SBML Model Report

Model name: "Cookson2011-_EnzymaticQueueingCoupling"

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 William Mather[2] at November third 2011 at 8:34 a. m. and last time modified at April sixth 2014 at 8:48 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	6
events	0	constraints	0
reactions	8	function definitions	1
global parameters	5	unit definitions	2
rules	0	initial assignments	0

Model Notes

This model is from the article:
Queueing up for enzymatic processing: correlated signaling through coupled degradation.
Natalie A Cookson, William H Mather, Tal Danino, Octavio Mondragn-Palomino, Ruth J Williams, Lev S Tsimring, & Jeff Hasty Molecular Systems Biology2011; 7:561; DOI:10.1038/msb.2011.94

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Abstract:
High-throughput technologies have led to the generation of complex wiring diagrams as a post-sequencing paradigm for depicting the interactions between vast and diverse cellular species. While these diagrams are useful for analyzing biological systems on a large scale, a detailed understanding of the molecular mechanisms that underlie the observed network connections is critical for the further development of systems and synthetic biology. Here, we use queueing theory to investigate how waiting lines can lead to correlations between protein customers that are coupled solely through a downstream set of enzymatic servers. Using the E. coli ClpXP degradation machine as a model processing system, we observe significant cross-talk between two networks that are indirectly coupled through a common set of processors. We further illustrate the implications of enzymatic queueing using a synthetic biology application, in which two independent synthetic networks demonstrate synchronized behavior when common ClpXP machinery is overburdened. Our results demonstrate that such post-translational processes can lead to dynamic connections in cellular networks and may provide a mechanistic understanding of existing but currently inexplicable links.

Note:
Individual stochastic trajectories for a queueing system in three different conditions, 1) Underloaded, 2) Balanced and 3) Overloaded, demonstrate correlation resonance. The parameter values in this model correspond to the Balanced Condition.

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 dimensionless

2.2 Unit `substance`

Name substance

Definition item

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_1	compartment		3	1	dimensionless	☑	

3.1 Compartment compartment_1

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

Name compartment

4 Species

This model contains six 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
species_1	x1	compartment_1	item $\cdot$ dimensionless^{-1}	⊟	⊟
species_2	x2	compartment_1	item $\cdot$ dimensionless^{-1}	⊟	⊟
species_3	E1	compartment_1	item $\cdot$ dimensionless^{-1}	⊟	⊟
species_4	E2	compartment_1	item $\cdot$ dimensionless^{-1}	⊟	⊟
species_5	E	compartment_1	item $\cdot$ dimensionless^{-1}	⊟	⊟
species_6	E+x1	compartment_1	item $\cdot$ dimensionless^{-1}	⊟	⊟

5 Parameters

This model contains five global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
parameter_1	lambda1	0000009	500.000		☑
parameter_2	lambda2	0000009	500.000		☑
parameter_3	mu	0000009	10.000		☑
parameter_4	Kp	0000009	1000.000		☑
parameter_5	g	0000009	0.035		☑

6 Function definition

This is an overview of one function definition.

6.1 Function definition function_1

Name Constant flux (irreversible)

Argument v

Mathematical Expression

$$v \tag{1}$$

7 Reactions

This model contains eight 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	`reaction_1`	binding1	species_1 + species_5 ⟶ species_3	0000344
2	`reaction_2`	binding2	species_2 + species_5 ⟶ species_4	0000344
3	`reaction_3`	production1	∅ ⟶ species_1	0000393
4	`reaction_4`	production2	∅ ⟶ species_2	0000393
5	`reaction_5`	degradation1	species_3 ⟶ species_5	0000179
6	`reaction_6`	degradation2	species_4 ⟶ species_5	0000179
7	`reaction_7`	dilution1	species_1 ⟶ ∅	0000179
8	`reaction_8`	dilution2	species_2 ⟶ ∅	0000179

7.1 Reaction reaction_1

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

Name binding1

SBO:0000344 molecular interaction

Reaction equation

$$\text{species\_1} + \text{species\_5} \longrightarrow \text{species\_3} \tag{2}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
species_1	x1	
species_5	E	

Product

Table 7: Properties of each product.

Id	Name	SBO
species_3	E1	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}(\text{compartment\_1}) \cdot \text{parameter\_4} \cdot [\text{species\_1}] \cdot [\text{species\_5}] \tag{3}$$

7.2 Reaction reaction_2

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

Name binding2

SBO:0000344 molecular interaction

Reaction equation

$$\text{species\_2} + \text{species\_5} \longrightarrow \text{species\_4} \tag{4}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
species_2	x2	
species_5	E	

Product

Table 9: Properties of each product.

Id	Name	SBO
species_4	E2	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}(\mathrm{compartment\_1}) \cdot \mathrm{parameter\_4} \cdot [\mathrm{species\_2}] \cdot [\mathrm{species\_5}] \tag{5}$$

7.3 Reaction reaction_3

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

Name production1

SBO:0000393 production

Reaction equation

$$\emptyset \longrightarrow \mathrm{species\_1} \tag{6}$$

Product

Table 10: Properties of each product.

