SBML Model Report

Model name: "Olsen2003_peroxidase"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Nicolas Le Novre[1] and Jacky L Snoep[2] at August 22nd 2005 at 10:49 p. m. and last time modified at April eighth 2016 at 3:21 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	16
events	0	constraints	0
reactions	15	function definitions	0
global parameters	0	unit definitions	1
rules	0	initial assignments	0

Model Notes

Notes of the BioModels curators:

The current model reproduce the figure 7, panel B of the paper. Note that there is a typo in the figure. The ordinates represent the concentration of peroxyde, as stated in the legend, and not of oxygen. The model has been tested in COPASI (http://www.copasi.org/, build 13).

Notes of the original version of the SBML file:

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SBML level 2 code generated for the JWS Online project by Jacky Snoep using PySCeS
Run this model online at http://jjj.biochem.sun.ac.za
To cite JWS Online please refer to: Olivier, B.G. and Snoep, J.L. (2004) Web-based modelling using JWS Online , Bioinformatics, 20:2143-2144

To cite BioModels Database, please use: Li C, Donizelli M, Rodriguez N, Dharuri H, Endler L, Chelliah V, Li L, He E, Henry A, Stefan MI, Snoep JL, Hucka M, Le Novre N, Laibe C (2010) BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models. BMC Syst Biol., 4:92.

2 Unit Definitions

This is an overview of five 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 `volume`

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

Definition l

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`			3	1	litre	☑	

3.1 Compartment `compartment`

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

4 Species

This model contains 16 species. The boundary condition of four of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 6 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
NADH		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
O2		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
H2O2		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
per3		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
coI		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
ArH		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
coII		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
Ar		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
NADrad		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
super		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
coIII		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
per2		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
NAD2		compartment	$\mu mol \cdot l^{-1}$	⊟	☑
NAD		compartment	$\mu mol \cdot l^{-1}$	⊟	☑
O2g		compartment	$\mu mol \cdot l^{-1}$	⊟	☑
NADHres		compartment	$\mu mol \cdot l^{-1}$	⊟	☑

5 Reactions

This model contains 15 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 4: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	v1		$NADH + O2 \longrightarrow H2O2 + NAD$	
2	v2		$per3 + H2O2 \longrightarrow coI$	
3	v3		$ArH + coI \longrightarrow Ar + coII$	
4	v4		$coII + ArH \longrightarrow per3 + Ar$	
5	v5		$NADrad + O2 \longrightarrow NAD + super$	
6	v6		$per3 + super \longrightarrow coIII$	
7	v7		$2\,super \longrightarrow H2O2 + O2$	
8	v8		$NADrad + coIII \longrightarrow NAD + coI$	
9	v9		$2\,NADrad \longrightarrow NAD2$	
10	v10		$per3 + NADrad \longrightarrow per2 + NAD$	
11	v11		$per2 + O2 \longrightarrow coIII$	
12	v12		$NADHres \longrightarrow NADH$	
13	v131		$O2g \longrightarrow O2$	
14	v132		$O2 \longrightarrow O2g$	
15	v14		$NADH + Ar \longrightarrow NADrad + ArH$	

5.1 Reaction v1

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

Reaction equation

$$\mathrm{NADH} + \mathrm{O2} \longrightarrow \mathrm{H2O2} + \mathrm{NAD} \tag{1}$$

Reactants

Table 5: Properties of each reactant.

Id	Name	SBO
NADH		
O2		

Products

Table 6: Properties of each product.

Id	Name	SBO
H2O2		
NAD		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k1} \cdot [\mathrm{NADH}] \cdot [\mathrm{O2}] \tag{2}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			$3 \cdot 10^{-6}$		☑

5.2 Reaction v2

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

Reaction equation

$$\mathrm{per3} + \mathrm{H2O2} \longrightarrow \mathrm{coI} \tag{3}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
per3		
H2O2		

Product

Table 9: Properties of each product.

Id	Name	SBO
coI		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k2} \cdot [\mathrm{H2O2}] \cdot [\mathrm{per3}] \tag{4}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k2			18.0		☑

5.3 Reaction v3

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

Reaction equation

$$\mathrm{ArH} + \mathrm{coI} \longrightarrow \mathrm{Ar} + \mathrm{coII} \tag{5}$$

Reactants

Table 11: Properties of each reactant.

Id	Name	SBO
ArH		
coI		

Products

Table 12: Properties of each product.

