SBML Model Report

Model name: “Koo2013 - Shear stress induced NO production - Model 4”

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following three authors: Nick Juty[1], Vijayalakshmi Chelliah[2] and Andrew Koo[3] at August 19th 2013 at 1:37 p. m. and last time modified at April seventh 2014 at 3:05 a. m. Table 1 shows 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	24	function definitions	0
global parameters	15	unit definitions	10
rules	0	initial assignments	0

2 Unit Definitions

This is an overview of ten unit definitions.

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2.1 Unit time

Name time

Definition s

2.2 Unit substance

Name substance

Definition 10^{-9} mol

2.3 Unit area

Name area

Definition m^2

2.4 Unit length

Name length

Definition m

2.5 Unit volume

Name volume

Definition l

2.6 Unit sub_sec

Name sub_sec

Definition $10^{-9}\,\text{mol} \cdot \text{s}^{-1}$

2.7 Unit inv_sec

Name inv_sec

Definition s^{-1}

2.8 Unit inv_sec_sub

Name inv_sec_sub

Definition $\left(10^{-9}\,\text{mol}\right)^{-1} \cdot \text{s}^{-1}$

2.9 Unit nM_inv_s

Name nM_inv_s

Definition $\mathrm{nmol} \cdot \mathrm{s}^{-1}$

2.10 Unit inv_nM_s

Name inv_nM_s

Definition $\mathrm{nmol}^{-1} \cdot \mathrm{s}^{-1}$

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
default			3	1	litre	☑	
c1	Cell		3	1	litre	☑	default

3.1 Compartment default

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

3.2 Compartment c1

This is a three dimensional compartment with a constant size of one litre, which is surrounded by default.

Name Cell

4 Species

This model contains 20 species. The boundary condition of one of these species is set to `true` so that this species' amount cannot be changed by any reaction. 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
s3	Ca_c	c1	10^{-9} mol	☑	☑
s27	pp-AKT:PI3P	c1	10^{-9} mol	☐	☐
s45	eNOS-CaM-Ca4	c1	10^{-9} mol	☐	☐
s47	CaM-Ca4	c1	10^{-9} mol	☐	☐
s48	CaM-Ca2	c1	10^{-9} mol	☐	☐
s50	eNOS-CaM-Ca2	c1	10^{-9} mol	☐	☐
s51	eNOS-Cav-1	c1	10^{-9} mol	☐	☐
s52	Calmodulin	c1	10^{-9} mol	☐	☐
s57	Hsp90	c1	10^{-9} mol	☐	☐
s58	Hsp90-eNOS-CaM-Ca4	c1	10^{-9} mol	☐	☐
s60	Hsp90-p-eNOS-CaM-Ca4	c1	10^{-9} mol	☐	☐
s61	Hsp90-eNOS-CaM-Ca2	c1	10^{-9} mol	☐	☐
s62	Hsp90-p-eNOS-CaM-Ca2	c1	10^{-9} mol	☐	☐
s63	L-Arg	c1	10^{-9} mol	☐	☐
s64	NO	c1	10^{-9} mol	☐	☐
s65	Hsp90-p-eNOS	c1	10^{-9} mol	☐	☐
s66	Hsp90-eNOS	c1	10^{-9} mol	☐	☐
s116	sa49_degraded	c1	10^{-9} mol	☐	☐
s117	s117	c1	10^{-9} mol	☐	☐
s118	s118	c1	10^{-9} mol	☐	☐

5 Parameters

This model contains 15 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.004	$\left(10^{-9}\ \mathrm{mol}\right)^{-1} \cdot \mathrm{s}^{-1}$	☑
k1r	k1r		10.300	s^{-1}	☑
k2	k2		0.080	$\left(10^{-9}\ \mathrm{mol}\right)^{-1} \cdot \mathrm{s}^{-1}$	☑
k2r	k2r		1152.000	s^{-1}	☑
k4	k4		0.015	$\left(10^{-9}\ \mathrm{mol}\right)^{-1} \cdot \mathrm{s}^{-1}$	☑
k3	k3		$1.5 \cdot 10^{-4}$	$\left(10^{-9}\ \mathrm{mol}\right)^{-1} \cdot \mathrm{s}^{-1}$	☑
k3r	k3r		1.500	s^{-1}	☑
k10	k10		0.100	s^{-1}	☑
Km10	Km10		5.000	$10^{-9}\ \mathrm{mol}$	☑
Km10r	Km10r		20.000	$10^{-9}\ \mathrm{mol}$	☑
V10r	V10r		4.000	$10^{-9}\ \mathrm{mol} \cdot \mathrm{s}^{-1}$	☑
k6	k6		0.002	$\left(10^{-9}\ \mathrm{mol}\right)^{-1} \cdot \mathrm{s}^{-1}$	☑
k7	k7		1.500	s^{-1}	☑
kD	kD		$9.45 \cdot 10^{-5}$	s^{-1}	☑
k5	k5		115.200	s^{-1}	☑

