SBML Model Report

Model name: “Koo2013 - Shear stress induced AKT and eNOS phosphorylation - Model 2”

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 1:35 p. m. and last time modified at April seventh 2014 at 2:59 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	2
species types	0	species	16
events	0	constraints	0
reactions	12	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.

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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 16 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
s14	PDK1	c1	10^{-9} mol	⊟	⊟
s15	PP2A	c1	10^{-9} mol	⊟	⊟
s16	AKT	c1	10^{-9} mol	⊟	⊟
s17	PI3P	c1	10^{-9} mol	⊟	⊟
s18	PTEN	c1	10^{-9} mol	⊟	⊟
s19	PIP2	c1	10^{-9} mol	⊟	⊟
s20	p-PI3K	c1	10^{-9} mol	⊟	⊟
s21	s3	c1	10^{-9} mol	⊟	⊟
s22	PI3K	c1	10^{-9} mol	⊟	⊟
s23	Time	c1	10^{-9} mol	⊟	⊟
s24	PDK2	c1	10^{-9} mol	⊟	⊟
s25	PDK1_cyto	c1	10^{-9} mol	⊟	⊟
s26	p-AKT:PI3P	c1	10^{-9} mol	⊟	⊟
s27	pp-AKT:PI3P	c1	10^{-9} mol	⊟	⊟
s28	AKT:PI3P	c1	10^{-9} mol	⊟	⊟
s119	Shear Stress	default	10^{-9} mol	⊟	⊟

5 Reactions

This model contains twelve 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

№	Id	Name	Reaction Equation	SBO
1	re57		$s22 \xrightleftharpoons{s23,\ s119,\ s23} s20$	
2	re58		$s19 \xrightarrow{s20,\ s19,\ s20} s17$	
3	re59		$s17 \xrightarrow{s18,\ s17,\ s18} s19$	
4	re60		$s17 + s16 \xrightleftharpoons{s17,\ s16,\ s28} s28$	
5	re61		$s28 \xrightarrow{s14,\ s28,\ s14} s26$	
6	re62		$s26 \xrightarrow{s24,\ s26,\ s24} s27$	
7	re63		$s26 \xrightarrow{s15,\ s26,\ s15} s28$	
8	re64		$s27 \xrightarrow{s15,\ s27,\ s15} s26$	
9	re65		$s27 \xrightarrow{s15,\ s27,\ s15} s17 + s16$	
10	re66		$s25 \xrightarrow{s17,\ s17,\ s25} s14$	
11	re67		$s14 \xrightarrow{s14} s25$	
12	re68		$s21 \longrightarrow s23$	

5.1 Reaction re57

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

Reaction equation

$$\mathrm{s22} \xrightleftharpoons{\mathrm{s23,\ s119,\ s23}} \mathrm{s20} \tag{1}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
s22	PI3K	

Modifiers

Table 6: Properties of each modifier.

Id	Name	SBO
s23	Time	
s119	Shear Stress	
s23	Time	

Product

Table 7: Properties of each product.

Id	Name	SBO
s20	p-PI3K	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \exp\left(\mathrm{unity} - \left(\frac{\mathrm{s23}}{\mathrm{tf}}\right)^{1.8}\right) \cdot \mathrm{normal} \cdot \left(\frac{\mathrm{s23}}{\mathrm{unimol}}\right)^{0.8} \cdot \left(\mathrm{unity} - \left(\frac{\mathrm{s23}}{\mathrm{tf}}\right)^{1.8}\right) \tag{2}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
normal			0.907	10^{-9} mol · s^{-1}	☑
unity			1.000	dimensionless	☑
unimol			1.000	10^{-9} mol	☑
tf			15.000	10^{-9} mol	☑

5.2 Reaction re58

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

Reaction equation

$$\text{s19} \xrightarrow{\text{s20, s19, s20}} \text{s17} \tag{3}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
s19	PIP2	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
s20	p-PI3K	
s19	PIP2	
s20	p-PI3K	

Product

Table 11: Properties of each product.

Id	Name	SBO
s17	PI3P	

Kinetic Law

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

$$v_2 = \frac{\mathrm{k2} \cdot \mathrm{s19} \cdot \mathrm{s20}}{\mathrm{Km2} + \mathrm{s19}} \tag{4}$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k2			0.2	s^{-1}	☑
Km2			6170.0	10^{-9} mol	☑

5.3 Reaction re59

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

Reaction equation

$$\mathrm{s17} \xrightarrow{\mathrm{s18,\ s17,\ s18}} \mathrm{s19} \tag{5}$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
s17	PI3P	

Modifiers

Table 14: Properties of each modifier.

Id	Name	SBO
s18	PTEN	
s17	PI3P	
s18	PTEN	

Product

Table 15: Properties of each product.

Id	Name	SBO
s19	PIP2	

Kinetic Law

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

$$v_3 = \frac{k3 \cdot s17 \cdot s18}{Km3 + s17} \tag{6}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k3			7.5	s^{-1}	☑
Km3			80.9	10^{-9} mol	☑

5.4 Reaction re60

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

Reaction equation

$$s17 + s16 \overset{s17,\ s16,\ s28}{\rightleftharpoons} s28 \tag{7}$$

Reactants

Table 17: Properties of each reactant.

