SBML Model Report

Model name: "Chance1952_Catalase_Mechanism"

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: Lukas Endler[1] and Kieran Smallbone[2] at October tenth 2010 at 10:10 a. m. and last time modified at April eighth 2016 at 4:53 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	6
events	0	constraints	0
reactions	3	function definitions	0
global parameters	4	unit definitions	3
rules	0	initial assignments	0

Model Notes

This model is described in the article:
The mechanism of catalase action. II. Electric analog computer studies.
Britton Chance, David S Greenstein, Joseph Higgins, CC Yang, Arch Biochem. 1952 37:322-39. PubmedID:14953444

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Summary:
An electric analog computer has been constructed for a study of the kinetics of catalase action. This computer gives results for the formation and disappearance of the catalase-hydrogen peroxide complex that are in good agreement with the experimental data. The computer study verifies an approximate method for the computation of the velocity constant for the combination of hydrogen peroxide and catalase and justifies the simple formula used previously to compute the velocity constant for the reaction of the catalase-hydrogen peroxide complex with donor molecules. Finally, the computer data show that the binding of peroxide to catalase is a practically irreversible reaction.

The reaction of the enzyme-substrate complex, p, with the electron donor, a, is bimolecular, although in the article, as a is assumed to be constant, it is modelled using an apparent rate constant consisting of the product of the rate constant, k4, and the concentration of a. In this implementation, the concentration of a is set to 1 and the value of k4 just adapted so that the product equals the values given for k4*a in the article. The specific parameter values are taken from Fig 3. The graphs do not exactly match those in the paper, this *may* be due to the different simulators used.

2 Unit Definitions

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

2.1 Unit `substance`

Name micromole

Definition μmol

2.2 Unit `per_uM_per_s`

Name per micromolar per second

Definition $\mu\text{mol}^{-1} \cdot \text{dal} \cdot \text{das}^{-1}$

2.3 Unit `per_s`

Name per second

Definition das^{-1}

2.4 Unit `volume`

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

Definition l

2.5 Unit area

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

Definition m^2

2.6 Unit length

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

Definition m

2.7 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
cell	cell	0000290	3	1	litre	☑	

3.1 Compartment cell

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

Name cell

SBO:0000290 physical compartment

4 Species

This model contains six species. The boundary condition of one of these species is set to `true` so that this species' amount cannot be changed by any reaction. 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
`e`	enzyme E (catalase)	`cell`	$\mu mol \cdot l^{-1}$	☐	☐
`x`	substrate S (hydrogen peroxide)	`cell`	$\mu mol \cdot l^{-1}$	☐	☐
`p`	enzyme-substrate complex ES (catalase - hydrogen peroxide)	`cell`	$\mu mol \cdot l^{-1}$	☐	☐
`p1`	product 1	`cell`	$\mu mol \cdot l^{-1}$	☐	☐
`a`	donor AH2	`cell`	$\mu mol \cdot l^{-1}$	☑	☑
`p2`	product 2	`cell`	$\mu mol \cdot l^{-1}$	☐	☐

5 Parameters

This model contains four global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1		0000339	11.00	$\mu mol^{-1} \cdot dal \cdot das^{-1}$	☑
k2		0000338	0.00	das^{-1}	☑
k4_prime		0000036	16.60	$\mu mol^{-1} \cdot dal \cdot das^{-1}$	☑
k4		0000036	0.72	$\mu mol^{-1} \cdot dal \cdot das^{-1}$	☑

6 Reactions

This model contains three 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	r1	$e + x \rightleftharpoons p$	0000177
2	r2	r2	$p + x \longrightarrow e + p1$	0000200
3	r3	r3	$p + a \longrightarrow e + p2$	0000200

6.1 Reaction r1

This is a reversible reaction of two reactants forming one product.

Name r1

SBO:0000177 non-covalent binding

Reaction equation

$$\mathrm{e} + \mathrm{x} \rightleftharpoons \mathrm{p} \tag{1}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
e	enzyme E (catalase)	
x	substrate S (hydrogen peroxide)	

Product

Table 7: Properties of each product.

