

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 Dharuri¹ 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: [BIOMD000000143](#).

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

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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 1

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	<input checked="" type="checkbox"/>	cytoplasm
cytoplasm	cytoplasm		3	10	l	<input checked="" type="checkbox"/>	

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

5 Parameters

This model contains 24 global parameters.

Table 4: Properties of each parameter.

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

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

Nº	Id	Name	Reaction Equation	SBO
1	R1	Myeloperoxidase reaction	$\text{per3_p} + \text{H2O2_p} \longrightarrow \text{coI_p}$	
2	R2	Melatonin-compound I reaction	$\text{MLTH_p} + \text{coI_p} \longrightarrow \text{MLT_p} + \text{coII_p}$	
3	R3	Melatonin-compound II reaction	$\text{MLTH_p} + \text{coII_p} \longrightarrow \text{MLT_p} + \text{per3_p}$	
4	R4	compound III formation	$\text{O2minus_p} + \text{per3_p} \longrightarrow \text{coIII_p}$	
5	R5	H2O2 formation	$2 \text{O2minus_p} + 2 \text{H_p} \longrightarrow \text{O2_p} + \text{H2O2_p}$	
6	R6	compound III-superoxide reaction	$\text{O2minus_p} + \text{coIII_p} \longrightarrow \text{O2_p} + \text{coI_p}$	
7	R7	NADPH autooxidation	$\text{O2_c} + \text{NADPH_c} \longrightarrow \text{H2O2_c} + \text{NADPplus_c}$	
8	R8	NADP radical-Oxygen reaction	$\text{O2_c} + \text{NADP_c} \longrightarrow \text{O2minus_c} + \text{NADPplus_c}$	
9	R9	H2O2 formation	$2 \text{O2minus_c} + 2 \text{H_c} \longrightarrow \text{O2_c} + \text{H2O2_c}$	
10	R10	NADP free radical formation	$\text{NADPH_c} + \text{MLT_c} \longrightarrow \text{NADP_c} + \text{MLTH_c}$	
11	R11	NADP dimer formation	$2 \text{NADP_c} \longrightarrow \text{NADP2_c}$	
12	R12	NADPH synthesis	$\emptyset \longrightarrow \text{NADPH_c}$	
13	R13a	Oxygen diffusion	$\emptyset \longrightarrow \text{O2_c}$	
14	R13b	Oxygen diffusion	$\text{O2_c} \longrightarrow \emptyset$	
15	R14	Oxygen diffusion- phagosome/cytoplasm	$\text{O2_p} \longrightarrow \text{O2_c}$	
16	R15	H2O2 diffusion phagosome/cytoplasm	$\text{H2O2_p} \longrightarrow \text{H2O2_c}$	
17	R16	Melatonin diffusion phagosome/cytoplasm	$\text{MLTH_p} \longrightarrow \text{MLTH_c}$	
18	R17	Melatonin free radical diffusion phagosome/cytoplasm	$\text{MLT_p} \longrightarrow \text{MLT_c}$	
19	R18	Superoxide diffusion phagosome/cytoplasm	$\text{O2minus_p} \longrightarrow \text{O2minus_c}$	
20	R19	NADPH oxidase activity	$2 \text{O2_p} + \text{NADPH_c} \longrightarrow 2 \text{O2minus_p} + \text{NADPplus_c}$	

6.1 Reaction R1

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

Name Myeloperoxidase reaction

Reaction equation



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

$$v_1 = \text{vol}(\text{phagosome}) \cdot (k_1 \cdot [\text{H2O2_p}] \cdot [\text{per3_p}] - k_{\text{minus1}} \cdot [\text{coI_p}]) \quad (2)$$

6.2 Reaction R2

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

Name Melatonin-compound I reaction

Reaction equation



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

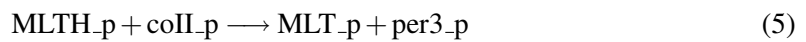
$$v_2 = \text{vol}(\text{phagosome}) \cdot k_2 \cdot [\text{coI_p}] \cdot [\text{MLTH_p}] \quad (4)$$

6.3 Reaction R3

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

Name Melatonin-compound II reaction

Reaction equation



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

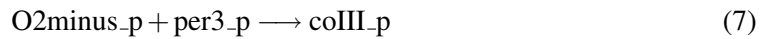
$$v_3 = \text{vol}(\text{phagosome}) \cdot k_3 \cdot [\text{coII_p}] \cdot [\text{MLTH_p}] \quad (6)$$

6.4 Reaction R4

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

Name compound III formation

Reaction equation



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

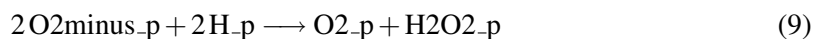
$$v_4 = \text{vol}(\text{phagosome}) \cdot k_4 \cdot [\text{per3_p}] \cdot [\text{O2minus_p}] \quad (8)$$

