

V11B

SBML und Modell- Erstellung

22. Januar 2015

Übersicht

Austausch und Archivierung von biochemischen Modellen
=> SBML

Diffusion plus Reaktionen
=> Virtual Cell

Komplexität der Modelle
=> BioNetGen

Systems Biology Markup Language



XML-Dialekt für Speicherung und Austausch
biochemischer Modelle

=> Archivierung

=> Transfer von Modellen in andere Softwaretools

Acknowledgements

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[von http://sbml.org/Acknowledgments](http://sbml.org/Acknowledgments)

SBML <= XML

XML = eXtensible Markup Language

- hierarchische Baumstruktur:
=> Schachtelung von <Object> ... </Object> oder <Objekt [Parameter...]/>
- genau ein Wurzelobjekt: <sbml...>

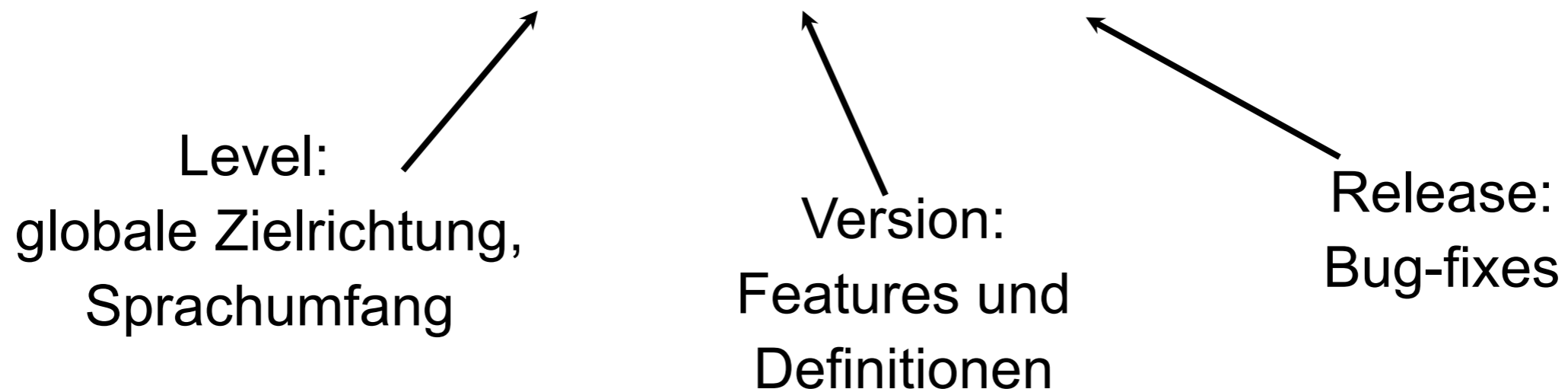
Aktuelle Dialekte: [siehe http://sbml.org/Documents/Specifications](http://sbml.org/Documents/Specifications)

SBML Level 1, Version 2

<http://www.sbml.org/specifications/sbml-level-1/version-2/sbml-level-1-v2.pdf>

SBML Level 2, Version 4, Release 1

<http://precedings.nature.com/documents/2715/version/1>



Was ist enthalten?

beginning of model definition
list of function definitions (optional)
list of unit definitions (optional)
list of compartment types (optional)
list of species types (optional)
list of compartments (optional)
list of species (optional)
list of parameters (optional)
list of initial assignments (optional)
list of rules (optional)
list of constraints (optional)
list of reactions (optional)
list of events (optional)
end of model definition