6 Reactions

This model contains 24 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	re37		$s51 + s47 \xrightarrow{s47,\ s51} s45$	
2	re38		$s48 + s51 \xrightleftharpoons{s51,\ s48,\ s50} s50$	
3	re41		$s52 \xrightleftharpoons{s3,\ s3,\ s52,\ s48} s48$	
4	re42		$s48 \xrightarrow{s3,\ s3,\ s48,\ s47} s47$	
5	re50		$s45 \xrightleftharpoons{s3,\ s45,\ s3,\ s50} s50$	
6	re51		$s45 + s57 \xrightarrow{s45,\ s57} s58$	
7	re52		$s58 \xrightleftharpoons{s3,\ s58,\ s3,\ s61} s61$	
8	re53		$s61 \xrightarrow{s61} s50 + s57$	
9	re54		$s60 \xrightleftharpoons{s3,\ s60,\ s3,\ s62} s62$	
10	re55		$s58 \xrightleftharpoons{s27,\ s58,\ s27,\ s60} s60$	
11	re56		$s61 \xrightleftharpoons{s27,\ s61,\ s27,\ s62} s62$	
12	re69		$s63 \xrightarrow{s45,\ s50,\ s61,\ s62,\ s58,\ s60,\ s65,\ s45,\ s58,\ s62,\ s65,\ s60} s64$	
13	re70		$s65 \xrightarrow{s65} s66$	
14	re71		$s66 \xrightarrow{s66} s51 + s57$	
15	re72		$s62 \xrightleftharpoons{s62,\ s65,\ s48} s65 + s48$	
16	re131		$s51 \xrightarrow{s51} s116$	

№	Id	Name	Reaction Equation	SBO
17	re132		$\mathrm{s45} \xrightarrow{\mathrm{s45}} \mathrm{s117} + \mathrm{s47}$	
18	re133		$\mathrm{s50} \xrightarrow{\mathrm{s50}} \mathrm{s117} + \mathrm{s48}$	
19	re134		$\mathrm{s66} \xrightarrow{\mathrm{s66}} \mathrm{s57} + \mathrm{s118}$	
20	re135		$\mathrm{s65} \xrightarrow{\mathrm{s65}} \mathrm{s118} + \mathrm{s57}$	
21	re136		$\mathrm{s61} \xrightarrow{\mathrm{s61}} \mathrm{s57} + \mathrm{s48}$	
22	re137		$\mathrm{s62} \xrightarrow{\mathrm{s62}} \mathrm{s57} + \mathrm{s48}$	
23	re138		$\mathrm{s58} \xrightarrow{\mathrm{s58}} \mathrm{s57} + \mathrm{s47}$	
24	re139		$\mathrm{s60} \xrightarrow{\mathrm{s60}} \mathrm{s57} + \mathrm{s47}$	

6.1 Reaction re37

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

Reaction equation

$$\mathrm{s51} + \mathrm{s47} \xrightarrow{\mathrm{s47,\ s51}} \mathrm{s45} \tag{1}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
s51	eNOS-Cav-1	
s47	CaM-Ca4	

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
s47	CaM-Ca4	
s51	eNOS-Cav-1	

Product

Table 8: Properties of each product.

Id	Name	SBO
s45	eNOS-CaM-Ca4	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot 10^{-9}\ \mathrm{mol}$

$$v_1 = \mathrm{k4} \cdot \mathrm{s47} \cdot \mathrm{s51} \tag{2}$$

6.2 Reaction re38

This is a reversible reaction of two reactants forming one product influenced by three modifiers.

