

SBML Model Report

Model name: “Kowald2006_SOD”



May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Enuo He¹ at March 28th 2007 at 12:43 a. m. and last time modified at October nineth 2014 at 3:46 p. m. Table 1 gives 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	9
events	0	constraints	0
reactions	17	function definitions	0
global parameters	18	unit definitions	0
rules	2	initial assignments	0

Model Notes

This model is according to the paper from Axel Kowald *Alternative pathways as mechanism for the negative effects associated with overexpression of superoxide dismutase*.

Reactions from 1 to 17 are listed in the paper, note that for clarity species whose concentrations are assumed to be constant (e.g. water, oxygen, protons, metal ions) are omitted from the diagram. In the paper, v16 is a fast reaction, but we do not use fast reaction in the model.

Figure2 has been reproduced by both SBMLodeSolver and Copasi4.0.20(development) . Figure 3 has been obtained with Copasi4.0.20(development) using parameter scan.

¹BNMC, enuo@caltech.edu

The steady-state of [LOO*] a little bit lower than showed on the paper, I guess it may be the simulation method used in the paper use fast reaction and also the reaction (5) listed on Page 831 on the paper is slightly different from equation (2) on Page 832. The rest of them are the quite the same.

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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 which are all predefined by SBML and not mentioned in the model.

2.1 Unit substance

Notes Mole is the predefined SBML unit for substance.

Definition mol

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 m²

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_0000001	cell		3	1	litre	<input checked="" type="checkbox"/>	

3.1 Compartment `compartment_0000001`

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

Name cell

4 Species

This model contains nine 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_0000001	O2*-	compartment_0000001	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
species_0000002	Cu(II)ZnSOD	compartment_0000001	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
species_0000006	H2O2	compartment_0000001	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
species_0000007	LOO*	compartment_0000001	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
species_0000008	HO*	compartment_0000001	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
species_0000009	LOOH	compartment_0000001	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
species_0000011	L*	compartment_0000001	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
species_0000016	SODtotal	compartment_0000001	$\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input type="checkbox"/>
species_0000017	Cat	compartment_0000001	$\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input type="checkbox"/>

5 Parameters

This model contains 18 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$6.6 \cdot 10^{-7}$		<input checked="" type="checkbox"/>
k2	k2		$1.6 \cdot 10^9$		<input checked="" type="checkbox"/>
k3	k3		$1.6 \cdot 10^9$		<input checked="" type="checkbox"/>
k4	k4		100000.000		<input checked="" type="checkbox"/>
k5	k5		20000.000		<input checked="" type="checkbox"/>
k6	k6		1.000		<input checked="" type="checkbox"/>
k7	k7		$3.4 \cdot 10^7$		<input checked="" type="checkbox"/>
k9	k9		1000000.000		<input checked="" type="checkbox"/>
k10	k10		1000.000		<input checked="" type="checkbox"/>
k11	k11		$2.5 \cdot 10^8$		<input checked="" type="checkbox"/>
k12	k12		0.380		<input checked="" type="checkbox"/>
k13a	k13a		0.009		<input checked="" type="checkbox"/>
k13b	k13b		0.009		<input checked="" type="checkbox"/>
k17	k17		30000.000		<input checked="" type="checkbox"/>
k18	k18		7.000		<input checked="" type="checkbox"/>
k19	k19		88000.000		<input checked="" type="checkbox"/>
H02star	HO2*		0.000		<input type="checkbox"/>
Cu_I_ZnSOD	Cu(I)ZnSOD		0.000		<input type="checkbox"/>

6 Rules

This is an overview of two rules.

6.1 Rule H02star

Rule H02star is an assignment rule for parameter H02star:

$$\text{H02star} = \frac{[\text{species_0000001}]}{100} \quad (1)$$

Notes HO2*=O2*/100

6.2 Rule Cu_I_ZnSOD

Rule Cu_I_ZnSOD is an assignment rule for parameter Cu_I_ZnSOD:

$$\text{Cu.I.ZnSOD} = [\text{species_0000016}] - [\text{species_0000002}] \quad (2)$$

