SBML Model Report

Model name: "Restif2006_Whooping_Cough"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Lukas Endler[1] at April 20th 2010 at 11:54 p. m. and last time modified at April eighth 2016 at 4:09 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	1
species types	0	species	9
events	0	constraints	0
reactions	20	function definitions	0
global parameters	21	unit definitions	4
rules	14	initial assignments	0

Model Notes

This is the model described in the article:
Integrating life history and cross-immunity into the evolutionary dynamics of pathogens.
Restif O, Grenfell BT. Proc Biol Sci. 2006 Feb 22;273(1585):409-16. PMID:16615206, doi:10.1098/rspb.2005.3335;
Abstract:
Models for the diversity and evolution of pathogens have branched into two main directions: the adaptive dynamics of quantitative life-history traits (notably virulence) and the maintenance and invasion of multiple, antigenically diverse strains that interact with the host's immune memory. In a first attempt to reconcile these two approaches, we developed a simple modelling

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framework where two strains of pathogens, defined by a pair of life-history traits (infectious period and infectivity), interfere through a given level of cross-immunity. We used whooping cough as a potential example, but the framework proposed here could be applied to other acute infectious diseases. Specifically, we analysed the effects of these parameters on the invasion dynamics of one strain into a population, where the second strain is endemic. Whereas the deterministic version of the model converges towards stable coexistence of the two strains in most cases, stochastic simulations showed that transient epidemic dynamics can cause the extinction of either strain. Thus ecological dynamics, modulated by the immune parameters, eventually determine the adaptive value of different pathogen genotypes. We advocate an integrative view of pathogen dynamics at the crossroads of immunology, epidemiology and evolution, as a way towards efficient control of infectious diseases.

This version of the model can be used for both the stochastic and the deterministic simulations described in the article. For deterministic interpretations with infinite population sizes, set the population size N = 1. The model reproduces the deterministic time courses. Stochastic interpretation with Copasi UI gave results similar to the article, but was not extensively tested. The initial conditions for competition simulations can be derived by equilibrating the system for one pathogen and then adding a starting concentration for the other.

Originally created by libAntimony v1.3 (using libSBML 4.1.0-b1)

2 Unit Definitions

This is an overview of seven unit definitions of which three are predefined by SBML and not mentioned in the model.

2.1 Unit `substance`

Name individuals

Definition item

2.2 Unit `time`

Name years

Definition $3.1536 \cdot 10^7$ s

2.3 Unit `days`

Name days

Definition 86400 s

2.4 Unit per_year

Name per_year

Definition $\left(3.1536 \cdot 10^{7}\ \mathrm{s}\right)^{-1}$

2.5 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

2.6 Unit area

Notes Square metre is the predefined SBML unit for area since SBML Level 2 Version 1.

Definition m^2

2.7 Unit length

Notes Metre is the predefined SBML unit for length since SBML Level 2 Version 1.

Definition m

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
env	environment	0000290	3	1	litre	☑	

3.1 Compartment env

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

Name environment

SBO:0000290 physical compartment

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
N		env	item	⊟	⊟
S		env	item	⊟	⊟
I_1		env	item	⊟	⊟
I_2		env	item	⊟	⊟
R_1		env	item	⊟	⊟
R_2		env	item	⊟	⊟
I_1p		env	item	⊟	⊟
I_2p		env	item	⊟	⊟
R_p		env	item	⊟	⊟