Reaction equation

$$\mathrm{s48} + \mathrm{s51} \rightleftharpoons^{\mathrm{s51,\ s48,\ s50}} \mathrm{s50} \tag{3}$$

Reactants

Table 9: Properties of each reactant.

Id	Name	SBO
s48	CaM-Ca2	
s51	eNOS-Cav-1	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
s51	eNOS-Cav-1	
s48	CaM-Ca2	
s50	eNOS-CaM-Ca2	

Product

Table 11: Properties of each product.

Id	Name	SBO
s50	eNOS-CaM-Ca2	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot 10^{-9}\ \mathrm{mol}$

$$v_2 = \mathrm{k3} \cdot \mathrm{s51} \cdot \mathrm{s48} - \mathrm{k3r} \cdot \mathrm{s50} \tag{4}$$

6.3 Reaction re41

This is a reversible reaction of one reactant forming one product influenced by four modifiers.

Reaction equation

$$\mathrm{s52} \rightleftharpoons^{\mathrm{s3,\ s3,\ s52,\ s48}} \mathrm{s48} \tag{5}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
s52	Calmodulin	

Modifiers

Table 13: Properties of each modifier.

Id	Name	SBO
s3	Ca_c	
s3	Ca_c	
s52	Calmodulin	
s48	CaM-Ca2	

Product

Table 14: Properties of each product.

Id	Name	SBO
s48	CaM-Ca2	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot 10^{-9}\ \mathrm{mol}$

$$v_3 = \mathrm{k1} \cdot \mathrm{s3} \cdot \mathrm{s52} - \mathrm{k1r} \cdot \mathrm{s48} \tag{6}$$

6.4 Reaction re42

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

Reaction equation

$$\mathrm{s48} \xrightarrow{\mathrm{s3,\ s3,\ s48,\ s47}} \mathrm{s47} \tag{7}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
s48	CaM-Ca2	

Modifiers

Table 16: Properties of each modifier.

Id	Name	SBO
s3	Ca_c	
s3	Ca_c	
s48	CaM-Ca2	
s47	CaM-Ca4	

Product

Table 17: Properties of each product.

Id	Name	SBO
s47	CaM-Ca4	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot 10^{-9}\ \mathrm{mol}$

$$v_4 = \mathrm{k2} \cdot \mathrm{s3} \cdot \mathrm{s48} - \mathrm{k2r} \cdot \mathrm{s47} \tag{8}$$

6.5 Reaction re50

This is a reversible reaction of one reactant forming one product influenced by four modifiers.

Reaction equation

$$\mathrm{s45} \underset{\text{s3, s45, s3, s50}}{\rightleftharpoons} \mathrm{s50} \tag{9}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
s45	eNOS-CaM-Ca4	

Modifiers

Table 19: Properties of each modifier.

Id	Name	SBO
s3	Ca_c	
s45	eNOS-CaM-Ca4	
s3	Ca_c	
s50	eNOS-CaM-Ca2	

Product

Table 20: Properties of each product.

Id	Name	SBO
s50	eNOS-CaM-Ca2	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot 10^{-9}\ \mathrm{mol}$

$$v_5 = \mathrm{k5} \cdot \mathrm{s45} - \mathrm{k2} \cdot \mathrm{s3} \cdot \mathrm{s50} \tag{10}$$

6.6 Reaction re51

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

Reaction equation

$$\mathrm{s45} + \mathrm{s57} \xrightarrow{\mathrm{s45,\ s57}} \mathrm{s58} \tag{11}$$

Reactants

Table 21: Properties of each reactant.

Id	Name	SBO
s45	eNOS-CaM-Ca4	
s57	Hsp90	

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
s45	eNOS-CaM-Ca4	
s57	Hsp90	

Product

Table 23: Properties of each product.

Id	Name	SBO
s58	Hsp90-eNOS-CaM-Ca4	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot 10^{-9}\ \mathrm{mol}$

$$v_6 = \mathrm{k6} \cdot \mathrm{s45} \cdot \mathrm{s57} \tag{12}$$

6.7 Reaction re52

This is a reversible reaction of one reactant forming one product influenced by four modifiers.