Derived unit $\text{mol} \cdot \text{l}^{-1}$

Notes $\text{Cu(I)ZnSOD} = \text{SOD}_{\text{total}} - \text{Cu(II)ZnSOD}$

7 Reactions

This model contains 17 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

Nº	Id	Name	Reaction Equation	SBO
1	reaction- _0000001	v1	$\emptyset \longrightarrow \text{species_0000001}$	
2	reaction_0	v2	$\text{species_0000001} + \text{species_0000002} \longrightarrow \emptyset$	
3	reaction_1	v3	$\text{species_0000001} \longrightarrow \text{species_0000006}$	+
4	reaction_2	v4	species_0000002 species_0000001 $\text{species_0000007} \longrightarrow \text{species_0000009}$	+
5	reaction_3	v5	species_0000001 $\text{species_0000006} \longrightarrow 2 \text{ species_0000008}$	+
6	reaction_4	v6	$\text{species_0000006} \xrightarrow{\text{species_0000002}} 2 \text{ species_0000008}$	
7	reaction_5	v7	$\text{species_0000006} \xrightarrow{\text{species_0000017}} \emptyset$	
8	reaction_6	v9	$\text{species_0000008} \longrightarrow \emptyset$	
9	reaction_7	v10	$\emptyset \longrightarrow \text{species_0000011} + \text{species_0000006}$	
10	reaction_8	v11	$\text{species_0000008} \longrightarrow \text{species_0000011}$	
11	reaction_9	v12	$\text{species_0000009} \longrightarrow \emptyset$	
12	reaction_10	v13a	$\emptyset \longrightarrow \text{species_0000002}$	
13	reaction_11	v13b	$\text{species_0000002} \longrightarrow \emptyset$	
14	reaction_12	v17	$\text{species_0000011} \longrightarrow \text{species_0000007}$	
15	reaction_13	v18	$\text{species_0000007} \longrightarrow \text{species_0000011}$ species_0000009	+
16	reaction_14	v19	$2 \text{ species_0000007} \longrightarrow \emptyset$	
17	fast	v16	$\text{species_0000001} \rightleftharpoons \emptyset$	

Nº	Id	Name	Reaction Equation	SBO
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7.1 Reaction `reaction_0000001`

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

Name `v1`

Reaction equation



Product

Table 6: Properties of each product.

Id	Name	SBO
species_0000001	O2*-	

Kinetic Law

Derived unit contains undeclared units

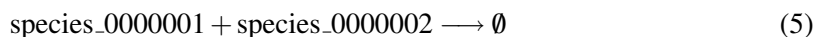
$$v_1 = \text{vol}(\text{compartment_0000001}) \cdot k_1 \quad (4)$$

7.2 Reaction `reaction_0`

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

Name `v2`

Reaction equation



Reactants

Table 7: Properties of each reactant.

Id	Name	SBO
species_0000001	O2*-	
species_0000002	Cu(II)ZnSOD	

Kinetic Law

Derived unit contains undeclared units

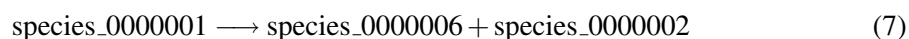
$$v_2 = \text{vol}(\text{compartment_0000001}) \cdot k_2 \cdot [\text{species_0000001}] \cdot [\text{species_0000002}] \quad (6)$$

7.3 Reaction `reaction_1`

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

Name `v3`

Reaction equation



Reactant

Table 8: Properties of each reactant.		
Id	Name	SBO
<code>species_0000001</code>	O2*-	

Products

Table 9: Properties of each product.		
Id	Name	SBO
<code>species_0000006</code>	H2O2	
<code>species_0000002</code>	Cu(II)ZnSOD	

Kinetic Law

Derived unit contains undeclared units

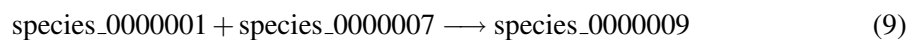
$$v_3 = \text{vol}(\text{compartment_0000001}) \cdot k_3 \cdot [\text{species_0000001}] \cdot \text{Cu_I_ZnSOD} \quad (8)$$

7.4 Reaction `reaction_2`

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

Name `v4`

Reaction equation



Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
species_0000001	O2*-	
species_0000007	LOO*	

Product

Table 11: Properties of each product.

Id	Name	SBO
species_0000009	LOOH	

Kinetic Law

Derived unit contains undeclared units

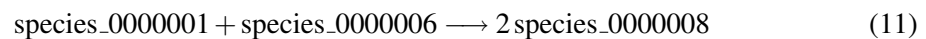
$$v_4 = \text{vol}(\text{compartment_0000001}) \cdot k_4 \cdot [\text{species_0000001}] \cdot [\text{species_0000007}] \quad (10)$$

7.5 Reaction `reaction_3`

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

Name `v5`

Reaction equation



Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
species_0000001	O2*-	
species_0000006	H2O2	

Product

Table 13: Properties of each product.