Ein Beispiel



```
<?xml version="1.0" encoding="UTF-8"?>
<sbml level="2" version="3" xmlns="http://www.sbml.org/sbml/level2/version3">
  <model name="EnzymaticReaction">
    <listOfUnitDefinitions>
      <unitDefinition id="per_second">
        <listOfUnits>
          <unit kind="second" exponent="-1"/>
        </listOfUnits>
      </unitDefinition>
      <unitDefinition id="litre_per_mole_per_second">
        <listOfUnits>
          <unit kind="mole" exponent="-1"/>
          <unit kind="litre" exponent="1"/>
          <unit kind="second" exponent="-1"/>
        </listOfUnits>
      </unitDefinition>
    </listOfUnitDefinitions>
    <listOfCompartments>
      <compartment id="cytosol" size="1e-14"/>
    </listOfCompartments>
    <listOfSpecies>
      <species compartment="cytosol" id="ES" initialAmount="0" name="ES"/>
      <species compartment="cytosol" id="P" initialAmount="0" name="P"/>
      <species compartment="cytosol" id="S" initialAmount="1e-20" name="S"/>
      <species compartment="cytosol" id="E" initialAmount="5e-21" name="E"/>
    </listOfSpecies>
    <listOfReactions>
      <reaction id="veq">
        <listOfReactants>
          <speciesReference species="E"/>
          <speciesReference species="S"/>
        </listOfReactants>
        <listOfProducts>
          <speciesReference species="ES"/>
        </listOfProducts>
        <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
            <math>k_{\text{off}} \cdot ES</math>
          </math>
        </kineticLaw>
      </reaction>
      <reaction id="vcat" reversible="false">
        <listOfReactants>
          <speciesReference species="ES"/>
        </listOfReactants>
        <listOfProducts>
          <speciesReference species="E"/>
          <speciesReference species="P"/>
        </listOfProducts>
        <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
            <math>k_{\text{cat}} \cdot ES</math>
          </math>
        </kineticLaw>
      </reaction>
    </listOfReactions>
  </model>
</sbml>
```

```
<ci>cytosol</ci>
<apply>
  <minus/>
  <apply>
    <times/>
    <ci>kon</ci>
    <ci>E</ci>
    <ci>S</ci>
  </apply>
</apply>
<apply>
  <times/>
  <ci>koff</ci>
  <ci>ES</ci>
</apply>
</apply>
</math>
<listOfParameters>
  <parameter id="kon" value="1000000" units="litre_per_mole_per_second"/>
  <parameter id="koff" value="0.2" units="per_second"/>
</listOfParameters>
</kineticLaw>
</reaction>
<reaction id="vcat" reversible="false">
  <listOfReactants>
    <speciesReference species="ES"/>
  </listOfReactants>
  <listOfProducts>
    <speciesReference species="E"/>
    <speciesReference species="P"/>
  </listOfProducts>
  <kineticLaw>
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <math>k_{\text{cat}} \cdot ES</math>
    </math>
    <listOfParameters>
      <parameter id="kcat" value="0.1" units="per_second"/>
    </listOfParameters>
  </kineticLaw>
</reaction>
</listOfReactions>
</model>
</sbml>
```

Nochmal:



```
<?xml version="1.0" encoding="UTF-8"?>
<sbml level="2" version="3" xmlns="http://www.sbml.org/sbml/level2/version3">
  <model name="EnzymaticReaction">
    <listOfUnitDefinitions>
      :
    </listOfUnitDefinitions>
    <listOfCompartments>
      <compartment id="cytosol" size="1e-14"/>
    </listOfCompartments>
    <listOfSpecies>
      <species compartment="cytosol" id="ES" initialAmount="0" name="ES"/>
      <species compartment="cytosol" id="P" initialAmount="0" name="P"/>
      <species compartment="cytosol" id="S" initialAmount="1e-20" name="S"/>
      <species compartment="cytosol" id="E" initialAmount="5e-21" name="E"/>
    </listOfSpecies>
    <listOfReactions>
      :
    </listOfReactions>
  </model>
```

Details: Einheiten

```
<listOfUnitDefinitions>
  <unitDefinition id="per_second">
    <listOfUnits>
      <unit kind="second" exponent="-1"/>
    </listOfUnits>
  </unitDefinition>
  <unitDefinition id="litre_per_mole_per_second">
    <listOfUnits>
      <unit kind="mole" exponent="-1"/>
      <unit kind="litre" exponent="1"/>
      <unit kind="second" exponent="-1"/>
    </listOfUnits>
  </unitDefinition>
</listOfUnitDefinitions>
```

per_seconds := s⁻¹

litre
mol s

SBML Software Guide/SBML Software Matrix - SBML.org

http://sbml.org/SBML_Software_Guide/SBML_Software_Matrix

SBML Software Matrix

This matrix provides an at-a-glance summary of software known to us to provide some degree of support for reading, writing, or otherwise working with SBML. The columns' meanings are explained below. For a list of longer descriptions grouped into themes, please see our [SBML Software Summary](#) page.

