SBML Model Report

Model name: "Kowald2006_SOD"

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1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Enuo He[1] 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.

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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.

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 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_0000001	cell		3	1	litre	☑	

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	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
species_0000002	Cu(II)ZnSOD	compartment_0000001	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
species_0000006	H2O2	compartment_0000001	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
species_0000007	LOO*	compartment_0000001	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
species_0000008	HO*	compartment_0000001	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
species_0000009	LOOH	compartment_0000001	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
species_0000011	L*	compartment_0000001	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
species_0000016	SODtotal	compartment_0000001	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	☐
species_0000017	Cat	compartment_0000001	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	☐

5 Parameters

This model contains 18 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$6.6 \cdot 10^{-7}$		☑
k2	k2		$1.6 \cdot 10^{9}$		☑
k3	k3		$1.6 \cdot 10^{9}$		☑
k4	k4		100000.000		☑
k5	k5		20000.000		☑
k6	k6		1.000		☑
k7	k7		$3.4 \cdot 10^{7}$		☑
k9	k9		1000000.000		☑
k10	k10		1000.000		☑
k11	k11		$2.5 \cdot 10^{8}$		☑
k12	k12		0.380		☑
k13a	k13a		0.009		☑
k13b	k13b		0.009		☑
k17	k17		30000.000		☑
k18	k18		7.000		☑
k19	k19		88000.000		☑
HO2star	HO2*		0.000		⊟
Cu_I_ZnSOD	Cu(I)ZnSOD		0.000		⊟

6 Rules

This is an overview of two rules.

6.1 Rule HO2star

Rule HO2star is an assignment rule for parameter HO2star:

$$\text{HO2star} = \frac{[\text{species\_0000001}]}{100} \tag{1}$$

Notes HO2*=O2*/100

6.2 Rule Cu_I_ZnSOD

Rule Cu_I_ZnSOD is an assignment rule for parameter Cu_I_ZnSOD:

$$\text{Cu\_I\_ZnSOD} = [\text{species\_0000016}] - [\text{species\_0000002}] \tag{2}$$

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

Notes Cu(I)ZnSOD=SODtotal-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

№	Id	Name	Reaction Equation	SBO
1	reaction-_0000001	v1	$\emptyset \longrightarrow$ species_0000001	
2	reaction_0	v2	species_0000001 + species_0000002 $\longrightarrow \emptyset$	
3	reaction_1	v3	species_0000001 $\longrightarrow$ species_0000006 + species_0000002	
4	reaction_2	v4	species_0000001 + species_0000007 $\longrightarrow$ species_0000009	
5	reaction_3	v5	species_0000001 + species_0000006 $\longrightarrow$ 2 species_0000008	
6	reaction_4	v6	species_0000006 $\xrightarrow{\text{species\_0000002}}$ 2 species_0000008	
7	reaction_5	v7	species_0000006 $\xrightarrow{\text{species\_0000017}} \emptyset$	
8	reaction_6	v9	species_0000008 $\longrightarrow \emptyset$	
9	reaction_7	v10	$\emptyset \longrightarrow$ species_0000011 + species_0000006	
10	reaction_8	v11	species_0000008 $\longrightarrow$ species_0000011	
11	reaction_9	v12	species_0000009 $\longrightarrow \emptyset$	
12	reaction_10	v13a	$\emptyset \longrightarrow$ species_0000002	
13	reaction_11	v13b	species_0000002 $\longrightarrow \emptyset$	
14	reaction_12	v17	species_0000011 $\longrightarrow$ species_0000007	
15	reaction_13	v18	species_0000007 $\longrightarrow$ species_0000011 + species_0000009	
16	reaction_14	v19	2 species_0000007 $\longrightarrow \emptyset$	
17	fast	v16	species_0000001 $\rightleftharpoons \emptyset$	

№	Id	Name	Reaction Equation	SBO

7.1 Reaction reaction_0000001

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

Name v1

Reaction equation

$$\emptyset \longrightarrow \text{species\_0000001} \tag{3}$$

Product

Table 6: Properties of each product.

