

SBML Model Report

Model name: “Koo2013 - Shear stress induced eNOS expression - Model 3”



May 5, 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 Juty¹, Vijayalakshmi Chelliah² and Andrew Koo³ at August 19th 2013 at 1:36 p. m. and last time modified at April seventh 2014 at three o’ clock in the morning. 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	3
species types	0	species	34
events	0	constraints	0
reactions	28	function definitions	0
global parameters	0	unit definitions	10
rules	0	initial assignments	0

2 Unit Definitions

This is an overview of ten unit definitions.

¹EMBL-EBI, juty@ebi.ac.uk

²EMBL-EBI, viji@ebi.ac.uk

³Massachusetts Institute of Technology, kooj@mit.edu

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 $(10^{-9} \text{ mol})^{-1} \cdot \text{s}^{-1}$

2.9 Unit `nM_inv_s`

Name `nM_inv_s`

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

2.10 Unit `inv_nM_s`

Name `inv_nM_s`

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

3 Compartments

This model contains three compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
default			3	1	litre	<input checked="" type="checkbox"/>	
c1	Cell		3	1	litre	<input checked="" type="checkbox"/>	default
c3	nucleus		3	1	litre	<input checked="" type="checkbox"/>	c1

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`

3.3 Compartment `c3`

This is a three dimensional compartment with a constant size of one litre, which is surrounded by `c1` (Cell).

Name `nucleus`

4 Species

This model contains 34 species. Section 6 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
s35	s35	c1	10^{-9} mol	\square	\square
s37	s37	c1	10^{-9} mol	\square	\square
s38	pre_time	c1	10^{-9} mol	\square	\square
s39	Time	c1	10^{-9} mol	\square	\square
s42	AP-1	c3	10^{-9} mol	\square	\square
s43	pp-JNKK	c1	10^{-9} mol	\square	\square
s44	pp-JNK	c1	10^{-9} mol	\square	\square
s49	KLF2	c1	10^{-9} mol	\square	\square
s51	eNOS-Cav-1	c1	10^{-9} mol	\square	\square
s91	Shc	c1	10^{-9} mol	\square	\square
s92	p-Src	c1	10^{-9} mol	\square	\square
s93	p-FAK	c1	10^{-9} mol	\square	\square
s94	Src	c1	10^{-9} mol	\square	\square
s95	FAK	c1	10^{-9} mol	\square	\square
s96	JNKK	c1	10^{-9} mol	\square	\square
s97	MEKK1	c1	10^{-9} mol	\square	\square
s98	p-Shc	c1	10^{-9} mol	\square	\square
s99	JNK	c1	10^{-9} mol	\square	\square
s100	p-JNKK	c1	10^{-9} mol	\square	\square
s101	p-MEKK1	c1	10^{-9} mol	\square	\square
s102	Ras:GTP	c1	10^{-9} mol	\square	\square
s103	Ras:GDP	c1	10^{-9} mol	\square	\square

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
s104	p-JNK	c1	10^{-9} mol	<input type="checkbox"/>	<input type="checkbox"/>
s105	KLF2	c1	10^{-9} mol	<input type="checkbox"/>	<input type="checkbox"/>
s106	eNOS	c1	10^{-9} mol	<input type="checkbox"/>	<input type="checkbox"/>
s107	aAP-1	c3	10^{-9} mol	<input type="checkbox"/>	<input type="checkbox"/>
s108	eNOS	c3	10^{-9} mol	<input type="checkbox"/>	<input type="checkbox"/>
s110	p-FAK:Shc	c1	10^{-9} mol	<input type="checkbox"/>	<input type="checkbox"/>
s111	Grb2:Sos	c1	10^{-9} mol	<input type="checkbox"/>	<input type="checkbox"/>
s112	p-FAK:p-Shc	c1	10^{-9} mol	<input type="checkbox"/>	<input type="checkbox"/>
s113	p-FAK:p-Shc:Grb2:Sos	c1	10^{-9} mol	<input type="checkbox"/>	<input type="checkbox"/>
s114	p-Shc:Grb2:Sos	c1	10^{-9} mol	<input type="checkbox"/>	<input type="checkbox"/>
s115	eNOS	c3	10^{-9} mol	<input type="checkbox"/>	<input type="checkbox"/>
s119	Shear Stress	default	10^{-9} mol	<input type="checkbox"/>	<input type="checkbox"/>

5 Reactions

This model contains 28 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 4: Overview of all reactions