	Capabilities					Frameworks						API	Dep.	Platforms	SBML		Availabil.			
	Creation	Simulation	Analysis	Database	Utility	ODE	DAE	PDE	Stochastic	Events	Logical				Other	Import	Export	Open source	Academic use	Commercial use
Cellware	•	•				•									L,W,M	•		•	F	\$
CL-SBML					•							•	LISP	LISP	L	•		•	F	F
CLEML															L,W	•	•		F	F
COBRA			•		•	•								MATLAB	L,W,M	•	•	•	F	F
ConsensusPathDB					•										B	•	•	•	F	F
COPASI	•	•	•		•	•			•				C++, Java, Python		L,W,M	•	•	•	F	\$
Cyto-Sim		•			•				•						L,W,M				F	F
Cytoscape	•				•								Java		L,W,M	•		•	F	F
DBSolve		•	•		•	•										•	•		F	F
Dizzy		•				•			•						L,W,M	•	•	•	F	F
E-CELL	•	•				•			•						L,W		•	•	F	F
ecellJ					•												•		F	F
EPE	•					•							Java		L,W, M	•			F	F
ESS		•							•					BSP				•	F	F

Import nach Copasi

The screenshot shows the COPASI 4.5 (Build 30) interface. The main window is titled "enzymatic - COPASI 4.5 (Build 30) /Users/.../V11/enzymatic.cps". The left sidebar shows a tree view of the model structure, with "Reactions" expanded and "veq" selected. The main panel displays the configuration for the reaction "veq".

Reaction Configuration:

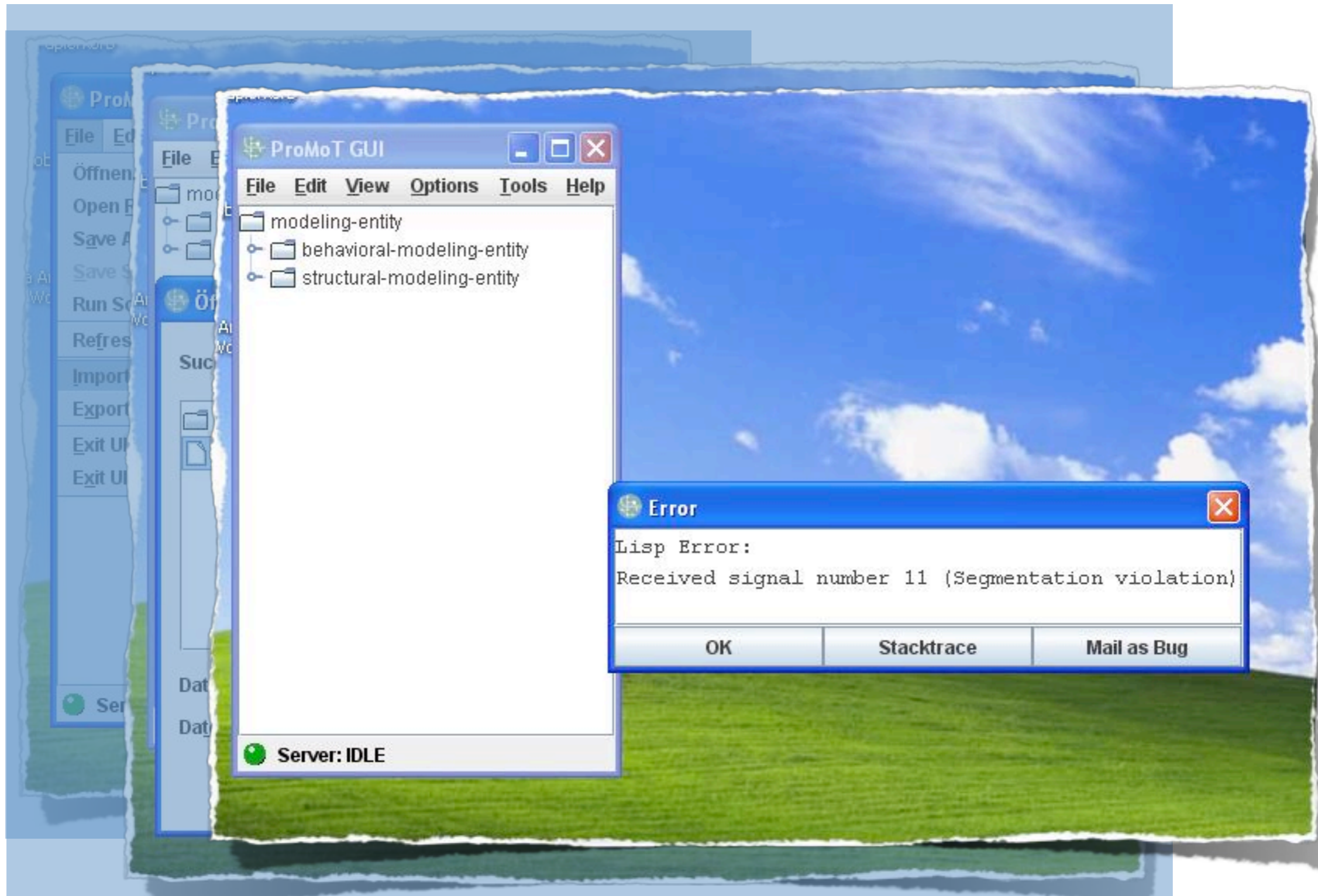
- Name: veq
- Chemical Equation: $E + S = ES$
- Reversible: Reversible, Multi Compartment
- Rate Law: Mass action (reversible)
- Flux (mol/s): 0

