SBML Model Report

Model name: "Field1974_Oregonator"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Nicolas Le Novre[1] and Bruce Shapiro[2] at June 28th 2005 at 1:58 p. m. and last time modified at April fourth 2014 at 5:35 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	5
events	0	constraints	0
reactions	5	function definitions	0
global parameters	1	unit definitions	0
rules	0	initial assignments	0

Model Notes

Field-Noyes Model of BZ Reaction

Citation
R.J.Field and R.M.Noyes,J.Chem.Phys.60,1877 (1974)

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Description
Field Noyes Version of Belousov-Zhabotinsky Reaction. BrO3 is held constant; HOBr is typically ignored, and can be replaced by an empty-set. The stoichiometry f is typically taken as 1/2 or 1..

Initially Generated by Cellerator Version 1.0 update 2.1220 using Mathematica 4.2 for Mac OS X (June 4, 2002), December 26, 2002 10:43:53, using (PowerMac,PowerPC,Mac OS X,MacOSX,Darwin). author=B.E.Shapiro

Modified with SBMLeditor by Nicolas Le Novre, to fit the original article.

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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 4: Properties of all compartments.

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

3.1 Compartment `BZ`

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

4 Species

This model contains five species. The boundary condition of two 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 5: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
`Br`	Br-	`BZ`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
`BrO3`	BrO3-	`BZ`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	☑
`Ce`	Ce4+	`BZ`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
`HBrO2`		`BZ`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
`HOBr`		`BZ`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	☑

5 Parameter

This model contains one global parameter.

Table 6: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
f			1.0		☑

6 Reactions

This model contains five 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 7: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	`Reaction1`	M1	$\mathrm{Br} + \mathrm{BrO3} \longrightarrow \mathrm{HBrO2} + \mathrm{HOBr}$	
2	`Reaction2`	M2	$\mathrm{Br} + \mathrm{HBrO2} \longrightarrow 2\,\mathrm{HOBr}$	
3	`Reaction3`	M3	$\mathrm{BrO3} + \mathrm{HBrO2} \longrightarrow \mathrm{Ce} + 2\,\mathrm{HBrO2}$	
4	`Reaction4`	M4	$2\,\mathrm{HBrO2} \longrightarrow \mathrm{BrO3} + \mathrm{HOBr}$	
5	`Reaction5`	M5	$\mathrm{Ce} \longrightarrow \mathrm{fBr}$	

6.1 Reaction Reaction1

This is an irreversible reaction of two reactants forming two products.

Name M1

Reaction equation

$$\mathrm{Br} + \mathrm{BrO3} \longrightarrow \mathrm{HBrO2} + \mathrm{HOBr} \tag{1}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
Br	Br-	
BrO3	BrO3-	

Products

Table 9: Properties of each product.

Id	Name	SBO
HBrO2		
HOBr		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = [\mathrm{Br}] \cdot [\mathrm{BrO3}] \cdot \mathrm{k1} \cdot \mathrm{vol}(\mathrm{BZ}) \tag{2}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	kM1		1.34		☑

6.2 Reaction Reaction2

This is an irreversible reaction of two reactants forming one product.

Name M2

Reaction equation

$$\mathrm{Br} + \mathrm{HBrO2} \longrightarrow 2\,\mathrm{HOBr} \tag{3}$$

Reactants

Table 11: Properties of each reactant.

Id	Name	SBO
Br	Br-	
HBrO2		

Product

Table 12: Properties of each product.

Id	Name	SBO
HOBr		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = [\mathrm{Br}] \cdot [\mathrm{HBrO2}] \cdot \mathrm{k2} \cdot \mathrm{vol}\,(\mathrm{BZ}) \tag{4}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k2	kM2		$1.6 \cdot 10^9$		☑

6.3 Reaction Reaction3

This is an irreversible reaction of two reactants forming two products.

Name M3

Reaction equation

$$\mathrm{BrO3} + \mathrm{HBrO2} \longrightarrow \mathrm{Ce} + 2\,\mathrm{HBrO2} \tag{5}$$

Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
BrO3	BrO3-	
HBrO2		

Products

Table 15: Properties of each product.

Id	Name	SBO
Ce	Ce4+	
HBrO2		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = [\mathrm{BrO3}] \cdot [\mathrm{HBrO2}] \cdot \mathrm{k3} \cdot \mathrm{vol}(\mathrm{BZ}) \tag{6}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k3	kM3		8000.0		☑

6.4 Reaction Reaction4

This is an irreversible reaction of one reactant forming two products.

Name M4

Reaction equation

$$2\,\mathrm{HBrO2} \longrightarrow \mathrm{BrO3} + \mathrm{HOBr} \tag{7}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
HBrO2		

Products

Table 18: Properties of each product.

Id	Name	SBO
BrO3	BrO3-	
HOBr		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = [\mathrm{HBrO2}]^2 \cdot \mathrm{k4} \cdot \mathrm{vol}\,(\mathrm{BZ}) \tag{8}$$

Table 19: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k4	kM4		$4 \cdot 10^7$		☑

6.5 Reaction Reaction5

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

Name M5

Reaction equation

$$\mathrm{Ce} \longrightarrow \mathrm{fBr} \tag{9}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
Ce	Ce4+	

Product

Table 21: Properties of each product.

Id	Name	SBO
Br	Br-	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = [\mathrm{Ce}] \cdot \mathrm{k5} \cdot \mathrm{vol}\,(\mathrm{BZ}) \tag{10}$$

Table 22: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k5	kM5		1.0		☑

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.

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.

7.1 Species Br

Name Br-

Initial concentration $10^{-7}\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in Reaction1, Reaction2 and as a product in Reaction5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Br} = \mathrm{f}\,v_5 - v_1 - v_2 \tag{11}$$

7.2 Species BrO3

Name BrO3-

Initial concentration $0.06\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in Reaction1, Reaction3 and as a product in Reaction4), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{BrO3} = 0 \tag{12}$$

7.3 Species Ce

Name Ce4+

Initial concentration $0.05\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in Reaction5 and as a product in Reaction3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ce} = v_3 - v_5 \tag{13}$$

7.4 Species HBrO2

Initial concentration $5\cdot 10^{-11}\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in Reaction2, Reaction3, Reaction4 and as a product in Reaction1, Reaction3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{HBrO2} = v_1 + 2\,v_3 - v_2 - v_3 - 2\,v_4 \tag{14}$$

7.5 Species HOBr

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a product in Reaction1, Reaction2, Reaction4), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{HOBr} = 0 \tag{15}$$

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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