5 Parameters

This model contains 21 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			0.0	$(3.1536 \cdot 10^7\ \mathrm{s})^{-1}$	⊟
l_e	life expectancy		50.0	$3.1536 \cdot 10^7\ \mathrm{s}$	☑
beta_1			0.0	$(3.1536 \cdot 10^7\ \mathrm{s})^{-1}$	⊟
R0_1			17.0	dimensionless	☑
gamma_1			0.0	$(3.1536 \cdot 10^7\ \mathrm{s})^{-1}$	⊟
beta_2			0.0	$(3.1536 \cdot 10^7\ \mathrm{s})^{-1}$	⊟
R0_2			17.0	dimensionless	☑
gamma_2			0.0	$(3.1536 \cdot 10^7\ \mathrm{s})^{-1}$	⊟
tInf_1	infectious period 1		21.0	86400 s	☑
tInf_2	infectious period 2		21.0	86400 s	☑
sigma			0.0	$(3.1536 \cdot 10^7\ \mathrm{s})^{-1}$	⊟
tImm	immune period		20.0	$3.1536 \cdot 10^7\ \mathrm{s}$	☑
Lambda_1			0.0	$(3.1536 \cdot 10^7\ \mathrm{s})^{-1}$	⊟
Lambda_2			0.0	$(3.1536 \cdot 10^7\ \mathrm{s})^{-1}$	⊟
I_1_frac			0.0	dimensionless	⊟
I_2_frac			0.0	dimensionless	⊟
S_frac			0.0	dimensionless	⊟
R1_frac			0.0	dimensionless	⊟
R2_frac			0.0	dimensionless	⊟
Rp_frac			0.0	dimensionless	⊟
psi			0.2	dimensionless	☑

6 Rules

This is an overview of 14 rules.

6.1 Rule mu

Rule mu is an assignment rule for parameter mu:

$$\mathrm{mu} = \frac{1}{\mathrm{l\_e}} \tag{1}$$

6.2 Rule beta_1

Rule beta_1 is an assignment rule for parameter beta_1:

$$\text{beta\_1} = \text{R0\_1} \cdot \text{gamma\_1} \tag{2}$$

Derived unit $\left(3.1536 \cdot 10^7\ \text{s}\right)^{-1}$

6.3 Rule gamma_1

Rule gamma_1 is an assignment rule for parameter gamma_1:

$$\text{gamma\_1} = \frac{365}{\text{tInf\_1}} \tag{3}$$

6.4 Rule beta_2

Rule beta_2 is an assignment rule for parameter beta_2:

$$\text{beta\_2} = \text{R0\_2} \cdot \text{gamma\_2} \tag{4}$$

Derived unit $\left(3.1536 \cdot 10^7\ \text{s}\right)^{-1}$

6.5 Rule gamma_2

Rule gamma_2 is an assignment rule for parameter gamma_2:

$$\text{gamma\_2} = \frac{365}{\text{tInf\_2}} \tag{5}$$

6.6 Rule sigma

Rule sigma is an assignment rule for parameter sigma:

$$\text{sigma} = \frac{1}{\text{tImm}} \tag{6}$$

6.7 Rule Lambda_1

Rule Lambda_1 is an assignment rule for parameter Lambda_1:

$$\text{Lambda\_1} = \frac{\text{beta\_1} \cdot (\text{I\_1} + \text{I\_1p})}{\text{N}} \tag{7}$$

Derived unit $\left(3.1536 \cdot 10^7\ \text{s}\right)^{-1}$

6.8 Rule Lambda_2

Rule Lambda_2 is an assignment rule for parameter Lambda_2:

$$\text{Lambda\_2} = \frac{\text{beta\_2} \cdot (\text{I\_2} + \text{I\_2p})}{\text{N}} \tag{8}$$

Derived unit $\left(3.1536 \cdot 10^7 \text{ s}\right)^{-1}$

6.9 Rule I_1_frac

Rule I_1_frac is an assignment rule for parameter I_1_frac:

$$\text{I\_1\_frac} = \frac{\text{I\_1} + \text{I\_1p}}{\text{N}} \tag{9}$$

Derived unit dimensionless

6.10 Rule I_2_frac

Rule I_2_frac is an assignment rule for parameter I_2_frac:

$$\text{I\_2\_frac} = \frac{\text{I\_2} + \text{I\_2p}}{\text{N}} \tag{10}$$

Derived unit dimensionless

6.11 Rule S_frac

Rule S_frac is an assignment rule for parameter S_frac:

$$\text{S\_frac} = \frac{\text{S}}{\text{N}} \tag{11}$$

Derived unit dimensionless

6.12 Rule R1_frac

Rule R1_frac is an assignment rule for parameter R1_frac:

$$\text{R1\_frac} = \frac{\text{R\_1} + \text{R\_p}}{\text{N}} \tag{12}$$

Derived unit dimensionless

6.13 Rule R2_frac

Rule R2_frac is an assignment rule for parameter R2_frac:

$$\text{R2\_frac} = \frac{\text{R\_2} + \text{R\_p}}{\text{N}} \tag{13}$$

Derived unit dimensionless

6.14 Rule Rp_frac

Rule Rp_frac is an assignment rule for parameter Rp_frac:

$$\mathrm{Rp\_frac} = \frac{\mathrm{R\_p}}{\mathrm{N}} \tag{14}$$

Derived unit dimensionless

7 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	Birth	$\emptyset \xrightarrow{\mathrm{N}} \mathrm{S}$	0000375
2	r2	Death in S	$\mathrm{S} \longrightarrow \emptyset$	0000375
3	r3	Death in I_1	$\mathrm{I\_1} \longrightarrow \emptyset$	0000375
4	r4	Death in I_2	$\mathrm{I\_2} \longrightarrow \emptyset$	0000375
5	r5	Death in R_1	$\mathrm{R\_1} \longrightarrow \emptyset$	0000375
6	r6	Death in R_2	$\mathrm{R\_2} \longrightarrow \emptyset$	0000375
7	r7	Death in I_1p	$\mathrm{I\_1p} \longrightarrow \emptyset$	0000375
8	r8	Death in I_2p	$\mathrm{I\_2p} \longrightarrow \emptyset$	0000375
9	r9	Death in R_p	$\mathrm{R\_p} \longrightarrow \emptyset$	0000375
10	r10	Primary Infection with strain 1	$\mathrm{S} \xrightarrow{\mathrm{I\_1,\ I\_1p,\ N}} \mathrm{I\_1}$	0000375
11	r11	Primary Infection with strain 2	$\mathrm{S} \xrightarrow{\mathrm{I\_2,\ I\_2p,\ N}} \mathrm{I\_2}$	0000375
12	r12	Secondary Infection with strain 1	$\mathrm{R\_2} \xrightarrow{\mathrm{I\_1,\ I\_1p,\ N}} \mathrm{I\_1p}$	0000375
13	r13	Secondary Infection with strain 2	$\mathrm{R\_1} \xrightarrow{\mathrm{I\_2,\ I\_2p,\ N}} \mathrm{I\_2p}$	0000375
14	r14	Recovery (I_1)	$\mathrm{I\_1} \longrightarrow \mathrm{R\_1}$	0000375
15	r15	Recovery (I_2)	$\mathrm{I\_2} \longrightarrow \mathrm{R\_2}$	0000375
16	r16	Recovery (I_1p)	$\mathrm{I\_1p} \longrightarrow \mathrm{R\_p}$	0000375
17	r17	Recovery (I_2p)	$\mathrm{I\_2p} \longrightarrow \mathrm{R\_p}$	0000375
18	r18	Loss of Immunity (R_1)	$\mathrm{R\_1} \longrightarrow \mathrm{S}$	0000375
19	r19	Loss of Immunity (R_2)	$\mathrm{R\_2} \longrightarrow \mathrm{S}$	0000375
20	r20	Loss of Immunity (R_p)	$\mathrm{R\_p} \longrightarrow \mathrm{S}$	0000375

7.1 Reaction r1

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

Name Birth

SBO:0000375 process

Reaction equation

$$\emptyset \xrightarrow{\mathrm{N}} \mathrm{S} \tag{15}$$

Modifier

Table 6: Properties of each modifier.

Id	Name	SBO
N		

Product

Table 7: Properties of each product.

Id	Name	SBO
S		

Kinetic Law

Derived unit $\left(3.1536 \cdot 10^{7}\ \mathrm{s}\right)^{-1} \cdot \mathrm{item}$

$$v_1 = \mathrm{mu} \cdot \mathrm{N} \tag{16}$$

7.2 Reaction r2

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

Name Death in S

SBO:0000375 process

Reaction equation

$$\mathrm{S} \longrightarrow \emptyset \tag{17}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
S		

Kinetic Law

Derived unit $\left(3.1536 \cdot 10^{7}\ \mathrm{s}\right)^{-1} \cdot \mathrm{item}$

$$v_2 = \mathrm{mu} \cdot \mathrm{S} \tag{18}$$

7.3 Reaction r3

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

Name Death in I_1

SBO:0000375 process

Reaction equation

$$\mathrm{I\_1} \longrightarrow \emptyset \tag{19}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
I_1		