Id	Name	SBO
species_0000001	O2*-	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}\left(\text{compartment\_0000001}\right) \cdot \text{k1} \tag{4}$$

7.2 Reaction reaction_0

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

Name v2

Reaction equation

$$\text{species\_0000001} + \text{species\_0000002} \longrightarrow \emptyset \tag{5}$$

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

$$v_2 = \mathrm{vol}\,(\mathrm{compartment\_0000001}) \cdot \mathrm{k2} \cdot [\mathrm{species\_0000001}] \cdot [\mathrm{species\_0000002}] \quad (6)$$

7.3 Reaction reaction_1

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

Name v3

Reaction equation

$$\mathrm{species\_0000001} \longrightarrow \mathrm{species\_0000006} + \mathrm{species\_0000002} \quad (7)$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
species_0000001	O2*-	

Products

Table 9: Properties of each product.

Id	Name	SBO
species_0000006	H2O2	
species_0000002	Cu(II)ZnSOD	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{compartment\_0000001}) \cdot \mathrm{k3} \cdot [\mathrm{species\_0000001}] \cdot \mathrm{Cu\_I\_ZnSOD} \quad (8)$$

7.4 Reaction reaction_2

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

Name v4

Reaction equation

$$\mathrm{species\_0000001} + \mathrm{species\_0000007} \longrightarrow \mathrm{species\_0000009} \quad (9)$$

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

$$v_4 = \mathrm{vol}\,(\mathrm{compartment\_0000001}) \cdot \mathrm{k4} \cdot [\mathrm{species\_0000001}] \cdot [\mathrm{species\_0000007}] \qquad (10)$$

7.5 Reaction reaction_3

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

Name v5

Reaction equation

$$\mathrm{species\_0000001} + \mathrm{species\_0000006} \longrightarrow 2\,\mathrm{species\_0000008} \qquad (11)$$

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

$$v_5 = \mathrm{vol}\,(\mathrm{compartment\_0000001}) \cdot \mathrm{k5} \cdot [\mathrm{species\_0000001}] \cdot [\mathrm{species\_0000006}] \qquad (12)$$

7.6 Reaction reaction_4

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

Name v6

Reaction equation

$$\mathrm{species\_0000006} \xrightarrow{\mathrm{species\_0000002}} 2\,\mathrm{species\_0000008} \qquad (13)$$

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

$$v_6 = \mathrm{vol}\,(\mathrm{compartment\_0000001}) \cdot \mathrm{k6} \cdot [\mathrm{species\_0000006}] \cdot [\mathrm{species\_0000002}] \qquad (14)$$

7.7 Reaction `reaction_5`

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

Name v7

Reaction equation

$$\mathrm{species\_0000006} \xrightarrow{\mathrm{species\_0000017}} \emptyset \qquad (15)$$

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

$$v_7 = \mathrm{vol}\,(\mathrm{compartment\_0000001}) \cdot \mathrm{k7} \cdot [\mathrm{species\_0000006}] \cdot [\mathrm{species\_0000017}] \qquad (16)$$

7.8 Reaction `reaction_6`

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

Name v9

Reaction equation

$$\text{species\_0000008} \longrightarrow \emptyset \tag{17}$$

Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
species_0000008	HO*	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{vol}\,(\text{compartment\_0000001}) \cdot \text{k9} \cdot [\text{species\_0000008}] \tag{18}$$

7.9 Reaction reaction_7

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

Name v10

Reaction equation

$$\emptyset \longrightarrow \text{species\_0000011} + \text{species\_0000006} \tag{19}$$

Products

Table 20: Properties of each product.

Id	Name	SBO
species_0000011	L*	
species_0000006	H2O2	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{vol}\,(\text{compartment\_0000001}) \cdot \text{k10} \cdot \text{HO2star} \tag{20}$$

7.10 Reaction reaction_8

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

Name v11

Reaction equation

$$\text{species\_0000008} \longrightarrow \text{species\_0000011} \tag{21}$$

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

$$v_{10} = \text{vol}\left(\text{compartment\_0000001}\right) \cdot \text{k11} \cdot [\text{species\_0000008}] \tag{22}$$

7.11 Reaction reaction_9

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

Name v12

Reaction equation

$$\text{species\_0000009} \longrightarrow \emptyset \tag{23}$$

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
species_0000009	LOOH	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{compartment\_0000001}) \cdot \mathrm{k12} \cdot [\mathrm{species\_0000009}] \tag{24}$$

7.12 Reaction `reaction_10`

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

Name v13a

Reaction equation

$$\emptyset \longrightarrow \mathrm{species\_0000002} \tag{25}$$

Product

Table 24: Properties of each product.