Id	Name	SBO
Ar		
coII		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}\,(\text{compartment}) \cdot \text{k3} \cdot [\text{coI}] \cdot [\text{ArH}] \tag{6}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k3			0.15		☑

5.4 Reaction v4

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

Reaction equation

$$\text{coII} + \text{ArH} \longrightarrow \text{per3} + \text{Ar} \tag{7}$$

Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
coII		
ArH		

Products

Table 15: Properties of each product.

Id	Name	SBO
per3		
Ar		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k4} \cdot [\mathrm{coII}] \cdot [\mathrm{ArH}] \tag{8}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k4			0.005		☑

5.5 Reaction v5

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

Reaction equation

$$\mathrm{NADrad} + \mathrm{O2} \longrightarrow \mathrm{NAD} + \mathrm{super} \tag{9}$$

Reactants

Table 17: Properties of each reactant.

Id	Name	SBO
NADrad		
O2		

Products

Table 18: Properties of each product.

Id	Name	SBO
NAD		

Id	Name	SBO
super		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k5} \cdot [\mathrm{NADrad}] \cdot [\mathrm{O2}] \tag{10}$$

Table 19: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k5			20.0		☑

5.6 Reaction v6

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

Reaction equation

$$\mathrm{per3} + \mathrm{super} \longrightarrow \mathrm{coIII} \tag{11}$$

Reactants

Table 20: Properties of each reactant.

Id	Name	SBO
per3		
super		

Product

Table 21: Properties of each product.

Id	Name	SBO
coIII		

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k6} \cdot [\mathrm{super}] \cdot [\mathrm{per3}] \tag{12}$$

Table 22: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k6			17.0		☑

5.7 Reaction v7

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

Reaction equation

$$2\,\mathrm{super} \longrightarrow \mathrm{H2O2} + \mathrm{O2} \tag{13}$$

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
super		

Products

Table 24: Properties of each product.

Id	Name	SBO
H2O2		
O2		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k7} \cdot [\mathrm{super}] \cdot [\mathrm{super}] \tag{14}$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k7			20.0		☑

5.8 Reaction v8

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

Reaction equation

$$\mathrm{NADrad} + \mathrm{coIII} \longrightarrow \mathrm{NAD} + \mathrm{coI} \tag{15}$$

Reactants

Table 26: Properties of each reactant.

Id	Name	SBO
NADrad		
coIII		

Products

Table 27: Properties of each product.

Id	Name	SBO
NAD		
coI		

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k8} \cdot [\mathrm{coIII}] \cdot [\mathrm{NADrad}] \tag{16}$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k8			40.0		☑

5.9 Reaction v9

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

Reaction equation

$$2\,\mathrm{NADrad} \longrightarrow \mathrm{NAD2} \tag{17}$$

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
NADrad		

Product

Table 30: Properties of each product.

Id	Name	SBO
NAD2		

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k9} \cdot [\mathrm{NADrad}] \cdot [\mathrm{NADrad}] \tag{18}$$

Table 31: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k9			60.0		☑

5.10 Reaction v10

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

Reaction equation

$$\mathrm{per3} + \mathrm{NADrad} \longrightarrow \mathrm{per2} + \mathrm{NAD} \tag{19}$$

Reactants

Table 32: Properties of each reactant.

Id	Name	SBO
per3		
NADrad		

Products

Table 33: Properties of each product.

Id	Name	SBO
per2		
NAD		

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k10} \cdot [\mathrm{per3}] \cdot [\mathrm{NADrad}] \tag{20}$$

Table 34: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k10			1.8		☑

5.11 Reaction v11

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

Reaction equation

$$\mathrm{per2} + \mathrm{O2} \longrightarrow \mathrm{coIII} \tag{21}$$

Reactants

Table 35: Properties of each reactant.

Id	Name	SBO
per2		
O2		

Product

Table 36: Properties of each product.

Id	Name	SBO
coIII		

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k11} \cdot [\mathrm{per2}] \cdot [\mathrm{O2}] \tag{22}$$

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k11			0.1		☑

5.12 Reaction v12

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

Reaction equation

$$\mathrm{NADHres} \longrightarrow \mathrm{NADH} \tag{23}$$

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
NADHres		

Product

Table 39: Properties of each product.

Id	Name	SBO
NADH		

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k12} \tag{24}$$

Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k12			0.08		☑

5.13 Reaction v131

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

Reaction equation

$$\mathrm{O2g} \longrightarrow \mathrm{O2} \tag{25}$$

Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
O2g		

Product

Table 42: Properties of each product.