Nº	Id	Name	Reaction Equation	SBO
1	re102		$s95 \xrightarrow{s39, s119, s39} s93$	
2	re103		$s94 \xrightarrow{s39, s119, s39} s92$	
3	re104		$s91 + s93 \xrightarrow{s91, s93, s110} s110$	
4	re105		$s110 \xrightarrow{s92, s110, s92, s112} s112$	
5	re106		$s112 + s111 \xrightarrow{s111, s112, s113} s113$	
6	re107		$s113 \xrightarrow{s113, s93, s114} s114 + s93$	
7	re108		$s98 \xrightarrow{s98} s91$	
8	re109		$s114 \xrightarrow{s114} s98 + s111$	
9	re110		$s115 \xrightarrow{s115} s106$	
10	re111		$s108 \xrightarrow{s107, s49, s107, s49} s115$	
11	re112		$s103 \xrightarrow{s114, s114, s103} s102$	
12	re113		$s102 \xrightarrow{s102} s103$	
13	re114		$s97 \xrightarrow{s102, s102, s97} s101$	
14	re115		$s101 \xrightarrow{s101} s97$	
15	re116		$s96 \xrightarrow{s101, s101, s96} s100$	
16	re117		$s100 \xrightarrow{s100} s96$	

Nº	Id	Name	Reaction Equation	SBO
17	re118		$s_{99} \xrightarrow{s_{43}, s_{99}, s_{43}} s_{104}$	
18	re119		$s_{104} \xrightarrow{s_{104}} s_{99}$	
19	re120		$s_{106} \xrightarrow{s_{106}} s_{35}$	
20	re121		$s_{37} \xrightarrow{s_{106}, s_{106}} s_{51}$	
21	re122		$s_{38} \longrightarrow s_{39}$	
22	re123		$s_{43} \xrightarrow{s_{43}} s_{100}$	
23	re124		$s_{100} \xrightarrow{s_{101}, s_{100}, s_{101}} s_{43}$	
24	re125		$s_{44} \xrightarrow{s_{44}} s_{104}$	
25	re126		$s_{104} \xrightarrow{s_{43}, s_{104}, s_{43}} s_{44}$	
26	re127		$s_{42} \xrightarrow{s_{44}, s_{44}, s_{42}} s_{107}$	
27	re128		$s_{107} \xrightarrow{s_{107}} s_{42}$	
28	re129		$s_{105} \xrightarrow{s_{39}, s_{39}} s_{49}$	

5.1 Reaction re102

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

Reaction equation



Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
s95	FAK	

Modifiers

Table 6: Properties of each modifier.

Id	Name	SBO
s39	Time	
s119	Shear Stress	
s39	Time	

Product

Table 7: Properties of each product.

Id	Name	SBO
s93	p-FAK	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \exp \left(\text{unity} - \left(\frac{s39}{\text{tf}} \right)^{0.35} \right) \cdot \text{normal} \cdot \left(\frac{s39 + \text{tiny_num}}{\text{unimol}} \right)^{-0.65} \cdot \left(\text{unity} - \left(\frac{s39}{\text{tf}} \right)^{0.35} \right) \quad (2)$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
normal			4.000	$\text{nmol} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>
tf			60.000	10^{-9} mol	<input checked="" type="checkbox"/>
unity			1.000	dimensionless	<input checked="" type="checkbox"/>
unimol			1.000	10^{-9} mol	<input checked="" type="checkbox"/>
tiny_num			10^{-6}	10^{-9} mol	<input checked="" type="checkbox"/>

5.2 Reaction re103

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

Reaction equation



Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
s94	Src	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
s39	Time	
s119	Shear Stress	
s39	Time	

Product

Table 11: Properties of each product.

Id	Name	SBO
s92	p-Src	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \exp\left(\text{unity} - \left(\frac{s39}{\text{tf}}\right)^{1.3}\right) \cdot \text{normal} \cdot \left(\frac{s39}{\text{unimol}}\right)^{0.3} \cdot \left(\text{unity} - \left(\frac{s39}{\text{tf}}\right)^{1.3}\right) \quad (4)$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
normal			0.026	nmol · s ⁻¹	✓
tf			540.000	10 ⁻⁹ mol	✓
unity			1.000	dimensionless	✓
unimol			1.000	10 ⁻⁹ mol	✓

5.3 Reaction re104

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

Reaction equation



Reactants

Table 13: Properties of each reactant.

Id	Name	SBO
s91	Shc	
s93	p-FAK	

Modifiers

Table 14: Properties of each modifier.

Id	Name	SBO
s91	Shc	
s93	p-FAK	
s110	p-FAK:Shc	

Product

Table 15: Properties of each product.

Id	Name	SBO
s110	p-FAK:Shc	

Kinetic Law

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

$$v_3 = k_3 \cdot s_{91} \cdot s_{93} - k_{r3} \cdot s_{110} \quad (6)$$

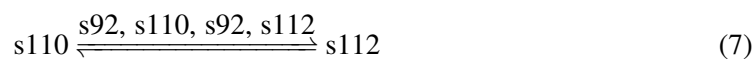
Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k3			0.1	$\text{nmol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>
kr3			1.0	s^{-1}	<input checked="" type="checkbox"/>

5.4 Reaction re105

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

Reaction equation



Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
s110	p-FAK:Shc	

Modifiers

Table 18: Properties of each modifier.