Kinetic Law

Derived unit $\left(3.1536 \cdot 10^{7}\ \mathrm{s}\right)^{-1} \cdot \mathrm{item}$

$$v_3 = \mathrm{mu} \cdot \mathrm{I\_1} \tag{20}$$

7.4 Reaction r4

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

Name Death in I_2

SBO:0000375 process

Reaction equation

$$\mathrm{I\_2} \longrightarrow \emptyset \tag{21}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
I_2		

Kinetic Law

Derived unit $\left(3.1536 \cdot 10^7\ \mathrm{s}\right)^{-1} \cdot \mathrm{item}$

$$v_4 = \mathrm{mu} \cdot \mathrm{I\_2} \tag{22}$$

7.5 Reaction r5

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

Name Death in R_1

SBO:0000375 process

Reaction equation

$$\mathrm{R\_1} \longrightarrow \emptyset \tag{23}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
R_1		

Kinetic Law

Derived unit $\left(3.1536 \cdot 10^7\ \mathrm{s}\right)^{-1} \cdot \mathrm{item}$

$$v_5 = \mathrm{mu} \cdot \mathrm{R\_1} \tag{24}$$

7.6 Reaction r6

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

Name Death in R_2

SBO:0000375 process

Reaction equation

$$\mathrm{R\_2} \longrightarrow \emptyset \tag{25}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
R_2		

Kinetic Law

Derived unit $\left(3.1536 \cdot 10^{7}\ \mathrm{s}\right)^{-1} \cdot \mathrm{item}$

$$v_6 = \mathrm{mu} \cdot \mathrm{R\_2} \tag{26}$$

7.7 Reaction r7

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

Name Death in I_1p

SBO:0000375 process

Reaction equation

$$\mathrm{I\_1p} \longrightarrow \emptyset \tag{27}$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
I_1p		

Kinetic Law

Derived unit $\left(3.1536 \cdot 10^{7}\ \mathrm{s}\right)^{-1} \cdot \mathrm{item}$

$$v_7 = \mathrm{mu} \cdot \mathrm{I\_1p} \tag{28}$$

7.8 Reaction r8

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

Name Death in I_2p

SBO:0000375 process

Reaction equation

$$\mathrm{I\_2p} \longrightarrow \emptyset \tag{29}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
I_2p		

Kinetic Law

Derived unit $\left(3.1536 \cdot 10^{7}\ \mathrm{s}\right)^{-1} \cdot \mathrm{item}$

$$v_8 = \mathrm{mu} \cdot \mathrm{I\_2p} \tag{30}$$

7.9 Reaction r9

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

Name Death in R_p

SBO:0000375 process

Reaction equation

$$\mathrm{R\_p} \longrightarrow \emptyset \tag{31}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
R_p		

Kinetic Law

Derived unit $\left(3.1536 \cdot 10^7 \text{ s}\right)^{-1} \cdot \text{item}$

$$v_9 = \text{mu} \cdot \text{R\_p} \tag{32}$$

7.10 Reaction r10

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

Name Primary Infection with strain 1

SBO:0000375 process

Reaction equation

$$\text{S} \xrightarrow{\text{I\_1, I\_1p, N}} \text{I\_1} \tag{33}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
S		

Modifiers

Table 17: Properties of each modifier.

Id	Name	SBO
I_1		
I_1p		
N		

Product

Table 18: Properties of each product.

Id	Name	SBO
I_1		

Kinetic Law

Derived unit $\left(3.1536 \cdot 10^7 \text{ s}\right)^{-1} \cdot \text{item}$

$$v_{10} = \text{beta\_1} \cdot \frac{\text{I\_1} + \text{I\_1p}}{\text{N}} \cdot \text{S} \tag{34}$$

7.11 Reaction r11

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

Name Primary Infection with strain 2

SBO:0000375 process

Reaction equation

$$\text{S} \xrightarrow{\text{I\_2, I\_2p, N}} \text{I\_2} \tag{35}$$

Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
S		

Modifiers

Table 20: Properties of each modifier.

Id	Name	SBO
I_2		
I_2p		
N		

Product

Table 21: Properties of each product.