Reaction equation

$$\mathrm{s58} \xrightleftharpoons{\mathrm{s3,\ s58,\ s3,\ s61}} \mathrm{s61} \tag{13}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
s58	Hsp90-eNOS-CaM-Ca4	

Modifiers

Table 25: Properties of each modifier.

Id	Name	SBO
s3	Ca_c	
s58	Hsp90-eNOS-CaM-Ca4	
s3	Ca_c	
s61	Hsp90-eNOS-CaM-Ca2	

Product

Table 26: Properties of each product.

Id	Name	SBO
s61	Hsp90-eNOS-CaM-Ca2	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot 10^{-9}\ \mathrm{mol}$

$$v_7 = \mathrm{k5} \cdot \mathrm{s58} - \mathrm{k2} \cdot \mathrm{s3} \cdot \mathrm{s61} \tag{14}$$

6.8 Reaction re53

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

Reaction equation

$$\mathrm{s61} \xrightarrow{\mathrm{s61}} \mathrm{s50} + \mathrm{s57} \tag{15}$$

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
s61	Hsp90-eNOS-CaM-Ca2	

Modifier

Table 28: Properties of each modifier.

Id	Name	SBO
s61	Hsp90-eNOS-CaM-Ca2	

Products

Table 29: Properties of each product.

Id	Name	SBO
s50	eNOS-CaM-Ca2	
s57	Hsp90	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9}$ mol

$$v_8 = k7 \cdot s61 \tag{16}$$

6.9 Reaction re54

This is a reversible reaction of one reactant forming one product influenced by four modifiers.

Reaction equation

$$s60 \xrightleftharpoons{s3,\ s60,\ s3,\ s62} s62 \tag{17}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
s60	Hsp90-p-eNOS-CaM-Ca4	

Modifiers

Table 31: Properties of each modifier.

Id	Name	SBO
s3	Ca_c	
s60	Hsp90-p-eNOS-CaM-Ca4	

Id	Name	SBO
s3	Ca_c	
s62	Hsp90-p-eNOS-CaM-Ca2	

Product

Table 32: Properties of each product.

Id	Name	SBO
s62	Hsp90-p-eNOS-CaM-Ca2	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot 10^{-9}\ \mathrm{mol}$

$$v_9 = \mathrm{k5} \cdot \mathrm{s60} - \mathrm{k2} \cdot \mathrm{s3} \cdot \mathrm{s62} \tag{18}$$

6.10 Reaction re55

This is a reversible reaction of one reactant forming one product influenced by four modifiers.

Reaction equation

$$\mathrm{s58} \underset{\mathrm{s27,\ s58,\ s27,\ s60}}{\rightleftharpoons} \mathrm{s60} \tag{19}$$

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
s58	Hsp90-eNOS-CaM-Ca4	

Modifiers

Table 34: Properties of each modifier.

Id	Name	SBO
s27	pp-AKT:PI3P	
s58	Hsp90-eNOS-CaM-Ca4	
s27	pp-AKT:PI3P	
s60	Hsp90-p-eNOS-CaM-Ca4	

Id	Name	SBO

Product

Table 35: Properties of each product.

Id	Name	SBO
s60	Hsp90-p-eNOS-CaM-Ca4	

Kinetic Law

Derived unit $s^{-1} \cdot 9.999999999999998 \cdot 10^{-10}\ mol$

$$v_{10} = \frac{k10 \cdot s58 \cdot s27}{s58 + Km10} - \frac{V10r \cdot s60}{s60 + Km10r} \tag{20}$$

6.11 Reaction re56

This is a reversible reaction of one reactant forming one product influenced by four modifiers.

Reaction equation

$$s61 \xrightleftharpoons{s27,\ s61,\ s27,\ s62} s62 \tag{21}$$

Reactant

Table 36: Properties of each reactant.

Id	Name	SBO
s61	Hsp90-eNOS-CaM-Ca2	

Modifiers

Table 37: Properties of each modifier.

Id	Name	SBO
s27	pp-AKT:PI3P	
s61	Hsp90-eNOS-CaM-Ca2	
s27	pp-AKT:PI3P	
s62	Hsp90-p-eNOS-CaM-Ca2	

Product

Table 38: Properties of each product.