6.5 Reaction R5

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

Name H2O2 formation

Reaction equation



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

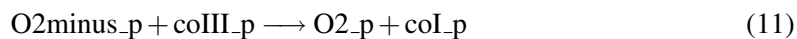
$$v_5 = \text{vol}(\text{phagosome}) \cdot k_5 \cdot [\text{O2minus_p}]^2 \quad (10)$$

6.6 Reaction R6

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

Name compound III-superoxide reaction

Reaction equation



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

$$v_6 = \text{vol}(\text{phagosome}) \cdot k_6 \cdot [\text{coIII_p}] \cdot [\text{O2minus_p}] \quad (12)$$

6.7 Reaction R7

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

Name NADPH autooxidation

Reaction equation



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

$$v_7 = \text{vol}(\text{cytoplasm}) \cdot k_7 \cdot [\text{NADPH}_c] \cdot [\text{O2}_c] \quad (14)$$

6.8 Reaction R8

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

Name NADP radical-Oxygen reaction

Reaction equation



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

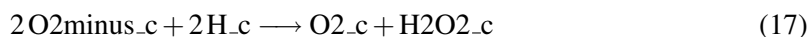
$$v_8 = \text{vol}(\text{cytoplasm}) \cdot k_8 \cdot [\text{NADP}_c] \cdot [\text{O2}_c] \quad (16)$$

6.9 Reaction R9

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

Name H2O2 formation

Reaction equation



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

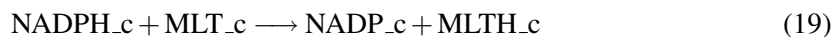
$$v_9 = \text{vol}(\text{cytoplasm}) \cdot k_9 \cdot [\text{O2minus_c}]^2 \quad (18)$$

6.10 Reaction R10

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

Name NADP free radical formation

Reaction equation



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

$$v_{10} = \text{vol}(\text{cytoplasm}) \cdot k_{10} \cdot [\text{MLT_c}] \cdot [\text{NADPH_c}] \quad (20)$$

6.11 Reaction R11

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

Name NADP dimer formation

Reaction equation



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

$$v_{11} = \text{vol}(\text{cytoplasm}) \cdot k_{11} \cdot [\text{NADP_c}]^2 \quad (22)$$

6.12 Reaction R12

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

Name NADPH synthesis

Reaction equation



Product

Table 28: Properties of each product.

Id	Name	SBO
NADPH_c	NADPH	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \text{vol}(\text{cytoplasm}) \cdot k_{12} \quad (24)$$

6.13 Reaction R13a

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

Name Oxygen diffusion

Reaction equation



Product

Table 29: Properties of each product.

Id	Name	SBO
02_c	Oxygen	

Kinetic Law

Derived unit contains undeclared units

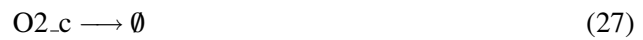
$$v_{13} = \text{vol}(\text{cytoplasm}) \cdot k_{13} \quad (26)$$

6.14 Reaction R13b

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

Name Oxygen diffusion

Reaction equation



Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
02_c	Oxygen	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \text{vol}(\text{cytoplasm}) \cdot k_{\text{minus13}} \cdot [\text{O2_c}] \quad (28)$$

6.15 Reaction R14

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

Name Oxygen diffusion- phagosome/cytoplasm

Reaction equation



Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
02_p	Oxygen	

Product

Table 32: Properties of each product.

Id	Name	SBO
02_c	Oxygen	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{vol}(\text{phagosome}) \cdot (k_{14} \cdot [\text{O2_p}] - k_{14} \cdot [\text{O2_c}]) \quad (30)$$

6.16 Reaction R15

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

Name H2O2 diffusion phagosome/cytoplasm

Reaction equation



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

$$v_{16} = \text{vol}(\text{phagosome}) \cdot (k_{15} \cdot [\text{H2O2}_p] - k_{15} \cdot [\text{H2O2}_c]) \quad (32)$$

6.17 Reaction R16

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

Name Melatonin diffusion phagosome/cytoplasm

Reaction equation



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

$$v_{17} = \text{vol}(\text{phagosome}) \cdot (k_{16} \cdot [\text{MLTH}_p] - k_{16} \cdot [\text{MLTH}_c]) \quad (34)$$

6.18 Reaction R17

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

Name Melatonin free radical diffusion phagosome/cytoplasm

Reaction equation



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

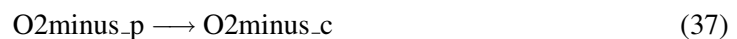
$$v_{18} = \text{vol}(\text{phagosome}) \cdot (k_{17} \cdot [\text{MLT_p}] - k_{17} \cdot [\text{MLT_c}]) \quad (36)$$

6.19 Reaction R18

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

Name Superoxide diffusion phagosome/cytoplasm

Reaction equation



Reactant

Table 39: Properties of each reactant.