Id	Name	SBO
s92	p-Src	

Id	Name	SBO
s110	p-FAK:Shc	
s92	p-Src	
s112	p-FAK:p-Shc	

Product

Table 19: Properties of each product.

Id	Name	SBO
s112	p-FAK:p-Shc	

Kinetic Law

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

$$v_4 = k_4 \cdot s110 \cdot s92 - kr_4 \cdot s112 \quad (8)$$

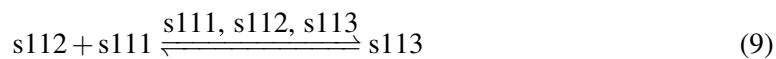
Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k4			8.33	$\text{nmol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>
kr4			5.00	s^{-1}	<input checked="" type="checkbox"/>

5.5 Reaction re106

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

Reaction equation



Reactants

Table 21: Properties of each reactant.

Id	Name	SBO
s112	p-FAK:p-Shc	
s111	Grb2:Sos	

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
s111	Grb2:Sos	
s112	p-FAK:p-Shc	
s113	p-FAK:p-Shc:Grb2:Sos	

Product

Table 23: Properties of each product.

Id	Name	SBO
s113	p-FAK:p-Shc:Grb2:Sos	

Kinetic Law

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

$$v_5 = k_5 \cdot s_{111} \cdot s_{112} - k_{r5} \cdot s_{113} \quad (10)$$

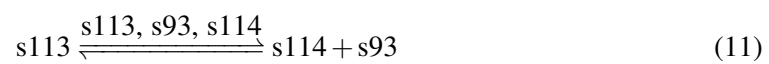
Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k5			60.0	$\text{nmol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>
kr5			546.0	s^{-1}	<input checked="" type="checkbox"/>

5.6 Reaction re107

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

Reaction equation



Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
s113	p-FAK:p-Shc:Grb2:Sos	

Modifiers

Table 26: Properties of each modifier.

Id	Name	SBO
s113	p-FAK:p-Shc:Grb2:Sos	
s93	p-FAK	
s114	p-Shc:Grb2:Sos	

Products

Table 27: Properties of each product.

Id	Name	SBO
s114	p-Shc:Grb2:Sos	
s93	p-FAK	

Kinetic Law

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

$$v_6 = k_6 \cdot s113 - kr_6 \cdot s93 \cdot s114 \quad (12)$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k6			2040.0	s^{-1}	<input checked="" type="checkbox"/>
kr6			15700.0	$\text{nmol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

5.7 Reaction re108

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

Reaction equation



Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
s98	p-Shc	

Modifier

Table 30: Properties of each modifier.

Id	Name	SBO
s98	p-Shc	

Product

Table 31: Properties of each product.

Id	Name	SBO
s91	Shc	

Kinetic Law

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

$$v_7 = \frac{V_8 \cdot s98}{K_{m8} + s98} \quad (14)$$

Table 32: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V8			154.0	$\text{nmol} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>
K _{m8}			340.0	10^{-9} mol	<input checked="" type="checkbox"/>

5.8 Reaction re109

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

Reaction equation



Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
s114	p-Shc:Grb2:Sos	

Modifier

Table 34: Properties of each modifier.

Id	Name	SBO
s114	p-Shc:Grb2:Sos	

Products

Table 35: Properties of each product.

Id	Name	SBO
s98	p-Shc	
s111	Grb2:Sos	

Kinetic Law

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

$$v_g = k7 \cdot s114 \quad (16)$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k7			40.8	s^{-1}	<input checked="" type="checkbox"/>

5.9 Reaction re110

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

Reaction equation



Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
s115	eNOS	

Modifier

Table 38: Properties of each modifier.

Id	Name	SBO
s115	eNOS	

Product

Table 39: Properties of each product.

Id	Name	SBO
s106	eNOS	

Kinetic Law

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

$$v_9 = k25 \cdot s115 \quad (18)$$

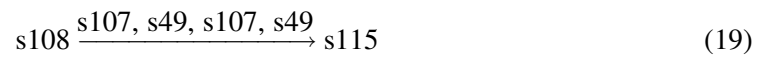
Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k25			0.001	s^{-1}	<input checked="" type="checkbox"/>

5.10 Reaction re111

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

Reaction equation



Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
s108	eNOS	

Modifiers

Table 42: Properties of each modifier.

Id	Name	SBO
s107	aAP-1	
s49	KLF2	
s107	aAP-1	
s49	KLF2	

Product

Table 43: Properties of each product.