Symbol Definition Table:

Description	Name	Value	Unit
Parameter	k1	1e+06	l/(mol*s)
Substrate	substrat		mol/l
		E	
		S	
Parameter	k2	0.2	1/s

Buttons at the bottom: Commit, Revert, New, Delete, Clear, Delete/Undelete, New.

Interoperabilität?



Details: eine Reaktion

<listOfReactions> :

```
<reaction id="vcat" reversible="false">  
  <listOfReactants>  
    <speciesReference species="ES"/>  
  </listOfReactants>  
  <listOfProducts>  
    <speciesReference species="E"/>  
    <speciesReference species="P"/>  
  </listOfProducts>
```

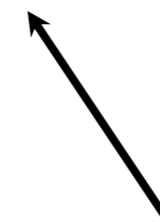
```
<kineticLaw>  
  <math xmlns="http://www.w3.org/1998/Math/MathML">  
    <apply>  
      <times/>  
      <ci>cytosol</ci>  
      <ci>kcat</ci>  
      <ci>ES</ci>  
    </apply>  
  </math>  
  <listOfParameters>  
    <parameter id="kcat" value="0.1" units="per_second"/>  
  </listOfParameters>  
</kineticLaw>
```

```
</reaction>
```

```
</listOfReactions>
```



$$\Rightarrow \frac{dN}{dt} = V_{\text{cytosol}} k_{\text{cat}} [ES]$$



lokaler Parameter!

SBML lesbar machen



convert

SBML file:

Report options

MIRIAM annotations:

Check SBML consistency:

Include predefined unit declarations:

Layout options

Convert to:

Set name in equations:

Landscape:

Font size:

Reaction participants in one table:

Set identifiers in typewriter font:

Paper size:

Create a title page:

<http://webservices.cs.uni-tuebingen.de/>

Dräger A, Planatscher H, Wouamba DM, Schröder A, Hucka M, Endler L, Golebiewski M, Müller W, and Zell A: "SBML2LaTeX: Conversion of SBML files into human-readable reports", Bioinformatics 2009

Drei Minuten später:

convert

Please download your result here:

[07ff0064-6af4-4eb5-bea1-906da1fbcd86-request.pdf](#)

SBML Model Report

Model name: "EnzymaticReaction"



June 30, 2009

1 General Overview

This is a document in SBML Level 2 Version 3 format. Table 1 gives an overview of the quantities of all components of this model.

Table 1: The SBML components in this model.
All components are described in more detail in the following sections.

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	4
events	0	constraints	0
reactions	2	function definitions	0
global parameters	0	unit definitions	2
rules	0	initial assignments	0

2 Unit Definitions

This is an overview of seven unit definitions. The units `substance`, `volume`, `area`, `length`, and `time` are predefined by SBML and not mentioned in the model.

