SBML Model Report

Model name: "Olsen2003_neutrophil-_oscillatory_metabolism"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Harish Dharuri[1] at July 27th 2007 at 8:45 a. m. and last time modified at June third 2014 at 1:27 p. 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	2
species types	0	species	20
events	0	constraints	0
reactions	20	function definitions	0
global parameters	24	unit definitions	1
rules	0	initial assignments	0

Model Notes

Olsen2003_neutrophil_oscillatory_metabolism

This model is described in the article:A model of the oscillatory metabolism of activated neutrophils.Olsen LF, Kummer U, Kindzelskii AL, Petty HR.Biophys. J. 2003 Jan; 84(1): 69-81

Abstract:

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We present a two-compartment model to explain the oscillatory behavior observed experimentally in activated neutrophils. Our model is based mainly on the peroxidase-oxidase reaction catalyzed by myeloperoxidase with melatonin as a cofactor and NADPH oxidase, a major protein in the phagosome membrane of the leukocyte. The model predicts that after activation of a neutrophil, an increase in the activity of the hexose monophosphate shunt and the delivery of myeloperoxidase into the phagosome results in oscillations in oxygen and NAD(P)H concentration. The period of oscillation changes from >200 s to 10-30 s. The model is consistent with previously reported oscillations in cell metabolism and oxidant production. Key features and predictions of the model were confirmed experimentally. The requirement of the hexose monophosphate pathway for 10 s oscillations was verified using 6-aminonicotinamide and dexamethasone, which are inhibitors of glucose-6-phosphate dehydrogenase. The role of the NADPH oxidase in promoting oscillations was confirmed by dose-response studies of the effect of diphenylene iodonium, an inhibitor of the NADPH oxidase. Moreover, the model predicted an increase in the amplitude of NADPH oscillations in the presence of melatonin, which was confirmed experimentally. Successful computer modeling of complex chemical dynamics within cells and their chemical perturbation will enhance our ability to identify new antiinflammatory compounds.

This model is hosted on BioModels Database and identified by: BIOMD0000000143.

To cite BioModels Database, please use: BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models.

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 micro mole

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 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
`phagosome`	phagosome		3	1	litre	☑	`cytoplasm`
`cytoplasm`	cytoplasm		3	10	l	☑	

3.1 Compartment `phagosome`

This is a three dimensional compartment with a constant size of one litre, which is surrounded by `cytoplasm` (cytoplasm).

Name phagosome

3.2 Compartment `cytoplasm`

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

Name cytoplasm

4 Species

This model contains 20 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
H2O2_p	H2O2	phagosome	$\mu mol \cdot l^{-1}$	⊟	⊟
per3_p	Ferric peroxidase	phagosome	$\mu mol \cdot l^{-1}$	⊟	⊟
coI_p	compound I	phagosome	$\mu mol \cdot l^{-1}$	⊟	⊟
MLTH_p	Melatonin	phagosome	$\mu mol \cdot l^{-1}$	⊟	⊟
coII_p	compound II	phagosome	$\mu mol \cdot l^{-1}$	⊟	⊟
MLT_p	Melatonin free radical	phagosome	$\mu mol \cdot l^{-1}$	⊟	⊟
O2minus_p	Superoxide	phagosome	$\mu mol \cdot l^{-1}$	⊟	⊟
H_p	Hydrogen	phagosome	$\mu mol \cdot l^{-1}$	⊟	⊟
O2_p	Oxygen	phagosome	$\mu mol \cdot l^{-1}$	⊟	⊟
NADPH_c	NADPH	cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
O2_c	Oxygen	cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
NADPplus_c	NADP	cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
H2O2_c	H2O2	cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
NADP_c	NADP	cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
O2minus_c	Superoxide	cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
H_c	Hydrogen	cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
MLT_c	Melatonin free radical	cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
MLTH_c	Melatonin	cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
coIII_p	compound III	phagosome	$\mu mol \cdot l^{-1}$	⊟	⊟
NADP2_c	NADP2	cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟

5 Parameters

This model contains 24 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Knadph			60.000		☑
k1			50.000		☑
kminus1			58.000		☑
k2			10.000		☑
k3			0.004		☑
k4			20.000		☑
k5			10.000		☑
k6			0.100		☑
k7			10^{-6}		☑
k8			50.000		☑
k9			500.000		☑
k10			10.000		☑
k11			60.000		☑
k12			25.000		☑
k13			12.500		☑
kminus13			0.045		☑
k14			30.000		☑
k15			30.000		☑
k16			10.000		☑
k17			10.000		☑
k18			2.000		☑
V			288.000		☑
L			550.000		☑
Ko			1.500		☑

6 Reactions

This model contains 20 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	Myeloperoxidase reaction	per3_p + H2O2_p ⟶ coI_p	
2	R2	Melatonin-compound I reaction	MLTH_p + coI_p ⟶ MLT_p + coII_p	
3	R3	Melatonin-compound II reaction	MLTH_p + coII_p ⟶ MLT_p + per3_p	
4	R4	compound III formation	O2minus_p + per3_p ⟶ coIII_p	
5	R5	H2O2 formation	2 O2minus_p + 2 H_p ⟶ O2_p + H2O2_p	
6	R6	compound III-superoxide reaction	O2minus_p + coIII_p ⟶ O2_p + coI_p	
7	R7	NADPH autooxidation	O2_c + NADPH_c ⟶ H2O2_c + NADPplus_c	
8	R8	NADP radical-Oxygen reaction	O2_c + NADP_c ⟶ O2minus_c + NADPplus_c	
9	R9	H2O2 formation	2 O2minus_c + 2 H_c ⟶ O2_c + H2O2_c	
10	R10	NADP free radical formation	NADPH_c + MLT_c ⟶ NADP_c + MLTH_c	
11	R11	NADP dimer formation	2 NADP_c ⟶ NADP2_c	
12	R12	NADPH synthesis	∅ ⟶ NADPH_c	
13	R13a	Oxygen diffusion	∅ ⟶ O2_c	
14	R13b	Oxygen diffusion	O2_c ⟶ ∅	
15	R14	Oxygen diffusion- phagosome/cytoplasm	O2_p ⟶ O2_c	
16	R15	H2O2 diffusion phagosome/cytoplasm	H2O2_p ⟶ H2O2_c	
17	R16	Melatonin diffusion phagosome/cytoplasm	MLTH_p ⟶ MLTH_c	
18	R17	Melatonin free radical diffusion phagosome/cytoplasm	MLT_p ⟶ MLT_c	
19	R18	Superoxide diffusion phagosome/cytoplasm	O2minus_p ⟶ O2minus_c	
20	R19	NADPH oxidase activity	2 O2_p + NADPH_c ⟶ 2 O2minus_p + NADPplus_c	

6.1 Reaction R1

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

Name Myeloperoxidase reaction

Reaction equation

$$\mathrm{per3\_p} + \mathrm{H2O2\_p} \longrightarrow \mathrm{coI\_p} \tag{1}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
per3_p	Ferric peroxidase	
H2O2_p	H2O2	

Product

Table 7: Properties of each product.

Id	Name	SBO
coI_p	compound I	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{phagosome}) \cdot (\mathrm{k1} \cdot [\mathrm{H2O2\_p}] \cdot [\mathrm{per3\_p}] - \mathrm{kminus1} \cdot [\mathrm{coI\_p}]) \tag{2}$$

6.2 Reaction R2

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

Name Melatonin-compound I reaction

Reaction equation

$$\mathrm{MLTH\_p} + \mathrm{coI\_p} \longrightarrow \mathrm{MLT\_p} + \mathrm{coII\_p} \tag{3}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
MLTH_p	Melatonin	
coI_p	compound I	

Products

Table 9: Properties of each product.

