SBML Model Report

Model name: “Koo2013 - Shear stress induced calcium influx and eNOS activation - Model 1”

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 Juty[1], Vijayalakshmi Chelliah[2] and Andrew Koo[3] at August 19th 2013 at 1:33 p. m. and last time modified at April seventh 2014 at 2:58 a. m. Table 1 gives 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	14
events	0	constraints	0
reactions	10	function definitions	0
global parameters	27	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 three 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
c2	ER		3	1	litre	☑	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 c2

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

Name ER

4 Species

This model contains 14 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
s1	Ca_ex	default	10^{-9} mol	⊟	⊟
s2	Ca_s	c2	10^{-9} mol	⊟	⊟
s3	Ca_c	c1	10^{-9} mol	⊟	⊟
s4	Ca_B	c1	10^{-9} mol	⊟	⊟
s5	s5	default	10^{-9} mol	⊟	⊟
s6	IP3	c1	10^{-9} mol	⊟	⊟
s7	s7	c1	10^{-9} mol	⊟	⊟
s8	s8	c1	10^{-9} mol	⊟	⊟
s9	s9	c1	10^{-9} mol	⊟	⊟
s10	s10	c1	10^{-9} mol	⊟	⊟
s11	s11	c1	10^{-9} mol	⊟	⊟
s12	TimeT	default	10^{-9} mol	⊟	⊟
s13	s13	default	10^{-9} mol	⊟	⊟
s119	Shear Stress	default	10^{-9} mol	⊟	⊟

5 Parameters

This model contains 27 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
R_T	R_T		44000.000	dimensionless	☑
k1	k1		$6 \cdot 10^{-4}$	$10^{-9}\ \mathrm{mol} \cdot \mathrm{s}^{-1}$	☑
k2	k2		1.000	s^{-1}	☑
k3	k3		3.320	s^{-1}	☑
k4	k4		2500.000	$10^{-9}\ \mathrm{mol} \cdot \mathrm{s}^{-1}$	☑
k5	k5		$5 \cdot 10^{-11}$	$\left(10^{-9}\ \mathrm{mol}\right)^{-1} \cdot \mathrm{s}^{-1}$	☑
k6	k6		0.050	$\left(10^{-9}\ \mathrm{mol}\right)^{-1} \cdot \mathrm{s}^{-1}$	☑
k7	k7		150.000	s^{-1}	☑
K1	K1		0.000	$10^{-9}\ \mathrm{mol}$	☑
K2	K2		200.000	$10^{-9}\ \mathrm{mol}$	☑
K3	K3		150.000	$10^{-9}\ \mathrm{mol}$	☑
K4	K4		80.000	$10^{-9}\ \mathrm{mol}$	☑
K5	K5		321.000	$10^{-9}\ \mathrm{mol}$	☑
K_hi	K_hi		380.000	$10^{-9}\ \mathrm{mol}$	☑
k_CICR	k_CICR		1.000	dimensionless	☑
K_CICR	K_CICR		0.000	$10^{-9}\ \mathrm{mol}$	☑
k_CCE	k_CCE		0.000	$\left(10^{-9}\ \mathrm{mol}\right)^{-1} \cdot \mathrm{s}^{-1}$	☑
B_T	B_T		120000.000	$10^{-9}\ \mathrm{mol}$	☑
dot_Vp	dot_Vp		815.000	$10^{-9}\ \mathrm{mol} \cdot \mathrm{s}^{-1}$	☑
dot_Vex	dot_Vex		9165.000	$10^{-9}\ \mathrm{mol} \cdot \mathrm{s}^{-1}$	☑
dot_Vhi	dot_Vhi		2380.000	$10^{-9}\ \mathrm{mol} \cdot \mathrm{s}^{-1}$	☑
dot_q_inpass	dot_q_inpass		3000.000	$10^{-9}\ \mathrm{mol} \cdot \mathrm{s}^{-1}$	☑
Cao	Cao		100.000	$10^{-9}\ \mathrm{mol}$	☑
tau_I	tau_I		66.000	$10^{-9}\ \mathrm{mol}$	☑
tau_II	tau_II		0.010	$10^{-9}\ \mathrm{mol}$	☑
half	half		0.500	dimensionless	☑
fracK	fracK		7071067.810	$10^{-9}\ \mathrm{mol}$	☑