Id	Name	SBO
`species_0000002`	Cu(II)ZnSOD	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}\,(\mathrm{compartment\_0000001}) \cdot \mathrm{k13a} \cdot \mathrm{Cu\_I\_ZnSOD} \tag{26}$$

7.13 Reaction `reaction_11`

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

Name v13b

Reaction equation

$$\mathrm{species\_0000002} \longrightarrow \emptyset \tag{27}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
species_0000002	Cu(II)ZnSOD	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}\,(\mathrm{compartment\_0000001}) \cdot \mathrm{k13b} \cdot [\mathrm{species\_0000002}] \tag{28}$$

7.14 Reaction reaction_12

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

Name v17

Reaction equation

$$\mathrm{species\_0000011} \longrightarrow \mathrm{species\_0000007} \tag{29}$$

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

$$v_{14} = \mathrm{vol}\,(\mathrm{compartment\_0000001}) \cdot \mathrm{k17} \cdot [\mathrm{species\_0000011}] \tag{30}$$

7.15 Reaction reaction_13

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

Name v18

Reaction equation

$$\text{species\_0000007} \longrightarrow \text{species\_0000011} + \text{species\_0000009} \tag{31}$$

Reactant

Table 28: Properties of each reactant.

Id	Name	SBO
species_0000007	LOO*	

Products

Table 29: Properties of each product.

Id	Name	SBO
species_0000011	L*	
species_0000009	LOOH	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{vol}\left(\text{compartment\_0000001}\right) \cdot \text{k18} \cdot [\text{species\_0000007}] \tag{32}$$

7.16 Reaction reaction_14

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

Name v19

Reaction equation

$$2\,\text{species\_0000007} \longrightarrow \emptyset \tag{33}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
species_0000007	LOO*	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}\,(\mathrm{compartment\_0000001}) \cdot \mathrm{k19} \cdot [\mathrm{species\_0000007}]^2 \tag{34}$$

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. HO2* =„ H+„ + „O2*-„. So in the equation (1) in the paper, you will see there is one item k10*„HO2*„ . 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

$$\mathrm{species\_0000001} \rightleftharpoons \emptyset \tag{35}$$

Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
species_0000001	O2*-	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{k10} \cdot \mathrm{HO2star} \cdot \mathrm{vol}\,(\mathrm{compartment\_0000001}) \tag{36}$$

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 $0\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_0000001} = v_1 - v_2 - v_3 - v_4 - v_5 - v_{17} \tag{37}$$

8.2 Species species_0000002

Name Cu(II)ZnSOD

Initial concentration $5 \cdot 10^{-6}\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_0000002} = v_3 + v_{12} - v_2 - v_{13} \tag{38}$$

8.3 Species species_0000006

Name H2O2

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

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_0000006} = v_3 + v_9 - v_5 - v_6 - v_7 \tag{39}$$

8.4 Species species_0000007

Name LOO*

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_0000007} = v_{14} - v_4 - v_{15} - 2\,v_{16} \tag{40}$$

8.5 Species species_0000008

Name HO*

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_0000008} = 2\,v_5 + 2\,v_6 - v_8 - v_{10} \tag{41}$$

8.6 Species species_0000009

Name LOOH

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_0000009} = v_4 + v_{15} - v_{11} \tag{42}$$

8.7 Species species_0000011

Name L*

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_0000011} = v_9 + v_{10} + v_{15} - v_{14} \tag{43}$$

8.8 Species species_0000016

Name SODtotal

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_0000016} = 0 \tag{44}$$

8.9 Species species_0000017

Name Cat

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_0000017} = 0 \tag{45}$$

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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