Id	Name	SBO
species_0000008	HO*	

Kinetic Law

Derived unit contains undeclared units

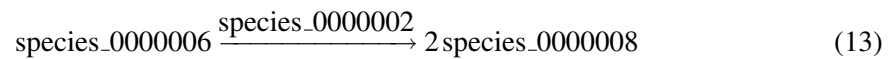
$$v_5 = \text{vol}(\text{compartment_0000001}) \cdot k_5 \cdot [\text{species_0000001}] \cdot [\text{species_0000006}] \quad (12)$$

7.6 Reaction `reaction_4`

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

Name `v6`

Reaction equation



Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
species_0000006	H2O2	

Modifier

Table 15: Properties of each modifier.

Id	Name	SBO
species_0000002	Cu(II)ZnSOD	

Product

Table 16: Properties of each product.

Id	Name	SBO
species_0000008	HO*	

Kinetic Law

Derived unit contains undeclared units

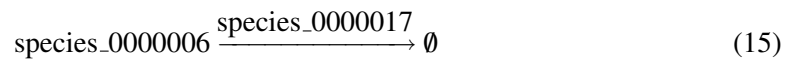
$$v_6 = \text{vol}(\text{compartment_0000001}) \cdot k_6 \cdot [\text{species_0000006}] \cdot [\text{species_0000002}] \quad (14)$$

7.7 Reaction `reaction_5`

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

Name `v7`

Reaction equation



Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
species_0000006	H2O2	

Modifier

Table 18: Properties of each modifier.

Id	Name	SBO
species_0000017	Cat	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{vol}(\text{compartment_0000001}) \cdot k_7 \cdot [\text{species_0000006}] \cdot [\text{species_0000017}] \quad (16)$$

7.8 Reaction `reaction_6`

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

Name `v9`

Reaction equation



Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
species_0000008	HO*	

Kinetic Law

Derived unit contains undeclared units

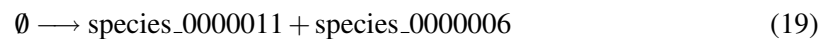
$$v_8 = \text{vol}(\text{compartment_0000001}) \cdot k_9 \cdot [\text{species_0000008}] \quad (18)$$

7.9 Reaction [reaction_7](#)

This is an irreversible reaction of no reactant forming two products.

Name v10

Reaction equation



Products

Table 20: Properties of each product.

Id	Name	SBO
species_0000011	L*	
species_0000006	H2O2	

Kinetic Law

Derived unit contains undeclared units

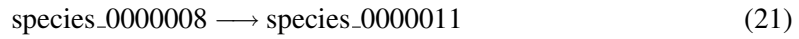
$$v_9 = \text{vol}(\text{compartment_0000001}) \cdot k_{10} \cdot \text{HO2star} \quad (20)$$

7.10 Reaction [reaction_8](#)

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

Name v11

Reaction equation



Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
species_0000008	HO*	

Product

Table 22: Properties of each product.

Id	Name	SBO
species_0000011	L*	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{vol}(\text{compartment_0000001}) \cdot k_{11} \cdot [\text{species_0000008}] \quad (22)$$

7.11 Reaction [reaction_9](#)

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

Name v12

Reaction equation



Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
species_0000009	LOOH	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \text{vol}(\text{compartment_0000001}) \cdot k_{12} \cdot [\text{species_0000009}] \quad (24)$$

7.12 Reaction [reaction_10](#)

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

Name v13a

Reaction equation



Product

Table 24: Properties of each product.

Id	Name	SBO
species_0000002	Cu(II)ZnSOD	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \text{vol}(\text{compartment_0000001}) \cdot k_{13a} \cdot \text{Cu_I_ZnSOD} \quad (26)$$

7.13 Reaction [reaction_11](#)

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

Name v13b

Reaction equation



Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
species_0000002	Cu(II)ZnSOD	

Kinetic Law**Derived unit** contains undeclared units

$$v_{13} = \text{vol}(\text{compartment_0000001}) \cdot k_{13b} \cdot [\text{species_0000002}] \quad (28)$$

7.14 Reaction [reaction_12](#)

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

Name v17**Reaction equation****Reactant**

Table 26: Properties of each reactant.

Id	Name	SBO
species_0000011	L*	

Product

Table 27: Properties of each product.

Id	Name	SBO
species_0000007	LOO*	

Kinetic Law**Derived unit** contains undeclared units

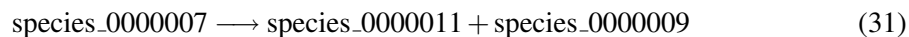
$$v_{14} = \text{vol}(\text{compartment_0000001}) \cdot k_{17} \cdot [\text{species_0000011}] \quad (30)$$

7.15 Reaction `reaction_13`

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

Name `v18`

Reaction equation



Reactant

Table 28: Properties of each reactant.

Id	Name	SBO
<code>species_0000007</code>	LOO*	

Products

Table 29: Properties of each product.

