SBML Model Report

Model name: "Murphy2016 - Differences in predictions of ODE models of tumor growth"

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: Emma Louise Fairbanks[1] and Matthew Grant Roberts[2] at June 14th 2017 at 2:46 p. m. and last time modified at March 16th 2018 at 2:40 p. 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	1
species types	0	species	7
events	0	constraints	0
reactions	0	function definitions	0
global parameters	14	unit definitions	0
rules	7	initial assignments	0

Model Notes

Murphy2016 - Differences in predictions ofODE models of tumor growthComparison of 7 ODE models for tumoursize. This models have been compared to experimental data.

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This model is described in the article:Differences in predictions of ODE models of tumor growth: a cautionary example.Murphy H, Jaafari H, Dobrovolny HM.BMC Cancer 2016 Feb; 16: 163

Abstract:

While mathematical models are often used to predict progression of cancer and treatment outcomes, there is still uncertainty over how to best model tumor growth. Seven ordinary differential equation (ODE) models of tumor growth (exponential, Mendelsohn, logistic, linear, surface, Gompertz, and Bertalanffy) have been proposed, but there is no clear guidance on how to choose the most appropriate model for a particular cancer.We examined all seven of the previously proposed ODE models in the presence and absence of chemotherapy. We derived equations for the maximum tumor size, doubling time, and the minimum amount of chemotherapy needed to suppress the tumor and used a sample data set to compare how these quantities differ based on choice of growth model.We find that there is a 12-fold difference in predicting doubling times and a 6-fold difference in the predicted amount of chemotherapy needed for suppression depending on which growth model was used.Our results highlight the need for careful consideration of model assumptions when developing mathematical models for use in cancer treatment planning.

This model is hosted on BioModels Database and identified by: BIOMD0000000671.

To cite BioModels Database, please use: Chelliah V et al. BioModels: ten-year anniversary. Nucl. Acids Res. 2015, 43(Database issue):D542-8.

2 Unit Definitions

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

2.1 Unit `substance`

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

Definition mol

2.2 Unit `volume`

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

Definition l

2.3 Unit `area`

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

Definition m^2

2.4 Unit `length`

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

Definition m

2.5 Unit `time`

Notes Second is the predefined SBML unit for `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
`tumour`	compartment		3	1	litre	☑	

3.1 Compartment `tumour`

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

Name compartment

4 Species

This model contains seven species. The boundary condition of seven of these species is set to `true` so that these species' amount cannot be changed by any reaction. 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
`V_exp`	V_exp	`tumour`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☑
`V_mend`	V_mend	`tumour`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☑
`V_log`	V_log	`tumour`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☑
`V_lin`	V_lin	`tumour`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☑
`V_surf`	V_surf	`tumour`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☑
`V_gomp`	V_gomp	`tumour`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☑
`V_bert`	V_bert	`tumour`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☑

5 Parameters

This model contains 14 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
a_exp	a_exp		0.025		☑
a_mend	a_mend		0.105		☑
a_log	a_log		0.030		☑
a_lin	a_lin		132.000		☑
a_surf	a_surf		0.291		☑
a_gomp	a_gomp		0.092		☑
a_bert	a_bert		0.234		☑
b_mend	b_mend		0.785		☑
b_log	b_log		6920.000		☑
b_lin	b_lin		4300.000		☑
b_surf	b_surf		708.000		☑
b_gomp	b_gomp		15500.000		☑
b_bert	b_bert		$3.46 \cdot 10^{-19}$		☑
c_gomp	c_gomp		10700.000		☑

6 Rules

This is an overview of seven rules.

6.1 Rule V_exp

Rule V_exp is a rate rule for species V_exp:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{V\_exp} = \mathrm{a\_exp} \cdot [\mathrm{V\_exp}] \tag{1}$$

6.2 Rule V_mend

Rule V_mend is a rate rule for species V_mend:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{V\_mend} = \mathrm{a\_mend} \cdot [\mathrm{V\_mend}]^{\mathrm{b\_mend}} \tag{2}$$

6.3 Rule V_log

Rule V_log is a rate rule for species V_log:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{V\_log} = \mathrm{a\_log} \cdot [\mathrm{V\_log}] \cdot \left(1 - \frac{[\mathrm{V\_log}]}{\mathrm{b\_log}}\right) \tag{3}$$

6.4 Rule V_lin

Rule V_lin is a rate rule for species V_lin:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{V\_lin} = \frac{\mathrm{a\_lin} \cdot [\mathrm{V\_lin}]}{[\mathrm{V\_lin}] + \mathrm{b\_lin}} \tag{4}$$

6.5 Rule V_surf

Rule V_surf is a rate rule for species V_surf:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{V\_surf} = \frac{\mathrm{a\_surf} \cdot [\mathrm{V\_surf}]}{([\mathrm{V\_surf}] + \mathrm{b\_surf})^{\frac{1}{3}}} \tag{5}$$

6.6 Rule V_gomp

Rule V_gomp is a rate rule for species V_gomp:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{V\_gomp} = \mathrm{a\_gomp} \cdot [\mathrm{V\_gomp}] \cdot \left(\frac{\mathrm{b\_gomp}}{[\mathrm{V\_gomp}] + \mathrm{c\_gomp}}\right) \tag{6}$$

6.7 Rule V_bert

Rule V_bert is a rate rule for species V_bert:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{V\_bert} = \mathrm{a\_bert} \cdot [\mathrm{V\_bert}]^{\frac{2}{3}} - \mathrm{b\_bert} \cdot [\mathrm{V\_bert}] \tag{7}$$

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 V_exp

Name V_exp

Initial concentration $220\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

Involved in rule V_exp

One rule determines the species' quantity.

7.2 Species V_mend

Name V_mend

Initial concentration $220\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

Involved in rule V_mend

One rule determines the species' quantity.

7.3 Species V_log

Name V_log

Initial concentration $220\ \text{mol}\cdot\text{l}^{-1}$

Involved in rule V_log

One rule determines the species' quantity.

7.4 Species V_lin

Name V_lin

Initial concentration $220\ \text{mol}\cdot\text{l}^{-1}$

Involved in rule V_lin

One rule determines the species' quantity.

7.5 Species V_surf

Name V_surf

Initial concentration $220\ \text{mol}\cdot\text{l}^{-1}$

Involved in rule V_surf

One rule determines the species' quantity.

7.6 Species V_gomp

Name V_gomp

Initial concentration $220\ \text{mol}\cdot\text{l}^{-1}$

Involved in rule V_gomp

One rule determines the species' quantity.

7.7 Species V_bert

Name V_bert

Initial concentration $220\ \text{mol}\cdot\text{l}^{-1}$

Involved in rule V_bert

One rule determines the species' quantity.

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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