1} \tag{27}$$

8.5 Reaction v3_cell_1

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

Name v3_cell_1

Reaction equation

$$\mathrm{S3\_\_Cell\_1\_} + \mathrm{A2\_\_Cell\_1\_} \longrightarrow \mathrm{S4\_\_Cell\_1\_} + 2\,\mathrm{A3\_\_Cell\_1\_} \tag{28}$$

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

$$v_5 = \mathrm{vol}\left(\mathrm{Cell\_1}\right) \cdot \mathrm{function\_for\_v3}\left(\mathrm{k3}, [\mathrm{S3\_\_Cell\_1\_}], [\mathrm{A2\_\_Cell\_1\_}]\right) \tag{29}$$

$$\mathrm{function\_for\_v3}\left(\mathrm{k3}, \mathrm{S3}, \mathrm{A2}\right) = \mathrm{k3} \cdot \mathrm{S3} \cdot \mathrm{A2} \tag{30}$$

$$\mathrm{function\_for\_v3}\left(\mathrm{k3}, \mathrm{S3}, \mathrm{A2}\right) = \mathrm{k3} \cdot \mathrm{S3} \cdot \mathrm{A2} \tag{31}$$

8.6 Reaction v3_cell_2

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

Name v3_cell_2

Reaction equation

$$\mathrm{S3\_\_Cell\_2\_} + \mathrm{A2\_\_Cell\_2\_} \longrightarrow \mathrm{S4\_\_Cell\_2\_} + 2\,\mathrm{A3\_\_Cell\_2\_} \tag{32}$$

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

$$v_6 = \mathrm{vol}\left(\mathrm{Cell\_2}\right) \cdot \mathrm{function\_for\_v3}\left(\mathrm{k3}, [\mathrm{S3\_\_Cell\_2\_}], [\mathrm{A2\_\_Cell\_2\_}]\right) \tag{33}$$

$$\mathrm{function\_for\_v3}\left(\mathrm{k3}, \mathrm{S3}, \mathrm{A2}\right) = \mathrm{k3} \cdot \mathrm{S3} \cdot \mathrm{A2} \tag{34}$$

$$\mathrm{function\_for\_v3}\left(\mathrm{k3}, \mathrm{S3}, \mathrm{A2}\right) = \mathrm{k3} \cdot \mathrm{S3} \cdot \mathrm{A2} \tag{35}$$

8.7 Reaction `v4_cell_1`

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

Name v4_cell_1

Reaction equation

$$\mathrm{S4\_\_Cell\_1\_} + \mathrm{N2\_\_Cell\_1\_} \longrightarrow \emptyset \tag{36}$$

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

$$v_7 = \mathrm{vol}\left(\mathrm{Cell\_1}\right) \cdot \mathrm{k4} \cdot [\mathrm{S4\_\_Cell\_1\_}] \cdot [\mathrm{N2\_\_Cell\_1\_}] \tag{37}$$

8.8 Reaction v4_cell_2

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

Name v4_cell_2

Reaction equation

$$\mathrm{S4\_\_Cell\_2\_} + \mathrm{N2\_\_Cell\_2\_} \longrightarrow \emptyset \tag{38}$$

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

$$v_8 = \mathrm{vol}\left(\mathrm{Cell\_2}\right) \cdot \mathrm{k4} \cdot [\mathrm{S4\_\_Cell\_2\_}] \cdot [\mathrm{N2\_\_Cell\_2\_}] \tag{39}$$

8.9 Reaction v5_cell_1

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

Name v5_cell_1

Reaction equation

$$\text{A3\_\_Cell\_1\_} \longrightarrow \emptyset \tag{40}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
A3__Cell_1_	A3	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{vol}\,(\text{Cell\_1}) \cdot \text{k5} \cdot [\text{A3\_\_Cell\_1\_}] \tag{41}$$

8.10 Reaction v5_cell_2

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

Name v5_cell_2

Reaction equation

$$\text{A3\_\_Cell\_2\_} \longrightarrow \emptyset \tag{42}$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
A3__Cell_2_	A3	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{vol}\,(\text{Cell\_2}) \cdot \text{k5} \cdot [\text{A3\_\_Cell\_2\_}] \tag{43}$$

8.11 Reaction v6_cell_1

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

Name v6_cell_1

Reaction equation

$$\text{S2\_\_Cell\_1\_} + \text{N2\_\_Cell\_1\_} \longrightarrow \emptyset \tag{44}$$

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

$$v_{11} = \text{vol}\left(\text{Cell\_1}\right) \cdot \text{k6} \cdot [\text{S2\_\_Cell\_1\_}] \cdot [\text{N2\_\_Cell\_1\_}] \tag{45}$$