2.1 Unit `per_second`

Definition s^{-1}

2.2 Unit `litre_per_mole_per_second`

Definition $\text{mol}^{-1} \cdot \text{l} \cdot \text{s}^{-1}$

2.3 Unit `substance`

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

Definition `mol`

2.4 Unit `volume`

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

Definition `l`

2.5 Unit `area`

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

Definition m^2

2.6 Unit `length`

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

Definition `m`

2.7 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
cytosol			3	10^{-14}	l	<input checked="" type="checkbox"/>	

3.1 Compartment cytosol

This is a three-dimensional compartment with a constant size of 10^{-14} litre.

4 Species

This model contains four 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
ES	ES	cytosol	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
P	P	cytosol	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
S	S	cytosol	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
E	E	cytosol	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>

5 Reactions

This model contains two reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by one or more modifiers, the identifiers of the modifier species are written above the reaction arrow.

Table 4: Overview of all reactions

Nº	Id	Name	Reaction Equation	SBO
1	veq		$E + S \rightleftharpoons ES$	
2	vcat		$ES \rightarrow E + P$	

5.1 Reaction veq

This is a reversible reaction of two reactants forming one product.

Reaction equation



Reactants

Table 5: Properties of each reactant.

Id	Name	SBO
E	E	
S	S	

Product

Table 6: Properties of each product.

Id	Name	SBO
ES	ES	

Kinetic Law

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

$$v_1 = \text{vol}(\text{cytosol}) \cdot (\text{kon} \cdot [E] \cdot [S] - \text{koff} \cdot [ES]) \quad (2)$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kon			1000000.0	$\text{mol}^{-1} \cdot \text{l} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>
koff			0.2	s^{-1}	<input checked="" type="checkbox"/>

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 ES

Name ES

Initial amount 0 mol

This species takes part in two reactions (as a reactant in *v_{cat}* and as a product in *v_{eq}*).

$$\frac{d}{dt}ES = v_1 - v_2$$

(5)

6.2 Species P

Name P

Initial amount 0 mol

This species takes part in one reaction (as a product in *v_{cat}*).

$$\frac{d}{dt}P = v_2$$

(6)

6.3 Species S

Name S

Initial amount 10^{-20} mol

This species takes part in one reaction (as a reactant in *v_{eq}*).

$$\frac{d}{dt}S = -v_1$$

(7)

6.4 Species E

Name E

Initial amount $5 \cdot 10^{-21}$ mol

This species takes part in two reactions (as a reactant in *v_{eq}* and as a product in *v_{cat}*).

$$\frac{d}{dt}E = v_2 - v_1$$

(8)

es gibt bereits sehr viele Modelle

The screenshot shows the BioModels Database website interface. At the top, there is a browser window with the address bar showing <http://www.ebi.ac.uk/biomodels-main/>. The website header includes the EMBL-EBI logo, an "EB-eye Search" box with a dropdown menu set to "All Databases" and a search input field containing "Enter Text Here". Navigation tabs include "Databases", "Tools", "EBI Groups", "Training", "Industry", "About Us", and "Help". A secondary navigation bar contains "BioModels Home", "Browse models", "Submit", "Sign in", "Support", and "About BioModels".

The main content area features a heading "BioModels Database - A Database of Annotated Published Models" and a descriptive paragraph: "BioModels Database is a data resource that allows biologists to store, search and retrieve published mathematical models of biological interests. Models present in BioModels Database are annotated and linked to relevant data resources, such as publications, databases of compounds and pathways, controlled vocabularies, etc." A search box with "Search" and "Go to the model" buttons is present, along with a link to "Advanced search".

On the left side, there are sections for "Browse models" (with sub-items: "Curated models (216)", "Browse models using GO", "Non-curated models (196)"), "Simulate in JWS Online", and "Submit a model".

On the right side, there is a "Model of the month" section for May 2009, featuring a diagram of sucrose accumulation in sugar cane. The diagram shows a central node labeled "Suc" with arrows pointing to it from below and away from it to the top-right (labeled "11") and bottom-right (labeled "8"). The text describes sucrose accumulation in *Saccharum officinarum* and includes a "Read more..." link. Below this is a "News" section with a date "16th June 2009" and a link for "Fourteenth release Download All Models Under SBML Format".

At the bottom, a footer link reads "Mirror at California Institute of Technology <http://biomodels.caltech.edu>". The browser's address bar at the very bottom shows <http://www.ebi.ac.uk/biomodels-main/modelmonth>.