Id	Name	SBO
s62	Hsp90-p-eNOS-CaM-Ca2	

Kinetic Law

Derived unit $s^{-1} \cdot 9.999999999999998 \cdot 10^{-10}$ mol

$$v_{11} = \frac{k10 \cdot s61 \cdot s27}{s61 + Km10} - \frac{V10r \cdot s62}{s62 + Km10r} \tag{22}$$

6.12 Reaction re69

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

Reaction equation

$$s63 \xrightarrow{s45,\ s50,\ s61,\ s62,\ s58,\ s60,\ s65,\ s45,\ s58,\ s62,\ s65,\ s60} s64 \tag{23}$$

Reactant

Table 39: Properties of each reactant.

Id	Name	SBO
s63	L-Arg	

Modifiers

Table 40: Properties of each modifier.

Id	Name	SBO
s45	eNOS-CaM-Ca4	
s50	eNOS-CaM-Ca2	
s61	Hsp90-eNOS-CaM-Ca2	
s62	Hsp90-p-eNOS-CaM-Ca2	
s58	Hsp90-eNOS-CaM-Ca4	
s60	Hsp90-p-eNOS-CaM-Ca4	
s65	Hsp90-p-eNOS	

Id	Name	SBO
s45	eNOS-CaM-Ca4	
s58	Hsp90-eNOS-CaM-Ca4	
s62	Hsp90-p-eNOS-CaM-Ca2	
s65	Hsp90-p-eNOS	
s60	Hsp90-p-eNOS-CaM-Ca4	

Product

Table 41: Properties of each product.

Id	Name	SBO
s64	NO	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot 10^{-9}\,\mathrm{mol}$

$$v_{12} = \mathrm{kCaM} \cdot (\mathrm{s45} + \mathrm{s58}) + \mathrm{kp} \cdot (\mathrm{s62} + \mathrm{s65}) + \mathrm{kpCaM} \cdot \mathrm{s60} \tag{24}$$

Table 42: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kCaM			17.0	s^{-1}	☑
kp			5.0	s^{-1}	☑
kpCaM			17.0	s^{-1}	☑

6.13 Reaction re70

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

Reaction equation

$$\mathrm{s65} \xrightarrow{\mathrm{s65}} \mathrm{s66} \tag{25}$$

Reactant

Table 43: Properties of each reactant.

Id	Name	SBO
s65	Hsp90-p-eNOS	

Modifier

Table 44: Properties of each modifier.

Id	Name	SBO
s65	Hsp90-p-eNOS	

Product

Table 45: Properties of each product.

Id	Name	SBO
s66	Hsp90-eNOS	

Kinetic Law

Derived unit $9.999999999999998 \cdot 10^{-10}\ \mathrm{mol} \cdot \mathrm{s}^{-1}$

$$v_{13} = \frac{\mathrm{V10r} \cdot \mathrm{s65}}{\mathrm{s65} + \mathrm{Km10r}} \tag{26}$$

6.14 Reaction re71

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

Reaction equation

$$\mathrm{s66} \xrightarrow{\mathrm{s66}} \mathrm{s51} + \mathrm{s57} \tag{27}$$

Reactant

Table 46: Properties of each reactant.

Id	Name	SBO
s66	Hsp90-eNOS	

Modifier

Table 47: Properties of each modifier.

Id	Name	SBO
s66	Hsp90-eNOS	

Products

Table 48: Properties of each product.

Id	Name	SBO
s51	eNOS-Cav-1	
s57	Hsp90	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot 10^{-9}\ \mathrm{mol}$

$$v_{14} = \mathrm{k7} \cdot \mathrm{s66} \tag{28}$$

6.15 Reaction re72

This is a reversible reaction of one reactant forming two products influenced by three modifiers.

Reaction equation

$$\mathrm{s62} \xrightleftharpoons{\mathrm{s62,\ s65,\ s48}} \mathrm{s65} + \mathrm{s48} \tag{29}$$

Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
s62	Hsp90-p-eNOS-CaM-Ca2	

Modifiers

Table 50: Properties of each modifier.

Id	Name	SBO
s62	Hsp90-p-eNOS-CaM-Ca2	
s65	Hsp90-p-eNOS	
s48	CaM-Ca2	

Products

Table 51: Properties of each product.