8.12 Reaction v6_cell_2

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

Name v6_cell_2

Reaction equation

$$\text{S2\_\_Cell\_2\_} + \text{N2\_\_Cell\_2\_} \longrightarrow \emptyset \tag{46}$$

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

$$v_{12} = \mathrm{vol}\left(\mathrm{Cell\_2}\right) \cdot \mathrm{k6} \cdot [\mathrm{S2\_\_Cell\_2\_}] \cdot [\mathrm{N2\_\_Cell\_2\_}] \qquad (47)$$

8.13 Reaction v7

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

Name v7

Reaction equation

$$\mathrm{S4\_ex} \longrightarrow \emptyset \qquad (48)$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
S4_ex	S4_ex	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}\left(\mathrm{Compartment}\right) \cdot \mathrm{k} \cdot [\mathrm{S4\_ex}] \qquad (49)$$

8.14 Reaction S1_cell_1_glucose_influx

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

Name S1_cell_1 glucose influx

Reaction equation

$$\emptyset \longrightarrow \mathrm{S1\_\_Cell\_1\_} \qquad (50)$$

Product

Table 25: Properties of each product.

Id	Name	SBO
S1__Cell_1_	S1	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{vol}\left(\mathrm{Cell\_1}\right) \cdot \mathrm{Constant\_flux\_\_irreversible}\left(\mathrm{J0}\right) \tag{51}$$

$$\mathrm{Constant\_flux\_\_irreversible}\left(\mathrm{v}\right) = \mathrm{v} \tag{52}$$

$$\mathrm{Constant\_flux\_\_irreversible}\left(\mathrm{v}\right) = \mathrm{v} \tag{53}$$

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

$$\emptyset \longrightarrow \mathrm{S1\_\_Cell\_2\_} \tag{54}$$

Product

Table 26: Properties of each product.

Id	Name	SBO
`S1__Cell_2_`	S1	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{vol}\left(\mathrm{Cell\_2}\right) \cdot \mathrm{Constant\_flux\_\_irreversible}\left(\mathrm{J0}\right) \tag{55}$$

$$\mathrm{Constant\_flux\_\_irreversible}\left(\mathrm{v}\right) = \mathrm{v} \tag{56}$$

$$\mathrm{Constant\_flux\_\_irreversible}\left(\mathrm{v}\right) = \mathrm{v} \tag{57}$$

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

$$\text{S4\_\_Cell\_1\_} \longrightarrow \emptyset \tag{58}$$

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
S4__Cell_1_	S4	

Kinetic Law

Derived unit contains undeclared units

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

$$\text{Constant\_flux\_\_irreversible}\left(\text{v}\right) = \text{v} \tag{60}$$

$$\text{Constant\_flux\_\_irreversible}\left(\text{v}\right) = \text{v} \tag{61}$$

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

$$\text{S4\_\_Cell\_2\_} \longrightarrow \emptyset \tag{62}$$

Reactant

Table 28: Properties of each reactant.

Id	Name	SBO
S4__Cell_2_	S4	

Kinetic Law

Derived unit contains undeclared units

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

$$\mathrm{Constant\_flux\_\_irreversible}\left(\mathrm{v}\right) = \mathrm{v} \quad (64)$$

$$\mathrm{Constant\_flux\_\_irreversible}\left(\mathrm{v}\right) = \mathrm{v} \quad (65)$$

8.18 Reaction `S4_ex_import`

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

Name S4_ex import

Reaction equation

$$\emptyset \longrightarrow \mathrm{S4\_ex} \quad (66)$$

Product

Table 29: Properties of each product.

Id	Name	SBO
`S4_ex`	S4_ex	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \mathrm{vol}\left(\mathrm{Compartment}\right) \cdot \mathrm{function\_for\_d\_dt\_S4\_ex}\left(\mathrm{phi}, \mathrm{J\_cell\_1}, \mathrm{j\_cell\_2}\right) \quad (67)$$

$$\mathrm{function\_for\_d\_dt\_S4\_ex}\left(\mathrm{phi}, \mathrm{J1}, \mathrm{J2}\right) = \frac{\mathrm{phi}}{2} \cdot \left(\mathrm{J1} + \mathrm{J2}\right) \quad (68)$$

$$\mathrm{function\_for\_d\_dt\_S4\_ex}\left(\mathrm{phi}, \mathrm{J1}, \mathrm{J2}\right) = \frac{\mathrm{phi}}{2} \cdot \left(\mathrm{J1} + \mathrm{J2}\right) \quad (69)$$

