SBML Model Report

Model name: "Giantsos-Adams2013 - Growth of glycocalyx under shear stress conditions"

September 28, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. Table 1 provides an overview of the quantities of all components of this model.

Table 1: Number of components in this model, which are described in the following sections.

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	7
events	0	constraints	0
reactions	7	function definitions	0
global parameters	0	unit definitions	5
rules	0	initial assignments	0

Model Notes

Giantsos-Adams2013 - Glycocalyx under shearstress conditions - Heparan Sulphate Endocytosis

This model is described in the article:Heparan Sulfate Regrowth Profiles Under Laminar Shear Flow Following Enzymatic Degradation.Giantsos-Adams KM, Koo AJ, Song S, Sakai J, Sankaran J, Shin JH, Garcia-Cardena G, Dewey CF.Cell Mol Bioeng 2013 Jun; 6(2): 160-174

Abstract:

The local hemodynamic shear stress waveforms present in an artery dictate the endothelial cell phenotype. The observed decrease of the apical glycocalyx layer on the endothelium in

atheroprone regions of the circulation suggests that the glycocalyx may have a central role in determining atherosclerotic plaque formation. However, the kinetics for the cells' ability to adapt its glycocalyx to the environment have not been quantitatively resolved. Here we report that the heparan sulfate component of the glycocalyx of HUVECs increases by 1.4-fold following the onset of high shear stress, compared to static cultured cells, with a time constant of 19h. Cell morphology experiments show that 12h are required for the cells to elongate, but only after 36h have the cells reached maximal alignment to the flow vector. Our findings demonstrate that following enzymatic degradation, heparan sulfate is restored to the cell surface within 12h under flow whereas the time required is 20h under static conditions. We also propose a model describing the contribution of endocytosis and exocytosis to apical heparan sulfate expression. The change in HS regrowth kinetics from static to high-shear EC phenotype implies a differential in the rate of endocytic and exocytic membrane turnover.

This model is hosted on BioModels Database and identified by: MODEL1609100000.

To cite BioModels Database, please use: BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models.

2 Unit Definitions

This is an overview of five unit definitions.

2.1 Unit `substance`

Name substance

Definition mol

2.2 Unit `volume`

Name volume

Definition l

2.3 Unit `area`

Name area

Definition m^2

2.4 Unit `length`

Name length

Definition m

2.5 Unit `time`

Name time

Definition s

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

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

3.1 Compartment `default`

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

4 Species

This model contains seven 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 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
`s1`	HS surface	`default`	mol	☐	☐
`s2`	early endosome	`default`	mol	☐	☐
`s3`	late endosome	`default`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
`s5`	s5	`default`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
`s6`	golgi	`default`	mol	☑	☑
`s8`	s8	`default`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
`s4`	lysosome	`default`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐

5 Reactions

This model contains seven 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	k_golgi	k3	s6 ⟶ s1	
2	k_endo	k1	s1 ⟶ s2	
3	k_exo	k2	s2 ⟶ s1	
4	k_le	k6	s2 ⟶ s3	
5	k_lys	k7	s3 ⟶ s4	
6	k_deg	k8	s4 ⟶ s5	
7	k_shed	k4	s1 ⟶ s8	

5.1 Reaction k_golgi

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

Name k3

Reaction equation

$$\mathrm{s6} \longrightarrow \mathrm{s1} \tag{1}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
s6	golgi	

Product

Table 6: Properties of each product.

Id	Name	SBO
s1	HS surface	

Kinetic Law

Derived unit mol^2

$$v_1 = \mathrm{s6} \cdot \mathrm{k3} \tag{2}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k3	k3		0.96	mol	☑

5.2 Reaction k_endo

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

Name k1

Reaction equation

$$\mathrm{s1} \longrightarrow \mathrm{s2} \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
s1	HS surface	

Product

Table 9: Properties of each product.