Id	Name	SBO
02minus_p	Superoxide	

Product

Table 40: Properties of each product.

Id	Name	SBO
02minus_c	Superoxide	

Kinetic Law

Derived unit contains undeclared units

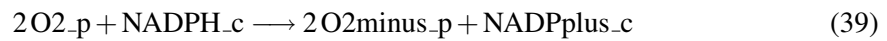
$$v_{19} = \text{vol}(\text{phagosome}) \cdot (k_{18} \cdot [\text{O2minus_p}] - k_{18} \cdot [\text{O2minus_c}]) \quad (38)$$

6.20 Reaction R19

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

Name NADPH oxidase activity

Reaction equation



Reactants

Table 41: Properties of each reactant.

Id	Name	SBO
02_p	Oxygen	
NADPH_c	NADPH	

Products

Table 42: Properties of each product.

Id	Name	SBO
02minus_p	Superoxide	

Id	Name	SBO
NADPplus_c	NADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \text{vol}(\text{phagosome}) \cdot \frac{\frac{V \cdot [\text{NADPH}_c]}{K_{\text{nadph}}} \cdot \left(1 + \frac{[\text{NADPH}_c]}{K_{\text{nadph}}}\right) \cdot [\text{O2}_p]}{\left(L + \left(1 + \frac{[\text{NADPH}_c]}{K_{\text{nadph}}}\right)^2\right) \cdot (K_o + [\text{O2}_p])} \quad (40)$$

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

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

$$\frac{d}{dt} \text{H2O2}_p = v_5 - v_1 - v_{16} \quad (41)$$

7.2 Species `per3_p`

Name Ferric peroxidase

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

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

$$\frac{d}{dt} \text{per3}_p = v_3 - v_1 - v_4 \quad (42)$$

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](#)).

$$\frac{d}{dt}\text{coI}_p = v_1 + v_6 - v_2 \quad (43)$$

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](#)).

$$\frac{d}{dt}\text{MLTH}_p = -v_2 - v_3 - v_{17} \quad (44)$$

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](#)).

$$\frac{d}{dt}\text{coII}_p = v_2 - v_3 \quad (45)$$

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](#)).

$$\frac{d}{dt}\text{MLT}_p = v_2 + v_3 - v_{18} \quad (46)$$

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](#)).

$$\frac{d}{dt}\text{O2minus}_p = 2v_{20} - v_4 - 2v_5 - v_6 - v_{19} \quad (47)$$

7.8 Species H_p

Name Hydrogen

Initial concentration 0 μmol · l⁻¹

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

$$\frac{d}{dt}H_p = -2 v_5 \quad (48)$$

7.9 Species O2_p

Name Oxygen

Initial concentration 0 μmol · l⁻¹

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

$$\frac{d}{dt}O2_p = v_5 + v_6 - v_{15} - 2 v_{20} \quad (49)$$

7.10 Species NADPH_c

Name NADPH

Initial concentration 0 μmol · l⁻¹

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

$$\frac{d}{dt}NADPH_c = v_{12} - v_7 - v_{10} - v_{20} \quad (50)$$

7.11 Species O2_c

Name Oxygen

Initial concentration 0 μmol · l⁻¹

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

$$\frac{d}{dt}O2_c = v_9 + v_{13} + v_{15} - v_7 - v_8 - v_{14} \quad (51)$$

7.12 Species NADPplus_c

Name NADP

Initial concentration 0 μmol · l⁻¹

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

$$\frac{d}{dt}NADPplus_c = v_7 + v_8 + v_{20} \quad (52)$$

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](#)).

$$\frac{d}{dt}\text{H2O2_c} = v_7 + v_9 + v_{16} \quad (53)$$

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](#)).

$$\frac{d}{dt}\text{NADP_c} = v_{10} - v_8 - 2 v_{11} \quad (54)$$

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](#)).

$$\frac{d}{dt}\text{O2minus_c} = v_8 + v_{19} - 2 v_9 \quad (55)$$

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](#)).

$$\frac{d}{dt}\text{H_c} = -2 v_9 \quad (56)$$

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](#)).

$$\frac{d}{dt}\text{MLT_c} = v_{18} - v_{10} \quad (57)$$

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).

$$\frac{d}{dt}\text{MLTH_c} = v_{10} + v_{17} \quad (58)$$

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).

$$\frac{d}{dt}\text{coIII_p} = v_4 - v_6 \quad (59)$$

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).

$$\frac{d}{dt}\text{NADP2_c} = v_{11} \quad (60)$$

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