Id	Name	SBO
O2		

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k13f} \cdot [\mathrm{O2g}] \tag{26}$$

Table 43: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k13f			0.006		☑

5.14 Reaction v132

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

Reaction equation

$$\mathrm{O2} \longrightarrow \mathrm{O2g} \tag{27}$$

Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
O2		

Product

Table 45: Properties of each product.

Id	Name	SBO
O2g		

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{vol}\left(\mathrm{compartment}\right) \cdot \mathrm{k13b} \cdot [\mathrm{O2}] \tag{28}$$

Table 46: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k13b			0.006		☑

5.15 Reaction v14

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

Reaction equation

$$\mathrm{NADH} + \mathrm{Ar} \longrightarrow \mathrm{NADrad} + \mathrm{ArH} \tag{29}$$

Reactants

Table 47: Properties of each reactant.

Id	Name	SBO
NADH		
Ar		

Products

Table 48: Properties of each product.

Id	Name	SBO
NADrad		
ArH		

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k14} \cdot [\mathrm{Ar}] \cdot [\mathrm{NADH}] \tag{30}$$

Table 49: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k14			0.7		☑

6 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.

6.1 Species `NADH`

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

This species takes part in three reactions (as a reactant in `v1`, `v14` and as a product in `v12`).

$$\frac{\text{d}}{\text{d}t}\text{NADH} = v_{12} - v_1 - v_{15} \tag{31}$$

6.2 Species `O2`

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

This species takes part in six reactions (as a reactant in `v1`, `v5`, `v11`, `v132` and as a product in `v7`, `v131`).

$$\frac{\text{d}}{\text{d}t}\text{O2} = v_7 + v_{13} - v_1 - v_5 - v_{11} - v_{14} \tag{32}$$

6.3 Species `H2O2`

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

This species takes part in three reactions (as a reactant in `v2` and as a product in `v1`, `v7`).

$$\frac{\text{d}}{\text{d}t}\text{H2O2} = v_1 + v_7 - v_2 \tag{33}$$

6.4 Species `per3`

Initial concentration $1.4\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in `v2`, `v6`, `v10` and as a product in `v4`).

$$\frac{\text{d}}{\text{d}t}\text{per3} = v_4 - v_2 - v_6 - v_{10} \tag{34}$$

6.5 Species `coI`

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

This species takes part in three reactions (as a reactant in `v3` and as a product in `v2`, `v8`).

$$\frac{\text{d}}{\text{d}t}\text{coI} = v_2 + v_8 - v_3 \tag{35}$$

6.6 Species ArH

Initial concentration 500 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in v3, v4 and as a product in v14).

$$\frac{\text{d}}{\text{d}t}\text{ArH} = v_{15} - v_3 - v_4 \tag{36}$$

6.7 Species coII

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

This species takes part in two reactions (as a reactant in v4 and as a product in v3).

$$\frac{\text{d}}{\text{d}t}\text{coII} = v_3 - v_4 \tag{37}$$

6.8 Species Ar

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

This species takes part in three reactions (as a reactant in v14 and as a product in v3, v4).

$$\frac{\text{d}}{\text{d}t}\text{Ar} = v_3 + v_4 - v_{15} \tag{38}$$

6.9 Species NADrad

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

This species takes part in five reactions (as a reactant in v5, v8, v9, v10 and as a product in v14).

$$\frac{\text{d}}{\text{d}t}\text{NADrad} = v_{15} - v_5 - v_8 - 2\,v_9 - v_{10} \tag{39}$$

6.10 Species super

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

This species takes part in three reactions (as a reactant in v6, v7 and as a product in v5).

$$\frac{\text{d}}{\text{d}t}\text{super} = v_5 - v_6 - 2\,v_7 \tag{40}$$

6.11 Species coIII

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

This species takes part in three reactions (as a reactant in v8 and as a product in v6, v11).

$$\frac{\text{d}}{\text{d}t}\text{coIII} = v_6 + v_{11} - v_8 \tag{41}$$

6.12 Species per2

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

This species takes part in two reactions (as a reactant in v11 and as a product in v10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{per2} = v_{10} - v_{11} \tag{42}$$

6.13 Species NAD2

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

This species takes part in one reaction (as a product in v9), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{NAD2} = 0 \tag{43}$$

6.14 Species NAD

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

This species takes part in four reactions (as a product in v1, v5, v8, v10), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{NAD} = 0 \tag{44}$$

6.15 Species O2g

Initial concentration $12\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in two reactions (as a reactant in v131 and as a product in v132), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{O2g} = 0 \tag{45}$$

6.16 Species NADHres

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

This species takes part in one reaction (as a reactant in v12), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{NADHres} = 0 \tag{46}$$

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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