Id	Name	SBO
s65	Hsp90-p-eNOS	
s48	CaM-Ca2	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot 10^{-9}\ \mathrm{mol}$

$$v_{15} = \mathrm{k3r} \cdot \mathrm{s62} - \mathrm{k3} \cdot \mathrm{s65} \cdot \mathrm{s48} \tag{30}$$

6.16 Reaction re131

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

Reaction equation

$$\mathrm{s51} \xrightarrow{\mathrm{s51}} \mathrm{s116} \tag{31}$$

Reactant

Table 52: Properties of each reactant.

Id	Name	SBO
s51	eNOS-Cav-1	

Modifier

Table 53: Properties of each modifier.

Id	Name	SBO
s51	eNOS-Cav-1	

Product

Table 54: Properties of each product.

Id	Name	SBO
s116	sa49_degraded	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9}$ mol

$$v_{16} = \text{kD} \cdot \text{s51} \tag{32}$$

6.17 Reaction re132

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

Reaction equation

$$\text{s45} \xrightarrow{\text{s45}} \text{s117} + \text{s47} \tag{33}$$

Reactant

Table 55: Properties of each reactant.

Id	Name	SBO
s45	eNOS-CaM-Ca4	

Modifier

Table 56: Properties of each modifier.

Id	Name	SBO
s45	eNOS-CaM-Ca4	

Products

Table 57: Properties of each product.

Id	Name	SBO
s117	s117	
s47	CaM-Ca4	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9}$ mol

$$v_{17} = \text{kD} \cdot \text{s45} \tag{34}$$

6.18 Reaction re133

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

Reaction equation

$$\text{s50} \xrightarrow{\text{s50}} \text{s117} + \text{s48} \tag{35}$$

Reactant

Table 58: Properties of each reactant.

Id	Name	SBO
s50	eNOS-CaM-Ca2	

Modifier

Table 59: Properties of each modifier.

Id	Name	SBO
s50	eNOS-CaM-Ca2	

Products

Table 60: Properties of each product.

Id	Name	SBO
s117	s117	
s48	CaM-Ca2	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9}$ mol

$$v_{18} = \text{kD} \cdot \text{s50} \tag{36}$$

6.19 Reaction re134

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

Reaction equation

$$\text{s66} \xrightarrow{\text{s66}} \text{s57} + \text{s118} \tag{37}$$

Reactant

Table 61: Properties of each reactant.

Id	Name	SBO
s66	Hsp90-eNOS	

Modifier

Table 62: Properties of each modifier.

Id	Name	SBO
s66	Hsp90-eNOS	

Products

Table 63: Properties of each product.

Id	Name	SBO
s57	Hsp90	
s118	s118	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot 10^{-9}\ \mathrm{mol}$

$$v_{19} = \mathrm{kD} \cdot \mathrm{s66} \tag{38}$$

6.20 Reaction `re135`

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

Reaction equation

$$\mathrm{s65} \xrightarrow{\mathrm{s65}} \mathrm{s118} + \mathrm{s57} \tag{39}$$

Reactant

Table 64: Properties of each reactant.

Id	Name	SBO
`s65`	Hsp90-p-eNOS	

Modifier

Table 65: Properties of each modifier.

Id	Name	SBO
`s65`	Hsp90-p-eNOS	

Products

Table 66: Properties of each product.

Id	Name	SBO
`s118`	s118	
`s57`	Hsp90	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot 10^{-9}\ \mathrm{mol}$

$$v_{20} = \mathrm{kD} \cdot \mathrm{s65} \tag{40}$$

6.21 Reaction re136

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

Reaction equation

$$\mathrm{s61} \xrightarrow{\mathrm{s61}} \mathrm{s57} + \mathrm{s48} \tag{41}$$

Reactant

Table 67: Properties of each reactant.

Id	Name	SBO
s61	Hsp90-eNOS-CaM-Ca2	

Modifier

Table 68: Properties of each modifier.

Id	Name	SBO
s61	Hsp90-eNOS-CaM-Ca2	

Products

Table 69: Properties of each product.