6 Reactions

This model contains ten 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	re3	re1	$s4 \xrightarrow{s3,\ s4,\ s3,\ s4} s3$	
2	re4		$s5 \xrightarrow{s1,\ s2,\ s1,\ s2,\ s1} s2$	
3	re5		$s7 \xrightarrow{s3,\ s12,\ s119,\ s12,\ s3,\ s12,\ s3} s6$	
4	re6		$s6 \xrightarrow{s6,\ s6} s8$	
5	re7		$s2 \xrightarrow{s6,\ s3,\ s6,\ s2,\ s3,\ s6,\ s2} s3$	
6	re8		$s3 \xrightarrow{s3,\ s3} s9$	
7	re9		$s3 \xrightarrow{s3,\ s3} s10$	
8	re10		$s11 \longrightarrow s3$	
9	re11		$s13 \longrightarrow s12$	
10	re12		$s3 \xrightarrow{s3,\ s3} s9$	

6.1 Reaction re3

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

Name re1

Reaction equation

$$\mathrm{s4} \xrightarrow{\mathrm{s3,\ s4,\ s3,\ s4}} \mathrm{s3} \tag{1}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
s4	Ca_B	

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
s3	Ca_c	
s4	Ca_B	
s3	Ca_c	
s4	Ca_B	

Product

Table 8: Properties of each product.

Id	Name	SBO
s3	Ca_c	

Kinetic Law

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

$$v_1 = \mathrm{k6} \cdot \mathrm{s3} \cdot (\mathrm{B\_T} - \mathrm{s4}) + \mathrm{k7} \cdot \mathrm{s4} \tag{2}$$

6.2 Reaction re4

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

Reaction equation

$$\mathrm{s5} \xrightarrow{\mathrm{s1,\ s2,\ s1,\ s2,\ s1}} \mathrm{s2} \tag{3}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
s5	s5	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
s1	Ca_ex	
s2	Ca_s	
s1	Ca_ex	
s2	Ca_s	
s1	Ca_ex	

Product

Table 11: Properties of each product.

Id	Name	SBO
s2	Ca_s	

Kinetic Law

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

$$v_2 = \mathrm{k\_CCE} \cdot \left(\frac{\mathrm{fracK} \cdot \mathrm{Cao}}{\mathrm{K3} + \mathrm{Cao}} - \mathrm{s2} \right) \cdot (\mathrm{s1} - \mathrm{s2}) \tag{4}$$

6.3 Reaction re5

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

Reaction equation

$$\mathrm{s7} \xrightarrow{\mathrm{s3,\ s12,\ s119,\ s12,\ s3,\ s12,\ s3}} \mathrm{s6} \tag{5}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
s7	s7	

Modifiers

Table 13: Properties of each modifier.

Id	Name	SBO
s3	Ca_c	
s12	TimeT	
s119	Shear Stress	
s12	TimeT	
s3	Ca_c	
s12	TimeT	
s3	Ca_c	

Product

Table 14: Properties of each product.