Id	Name	SBO
MLT_p	Melatonin free radical	
coII_p	compound II	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{phagosome}) \cdot \mathrm{k2} \cdot [\mathrm{coI\_p}] \cdot [\mathrm{MLTH\_p}] \tag{4}$$

6.3 Reaction R3

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

Name Melatonin-compound II reaction

Reaction equation

$$\mathrm{MLTH\_p} + \mathrm{coII\_p} \longrightarrow \mathrm{MLT\_p} + \mathrm{per3\_p} \tag{5}$$

Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
MLTH_p	Melatonin	
coII_p	compound II	

Products

Table 11: Properties of each product.

Id	Name	SBO
MLT_p	Melatonin free radical	
per3_p	Ferric peroxidase	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{phagosome}) \cdot \mathrm{k3} \cdot [\mathrm{coII\_p}] \cdot [\mathrm{MLTH\_p}] \tag{6}$$

6.4 Reaction R4

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

Name compound III formation

Reaction equation

$$\mathrm{O2minus\_p} + \mathrm{per3\_p} \longrightarrow \mathrm{coIII\_p} \tag{7}$$

Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
O2minus_p	Superoxide	
per3_p	Ferric peroxidase	

Product

Table 13: Properties of each product.

Id	Name	SBO
coIII_p	compound III	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{phagosome}) \cdot \mathrm{k4} \cdot [\mathrm{per3\_p}] \cdot [\mathrm{O2minus\_p}] \tag{8}$$

6.5 Reaction R5

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

Name H2O2 formation

Reaction equation

$$2\,\mathrm{O2minus\_p} + 2\,\mathrm{H\_p} \longrightarrow \mathrm{O2\_p} + \mathrm{H2O2\_p} \tag{9}$$

Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
O2minus_p	Superoxide	
H_p	Hydrogen	

Products

Table 15: Properties of each product.

Id	Name	SBO
O2_p	Oxygen	
H2O2_p	H2O2	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{phagosome}) \cdot \mathrm{k5} \cdot [\mathrm{O2minus\_p}]^2 \tag{10}$$

6.6 Reaction R6

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

Name compound III-superoxide reaction

Reaction equation

$$\mathrm{O2minus\_p} + \mathrm{coIII\_p} \longrightarrow \mathrm{O2\_p} + \mathrm{coI\_p} \tag{11}$$

Reactants

Table 16: Properties of each reactant.

Id	Name	SBO
O2minus_p	Superoxide	
coIII_p	compound III	

Products

Table 17: Properties of each product.

Id	Name	SBO
O2_p	Oxygen	
coI_p	compound I	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{phagosome}) \cdot \mathrm{k6} \cdot [\mathrm{coIII\_p}] \cdot [\mathrm{O2minus\_p}] \tag{12}$$

6.7 Reaction R7

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

Name NADPH autooxidation

Reaction equation

$$\mathrm{O2\_c} + \mathrm{NADPH\_c} \longrightarrow \mathrm{H2O2\_c} + \mathrm{NADPplus\_c} \tag{13}$$

Reactants

Table 18: Properties of each reactant.

Id	Name	SBO
O2_c	Oxygen	
NADPH_c	NADPH	

Products

Table 19: Properties of each product.

Id	Name	SBO
H2O2_c	H2O2	
NADPplus_c	NADP	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{k7} \cdot [\mathrm{NADPH\_c}] \cdot [\mathrm{O2\_c}] \tag{14}$$

6.8 Reaction R8

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

Name NADP radical-Oxygen reaction

Reaction equation

$$\mathrm{O2\_c} + \mathrm{NADP\_c} \longrightarrow \mathrm{O2minus\_c} + \mathrm{NADPplus\_c} \tag{15}$$

Reactants

Table 20: Properties of each reactant.

Id	Name	SBO
O2_c	Oxygen	
NADP_c	NADP	

Products

Table 21: Properties of each product.