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 $5.8 \text{ mmol} \cdot \text{ml}^{-1}$

This species takes part in two reactions (as a reactant in `v1_cell_1` and as a product in `S1_cell_1_glucose_influx`).

$$\frac{\mathrm{d}}{\mathrm{d}t} \text{S1\_\_Cell\_1\_} = v_{14} - v_{1} \tag{70}$$

9.2 Species `S1__Cell_2_`

Name S1

Initial concentration $2.9 \text{ mmol} \cdot \text{ml}^{-1}$

This species takes part in two reactions (as a reactant in `v1_cell_2` and as a product in `S1_cell_2_glucose_influx`).

$$\frac{\mathrm{d}}{\mathrm{d}t} \text{S1\_\_Cell\_2\_} = v_{15} - v_{2} \tag{71}$$

9.3 Species `S2__Cell_1_`

Name S2

Initial concentration $0.9 \text{ mmol} \cdot \text{ml}^{-1}$

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`).

$$\frac{\mathrm{d}}{\mathrm{d}t} \text{S2\_\_Cell\_1\_} = 2\, v_{1} - v_{3} - v_{11} \tag{72}$$

9.4 Species `S2__Cell_2_`

Name S2

Initial concentration $0.45 \text{ mmol} \cdot \text{ml}^{-1}$

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`).

$$\frac{\mathrm{d}}{\mathrm{d}t} \text{S2\_\_Cell\_2\_} = 2\, v_{2} - v_{4} - v_{12} \tag{73}$$

9.5 Species S3__Cell_1_

Name S3

Initial concentration $0.2\ \text{mmol} \cdot \text{ml}^{-1}$

This species takes part in two reactions (as a reactant in v3_cell_1 and as a product in v2_cell_1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{S3\_\_Cell\_1\_} = v_3 - v_5 \tag{74}$$

9.6 Species S3__Cell_2_

Name S3

Initial concentration $0.1\ \text{mmol} \cdot \text{ml}^{-1}$

This species takes part in two reactions (as a reactant in v3_cell_2 and as a product in v2_cell_2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{S3\_\_Cell\_2\_} = v_4 - v_6 \tag{75}$$

9.7 Species S4__Cell_1_

Name S4

Initial concentration $0.2\ \text{mmol} \cdot \text{ml}^{-1}$

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{S4\_\_Cell\_1\_} = v_5 - v_7 - v_{16} \tag{76}$$

9.8 Species S4__Cell_2_

Name S4

Initial concentration $0.1\ \text{mmol} \cdot \text{ml}^{-1}$

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{S4\_\_Cell\_2\_} = v_6 - v_8 - v_{17} \tag{77}$$

9.9 Species N2__Cell_1_

Name N2

Initial concentration $0.1\ \mathrm{mmol} \cdot \mathrm{ml}^{-1}$

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{N2\_\_Cell\_1\_} = v_3 - v_7 - v_{11} \tag{78}$$

9.10 Species N2__Cell_2_

Name N2

Initial concentration $0.05\ \mathrm{mmol} \cdot \mathrm{ml}^{-1}$

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{N2\_\_Cell\_2\_} = v_4 - v_8 - v_{12} \tag{79}$$

9.11 Species A3__Cell_1_

Name A3

Initial concentration $3.2\ \mathrm{mmol} \cdot \mathrm{ml}^{-1}$

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A3\_\_Cell\_1\_} = 2\,v_5 - 2\,v_1 - v_9 \tag{80}$$

9.12 Species A3__Cell_2_

Name A3

Initial concentration $0.2\ \mathrm{mmol} \cdot \mathrm{ml}^{-1}$

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A3\_\_Cell\_2\_} = 2\,v_6 - 2\,v_2 - v_{10} \tag{81}$$

9.13 Species S4_ex

Name S4_ex

Initial concentration $0.1\ \mathrm{mmol} \cdot \mathrm{ml}^{-1}$

This species takes part in two reactions (as a reactant in v7 and as a product in S4_ex_import).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S4\_ex} = v_{18} - v_{13} \tag{82}$$

9.14 Species A

Name A

Initial concentration $4\ \mathrm{mmol} \cdot \mathrm{ml}^{-1}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A} = 0 \tag{83}$$

9.15 Species N

Name N

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{N} = 0 \tag{84}$$

9.16 Species N1__Cell_1_

Name N1

Initial concentration $0.9\ \mathrm{mmol} \cdot \mathrm{ml}^{-1}$

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 $0.95\ \mathrm{mmol} \cdot \mathrm{ml}^{-1}$

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.

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