Id	Name	SBO
s6	IP3	

Kinetic Law

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

$$v_3 = \frac{\mathrm{k1} \cdot \left(\mathrm{R\_T} - \mathrm{half} \cdot \mathrm{R\_T} \cdot \left(\exp\left(\frac{\mathrm{s12}}{\mathrm{tau\_I}}\right) + \exp\left(\frac{\mathrm{s12}}{\mathrm{tau\_II}}\right) + \frac{\left(\exp\left(\frac{\mathrm{s12}}{\mathrm{tau\_I}}\right) - \exp\left(\frac{\mathrm{s12}}{\mathrm{tau\_II}}\right)\right) \cdot (\mathrm{tau\_I} + \mathrm{tau\_II})}{\mathrm{tau\_I} - \mathrm{tau\_II}} \right) \right) \cdot \mathrm{s3}}{\mathrm{K1} + \mathrm{s3}} \tag{6}$$

6.4 Reaction re6

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

Reaction equation

$$\mathrm{s6} \xrightarrow{\mathrm{s6,\ s6}} \mathrm{s8} \tag{7}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
s6	IP3	

Modifiers

Table 16: Properties of each modifier.

Id	Name	SBO
s6	IP3	
s6	IP3	

Product

Table 17: Properties of each product.

Id	Name	SBO
s8	s8	

Kinetic Law

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

$$v_4 = \mathrm{k2} \cdot \mathrm{s6} \tag{8}$$

6.5 Reaction re7

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

Reaction equation

$$\mathrm{s2} \xrightarrow{\mathrm{s6,\ s3,\ s6,\ s2,\ s3,\ s6,\ s2}} \mathrm{s3} \tag{9}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
s2	Ca_s	

Modifiers

Table 19: Properties of each modifier.

Id	Name	SBO
s6	IP3	
s3	Ca_c	
s6	IP3	
s2	Ca_s	
s3	Ca_c	
s6	IP3	
s2	Ca_s	

Product

Table 20: Properties of each product.

Id	Name	SBO
s3	Ca_c	

Kinetic Law

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

$$v_5 = \mathrm{k3} \cdot \frac{\mathrm{k\_CICR} \cdot \mathrm{s3}}{\mathrm{K\_CICR} + \mathrm{s3}} \cdot \left(\frac{\mathrm{s6}}{\mathrm{K2} + \mathrm{s6}}\right)^3 \cdot \mathrm{s2} - \mathrm{k4} \cdot \left(\frac{\mathrm{s3}}{\mathrm{K3} + \mathrm{s3}}\right)^2 + \mathrm{k5} \cdot \mathrm{s2} \cdot \mathrm{s2} \tag{10}$$

6.6 Reaction re8

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

Reaction equation

$$\mathrm{s3} \xrightarrow{\mathrm{s3,\ s3}} \mathrm{s9} \tag{11}$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
s3	Ca_c	

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
s3	Ca_c	
s3	Ca_c	

Product

Table 23: Properties of each product.

Id	Name	SBO
s9	s9	

Kinetic Law

Derived unit $9.99999999999994 \cdot 10^{-10}\ \mathrm{mol} \cdot \mathrm{s}^{-1}$

$$v_6 = \frac{\mathrm{dot\_Vhi} \cdot \mathrm{s3}^4}{\mathrm{K\_hi}^4 + \mathrm{s3}^4} \tag{12}$$

6.7 Reaction re9

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

Reaction equation

$$\mathrm{s3} \xrightarrow{\mathrm{s3,\ s3}} \mathrm{s10} \tag{13}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
s3	Ca_c	

Modifiers

Table 25: Properties of each modifier.

Id	Name	SBO
s3	Ca_c	
s3	Ca_c	

Product

Table 26: Properties of each product.

Id	Name	SBO
s10	s10	

Kinetic Law

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

$$v_7 = \frac{\mathrm{dot\_Vex} \cdot \mathrm{s3}}{\mathrm{K5} + \mathrm{s3}} \tag{14}$$

6.8 Reaction re10

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

Reaction equation

$$\mathrm{s11} \longrightarrow \mathrm{s3} \tag{15}$$

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
s11	s11	

Product

Table 28: Properties of each product.

Id	Name	SBO
s3	Ca_c	

Kinetic Law

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

$$v_8 = \mathrm{dot\_q\_inpass} \tag{16}$$

6.9 Reaction re11

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

Reaction equation

$$\mathrm{s13} \longrightarrow \mathrm{s12} \tag{17}$$

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
s13	s13	

Product

Table 30: Properties of each product.