Id	Name	SBO
s115	eNOS	

Kinetic Law

Derived unit $(10^{-9} \text{ mol})^2 \cdot \text{s}^{-1}$

$$v_{10} = k_{24t1} \cdot s107 + k_{24t2} \cdot s49 \quad (20)$$

Table 44: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k24t1			$1.2 \cdot 10^{-4}$	$\text{nmol} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>
k24t2			$9 \cdot 10^{-6}$	$\text{nmol} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

5.11 Reaction re112

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

Reaction equation



Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
s103	Ras:GDP	

Modifiers

Table 46: Properties of each modifier.

Id	Name	SBO
s114	p-Shc:Grb2:Sos	
s114	p-Shc:Grb2:Sos	
s103	Ras:GDP	

Product

Table 47: Properties of each product.

Id	Name	SBO
s102	Ras:GTP	

Kinetic Law

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

$$v_{11} = \frac{k9 \cdot s114 \cdot s103}{s103 + Km9} \quad (22)$$

Table 48: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k9			0.222	s ⁻¹	<input checked="" type="checkbox"/>
Km9			0.181	10 ⁻⁹ mol	<input checked="" type="checkbox"/>

5.12 Reaction re113

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

Reaction equation



Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
s102	Ras:GTP	

Modifier

Table 50: Properties of each modifier.

Id	Name	SBO
s102	Ras:GTP	

Product

Table 51: Properties of each product.

Id	Name	SBO
s103	Ras:GDP	

Kinetic Law

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

$$v_{12} = \frac{V10 \cdot s102}{Km10 + s102} \quad (24)$$

Table 52: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V10			0.289	$\text{nmol} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>
Km10			0.057	10^{-9} mol	<input checked="" type="checkbox"/>

5.13 Reaction re114

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

Reaction equation



Reactant

Table 53: Properties of each reactant.

Id	Name	SBO
s97	MEKK1	

Modifiers

Table 54: Properties of each modifier.

Id	Name	SBO
s102	Ras:GTP	
s102	Ras:GTP	
s97	MEKK1	

Product

Table 55: Properties of each product.

Id	Name	SBO
s101	p-MEKK1	

Kinetic Law

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

$$v_{13} = \frac{k_{11} \cdot s_{102} \cdot s_{97}}{K_{m11} + s_{97}} \quad (26)$$

Table 56: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k11			0.035	s^{-1}	<input checked="" type="checkbox"/>
Km11			10.000	10^{-9} mol	<input checked="" type="checkbox"/>

5.14 Reaction re115

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

Reaction equation



Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
s101	p-MEKK1	

Modifier

Table 58: Properties of each modifier.

Id	Name	SBO
s101	p-MEKK1	

Product

Table 59: Properties of each product.

Id	Name	SBO
s97	MEKK1	

Kinetic Law

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

$$v_{14} = \frac{V12 \cdot s101}{Km12 + s101} \quad (28)$$

Table 60: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km12			8.000	10^{-9} mol	<input checked="" type="checkbox"/>
V12			0.125	$\text{nmol} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

5.15 Reaction re116

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

Reaction equation



Reactant

Table 61: Properties of each reactant.

Id	Name	SBO
s96	JNKK	

Modifiers

Table 62: Properties of each modifier.

Id	Name	SBO
s101	p-MEKK1	
s101	p-MEKK1	
s96	JNKK	

Product

Table 63: Properties of each product.

Id	Name	SBO
s100	p-JNKK	

Kinetic Law

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

$$v_{15} = \frac{k_{13} \cdot s_{101} \cdot s_{96}}{K_{m13} + s_{96}} \quad (30)$$

Table 64: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k13			0.005	s^{-1}	<input checked="" type="checkbox"/>
Km13			15.000	10^{-9} mol	<input checked="" type="checkbox"/>

5.16 Reaction re117

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

Reaction equation



Reactant

Table 65: Properties of each reactant.

Id	Name	SBO
s100	p-JNKK	

Id	Name	SBO
----	------	-----

Modifier

Table 66: Properties of each modifier.

Id	Name	SBO
s100	p-JNKK	

Product

Table 67: Properties of each product.

Id	Name	SBO
s96	JNKK	

Kinetic Law

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

$$v_{16} = \frac{V14 \cdot s100}{s100 + Km14} \quad (32)$$

Table 68: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km14			15.000	10^{-9} mol	<input checked="" type="checkbox"/>
V14			0.375	$\text{nmol} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

5.17 Reaction re118

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

Reaction equation



Reactant

Table 69: Properties of each reactant.

Id	Name	SBO
s99	JNK	

Modifiers

Table 70: Properties of each modifier.

Id	Name	SBO
s43	pp-JNKK	
s99	JNK	
s43	pp-JNKK	

Product

Table 71: Properties of each product.

Id	Name	SBO
s104	p-JNK	

Kinetic Law

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

$$v_{17} = \frac{k_{17} \cdot s_{99} \cdot s_{43}}{s_{99} + K_{m17}} \quad (34)$$

Table 72: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k17			0.002	s^{-1}	<input checked="" type="checkbox"/>
Km17			30.000	10^{-9} mol	<input checked="" type="checkbox"/>

5.18 Reaction re119

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

Reaction equation



Reactant

Table 73: Properties of each reactant.