Id	Name	SBO
O2minus_c	Superoxide	
NADPplus_c	NADP	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{k8} \cdot [\mathrm{NADP\_c}] \cdot [\mathrm{O2\_c}] \tag{16}$$

6.9 Reaction R9

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

Name H2O2 formation

Reaction equation

$$2\,\mathrm{O2minus\_c} + 2\,\mathrm{H\_c} \longrightarrow \mathrm{O2\_c} + \mathrm{H2O2\_c} \tag{17}$$

Reactants

Table 22: Properties of each reactant.

Id	Name	SBO
O2minus_c	Superoxide	
H_c	Hydrogen	

Products

Table 23: Properties of each product.

Id	Name	SBO
O2_c	Oxygen	
H2O2_c	H2O2	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{k9} \cdot [\mathrm{O2minus\_c}]^2 \tag{18}$$

6.10 Reaction R10

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

Name NADP free radical formation

Reaction equation

$$\mathrm{NADPH\_c} + \mathrm{MLT\_c} \longrightarrow \mathrm{NADP\_c} + \mathrm{MLTH\_c} \tag{19}$$

Reactants

Table 24: Properties of each reactant.

Id	Name	SBO
NADPH_c	NADPH	
MLT_c	Melatonin free radical	

Products

Table 25: Properties of each product.

Id	Name	SBO
NADP_c	NADP	
MLTH_c	Melatonin	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{k10} \cdot [\mathrm{MLT\_c}] \cdot [\mathrm{NADPH\_c}] \tag{20}$$

6.11 Reaction R11

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

Name NADP dimer formation

Reaction equation

$$2\,\mathrm{NADP\_c} \longrightarrow \mathrm{NADP2\_c} \tag{21}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
NADP_c	NADP	

Product

Table 27: Properties of each product.

Id	Name	SBO
NADP2_c	NADP2	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{k11} \cdot [\mathrm{NADP\_c}]^2 \tag{22}$$

6.12 Reaction R12

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

Name NADPH synthesis

Reaction equation

$$\emptyset \longrightarrow \mathrm{NADPH\_c} \tag{23}$$

Product

Table 28: Properties of each product.

Id	Name	SBO
NADPH_c	NADPH	

Kinetic Law

Derived unit contains undeclared units

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

6.13 Reaction R13a

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

Name Oxygen diffusion

Reaction equation

$$\emptyset \longrightarrow \mathrm{O2\_c} \tag{25}$$

Product

Table 29: Properties of each product.

Id	Name	SBO
O2_c	Oxygen	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{k13} \tag{26}$$

6.14 Reaction R13b

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

Name Oxygen diffusion

Reaction equation

$$\mathrm{O2\_c} \longrightarrow \emptyset \tag{27}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
O2_c	Oxygen	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{kminus13} \cdot [\mathrm{O2\_c}] \tag{28}$$

6.15 Reaction R14

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

Name Oxygen diffusion- phagosome/cytoplasm

Reaction equation

$$\mathrm{O2\_p} \longrightarrow \mathrm{O2\_c} \tag{29}$$

Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
O2_p	Oxygen	

Product

Table 32: Properties of each product.

Id	Name	SBO
O2_c	Oxygen	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{vol}\,(\mathrm{phagosome}) \cdot (\mathrm{k14} \cdot [\mathrm{O2\_p}] - \mathrm{k14} \cdot [\mathrm{O2\_c}]) \tag{30}$$

6.16 Reaction R15

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

Name H2O2 diffusion phagosome/cytoplasm

Reaction equation

$$\mathrm{H2O2\_p} \longrightarrow \mathrm{H2O2\_c} \tag{31}$$

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
H2O2_p	H2O2	

Product

Table 34: Properties of each product.

Id	Name	SBO
H2O2_c	H2O2	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}\,(\mathrm{phagosome}) \cdot (\mathrm{k15} \cdot [\mathrm{H2O2\_p}] - \mathrm{k15} \cdot [\mathrm{H2O2\_c}]) \tag{32}$$

6.17 Reaction R16

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

Name Melatonin diffusion phagosome/cytoplasm

Reaction equation

$$\mathrm{MLTH\_p} \longrightarrow \mathrm{MLTH\_c} \tag{33}$$

Reactant

Table 35: Properties of each reactant.