Id	Name	SBO
s57	Hsp90	
s48	CaM-Ca2	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot 10^{-9}\ \mathrm{mol}$

$$v_{21} = \mathrm{kD} \cdot \mathrm{s61} \tag{42}$$

6.22 Reaction re137

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

Reaction equation

$$\mathrm{s62} \xrightarrow{\mathrm{s62}} \mathrm{s57} + \mathrm{s48} \tag{43}$$

Reactant

Table 70: Properties of each reactant.

Id	Name	SBO
s62	Hsp90-p-eNOS-CaM-Ca2	

Modifier

Table 71: Properties of each modifier.

Id	Name	SBO
s62	Hsp90-p-eNOS-CaM-Ca2	

Products

Table 72: Properties of each product.

Id	Name	SBO
s57	Hsp90	
s48	CaM-Ca2	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot 10^{-9}\ \mathrm{mol}$

$$v_{22} = \mathrm{kD} \cdot \mathrm{s62} \tag{44}$$

6.23 Reaction re138

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

Reaction equation

$$\mathrm{s58} \xrightarrow{\mathrm{s58}} \mathrm{s57} + \mathrm{s47} \tag{45}$$

Reactant

Table 73: Properties of each reactant.

Id	Name	SBO
s58	Hsp90-eNOS-CaM-Ca4	

Modifier

Table 74: Properties of each modifier.

Id	Name	SBO
s58	Hsp90-eNOS-CaM-Ca4	

Products

Table 75: Properties of each product.

Id	Name	SBO
s57	Hsp90	
s47	CaM-Ca4	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot 10^{-9}\ \mathrm{mol}$

$$v_{23} = \mathrm{kD} \cdot \mathrm{s58} \tag{46}$$

6.24 Reaction re139

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

Reaction equation

$$\mathrm{s60} \xrightarrow{\mathrm{s60}} \mathrm{s57} + \mathrm{s47} \tag{47}$$

Reactant

Table 76: Properties of each reactant.

Id	Name	SBO
s60	Hsp90-p-eNOS-CaM-Ca4	

Modifier

Table 77: Properties of each modifier.

Id	Name	SBO
s60	Hsp90-p-eNOS-CaM-Ca4	

Products

Table 78: Properties of each product.

Id	Name	SBO
s57	Hsp90	
s47	CaM-Ca4	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot 10^{-9}\ \mathrm{mol}$

$$v_{24} = \mathrm{kD} \cdot \mathrm{s60} \tag{48}$$

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.

7.1 Species s3

Name Ca_c

Initial amount 117.2

Charge 0

This species takes part in ten reactions (as a modifier in re41, re41, re42, re42, re50, re50, re52, re52, re54, re54), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s3} = 0 \tag{49}$$

7.2 Species s27

Name pp-AKT:PI3P

Initial amount 1.723

Charge 0

This species takes part in four reactions (as a modifier in re55, re55, re56, re56).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s27} = 0 \tag{50}$$

7.3 Species s45

Name eNOS-CaM-Ca4

SBO:0000297 protein complex

Initial amount 0.0415

Charge 0

This species takes part in nine reactions (as a reactant in re50, re51, re132 and as a product in re37 and as a modifier in re50, re51, re69, re69, re132).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s45} = v_1 - v_5 - v_6 - v_{17} \tag{51}$$

7.4 Species s47

Name CaM-Ca4

SBO:0000297 protein complex

Initial amount 2.827

Charge 0

This species takes part in seven reactions (as a reactant in re37 and as a product in re42, re132, re138, re139 and as a modifier in re37, re42).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s47} = v_4 + v_{17} + v_{23} + v_{24} - v_1 \tag{52}$$

7.5 Species s48

Name CaM-Ca2

SBO:0000297 protein complex

Initial amount 347.52

Charge 0

This species takes part in eleven reactions (as a reactant in re38, re42 and as a product in re41, re72, re133, re136, re137 and as a modifier in re38, re41, re42, re72).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s48} = v_3 + v_{15} + v_{18} + v_{21} + v_{22} - v_2 - v_4 \tag{53}$$

7.6 Species s50

Name eNOS-CaM-Ca2

SBO:0000297 protein complex

Initial amount 2.12

Charge 0

This species takes part in eight reactions (as a reactant in re133 and as a product in re38, re50, re53 and as a modifier in re38, re50, re69, re133).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s50} = v_2 + v_5 + v_8 - v_{18} \tag{54}$$