Id	Name	SBO
s104	p-JNK	

Modifier

Table 74: Properties of each modifier.

Id	Name	SBO
s104	p-JNK	

Product

Table 75: Properties of each product.

Id	Name	SBO
s99	JNK	

Kinetic Law

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

$$v_{18} = \frac{V18 \cdot s104}{s104 + Km18} \quad (36)$$

Table 76: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km18			15.00	10^{-9} mol	<input checked="" type="checkbox"/>
V18			0.05	$\text{nmol} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

5.19 Reaction re120

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

Reaction equation



Reactant

Table 77: Properties of each reactant.

Id	Name	SBO
s106	eNOS	

Modifier

Table 78: Properties of each modifier.

Id	Name	SBO
s106	eNOS	

Product

Table 79: Properties of each product.

Id	Name	SBO
s35	s35	

Kinetic Law

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

$$v_{19} = k26 \cdot s106 \quad (38)$$

Table 80: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k26			$2.8 \cdot 10^{-5}$	s^{-1}	<input checked="" type="checkbox"/>

5.20 Reaction re121

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

Reaction equation



Reactant

Table 81: Properties of each reactant.

Id	Name	SBO
s37	s37	

Modifiers

Table 82: Properties of each modifier.

Id	Name	SBO
s106	eNOS	
s106	eNOS	

Product

Table 83: Properties of each product.

Id	Name	SBO
s51	eNOS-Cav-1	

Kinetic Law

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

$$v_{20} = \frac{V27 \cdot s106}{s106 + Km27} \quad (40)$$

Table 84: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V27			0.028	$\text{nmol} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>
Km27			16.000	10^{-9} mol	<input checked="" type="checkbox"/>

5.21 Reaction re122

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

Reaction equation



Reactant

Table 85: Properties of each reactant.

Id	Name	SBO
s38	pre_time	

Product

Table 86: Properties of each product.

Id	Name	SBO
s39	Time	

Kinetic Law

Derived unit $\text{nmol} \cdot \text{s}^{-1}$

$$v_{21} = \text{unitime} \quad (42)$$

Table 87: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
unitime			1.0	$\text{nmol} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

5.22 Reaction re123

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

Reaction equation



Reactant

Table 88: Properties of each reactant.

Id	Name	SBO
s43	pp-JNKK	

Modifier

Table 89: Properties of each modifier.

Id	Name	SBO
s43	pp-JNKK	

Product

Table 90: Properties of each product.

Id	Name	SBO
s100	p-JNKK	

Kinetic Law

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

$$v_{22} = \frac{V16 \cdot s43}{s43 + Km16} \quad (44)$$

Table 91: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V16			0.375	$\text{nmol} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>
Km16			15.000	10^{-9} mol	<input checked="" type="checkbox"/>

5.23 Reaction re124

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

Reaction equation



Reactant

Table 92: Properties of each reactant.

Id	Name	SBO
s100	p-JNKK	

Modifiers

Table 93: Properties of each modifier.

Id	Name	SBO
s101	p-MEKK1	
s100	p-JNKK	
s101	p-MEKK1	

Product

Table 94: Properties of each product.

Id	Name	SBO
s43	pp-JNKK	

Kinetic Law

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

$$v_{23} = \frac{k15 \cdot s100 \cdot s101}{Km15 + s100} \quad (46)$$

Table 95: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k15			0.005	s^{-1}	<input checked="" type="checkbox"/>
Km15			15.000	10^{-9} mol	<input checked="" type="checkbox"/>

5.24 Reaction re125

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

Reaction equation



Reactant

Table 96: Properties of each reactant.

Id	Name	SBO
s44	pp-JNK	

Modifier

Table 97: Properties of each modifier.

Id	Name	SBO
s44	pp-JNK	

Product

Table 98: Properties of each product.

Id	Name	SBO
s104	p-JNK	

Kinetic Law

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

$$v_{24} = \frac{V20 \cdot s44}{Km20 + s44} \quad (48)$$

Table 99: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V20			0.05	$\text{nmol} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>
Km20			15.00	10^{-9} mol	<input checked="" type="checkbox"/>

5.25 Reaction re126

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

Reaction equation



Reactant

Table 100: Properties of each reactant.

Id	Name	SBO
s104	p-JNK	

Modifiers

Table 101: Properties of each modifier.

Id	Name	SBO
s43	pp-JNKK	
s104	p-JNK	
s43	pp-JNKK	

Product

Table 102: Properties of each product.