Id	Name	SBO
s17	PI3P	
s16	AKT	

Modifiers

Table 18: Properties of each modifier.

Id	Name	SBO
s17	PI3P	

Id	Name	SBO
s16	AKT	
s28	AKT:PI3P	

Product

Table 19: Properties of each product.

Id	Name	SBO
s28	AKT:PI3P	

Kinetic Law

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

$$v_4 = \mathrm{k4} \cdot \mathrm{s17} \cdot \mathrm{s16} - \mathrm{kr4} \cdot \mathrm{s28} \tag{8}$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k4			0.045	$\left(10^{-9}\ \mathrm{mol}\right)^{-1} \cdot \mathrm{s}^{-1}$	☑
kr4			0.089	s^{-1}	☑

5.5 Reaction re61

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

Reaction equation

$$\mathrm{s28} \xrightarrow{\mathrm{s14,\ s28,\ s14}} \mathrm{s26} \tag{9}$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
s28	AKT:PI3P	

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
s14	PDK1	
s28	AKT:PI3P	
s14	PDK1	

Product

Table 23: Properties of each product.

Id	Name	SBO
s26	p-AKT:PI3P	

Kinetic Law

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

$$v_5 = \frac{\mathrm{k8} \cdot \mathrm{s28} \cdot \mathrm{s14}}{\mathrm{Km8} + \mathrm{s28}} \tag{10}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k8			20.0	s^{-1}	☑
Km8			80000.0	10^{-9} mol	☑

5.6 Reaction re62

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

Reaction equation

$$\mathrm{s26} \xrightarrow{\mathrm{s24,\ s26,\ s24}} \mathrm{s27} \tag{11}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
s26	p-AKT:PI3P	

Id	Name	SBO

Modifiers

Table 26: Properties of each modifier.

Id	Name	SBO
s24	PDK2	
s26	p-AKT:PI3P	
s24	PDK2	

Product

Table 27: Properties of each product.

Id	Name	SBO
s27	pp-AKT:PI3P	

Kinetic Law

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

$$v_6 = \frac{\mathrm{k10} \cdot \mathrm{s26} \cdot \mathrm{s24}}{\mathrm{Km10} + \mathrm{s26}} \tag{12}$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k10			20.0	s^{-1}	☑
Km10			80000.0	10^{-9} mol	☑

5.7 Reaction re63

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

Reaction equation

$$\mathrm{s26} \xrightarrow{\mathrm{s15,\ s26,\ s15}} \mathrm{s28} \tag{13}$$

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
s26	p-AKT:PI3P	

Modifiers

Table 30: Properties of each modifier.

Id	Name	SBO
s15	PP2A	
s26	p-AKT:PI3P	
s15	PP2A	

Product

Table 31: Properties of each product.

Id	Name	SBO
s28	AKT:PI3P	

Kinetic Law

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

$$v_7 = \frac{\mathrm{k7} \cdot \mathrm{s26} \cdot \mathrm{s15}}{\mathrm{Km7} + \mathrm{s26}} \tag{14}$$

Table 32: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k7			0.037	s^{-1}	☑
Km7			8800.000	10^{-9} mol	☑

5.8 Reaction re64

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

Reaction equation

$$\text{s27} \xrightarrow{\text{s15, s27, s15}} \text{s26} \tag{15}$$

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
s27	pp-AKT:PI3P	

Modifiers

Table 34: Properties of each modifier.

Id	Name	SBO
s15	PP2A	
s27	pp-AKT:PI3P	
s15	PP2A	

Product

Table 35: Properties of each product.

Id	Name	SBO
s26	p-AKT:PI3P	

Kinetic Law

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

$$v_8 = \frac{\text{k9} \cdot \text{s27} \cdot \text{s15}}{\text{Km9} + \text{s27}} \tag{16}$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k9			0.04	s^{-1}	☑
Km9			48000.00	10^{-9} mol	☑

5.9 Reaction re65

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

Reaction equation

$$\mathrm{s27} \xrightarrow{\mathrm{s15,\ s27,\ s15}} \mathrm{s17} + \mathrm{s16} \tag{17}$$

Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
s27	pp-AKT:PI3P	

Modifiers

Table 38: Properties of each modifier.

Id	Name	SBO
s15	PP2A	
s27	pp-AKT:PI3P	
s15	PP2A	

Products

Table 39: Properties of each product.

Id	Name	SBO
s17	PI3P	
s16	AKT	

Kinetic Law

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

$$v_9 = \frac{\mathrm{k11} \cdot \mathrm{s27} \cdot \mathrm{s15}}{\mathrm{Km11} + \mathrm{s27}} \tag{18}$$

Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k11			0.163	s^{-1}	☑
Km11			48000.000	10^{-9} mol	☑

5.10 Reaction re66

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

Reaction equation

$$s25 \xrightarrow{s17,\ s17,\ s25} s14 \tag{19}$$

Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
s25	PDK1_cyto	

Modifiers

Table 42: Properties of each modifier.