Id	Name	SBO
MLTH_p	Melatonin	

Product

Table 36: Properties of each product.

Id	Name	SBO
MLTH_c	Melatonin	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{vol}\,(\mathrm{phagosome}) \cdot (\mathrm{k16} \cdot [\mathrm{MLTH\_p}] - \mathrm{k16} \cdot [\mathrm{MLTH\_c}]) \tag{34}$$

6.18 Reaction R17

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

Name Melatonin free radical diffusion phagosome/cytoplasm

Reaction equation

$$\text{MLT\_p} \longrightarrow \text{MLT\_c} \tag{35}$$

Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
MLT_p	Melatonin free radical	

Product

Table 38: Properties of each product.

Id	Name	SBO
MLT_c	Melatonin free radical	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \text{vol}\,(\text{phagosome}) \cdot (\text{k17} \cdot [\text{MLT\_p}] - \text{k17} \cdot [\text{MLT\_c}]) \tag{36}$$

6.19 Reaction R18

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

Name Superoxide diffusion phagosome/cytoplasm

Reaction equation

$$\text{O2minus\_p} \longrightarrow \text{O2minus\_c} \tag{37}$$

Reactant

Table 39: Properties of each reactant.

Id	Name	SBO
O2minus_p	Superoxide	

Product

Table 40: Properties of each product.

Id	Name	SBO
O2minus_c	Superoxide	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \mathrm{vol}\,(\mathrm{phagosome}) \cdot (\mathrm{k18} \cdot [\mathrm{O2minus\_p}] - \mathrm{k18} \cdot [\mathrm{O2minus\_c}]) \tag{38}$$

6.20 Reaction R19

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

Name NADPH oxidase activity

Reaction equation

$$2\,\mathrm{O2\_p} + \mathrm{NADPH\_c} \longrightarrow 2\,\mathrm{O2minus\_p} + \mathrm{NADPplus\_c} \tag{39}$$

Reactants

Table 41: Properties of each reactant.

Id	Name	SBO
O2_p	Oxygen	
NADPH_c	NADPH	

Products

Table 42: Properties of each product.

Id	Name	SBO
O2minus_p	Superoxide	

Id	Name	SBO
NADPplus_c	NADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \mathrm{vol}\,(\mathrm{phagosome}) \cdot \frac{\frac{\mathrm{V}\cdot[\mathrm{NADPH\_c}]}{\mathrm{Knadph}} \cdot \left(1 + \frac{[\mathrm{NADPH\_c}]}{\mathrm{Knadph}}\right) \cdot [\mathrm{O2\_p}]}{\left(\mathrm{L} + \left(1 + \frac{[\mathrm{NADPH\_c}]}{\mathrm{Knadph}}\right)^2\right) \cdot (\mathrm{Ko} + [\mathrm{O2\_p}])} \tag{40}$$

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 H2O2_p

Name H2O2

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

This species takes part in three reactions (as a reactant in R1, R15 and as a product in R5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{H2O2\_p} = v_5 - v_1 - v_{16} \tag{41}$$

7.2 Species per3_p

Name Ferric peroxidase

Initial concentration $300\ \mu\mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in R1, R4 and as a product in R3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{per3\_p} = v_3 - v_1 - v_4 \tag{42}$$

7.3 Species coI_p

Name compound I

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

This species takes part in three reactions (as a reactant in R2 and as a product in R1, R6).

$$\frac{\text{d}}{\text{d}t}\text{coI\_p} = v_1 + v_6 - v_2 \tag{43}$$

7.4 Species MLTH_p

Name Melatonin

Initial concentration $300\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in three reactions (as a reactant in R2, R3, R16).

$$\frac{\text{d}}{\text{d}t}\text{MLTH\_p} = -v_2 - v_3 - v_{17} \tag{44}$$

7.5 Species coII_p

Name compound II

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

This species takes part in two reactions (as a reactant in R3 and as a product in R2).