Id	Name	SBO
s44	pp-JNK	

Kinetic Law

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

$$v_{25} = \frac{k19 \cdot s104 \cdot s43}{Km19 + s104} \quad (50)$$

Table 103: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k19			0.002	s ⁻¹	<input checked="" type="checkbox"/>
Km19			30.000	10 ⁻⁹ mol	<input checked="" type="checkbox"/>

5.26 Reaction re127

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

Reaction equation



Reactant

Table 104: Properties of each reactant.

Id	Name	SBO
s42	AP-1	

Modifiers

Table 105: Properties of each modifier.

Id	Name	SBO
s44	pp-JNK	
s44	pp-JNK	
s42	AP-1	

Product

Table 106: Properties of each product.

Id	Name	SBO
s107	aAP-1	

Kinetic Law

Derived unit 9.999999999999998 · 10⁻¹⁰ mol · s⁻¹

$$v_{26} = \frac{s_{44} \cdot s_{42} \cdot k_{21}}{K_{m21} + s_{42}} \quad (52)$$

Table 107: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km21			25.000	10 ⁻⁹ mol	<input checked="" type="checkbox"/>
k21			4 · 10 ⁻⁵	s ⁻¹	<input checked="" type="checkbox"/>

5.27 Reaction re128

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

Reaction equation



Reactant

Table 108: Properties of each reactant.

Id	Name	SBO
s107	aAP-1	

Modifier

Table 109: Properties of each modifier.

Id	Name	SBO
s107	aAP-1	

Product

Table 110: Properties of each product.

Id	Name	SBO
s42	AP-1	

Kinetic Law

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

$$v_{27} = \frac{V_{22} \cdot s_{107}}{s_{107} + K_{m22}} \quad (54)$$

Table 111: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km22			5.000	10^{-9} mol	<input checked="" type="checkbox"/>
V22			0.002	$\text{nmol} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

5.28 Reaction [re129](#)

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

Reaction equation



Reactant

Table 112: Properties of each reactant.

Id	Name	SBO
s105	KLF2	

Modifiers

Table 113: Properties of each modifier.

Id	Name	SBO
s39	Time	
s39	Time	

Product

Table 114: Properties of each product.

Id	Name	SBO
s49	KLF2	

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \frac{\frac{\exp\left(\tau \cdot \left(\text{delay} - \frac{s_{39}}{t_c}\right)\right)}{1 + 2 \cdot \exp\left(\tau \cdot \left(\text{delay} - \frac{s_{39}}{t_c}\right)\right) + \exp\left(2 \cdot \tau \cdot \left(\text{delay} - \frac{s_{39}}{t_c}\right)\right)}}{uc} \cdot 29.256 \quad (56)$$

Table 115: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
tau			0.55	dimensionless	✓
tc			3600.00	10 ⁻⁹ mol	✓
uc			3600.00	dimensionless	✓
delay			5.00	dimensionless	✓
unity			20.00	nmol · s ⁻¹	✓

6 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.

6.1 Species s35

Name s35

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in one reaction (as a product in [re120](#)).

$$\frac{d}{dt}s_{35} = v_{19} \quad (57)$$

6.2 Species [s37](#)

Name [s37](#)

SBO:0000291 empty set

Initial amount 10000

Charge 0

This species takes part in one reaction (as a reactant in [re121](#)).

$$\frac{d}{dt}s_{37} = -v_{20} \quad (58)$$

6.3 Species [s38](#)

Name [pre_time](#)

SBO:0000347 duration

Initial amount 0

Charge 0

This species takes part in one reaction (as a reactant in [re122](#)).

$$\frac{d}{dt}s_{38} = -v_{21} \quad (59)$$

6.4 Species [s39](#)

Name [Time](#)

Initial amount 0

Charge 0

This species takes part in seven reactions (as a product in [re122](#) and as a modifier in [re102](#), [re102](#), [re103](#), [re103](#), [re129](#), [re129](#)).

$$\frac{d}{dt}s_{39} = v_{21} \quad (60)$$

6.5 Species s42

Name AP-1

Initial amount 50

Charge 0

This species takes part in three reactions (as a reactant in [re127](#) and as a product in [re128](#) and as a modifier in [re127](#)).

$$\frac{d}{dt}s_{42} = v_{27} - v_{26} \quad (61)$$

6.6 Species s43

Name pp-JNKK

Initial amount 0.0060

Charge 0

This species takes part in seven reactions (as a reactant in [re123](#) and as a product in [re124](#) and as a modifier in [re118](#), [re118](#), [re123](#), [re126](#), [re126](#)).

$$\frac{d}{dt}s_{43} = v_{23} - v_{22} \quad (62)$$

6.7 Species s44

Name pp-JNK

Initial amount 0

Charge 0

This species takes part in five reactions (as a reactant in [re125](#) and as a product in [re126](#) and as a modifier in [re125](#), [re127](#), [re127](#)).