Id	Name	SBO
s17	PI3P	
s17	PI3P	
s25	PDK1_cyto	

Product

Table 43: Properties of each product.

Id	Name	SBO
s14	PDK1	

Kinetic Law

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

$$v_{10} = \mathrm{k5} \cdot \mathrm{s17} \cdot \mathrm{s25} \tag{20}$$

Table 44: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k5			$7 \cdot 10^{-4}$	$\left(10^{-9}\ \mathrm{mol}\right)^{-1} \cdot \mathrm{s}^{-1}$	☑

5.11 Reaction re67

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

Reaction equation

$$\mathrm{s14} \xrightarrow{\mathrm{s14}} \mathrm{s25} \tag{21}$$

Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
s14	PDK1	

Modifier

Table 46: Properties of each modifier.

Id	Name	SBO
s14	PDK1	

Product

Table 47: Properties of each product.

Id	Name	SBO
s25	PDK1_cyto	

Kinetic Law

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

$$v_{11} = \mathrm{k6} \cdot \mathrm{s14} \tag{22}$$

Table 48: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k6			0.98	s^{-1}	☑

5.12 Reaction re68

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

Reaction equation

$$\mathrm{s21} \longrightarrow \mathrm{s23} \tag{23}$$

Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
s21	s3	

Product

Table 50: Properties of each product.

Id	Name	SBO
s23	Time	

Kinetic Law

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

$$v_{12} = \mathrm{unitime} \tag{24}$$

Table 51: Properties of each parameter.

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

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.

6.1 Species s14

Name PDK1

Initial amount 0.246

Charge 0

This species takes part in five reactions (as a reactant in re67 and as a product in re66 and as a modifier in re61, re61, re67).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s14} = v_{10} - v_{11} \tag{25}$$

6.2 Species s15

Name PP2A

Initial amount 150

Charge 0

This species takes part in six reactions (as a modifier in re63, re63, re64, re64, re65, re65).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s15} = 0 \tag{26}$$

6.3 Species s16

Name AKT

Initial amount 167.616

Charge 0

This species takes part in three reactions (as a reactant in re60 and as a product in re65 and as a modifier in re60).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s16} = v_{9} - v_{4} \tag{27}$$

6.4 Species s17

Name PI3P

Initial amount 0.345

Charge 0

This species takes part in eight reactions (as a reactant in re59, re60 and as a product in re58, re65 and as a modifier in re59, re60, re66, re66).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s17} = v_2 + v_9 - v_3 - v_4 \tag{28}$$

6.5 Species s18

Name PTEN

Initial amount 0.1

Charge 0

This species takes part in two reactions (as a modifier in re59, re59).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s18} = 0 \tag{29}$$

6.6 Species s19

Name PIP2

Initial amount 6967.271

Charge 0

This species takes part in three reactions (as a reactant in re58 and as a product in re59 and as a modifier in re58).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s19} = v_3 - v_2 \tag{30}$$

6.7 Species s20

Name p-PI3K

Initial amount 0.03

Charge 0

This species takes part in three reactions (as a product in re57 and as a modifier in re58, re58).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s20} = v_1 \tag{31}$$

6.8 Species s21

Name s3

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in one reaction (as a reactant in re68).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s21} = -v_{12} \tag{32}$$

6.9 Species s22

Name PI3K

Initial amount 99.97

Charge 0

This species takes part in one reaction (as a reactant in re57).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s22} = -v_{1} \tag{33}$$

6.10 Species s23

Name Time

Initial amount 0

Charge 0

This species takes part in three reactions (as a product in re68 and as a modifier in re57, re57).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s23} = v_{12} \tag{34}$$

6.11 Species s24

Name PDK2

Initial amount 3

Charge 0

This species takes part in two reactions (as a modifier in re62, re62).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s24} = 0 \tag{35}$$

6.12 Species s25

Name PDK1_cyto

Initial amount 999.754

Charge 0

This species takes part in three reactions (as a reactant in re66 and as a product in re67 and as a modifier in re66).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s25} = v_{11} - v_{10} \tag{36}$$

6.13 Species s26

Name p-AKT:PI3P

Initial amount 1.457

Charge 0

This species takes part in six reactions (as a reactant in re62, re63 and as a product in re61, re64 and as a modifier in re62, re63).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s26} = v_5 + v_8 - v_6 - v_7 \tag{37}$$

6.14 Species s27

Name pp-AKT:PI3P

Initial amount 1.723

Charge 0

This species takes part in five reactions (as a reactant in re64, re65 and as a product in re62 and as a modifier in re64, re65).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s27} = v_6 - v_8 - v_9 \tag{38}$$

6.15 Species s28

Name AKT:PI3P

Initial amount 29.203

Charge 0

This species takes part in five reactions (as a reactant in re61 and as a product in re60, re63 and as a modifier in re60, re61).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s28} = v_4 + v_7 - v_5 \tag{39}$$

6.16 Species s119

Name Shear Stress

Initial amount 0

Charge 0

This species takes part in one reaction (as a modifier in re57).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s119} = 0 \tag{40}$$

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.

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