Id	Name	SBO
I_2		

Kinetic Law

Derived unit $\left(3.1536 \cdot 10^7 \text{ s}\right)^{-1} \cdot \text{item}$

$$v_{11} = \text{beta\_2} \cdot \frac{\text{I\_2} + \text{I\_2p}}{\text{N}} \cdot \text{S} \tag{36}$$

7.12 Reaction r12

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

Name Secondary Infection with strain 1

SBO:0000375 process

Reaction equation

$$\text{R\_2} \xrightarrow{\text{I\_1, I\_1p, N}} \text{I\_1p} \tag{37}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
R_2		

Modifiers

Table 23: Properties of each modifier.

Id	Name	SBO
I_1		
I_1p		
N		

Product

Table 24: Properties of each product.

Id	Name	SBO
I_1p		

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \frac{(1 - \text{psi}) \cdot \text{beta\_1} \cdot (\text{I\_1} + \text{I\_1p})}{\text{N}} \cdot \text{R\_2} \tag{38}$$

7.13 Reaction r13

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

Name Secondary Infection with strain 2

SBO:0000375 process

Reaction equation

$$\text{R\_1} \xrightarrow{\text{I\_2, I\_2p, N}} \text{I\_2p} \tag{39}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
R_1		

Modifiers

Table 26: Properties of each modifier.

Id	Name	SBO
I_2		
I_2p		
N		

Product

Table 27: Properties of each product.

Id	Name	SBO
I_2p		

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \frac{(1 - \text{psi}) \cdot \text{beta\_2} \cdot (\text{I\_2} + \text{I\_2p})}{\text{N}} \cdot \text{R\_1} \tag{40}$$

7.14 Reaction r14

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

Name Recovery (I_1)

SBO:0000375 process

Reaction equation

$$\text{I\_1} \longrightarrow \text{R\_1} \tag{41}$$

Reactant

Table 28: Properties of each reactant.

Id	Name	SBO
I_1		

Product

Table 29: Properties of each product.

Id	Name	SBO
R_1		

Kinetic Law

Derived unit $\left(3.1536 \cdot 10^7 \text{ s}\right)^{-1} \cdot \text{item}$

$$v_{14} = \text{gamma\_1} \cdot \text{I\_1} \tag{42}$$

7.15 Reaction r15

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

Name Recovery (I_2)

SBO:0000375 process

Reaction equation

$$\mathrm{I\_2} \longrightarrow \mathrm{R\_2} \tag{43}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
I_2		

Product

Table 31: Properties of each product.

Id	Name	SBO
R_2		

Kinetic Law

Derived unit $\left(3.1536 \cdot 10^{7}\ \mathrm{s}\right)^{-1} \cdot \mathrm{item}$

$$v_{15} = \mathrm{gamma\_2} \cdot \mathrm{I\_2} \tag{44}$$

7.16 Reaction r16

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

Name Recovery (I_1p)

SBO:0000375 process

Reaction equation

$$\mathrm{I\_1p} \longrightarrow \mathrm{R\_p} \tag{45}$$

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
I_1p		

Product

Table 33: Properties of each product.

Id	Name	SBO
R_p		

Kinetic Law

Derived unit $\left(3.1536 \cdot 10^{7}\ \mathrm{s}\right)^{-1} \cdot \mathrm{item}$

$$v_{16} = \mathrm{gamma\_1} \cdot \mathrm{I\_1p} \tag{46}$$

7.17 Reaction r17

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

Name Recovery (I_2p)

SBO:0000375 process

Reaction equation

$$\mathrm{I\_2p} \longrightarrow \mathrm{R\_p} \tag{47}$$

Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
I_2p		

Product

Table 35: Properties of each product.

Id	Name	SBO
R_p		

Kinetic Law

Derived unit $\left(3.1536 \cdot 10^7 \text{ s}\right)^{-1} \cdot \text{item}$

$$v_{17} = \text{gamma\_2} \cdot \text{I\_2p} \tag{48}$$

7.18 Reaction r18

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

Name Loss of Immunity (R_1)

SBO:0000375 process

Reaction equation

$$\text{R\_1} \longrightarrow \text{S} \tag{49}$$

Reactant

Table 36: Properties of each reactant.

Id	Name	SBO
R_1		

Product

Table 37: Properties of each product.