$$\frac{d}{dt}s_{44} = v_{25} - v_{24} \quad (63)$$

6.8 Species s49

Name KLF2

SBO:0000252 polypeptide chain

Initial amount 10

Charge 0

This species takes part in three reactions (as a product in [re129](#) and as a modifier in [re111](#), [re111](#)).

$$\frac{d}{dt}s_{49} = v_{28} \quad (64)$$

6.9 Species [s51](#)

Name eNOS-Cav-1

Initial amount 34.98

Charge 0

This species takes part in one reaction (as a product in [re121](#)).

$$\frac{d}{dt}s_{51} = v_{20} \quad (65)$$

6.10 Species [s91](#)

Name Shc

Initial amount 819.25

Charge 0

This species takes part in three reactions (as a reactant in [re104](#) and as a product in [re108](#) and as a modifier in [re104](#)).

$$\frac{d}{dt}s_{91} = v_7 - v_3 \quad (66)$$

6.11 Species [s92](#)

Name p-Src

Initial amount 18

Charge 0

This species takes part in three reactions (as a product in [re103](#) and as a modifier in [re105](#), [re105](#)).

$$\frac{d}{dt}s_{92} = v_2 \quad (67)$$

6.12 Species s93

Name p-FAK

Initial amount 0.605

Charge 0

This species takes part in five reactions (as a reactant in [re104](#) and as a product in [re102](#), [re107](#) and as a modifier in [re104](#), [re107](#)).

$$\frac{d}{dt}s_{93} = v_1 + v_6 - v_3 \quad (68)$$

6.13 Species s94

Name Src

Initial amount 72

Charge 0

This species takes part in one reaction (as a reactant in [re103](#)).

$$\frac{d}{dt}s_{94} = -v_2 \quad (69)$$

6.14 Species s95

Name FAK

Initial amount 57

Charge 0

This species takes part in one reaction (as a reactant in [re102](#)).

$$\frac{d}{dt}s_{95} = -v_1 \quad (70)$$

6.15 Species s96

Name JNKK

Initial amount 299.706

Charge 0

This species takes part in three reactions (as a reactant in [re116](#) and as a product in [re117](#) and as a modifier in [re116](#)).

$$\frac{d}{dt}s_{96} = v_{16} - v_{15} \quad (71)$$

6.16 Species s97

Name MEKK1

Initial amount 98.514

Charge 0

This species takes part in three reactions (as a reactant in [re114](#) and as a product in [re115](#) and as a modifier in [re114](#)).

$$\frac{d}{dt}s97 = v_{14} - v_{13} \quad (72)$$

6.17 Species s98

Name p-Shc

Initial amount 157.162

Charge 0

This species takes part in three reactions (as a reactant in [re108](#) and as a product in [re109](#) and as a modifier in [re108](#)).

$$\frac{d}{dt}s98 = v_8 - v_7 \quad (73)$$

6.18 Species s99

Name JNK

Initial amount 299.997

Charge 0

This species takes part in three reactions (as a reactant in [re118](#) and as a product in [re119](#) and as a modifier in [re118](#)).

$$\frac{d}{dt}s99 = v_{18} - v_{17} \quad (74)$$

6.19 Species s100

Name p-JNKK

Initial amount 0.288

Charge 0

This species takes part in six reactions (as a reactant in [re117](#), [re124](#) and as a product in [re116](#), [re123](#) and as a modifier in [re117](#), [re124](#)).

$$\frac{d}{dt}s100 = v_{15} + v_{22} - v_{16} - v_{23} \quad (75)$$

6.20 Species s101

Name p-MEKK1

Initial amount 1.486

Charge 0

This species takes part in seven reactions (as a reactant in [re115](#) and as a product in [re114](#) and as a modifier in [re115](#), [re116](#), [re116](#), [re124](#), [re124](#)).

$$\frac{d}{dt}s_{101} = v_{13} - v_{14} \quad (76)$$

6.21 Species s102

Name Ras:GTP

Initial amount 0.616

Charge 0

This species takes part in five reactions (as a reactant in [re113](#) and as a product in [re112](#) and as a modifier in [re113](#), [re114](#), [re114](#)).

$$\frac{d}{dt}s_{102} = v_{11} - v_{12} \quad (77)$$

6.22 Species s103

Name Ras:GDP

Initial amount 119.384

Charge 0

This species takes part in three reactions (as a reactant in [re112](#) and as a product in [re113](#) and as a modifier in [re112](#)).

$$\frac{d}{dt}s_{103} = v_{12} - v_{11} \quad (78)$$

6.23 Species s104

Name p-JNK

Initial amount 0.0030

Charge 0

This species takes part in six reactions (as a reactant in [re119](#), [re126](#) and as a product in [re118](#), [re125](#) and as a modifier in [re119](#), [re126](#)).

