# **SBML Model Report**

# Model name: "Waugh2006 - Diabetic Wound Healing - Treated and Untreated Macrophage Dynamics"



May 17, 2018

#### 1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Matthew Grant Roberts<sup>1</sup> and Catherine Lloyd<sup>2</sup> at June 25<sup>th</sup> 2010 at 12:01 a.m. and last time modified at March first 2018 at 1:07 p.m. 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	4
events	1	constraints	0
reactions	0	function definitions	0
global parameters	13	unit definitions	9
rules	5	initial assignments	0

#### **Model Notes**

This a model from the article:

Macrophage dynamics in diabetic wound dealing.

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Waugh HV, Sherratt JA. Bull Math Biol 2006 Jan;68(1):197-207 16794927,

#### **Abstract:**

Wound healing in diabetes is a complex process, characterised by a chronicinflammation phase. The exact mechanism by which this occurs is not fullyunderstood, and whilst several treatments for healing diabetic wounds exist, very little research has been conducted towards the causes of the extendedinflammation phase. We describe a mathematical model which offers a possible-explanation for diabetic wound healing in terms of the distribution ofmacrophage phenotypes being altered in the diabetic patient compared to normalwound repair. As a consequence of this, we put forward a suggestion fortreatment based on rectifying the macrophage phenotype imbalance.

This model was taken from the CellML repository and automatically converted to SBML. The original model was: Waugh HV, Sherratt JA. (2006) - version=1.0

The original CellML model was created by:

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To cite BioModels Database, please use: Li C, Donizelli M, Rodriguez N, Dharuri H, Endler L, Chelliah V, Li L, He E, Henry A, Stefan MI, Snoep JL, Hucka M, Le Novre N, Laibe C (2010) BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models. BMC Syst Biol., 4:92.

#### 2 Unit Definitions

This is an overview of 13 unit definitions of which four are predefined by SBML and not mentioned in the model.

#### 2.1 Unit time

Name time

**Definition** 86400 s

#### 2.2 Unit unit\_0

Name  $8.64e-11*m\hat{6}/(g*s)$ 

**Definition**  $(8.64 \cdot 10^{-11} \text{ m})^6 \cdot \text{g}^{-3} \cdot \text{s}^{-1}$ 

#### 2.3 Unit unit\_1

Name 0.0864\*mm/(g\*s)

**Definition**  $(0.0864 \text{ mm})^3 \cdot g^{-2} \cdot s^{-1}$ 

#### 2.4 Unit unit\_2

Name 1/(11.5741\*Mg\*s)

**Definition**  $(11.5741 \text{ Mg})^{-1} \cdot \text{s}^{-1}$ 

#### 2.5 Unit unit\_3

Name 1/(0.0115741\*m\*s)

**Definition**  $(0.0115741 \text{ m})^{-3} \cdot s^{-1}$ 

#### 2.6 Unit unit\_4

Name 1

**Definition** dimensionless<sup>0</sup>

#### 2.7 Unit unit\_5

Name 1/(0.0115741\*ms)

**Definition**  $(0.0115741 \text{ ms})^{-1}$ 

#### 2.8 Unit unit\_6

Name 0.001\*m

**Definition**  $(0.0010 \text{ m})^3$ 

#### 2.9 Unit unit\_7

Name 0.0864\*g/s

**Definition**  $(0.0864 \ 10^{-6} \ dimensionless)^0 \cdot 0.0864 \ g \cdot s^{-1}$ 

#### 2.10 Unit substance

**Notes** Mole is the predefined SBML unit for substance.

**Definition** mol

#### 2.11 Unit volume

**Notes** Litre is the predefined SBML unit for volume.

**Definition** 1

#### 2.12 Unit area

**Notes** Square metre is the predefined SBML unit for area since SBML Level 2 Version 1.

**Definition**  $m^2$ 

#### 2.13 Unit length

**Notes** Metre is the predefined SBML unit for length since SBML Level 2 Version 1.

**Definition** m

# 3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
COMpartment	Wound		3	1	litre	Ø	

## 3.1 Compartment COMpartment

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

Name Wound

# 4 Species

This model contains four species. The boundary condition of four of these species is set to true so that these species' amount cannot be changed by any reaction. Section 8 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

		Tueste et l'apperente et euten species.			
Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
K_T	K₋T	COMpartment	$\text{mol} \cdot 1^{-1}$		
$\mathtt{phi}_{-}\mathtt{I}$	phi_I	COMpartment	$\text{mol} \cdot l^{-1}$		
$phi_R$	phi_R	${\tt COMpartment}$	$\text{mol} \cdot l^{-1}$		$\square$
T	T	${\tt COMpartment}$	$\text{mol} \cdot l^{-1}$		$\square$

### **5 Parameters**

This model contains 13 global parameters.