7.7 Species s51

Name eNOS-Cav-1

SBO:0000297 protein complex

Initial amount 34.98

Charge 0

This species takes part in seven reactions (as a reactant in re37, re38, re131 and as a product in re71 and as a modifier in re37, re38, re131).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s51} = v_{14} - v_1 - v_2 - v_{16} \tag{55}$$

7.8 Species s52

Name Calmodulin

Initial amount 7635.36

Charge 0

This species takes part in two reactions (as a reactant in re41 and as a modifier in re41).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s52} = -v_3 \tag{56}$$

7.9 Species s57

Name Hsp90

Initial amount 199987

Charge 0

This species takes part in ten reactions (as a reactant in re51 and as a product in re53, re71, re134, re135, re136, re137, re138, re139 and as a modifier in re51).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s57} = v_8 + v_{14} + v_{19} + v_{20} + v_{21} + v_{22} + v_{23} + v_{24} - v_6 \tag{57}$$

7.10 Species s58

Name Hsp90-eNOS-CaM-Ca4

SBO:0000297 protein complex

Initial amount 1.037

Charge 0

This species takes part in nine reactions (as a reactant in re52, re55, re138 and as a product in re51 and as a modifier in re52, re55, re69, re69, re138).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s58} = v_6 - v_7 - v_{10} - v_{23} \tag{58}$$

7.11 Species s60

Name Hsp90-p-eNOS-CaM-Ca4

SBO:0000297 protein complex

Initial amount 0.0089

Charge 0

This species takes part in eight reactions (as a reactant in re54, re139 and as a product in re55 and as a modifier in re54, re55, re69, re69, re139).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s60} = v_{10} - v_9 - v_{24} \tag{59}$$

7.12 Species s61

Name Hsp90-eNOS-CaM-Ca2

SBO:0000297 protein complex

Initial amount 10.98

Charge 0

This species takes part in nine reactions (as a reactant in re53, re56, re136 and as a product in re52 and as a modifier in re52, re53, re56, re69, re136).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s61} = v_7 - v_8 - v_{11} - v_{21} \tag{60}$$

7.13 Species s62

Name Hsp90-p-eNOS-CaM-Ca2

SBO:0000297 protein complex

Initial amount 0.106

Charge 0

This species takes part in ten reactions (as a reactant in re72, re137 and as a product in re54, re56 and as a modifier in re54, re56, re69, re69, re72, re137).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s62} = v_9 + v_{11} - v_{15} - v_{22} \tag{61}$$

7.14 Species s63

Name L-Arg

SBO:0000291 empty set

Initial amount 500000

Charge 0

This species takes part in one reaction (as a reactant in re69).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s63} = -v_{12} \tag{62}$$

7.15 Species s64

Name NO

Initial amount 0

Charge 0

This species takes part in one reaction (as a product in re69).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s64} = v_{12} \tag{63}$$

7.16 Species s65

Name Hsp90-p-eNOS

SBO:0000297 protein complex

Initial amount 0.643

Charge 0

This species takes part in eight reactions (as a reactant in re70, re135 and as a product in re72 and as a modifier in re69, re69, re70, re72, re135).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s65} = v_{15} - v_{13} - v_{20} \tag{64}$$

7.17 Species s66

Name Hsp90-eNOS

SBO:0000297 protein complex

Initial amount 0.083

Charge 0

This species takes part in five reactions (as a reactant in re71, re134 and as a product in re70 and as a modifier in re71, re134).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s66} = v_{13} - v_{14} - v_{19} \tag{65}$$

7.18 Species s116

Name sa49_degraded

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in one reaction (as a product in re131).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s116} = v_{16} \tag{66}$$

7.19 Species s117

Name s117

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in two reactions (as a product in re132, re133).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s117} = v_{17} + v_{18} \tag{67}$$

7.20 Species s118

Name s118

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in two reactions (as a product in re134, re135).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s118} = v_{19} + v_{20} \tag{68}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000291 empty set: Entity defined by the absence of any actual object. An empty set is often used to represent the source of a creation process or the result of a degradation process.

SBO:0000297 protein complex: Macromolecular complex containing one or more polypeptide chains possibly associated with simple chemicals. CHEBI:3608

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