Id	Name	SBO
S		

Kinetic Law

Derived unit $\left(3.1536 \cdot 10^7 \text{ s}\right)^{-1} \cdot \text{item}$

$$v_{18} = \text{sigma} \cdot \text{R\_1} \tag{50}$$

7.19 Reaction r19

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

Name Loss of Immunity (R_2)

SBO:0000375 process

Reaction equation

$$\mathrm{R\_2} \longrightarrow \mathrm{S} \tag{51}$$

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
R_2		

Product

Table 39: Properties of each product.

Id	Name	SBO
S		

Kinetic Law

Derived unit $\left(3.1536 \cdot 10^{7}\ \mathrm{s}\right)^{-1} \cdot \mathrm{item}$

$$v_{19} = \mathrm{sigma} \cdot \mathrm{R\_2} \tag{52}$$

7.20 Reaction r20

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

Name Loss of Immunity (R_p)

SBO:0000375 process

Reaction equation

$$\mathrm{R\_p} \longrightarrow \mathrm{S} \tag{53}$$

Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
R_p		

Product

Table 41: Properties of each product.

Id	Name	SBO
S		

Kinetic Law

Derived unit $\left(3.1536 \cdot 10^{7}\ \mathrm{s}\right)^{-1} \cdot \mathrm{item}$

$$v_{20} = \mathrm{sigma} \cdot \mathrm{R\_p} \tag{54}$$

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.

8.1 Species N

SBO:0000240 material entity

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

This species takes part in five reactions (as a modifier in r1, r10, r11, r12, r13).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{N} = 0 \tag{55}$$

8.2 Species S

SBO:0000240 material entity

Initial concentration $0.0588912\ \mathrm{item} \cdot \mathrm{l}^{-1}$

This species takes part in seven reactions (as a reactant in r2, r10, r11 and as a product in r1, r18, r19, r20).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S} = v_1 + v_{18} + v_{19} + v_{20} - v_2 - v_{10} - v_{11} \tag{56}$$

8.3 Species I_1

SBO:0000240 material entity

Initial concentration $0.003775\ \text{item} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in r3, r14 and as a product in r10 and as a modifier in r10, r12).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{I\_1} = v_{10} - v_3 - v_{14} \tag{57}$$

8.4 Species I_2

SBO:0000240 material entity

Initial concentration $10^{-6}\ \text{item} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in r4, r15 and as a product in r11 and as a modifier in r11, r13).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{I\_2} = v_{11} - v_4 - v_{15} \tag{58}$$

8.5 Species R_1

SBO:0000240 material entity

Initial concentration $0.93733\ \text{item} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in r5, r13, r18 and as a product in r14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{R\_1} = v_{14} - v_5 - v_{13} - v_{18} \tag{59}$$

8.6 Species R_2

SBO:0000240 material entity

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

This species takes part in four reactions (as a reactant in r6, r12, r19 and as a product in r15).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{R\_2} = v_{15} - v_6 - v_{12} - v_{19} \tag{60}$$

8.7 Species I_1p

SBO:0000240 material entity

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

This species takes part in five reactions (as a reactant in r7, r16 and as a product in r12 and as a modifier in r10, r12).

$$\frac{\text{d}}{\text{d}t}\text{I\_1p} = v_{12} - v_7 - v_{16} \tag{61}$$

8.8 Species I_2p

SBO:0000240 material entity

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

This species takes part in five reactions (as a reactant in r8, r17 and as a product in r13 and as a modifier in r11, r13).

$$\frac{\text{d}}{\text{d}t}\text{I\_2p} = v_{13} - v_8 - v_{17} \tag{62}$$

8.9 Species R_p

SBO:0000240 material entity

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

This species takes part in four reactions (as a reactant in r9, r20 and as a product in r16, r17).

$$\frac{\text{d}}{\text{d}t}\text{R\_p} = v_{16} + v_{17} - v_9 - v_{20} \tag{63}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000240 material entity: A real thing that is defined by its physico-chemical structure.

SBO:0000290 physical compartment: Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions

SBO:0000375 process: A sequential series of actions, motions, or occurrences, such as chemical reactions, that affect one or more entities in a phenomenologically characteristic manner

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