Table 4: Properties of each parameter.

rable 4. Froperties of each parameter.					
Id	Name	SBO	Value	Unit	Constant
tau1	tau1		-2.470	$(8.64 \cdot 10^{-11} \text{ m})^6 \cdot g^{-3} \cdot s^{-1}$	$\square$
tau2	tau2		21.940	$(0.0864 \text{ mm})^3 \qquad \cdot \\ g^{-2} \cdot s^{-1}$	
tau3	tau3		6.410	$(11.5741 \text{ Mg})^{-1} \cdot \text{s}^{-1}$	$\square$
tau4	tau4		1.750	$(0.0115741 \text{ m})^{-3} \cdot \text{s}^{-1}$	$\square$
alpha	alpha		0.800	dimensionless <sup>0</sup>	
k1	k1		0.050	dimensionless <sup>0</sup>	
k2	k2		0.693	$(0.0115741 \text{ ms})^{-1}$	
k3	k3		0.002	$(0.0010 \mathrm{m})^3$	
k4	k4		0.070	$(0.0864 \ 10^{-6} \ \text{dimen})$	$(sionless)^0$
				$0.0864 \text{ g} \cdot \text{s}^{-1}$	
d1	d1		0.200	$(0.0115741 \text{ ms})^{-1}$	
d2	d2		9.100	$(0.0115741 \text{ ms})^{-1}$	$\overline{\mathscr{L}}$
${\tt total\_M}$	$total\_M$		400.000	•	
dummy-	dummy_variable		0.000		
$_{ t variable}$					

# 6 Rules

This is an overview of five rules.

#### **6.1 Rule** K\_T

Rule K\_T is an assignment rule for species K\_T:

$$K_{-}T = tau1 \cdot [T]^3 + tau2 \cdot [T]^2 + tau3 \cdot [T] + tau4$$
 (1)

Derived unit  $\left(8.64\cdot10^{-11}\;m\right)^6\cdot g^{-3}\cdot s^{-1}\cdot mol^3\cdot l^{-3}$ 

#### 6.2 Rule total\_M

Rule total\_M is an assignment rule for parameter total\_M:

$$total_M = 0 \cdot [K_T] + [phi_I] + [phi_R]$$
 (2)

#### 6.3 Rule phi\_I

Rule phi\_I is a rate rule for species phi\_I:

$$\frac{d}{d\textit{t}} phi\_I = alpha \cdot [K\_T] + k1 \cdot k2 \cdot [phi\_I] \cdot (1 - k3 \cdot ([phi\_I] + [phi\_R])) - d1 \cdot [phi\_I] \quad (3)$$

#### 6.4 Rule phi\_R

Rule phi\_R is a rate rule for species phi\_R:

$$\frac{d}{dt}phi\_R = (1 - alpha) \cdot [K\_T] + k1 \cdot k2 \cdot [phi\_R] \cdot (1 - k3 \cdot ([phi\_I] + [phi\_R])) - d1 \cdot [phi\_R] \quad (4)$$

#### 6.5 Rule T

Rule T is a rate rule for species T:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{T} = \mathbf{k}4 \cdot [\mathbf{phi}.\mathbf{I}] - \mathbf{d}2 \cdot [\mathbf{T}] \tag{5}$$

Derived unit  $0.0864~g\cdot s^{-1}\cdot mol\cdot l^{-1}$ 

#### 7 Event

This is an overview of one event. Each event is initiated whenever its trigger condition switches from false to true. A delay function postpones the effects of an event to a later time point. At the time of execution, an event can assign values to species, parameters or compartments if these are not set to constant.

#### 7.1 Event event

Name event

**Trigger condition** 

time 
$$> 22$$
 (6)

**Assignment** 

$$alpha = 0.2 + 0.6 \cdot dummy\_variable \tag{7}$$

# 8 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.

```
8.1 Species K_T
Name K_T
Initial concentration 296.53 \text{ mol} \cdot l^{-1}
Involved in rule K_T
One rule determines the species' quantity.
8.2 Species phi_I
Name phi_I
Initial concentration 200 \text{ mol} \cdot l^{-1}
Involved in rule phi_I
One rule determines the species' quantity.
8.3 Species phi_R
Name phi_R
Initial concentration 200 mol·l<sup>-1</sup>
Involved in rule phi_R
One rule determines the species' quantity.
8.4 Species T
Name T
Initial concentration 6 \text{ mol} \cdot l^{-1}
Involved in rule T
```

One rule determines the species' quantity.

BML2ATEX was developed by Andreas Dräger<sup>a</sup>, Hannes Planatscher<sup>a</sup>, Dieudonné M Wouamba<sup>a</sup>, Adrian Schröder<sup>a</sup>, Michael Hucka<sup>b</sup>, Lukas Endler<sup>c</sup>, Martin Golebiewski<sup>d</sup> and Andreas Zell<sup>a</sup>. Please see http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX for more information.

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