Id	Name	SBO
species_1	x1	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_1}\left(\mathrm{parameter\_1}\right) \tag{7}$$

$$\mathrm{function\_1}\left(\mathrm{v}\right) = \mathrm{v} \tag{8}$$

$$\mathrm{function\_1}\left(\mathrm{v}\right) = \mathrm{v} \tag{9}$$

7.4 Reaction `reaction_4`

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

Name production2

SBO:0000393 production

Reaction equation

$$\emptyset \longrightarrow \mathrm{species\_2} \tag{10}$$

Product

Table 11: Properties of each product.

Id	Name	SBO
`species_2`	x2	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_1}\left(\mathrm{parameter\_2}\right) \tag{11}$$

$$\mathrm{function\_1}\left(\mathrm{v}\right) = \mathrm{v} \tag{12}$$

$$\mathrm{function\_1}\left(\mathrm{v}\right) = \mathrm{v} \tag{13}$$

7.5 Reaction `reaction_5`

This is an irreversible reaction of one reactant forming one product.

Name degradation1

SBO:0000179 degradation

Reaction equation

$$\text{species\_3} \longrightarrow \text{species\_5} \tag{14}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
species_3	E1	

Product

Table 13: Properties of each product.

Id	Name	SBO
species_5	E	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{vol}\left(\text{compartment\_1}\right) \cdot \text{parameter\_3} \cdot [\text{species\_3}] \tag{15}$$

7.6 Reaction reaction_6

This is an irreversible reaction of one reactant forming one product.

Name degradation2

SBO:0000179 degradation

Reaction equation

$$\text{species\_4} \longrightarrow \text{species\_5} \tag{16}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
species_4	E2	

Product

Table 15: Properties of each product.

Id	Name	SBO
species_5	E	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{parameter\_3} \cdot [\mathrm{species\_4}] \tag{17}$$

7.7 Reaction reaction_7

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

Name dilution1

SBO:0000179 degradation

Reaction equation

$$\mathrm{species\_1} \longrightarrow \emptyset \tag{18}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
species_1	x1	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{parameter\_5} \cdot [\mathrm{species\_1}] \tag{19}$$

7.8 Reaction reaction_8

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

Name dilution2

SBO:0000179 degradation

Reaction equation

$$\text{species\_2} \longrightarrow \emptyset \tag{20}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
species_2	x2	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{vol}\left(\text{compartment\_1}\right) \cdot \text{parameter\_5} \cdot [\text{species\_2}] \tag{21}$$

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 species_1

Name x1

SBO:0000252 polypeptide chain

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

This species takes part in three reactions (as a reactant in reaction_1, reaction_7 and as a product in reaction_3).

$$\frac{\text{d}}{\text{d}t}\text{species\_1} = v_3 - v_1 - v_7 \tag{22}$$

8.2 Species species_2

Name x2

SBO:0000252 polypeptide chain

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

This species takes part in three reactions (as a reactant in reaction_2, reaction_8 and as a product in reaction_4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_2} = v_4 - v_2 - v_8 \tag{23}$$

8.3 Species species_3

Name E1

SBO:0000014 enzyme

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

This species takes part in two reactions (as a reactant in reaction_5 and as a product in reaction_1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_3} = v_1 - v_5 \tag{24}$$

8.4 Species species_4

Name E2

SBO:0000014 enzyme

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

This species takes part in two reactions (as a reactant in reaction_6 and as a product in reaction_2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_4} = v_2 - v_6 \tag{25}$$

8.5 Species species_5

Name E

SBO:0000014 enzyme

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

This species takes part in four reactions (as a reactant in reaction_1, reaction_2 and as a product in reaction_5, reaction_6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_5} = v_5 + v_6 - v_1 - v_2 \tag{26}$$

8.6 Species species_6

Name E+x1

SBO:0000296 macromolecular complex

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

This species does not take part in any reactions. Its quantity does hence not change over time:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_6} = 0 \tag{27}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000009 kinetic constant: Numerical parameter that quantifies the velocity of a chemical reaction

SBO:0000014 enzyme: A protein that catalyzes a chemical reaction. The word comes from en “a” or“i”) and simo “leave” or“yeas”)

SBO:0000179 degradation: Complete disappearance of a physical entity

SBO:0000252 polypeptide chain: Naturally occurring macromolecule formed by the repetition of amino-acid residues linked by peptidic bonds. A polypeptide chain is synthesized by the ribosome. CHEBI:1654

SBO:0000296 macromolecular complex: Non-covalent complex of one or more macromolecules and zero or more simple chemicals

SBO:0000344 molecular interaction: Relationship between molecular entities, based on contacts, direct or indirect.

SBO:0000393 production: Generation 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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