$$\frac{d}{dt}s_{104} = v_{17} + v_{24} - v_{18} - v_{25} \quad (79)$$

6.24 Species s105

Name KLF2

SBO:0000278 messenger RNA

Initial amount 0

Charge 0

This species takes part in one reaction (as a reactant in [re129](#)).

$$\frac{d}{dt}s_{105} = -v_{28} \quad (80)$$

6.25 Species s106

Name eNOS

SBO:0000278 messenger RNA

Initial amount 3.214

Charge 0

This species takes part in five reactions (as a reactant in [re120](#) and as a product in [re110](#) and as a modifier in [re120](#), [re121](#), [re121](#)).

$$\frac{d}{dt}s_{106} = v_9 - v_{19} \quad (81)$$

6.26 Species s107

Name aAP-1

Initial amount 0

Charge 0

This species takes part in five reactions (as a reactant in [re128](#) and as a product in [re127](#) and as a modifier in [re111](#), [re111](#), [re128](#)).

$$\frac{d}{dt}s_{107} = v_{26} - v_{27} \quad (82)$$

6.27 Species s108

Name eNOS

SBO:0000243 gene

Initial amount 0

Charge 0

This species takes part in one reaction (as a reactant in [re111](#)).

$$\frac{d}{dt}s108 = -v_{10} \quad (83)$$

6.28 Species s110

Name p-FAK:Shc

SBO:0000297 protein complex

Initial amount 0.857

Charge 0

This species takes part in four reactions (as a reactant in [re105](#) and as a product in [re104](#) and as a modifier in [re104](#), [re105](#)).

$$\frac{d}{dt}s110 = v_3 - v_4 \quad (84)$$

6.29 Species s111

Name Grb2:Sos

SBO:0000344 molecular interaction

Initial amount 3.23

Charge 0

This species takes part in three reactions (as a reactant in [re106](#) and as a product in [re109](#) and as a modifier in [re106](#)).

$$\frac{d}{dt}s111 = v_8 - v_5 \quad (85)$$

6.30 Species s112

Name p-FAK:p-Shc

SBO:0000297 protein complex

Initial amount 15.962

Charge 0

This species takes part in four reactions (as a reactant in [re106](#) and as a product in [re105](#) and as a modifier in [re105](#), [re106](#)).

$$\frac{d}{dt}s112 = v_4 - v_5 \quad (86)$$

6.31 Species s113

Name p-FAK:p-Shc:Grb2:Sos

SBO:0000297 protein complex

Initial amount 5.577

Charge 0

This species takes part in four reactions (as a reactant in [re107](#) and as a product in [re106](#) and as a modifier in [re106](#), [re107](#)).

$$\frac{d}{dt}s113 = v_5 - v_6 \quad (87)$$

6.32 Species s114

Name p-Shc:Grb2:Sos

Initial amount 1.193

Charge 0

This species takes part in six reactions (as a reactant in [re109](#) and as a product in [re107](#) and as a modifier in [re107](#), [re109](#), [re112](#), [re112](#)).

$$\frac{d}{dt}s114 = v_6 - v_8 \quad (88)$$

6.33 Species s115

Name eNOS

SBO:0000278 messenger RNA

Initial amount 0.09

Charge 0

This species takes part in three reactions (as a reactant in [re110](#) and as a product in [re111](#) and as a modifier in [re110](#)).

$$\frac{d}{dt}s_{115} = v_{10} - v_9 \quad (89)$$

6.34 Species s119

Name Shear Stress

Initial amount 0

Charge 0

This species takes part in two reactions (as a modifier in [re102](#), [re103](#)).

$$\frac{d}{dt}s_{119} = 0 \quad (90)$$

A Glossary of Systems Biology Ontology Terms

SBO:0000243 gene: A locatable region of genomic sequence, corresponding to a unit of inheritance, which is associated with regulatory regions, transcribed regions and/or other functional sequence regions. Sequence Ontology SO:000070

SBO:0000252 polypeptide chain: Naturally occurring macromolecule formed by the repetition of amino-acid residues linked by peptidic bonds. A polypeptide chain is synthesized by the ribosome. CHEBI:1654

SBO:0000278 messenger RNA: A messenger RNA is a ribonucleic acid synthesized during the transcription of a gene, and that carries the information to encode one or several proteins

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

SBO:0000344 molecular interaction: Relationship between molecular entities, based on contacts, direct or indirect.

SBO:0000347 duration: Amount of time during which an event persists

SBML²TeX was developed by Andreas Dräger^a, Hannes Planatscher^a, Dieudonné M Wouamba^a, Adrian Schröder^a, Michael Hucka^b, Lukas Endler^c, Martin Golebiewski^d and Andreas Zell^a. Please see <http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX> for more information.

^aCenter for Bioinformatics Tübingen (ZBIT), Germany

^bCalifornia Institute of Technology, Beckman Institute BNMC, Pasadena, United States

^cEuropean Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom

^dEML Research gGmbH, Heidelberg, Germany