$$\frac{\text{d}}{\text{d}t}\text{coII\_p} = v_2 - v_3 \tag{45}$$

7.6 Species MLT_p

Name Melatonin free radical

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

This species takes part in three reactions (as a reactant in R17 and as a product in R2, R3).

$$\frac{\text{d}}{\text{d}t}\text{MLT\_p} = v_2 + v_3 - v_{18} \tag{46}$$

7.7 Species O2minus_p

Name Superoxide

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

This species takes part in five reactions (as a reactant in R4, R5, R6, R18 and as a product in R19).

$$\frac{\text{d}}{\text{d}t}\text{O2minus\_p} = 2\,v_{20} - v_4 - 2\,v_5 - v_6 - v_{19} \tag{47}$$

7.8 Species H_p

Name Hydrogen

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

This species takes part in one reaction (as a reactant in R5).

$$\frac{\text{d}}{\text{d}t}\text{H\_p} = -2\,v_5 \tag{48}$$

7.9 Species O2_p

Name Oxygen

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

This species takes part in four reactions (as a reactant in R14, R19 and as a product in R5, R6).

$$\frac{\text{d}}{\text{d}t}\text{O2\_p} = v_5 + v_6 - v_{15} - 2\,v_{20} \tag{49}$$

7.10 Species NADPH_c

Name NADPH

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

This species takes part in four reactions (as a reactant in R7, R10, R19 and as a product in R12).

$$\frac{\text{d}}{\text{d}t}\text{NADPH\_c} = v_{12} - v_7 - v_{10} - v_{20} \tag{50}$$

7.11 Species O2_c

Name Oxygen

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

This species takes part in six reactions (as a reactant in R7, R8, R13b and as a product in R9, R13a, R14).

$$\frac{\text{d}}{\text{d}t}\text{O2\_c} = v_9 + v_{13} + v_{15} - v_7 - v_8 - v_{14} \tag{51}$$

7.12 Species NADPplus_c

Name NADP

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

This species takes part in three reactions (as a product in R7, R8, R19).

$$\frac{\text{d}}{\text{d}t}\text{NADPplus\_c} = v_7 + v_8 + v_{20} \tag{52}$$

7.13 Species H2O2_c

Name H2O2

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

This species takes part in three reactions (as a product in R7, R9, R15).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{H2O2\_c} = v_7 + v_9 + v_{16} \tag{53}$$

7.14 Species NADP_c

Name NADP

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

This species takes part in three reactions (as a reactant in R8, R11 and as a product in R10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{NADP\_c} = v_{10} - v_8 - 2\,v_{11} \tag{54}$$

7.15 Species O2minus_c

Name Superoxide

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

This species takes part in three reactions (as a reactant in R9 and as a product in R8, R18).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{O2minus\_c} = v_8 + v_{19} - 2\,v_9 \tag{55}$$

7.16 Species H_c

Name Hydrogen

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

This species takes part in one reaction (as a reactant in R9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{H\_c} = -2\,v_9 \tag{56}$$

7.17 Species MLT_c

Name Melatonin free radical

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

This species takes part in two reactions (as a reactant in R10 and as a product in R17).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{MLT\_c} = v_{18} - v_{10} \tag{57}$$

7.18 Species MLTH_c

Name Melatonin

Initial concentration $300\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a product in R10, R16).

$$\frac{\text{d}}{\text{d}t}\text{MLTH\_c} = v_{10} + v_{17} \tag{58}$$

7.19 Species coIII_p

Name compound III

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

This species takes part in two reactions (as a reactant in R6 and as a product in R4).

$$\frac{\text{d}}{\text{d}t}\text{coIII\_p} = v_4 - v_6 \tag{59}$$

7.20 Species NADP2_c

Name NADP2

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

This species takes part in one reaction (as a product in R11).

$$\frac{\text{d}}{\text{d}t}\text{NADP2\_c} = v_{11} \tag{60}$$

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