Id	Name	SBO
s2	early endosome	

Kinetic Law

Derived unit mol^2

$$v_2 = \mathrm{s1} \cdot \mathrm{k1} \tag{4}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.025	mol	☑

5.3 Reaction k_exo

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

Name k2

Reaction equation

$$\mathrm{s2} \longrightarrow \mathrm{s1} \tag{5}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
s2	early endosome	

Product

Table 12: Properties of each product.

Id	Name	SBO
s1	HS surface	

Kinetic Law

Derived unit mol^2

$$v_3 = \text{s2} \cdot \text{k2} \tag{6}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k2	k2		0.075	mol	☑

5.4 Reaction k_le

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

Name k6

Reaction equation

$$\text{s2} \longrightarrow \text{s3} \tag{7}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
s2	early endosome	

Product

Table 15: Properties of each product.

Id	Name	SBO
s3	late endosome	

Kinetic Law

Derived unit mol^2

$$v_4 = \text{s2} \cdot \text{k6} \tag{8}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k6	k6		0.01	mol	☑

5.5 Reaction k_lys

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

Name k7

Reaction equation

$$\text{s3} \longrightarrow \text{s4} \tag{9}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
s3	late endosome	

Product

Table 18: Properties of each product.

Id	Name	SBO
s4	lysosome	

Kinetic Law

Derived unit $\mathrm{mol}^2 \cdot \mathrm{l}^{-1}$

$$v_5 = [\mathrm{s3}] \cdot \mathrm{k7} \tag{10}$$

Table 19: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k7	k7		0.01	mol	☑

5.6 Reaction k_deg

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

Name k8

Reaction equation

$$\mathrm{s4} \longrightarrow \mathrm{s5} \tag{11}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
s4	lysosome	

Product

Table 21: Properties of each product.

Id	Name	SBO
s5	s5	

Kinetic Law

Derived unit $\mathrm{mol}^2 \cdot \mathrm{l}^{-1}$

$$v_6 = [\mathrm{s4}] \cdot \mathrm{k8} \tag{12}$$

Table 22: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k8	k8		0.005	mol	☑

5.7 Reaction k_shed

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

Name k4

Reaction equation

$$\mathrm{s1} \longrightarrow \mathrm{s8} \tag{13}$$

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
s1	HS surface	

Product

Table 24: Properties of each product.

Id	Name	SBO
s8	s8	

Kinetic Law

Derived unit mol^2

$$v_7 = \mathrm{s1} \cdot \mathrm{k4} \tag{14}$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k4	k4		0.1	mol	☑

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 `s1`

Name HS surface

Initial amount 0.1 mol

Charge 0

This species takes part in four reactions (as a reactant in `k_endo`, `k_shed` and as a product in `k_golgi`, `k_exo`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s1} = v_1 + v_3 - v_2 - v_7 \tag{15}$$

6.2 Species `s2`

Name early endosome

Initial amount 0.4 mol

Charge 0

This species takes part in three reactions (as a reactant in `k_exo`, `k_le` and as a product in `k_endo`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s2} = v_2 - v_3 - v_4 \tag{16}$$

6.3 Species `s3`

Name late endosome

Initial amount 0.4 mol

This species takes part in two reactions (as a reactant in `k_lys` and as a product in `k_le`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s3} = v_4 - v_5 \tag{17}$$

6.4 Species s5

Name s5

Initial amount 0 mol

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s5} = v_6 \tag{18}$$

6.5 Species s6

Name golgi

Initial amount 0.155 mol

Charge 0

This species takes part in one reaction (as a reactant in k_golgi), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s6} = 0 \tag{19}$$

6.6 Species s8

Name s8

Initial amount 0 mol

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s8} = v_7 \tag{20}$$

6.7 Species s4

Name lysosome

Initial amount 0.85 mol

This species takes part in two reactions (as a reactant in k_deg and as a product in k_lys).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s4} = v_5 - v_6 \tag{21}$$

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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