Id	Name	SBO
s12	TimeT	

Kinetic Law

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

$$v_9 = \mathrm{unisec} \tag{18}$$

Table 31: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
unisec			1.0	$10^{-9}\ \mathrm{mol}\cdot\mathrm{s}^{-1}$	☑

6.10 Reaction re12

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

Reaction equation

$$\mathrm{s3} \xrightarrow{\mathrm{s3},\ \mathrm{s3}} \mathrm{s9} \tag{19}$$

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
s3	Ca_c	

Modifiers

Table 33: Properties of each modifier.

Id	Name	SBO
s3	Ca_c	
s3	Ca_c	

Product

Table 34: Properties of each product.

Id	Name	SBO
s9	s9	

Kinetic Law

Derived unit $1.0000000000000038 \cdot 10^{-9}\ \mathrm{mol}\cdot\mathrm{s}^{-1}$

$$v_{10} = \frac{\mathrm{dot\_Vp}\cdot \mathrm{s3}^2}{\mathrm{K4}^2 + \mathrm{s3}^2} \tag{20}$$

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 s1

Name Ca_ex

Initial amount 1500000

Charge 0

This species takes part in three reactions (as a modifier in re4, re4, re4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s1} = 0 \tag{21}$$

7.2 Species s2

Name Ca_s

Initial amount 2830000

Charge 0

This species takes part in six reactions (as a reactant in re7 and as a product in re4 and as a modifier in re4, re4, re7, re7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s2} = v_2 - v_5 \tag{22}$$

7.3 Species s3

Name Ca_c

Initial amount 117.2

Charge 0

This species takes part in 19 reactions (as a reactant in re8, re9, re12 and as a product in re3, re7, re10 and as a modifier in re3, re3, re5, re5, re5, re7, re7, re8, re8, re9, re9, re12, re12).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s3} = v_1 + v_5 + v_8 - v_6 - v_7 - v_{10} \tag{23}$$

7.4 Species s4

Name Ca_B

SBO:0000297 protein complex

Initial amount 3870

Charge 0

This species takes part in three reactions (as a reactant in re3 and as a modifier in re3, re3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s4} = -v_1 \tag{24}$$

7.5 Species s5

Name s5

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in one reaction (as a reactant in re4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s5} = -v_2 \tag{25}$$

7.6 Species s6

Name IP3

Initial amount 0

Charge 0

This species takes part in seven reactions (as a reactant in re6 and as a product in re5 and as a modifier in re6, re6, re7, re7, re7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s6} = v_3 - v_4 \tag{26}$$

7.7 Species s7

Name s7

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in one reaction (as a reactant in re5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s7} = -v_3 \tag{27}$$

7.8 Species s8

Name s8

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in one reaction (as a product in re6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s8} = v_4 \tag{28}$$

7.9 Species s9

Name s9

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in two reactions (as a product in re8, re12).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s9} = v_6 + v_{10} \tag{29}$$

7.10 Species s10

Name s10

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in one reaction (as a product in re9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s10} = v_7 \tag{30}$$

7.11 Species s11

Name s11

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in one reaction (as a reactant in re10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s11} = -v_8 \tag{31}$$

7.12 Species s12

Name TimeT

SBO:0000331 half-life

Initial amount 0

Charge 0

This species takes part in four reactions (as a product in re11 and as a modifier in re5, re5, re5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s12} = v_9 \tag{32}$$

7.13 Species s13

Name s13

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in one reaction (as a reactant in re11).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s13} = -v_9 \tag{33}$$

7.14 Species s119

Name Shear Stress

Initial amount 0

Charge 0

This species takes part in one reaction (as a modifier in re5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s119} = 0 \tag{34}$$

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

SBO:0000331 half-life: Time interval over which a quantified entity is reduced to half its original value

SBML2LaTeX 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.

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