Id	Name	SBO
<code>species_0000011</code>	L*	
<code>species_0000009</code>	LOOH	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{vol}(\text{compartment_0000001}) \cdot k_{18} \cdot [\text{species_0000007}] \quad (32)$$

7.16 Reaction `reaction_14`

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

Name `v19`

Reaction equation



Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
species_0000007	LOO*	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \text{vol}(\text{compartment_0000001}) \cdot k_{19} \cdot [\text{species_0000007}]^2 \quad (34)$$

7.17 Reaction fast

This is a reversible reaction of one reactant forming no product.

Name v16

Notes Reaction16 showed in the paper is a fast equilibrium reaction. $\text{HO}_2^* =, \text{H}^+, +, \text{O}_2^{*-},,$. So in the equation (1) in the paper, you will see there is one item $k_{10}^*, \text{HO}_2^*, .$ However, most simulation software does not support fast reaction yet, so curator creat this fake v16 reaction in order to make the final ODE correct.

Reaction equation



Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
species_0000001	O2*-	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = k_{10} \cdot \text{HO2star} \cdot \text{vol}(\text{compartment_0000001}) \quad (36)$$

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_0000001`

Name O2*-

Initial concentration 0 mol · l⁻¹

This species takes part in six reactions (as a reactant in `reaction_0`, `reaction_1`, `reaction_2`, `reaction_3`, `fast` and as a product in `reaction_0000001`).

$$\frac{d}{dt}\text{species_0000001} = v_1 - v_2 - v_3 - v_4 - v_5 - v_{17} \quad (37)$$

8.2 Species `species_0000002`

Name Cu(II)ZnSOD

Initial concentration 5 · 10⁻⁶ mol · l⁻¹

This species takes part in five reactions (as a reactant in `reaction_0`, `reaction_11` and as a product in `reaction_1`, `reaction_10` and as a modifier in `reaction_4`).

$$\frac{d}{dt}\text{species_0000002} = v_3 + v_{12} - v_2 - v_{13} \quad (38)$$

8.3 Species `species_0000006`

Name H2O2

Initial concentration 0 mol · l⁻¹

This species takes part in five reactions (as a reactant in `reaction_3`, `reaction_4`, `reaction_5` and as a product in `reaction_1`, `reaction_7`).

$$\frac{d}{dt}\text{species_0000006} = v_3 + v_9 - v_5 - v_6 - v_7 \quad (39)$$

8.4 Species `species_0000007`

Name LOO*

Initial concentration 0 mol · l⁻¹

This species takes part in four reactions (as a reactant in [reaction_2](#), [reaction_13](#), [reaction_14](#) and as a product in [reaction_12](#)).

$$\frac{d}{dt}\text{species_0000007} = v_{14} - v_4 - v_{15} - 2 v_{16} \quad (40)$$

8.5 Species `species_0000008`

Name HO*

Initial concentration 0 mol · l⁻¹

This species takes part in four reactions (as a reactant in [reaction_6](#), [reaction_8](#) and as a product in [reaction_3](#), [reaction_4](#)).

$$\frac{d}{dt}\text{species_0000008} = 2 v_5 + 2 v_6 - v_8 - v_{10} \quad (41)$$

8.6 Species `species_0000009`

Name LOOH

Initial concentration 0 mol · l⁻¹

This species takes part in three reactions (as a reactant in [reaction_9](#) and as a product in [reaction_2](#), [reaction_13](#)).

$$\frac{d}{dt}\text{species_0000009} = v_4 + v_{15} - v_{11} \quad (42)$$

8.7 Species `species_0000011`

Name L*

Initial concentration 0 mol · l⁻¹

This species takes part in four reactions (as a reactant in [reaction_12](#) and as a product in [reaction_7](#), [reaction_8](#), [reaction_13](#)).

$$\frac{d}{dt}\text{species_0000011} = v_9 + v_{10} + v_{15} - v_{14} \quad (43)$$

8.8 Species `species_0000016`

Name SODtotal

Initial concentration $10^{-5} \text{ mol} \cdot \text{l}^{-1}$

$$\frac{d}{dt} \text{species_0000016} = 0 \quad (44)$$

8.9 Species `species_0000017`

Name Cat

Initial concentration $10^{-5} \text{ mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a modifier in [reaction_5](#)).

$$\frac{d}{dt} \text{species_0000017} = 0 \quad (45)$$

SBML2^{AT}EX 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.

^aCenter for Bioinformatics Tübingen (ZBIT), Germany

^bCalifornia Institute of Technology, Beckman Institute BNMC, Pasadena, United States

^cEuropean Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom

^dEML Research gGmbH, Heidelberg, Germany