Id	Name	SBO
p	enzyme-substrate complex ES (catalase - hydrogen peroxide)	

Kinetic Law

Derived unit $\mathrm{das}^{-1} \cdot \mu\mathrm{mol}$

$$v_1 = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k1} \cdot [\mathrm{e}] \cdot [\mathrm{x}] - \mathrm{k2} \cdot [\mathrm{p}]) \tag{2}$$

6.2 Reaction r2

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

Name r2

SBO:0000200 redox reaction

Reaction equation

$$\mathrm{p} + \mathrm{x} \longrightarrow \mathrm{e} + \mathrm{p1} \tag{3}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
p	enzyme-substrate complex ES (catalase - hydrogen peroxide)	
x	substrate S (hydrogen peroxide)	

Products

Table 9: Properties of each product.

Id	Name	SBO
e	enzyme E (catalase)	
p1	product 1	

Kinetic Law

Derived unit $\mathrm{das}^{-1} \cdot \mu\mathrm{mol}$

$$v_2 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k4\_prime} \cdot [\mathrm{p}] \cdot [\mathrm{x}] \tag{4}$$

6.3 Reaction r3

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

Name r3

SBO:0000200 redox reaction

Reaction equation

$$\mathrm{p} + \mathrm{a} \longrightarrow \mathrm{e} + \mathrm{p2} \tag{5}$$

Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
p	enzyme-substrate complex ES (catalase - hydrogen peroxide)	
a	donor AH2	

Products

Table 11: Properties of each product.

Id	Name	SBO
e	enzyme E (catalase)	
p2	product 2	

Kinetic Law

Derived unit $\mathrm{das}^{-1} \cdot \mu\mathrm{mol}$

$$v_3 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k4} \cdot [\mathrm{p}] \cdot [\mathrm{a}] \tag{6}$$

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 e

Name enzyme E (catalase)

SBO:0000252 polypeptide chain

Initial concentration $1.36\ \mu\mathrm{mol} \cdot \mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e} = v_2 + v_3 - v_1 \tag{7}$$

7.2 Species x

Name substrate S (hydrogen peroxide)

SBO:0000247 simple chemical

Initial concentration $2\ \mu\mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in r1, r2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x} = -v_1 - v_2 \tag{8}$$

7.3 Species p

Name enzyme-substrate complex ES (catalase - hydrogen peroxide)

SBO:0000297 protein complex

Initial concentration $0\ \mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{p} = v_1 - v_2 - v_3 \tag{9}$$

7.4 Species p1

Name product 1

SBO:0000247 simple chemical

Initial concentration $0\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in r2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{p1} = v_2 \tag{10}$$

7.5 Species a

Name donor AH2

SBO:0000247 simple chemical

Initial concentration $0\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a reactant in r3), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{a} = 0 \tag{11}$$

7.6 Species p2

Name product 2

SBO:0000247 simple chemical

Initial concentration $0\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in r3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{p2} = v_3 \tag{12}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000036 forward bimolecular rate constant, continuous case: Numerical parameter that quantifies the forward velocity of a chemical reaction involving two reactants. This parameter encompasses all the contributions to the velocity except the quantity of the reactants. It is to be used in a reaction modelled using a continuous framework

SBO:0000177 non-covalent binding: Interaction between several biochemical entities that results in the formation of a non-covalent comple

SBO:0000200 redox reaction: Chemical process in which atoms have their oxidation number (oxidation state) changed

SBO:0000247 simple chemical: Simple, non-repetitive chemical 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:0000290 physical compartment: Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions

SBO:0000297 protein complex: Macromolecular complex containing one or more polypeptide chains possibly associated with simple chemicals. CHEBI:3608

SBO:0000338 dissociation rate constant: Rate with which a complex dissociates into its components

SBO:0000339 bimolecular association rate constant: Rate with which two components associate into a complex

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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