SBML Model Report

Model name: "Chance1943_Peroxidase_ES_Kinetics"

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 seventh 2014 at 1:31 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	1
species types	0	species	4
events	0	constraints	0
reactions	2	function definitions	0
global parameters	2	unit definitions	3
rules	0	initial assignments	0

Model Notes

Default parameter values are those in the right hand panel of Fig 12. The other panels may be obtained by setting X to 1, 2 or 4, and K3 to 0, 1/2 or 1.

This model is described in:

The kinetics of the enzyme-substrate compound of peroxidase.

[1]EMBL-EBI, lukas@ebi.ac.uk
[2]University of Manchester, kieran.smallbone@manchester.ac.uk

Britton Chance, Journal of Biological Chemistry, 151, 553-577, 1943. PDF at JBC
reprinted in: Adv Enzymol Relat Areas Mol Biol. 1999;73:3-23. PubmedID:10218104>
Abstract:
Under the narrow range of experimental conditions, and at a temperature of approximately 25 degrees, the following data were obtained. 1. The equilibrium constant of peroxidase and hydrogen peroxide has a minimum value of 2 x 10(-8). 2. The velocity constant for the formation of peroxidase-H2O2 Complex I is 1.2 x 10(7) liter mole-1 sec.-1, +/- 0.4 x 10(7). 3. The velocity constant for the reversible breakdown of peroxidase-H2O2 Complex I is a negligible factor in the enzyme-substrate kinetics and is calculated to be less than 0.2 sec.-1. 4. The velocity constant, k3, for the enzymatic breakdown of peroxidase-H2O2 Complex I varies from nearly zero to higher than 5 sec.-1, depending upon the acceptor and its concentration. The quotient of k3 and the leucomalachite green concentration is 3.0 x 10(4) liter mole-1 sec.-1. For ascorbic acid this has a value of 1.8 x 10(5) liter mole-1 sec.-1. 5. For a particular acceptor concentration, k3 is determined solely from the enzyme-substrate kinetics and is found to be 4.2 sec.-1. 6. For the same conditions, k3 is determined from a simple relationship derived from mathematical solutions of the Michaelis theory and is found to be 5.2 sec.-1. 7. For the same conditions, k3 is determined from the over-all enzyme action and is found to be 5.1 sec.-1. 8. The Michaelis constant determined from kinetic data alone is found to be 0.44 x 10(-6). 9. The Michaelis constant determined from steady state measurements is found to be 0.41 x 10(-6). 10. The Michaelis constant determined from measurement of the overall enzyme reaction is found to be 0.50 x 10(-6). 11. The kinetics of the enzyme-substrate compound closely agree with mathematical solutions of an extension of the Michaelis theory obtained for experimental values of concentrations and reaction velocity constants. 12. The adequacy of the criteria by which experiment and theory were correlated has been examined critically and the mathematical solutions have been found to be sensitive to variations in the experimental conditions. 13. The critical features of the enzyme-substrate kinetics are Pmax, and curve shape, rather than t1/2. t1/2 serves as a simple measure of dx/dt. 14. A second order combination of enzyme and substrate to form the enzyme-substrate compound, followed by a first order breakdown of the compound, describes the activity of peroxidase for a particular acceptor concentration. 15. The kinetic data indicate a bimolecular combination of acceptor and enzyme-substrate compound.

This model is the one described in the appendix of the article. It reproduces, amongst others, figure 12. The parameters and concentrations used are rescaled as stated in the article. K2 and K3 stand for k2 and k3, respectively, divided by k1.

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
`cell`	cell	0000290	3	1	dimensionless	☑	

3.1 Compartment `cell`

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

Name cell

SBO:0000290 physical compartment

4 Species

This model contains four species. 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
X	X	cell	dimensionless $\cdot$ dimensionless^{-1}	⊟	⊟
E	E	cell	dimensionless $\cdot$ dimensionless^{-1}	⊟	⊟
P	P	cell	dimensionless $\cdot$ dimensionless^{-1}	⊟	⊟
Q	Q	cell	dimensionless $\cdot$ dimensionless^{-1}	⊟	⊟

5 Parameters

This model contains two global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K2			0.0	dimensionless	☑
K3			0.5	dimensionless	☑

6 Reactions

This model contains two 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	$X + E \rightleftharpoons P$	0000177
2	r2	r2	$P \longrightarrow E + Q$	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

$$\mathrm{X} + \mathrm{E} \rightleftharpoons \mathrm{P} \tag{1}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
X	X	
E	E	

Product

Table 7: Properties of each product.

Id	Name	SBO
P	P	

Kinetic Law

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

$$v_1 = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{E}] \cdot [\mathrm{X}] - \mathrm{K2} \cdot [\mathrm{P}]) \tag{2}$$

6.2 Reaction r2

This is an irreversible reaction of one reactant forming two products.

Name r2

SBO:0000200 redox reaction

Reaction equation

$$\mathrm{P} \longrightarrow \mathrm{E} + \mathrm{Q} \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
P	P	

Products

Table 9: Properties of each product.

Id	Name	SBO
E	E	
Q	Q	

Kinetic Law

Derived unit dimensionless^{-1}

$$v_2 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{K3} \cdot [\mathrm{P}] \tag{4}$$

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.

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.

7.1 Species X

Name X

SBO:0000247 simple chemical

Initial concentration 8 dimensionless $\cdot$ dimensionless^{-1}

This species takes part in one reaction (as a reactant in `r1`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X} = -v_1 \tag{5}$$

7.2 Species E

Name E

SBO:0000252 polypeptide chain

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E} = v_2 - v_1 \tag{6}$$

7.3 Species P

Name P

SBO:0000297 protein complex

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P} = v_1 - v_2 \tag{7}$$

7.4 Species Q

Name Q

SBO:0000247 simple chemical

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Q} = v_2 \tag{8}$$

A Glossary of Systems Biology Ontology Terms

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

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.

[a]Center for Bioinformatics Tübingen (ZBIT), Germany
[b]California Institute of Technology, Beckman Institute BNMC, Pasadena, United States
[c]European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom
[d]EML Research gGmbH, Heidelberg, Germany