1.2 Scope and Limitations

SBML Level 1 is meant to support non-spatial biochemical models and the kinds of operations that are

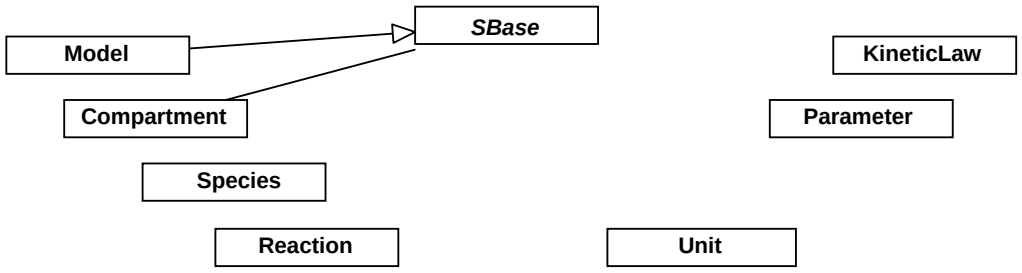
SBase
Model
KineticLaw
Compartment
Parameter
Species
Reaction
Unit

Figure 1:

reference is “http://www.mysim.org/ns” and the prefix is mysim

```
letter   ::= 'a'..'z','A'..'Z'
digit    ::= '0'..'9'
name     ::= ( letter | '_' ) ( letter | digit | '_' )*
```

Figure 3: *The definition of the type SName, expressed in the variant of Extended Backus-Naur Form (EBNF) used by the XML 1.0 specification (Bray et al., 2000). The characters (*

Name	Allowable Units	Default Units
`substance`	moles *or* number of molecules	moles
`volume`	liters	liters
`time`	seconds	seconds

The optional boolean field `boundaryCondition`

The following is an example of parameters defined at the `Model` level:

```
<model>
    ...
    <listOfSpecies>
        ...
    </listOfSpecies>
    <listOfParameters>
        <parameter name="Km1" value="2.3" units="second"/>
        <parameter name="Km2" value="10.7" units="second"/>
    </listOfParameters>
    <listOfReactions>
        ...
    </listOfReactions>
    ...
</model>
```

Figure 10: *The definitions of* `Reaction`, `KineticLaw` *and*

4.7.2 KineticLaw

A kineticLaw

```
                </listOfProducts>
                <kineticLaw formula="(vm * s1)/(km + s1)"/>
            </reaction>
            <reaction name="v2">
                <listOfReactants>
                    <speciesReference species="s1"/>
                </listOfReactants>
                <listOfProducts>
                    <speciesReference species="s2"/>
                </listOfProducts>
                <kineticLaw formula="(vm * s2)/(km + s2)"/>
            </reaction>
            <reaction name="v3">
                <listOfReactants>
                    <speciesReference species="s2"/>
                </listOfReactants>
                <listOfProducts>
                    <speciesReference species="x1"/>
                </listOfProducts>
                <kineticLaw formula="(vm * s1)/(km + s1)"/>
            </reaction>
        </listOfReactions>
    </model>
</sbml>
```

5.3 An Example of Using Rules

This section contains a model which simulates a system containing a fast reaction. This model uses rules to express the mathematics of the fast react explicitly rather than using the implicit fast field on a reaction element. The system modeled is

$$X_0 \xrightarrow{k_1 X_0} S_1$$

$$S_1 \xrightarrow{k_f S_1 - k_r S_2} S_2$$

$$S_2 \xrightarrow{k_2 S_1} X_1$$

$$k_1 = 0.1, \quad k_2 = 0.15, \quad k_f = K_{eq}10000, \quad k_r = 10000, \quad K_{eq} = 2.5.$$

Our vision for SBML is to create an open standard that will enable simulation software to exchange models. SBML is not static; we continue to develop and experiment with it, and we interact with other groups who seek to develop similar markup languages. We plan on continuing to evolve SBML with the help of the systems biology community to make SBML increasingly more powerful, flexible and useful.

6.1 Future Enhancements to SBML: Level 2 and Beyond

As mentioned above, SBML Level 1 is intended to provide the most basic foundations for modeling bio-
eion

SBML is closer to the internal object model used in a number of common model simulation packages. Because SBML Level 1 is being developed in the context of interacting with a number of existing software packages, it is a more concrete language than CellML and may be better suited to its purpose of enabling interoperability with existing simulation tools. However, CellML o□ers viable alternative ideas and the developers of SBML and CellML are actively engaged in ensuring that the two representations can be translated between each

Appendix

A Summary of Notation

```
  </xsd:annotation>
  <xsd:restriction base="xsd:string">
    <xsd:pattern value="(_|[a-z]|[A-Z])(_|[a-z]|[A-Z]|[0-9])*"/>
  </xsd:restriction>
</xsd:simpleType>
<!--The definition of SBase follows.-->
<xsd:complexType name="SBase" abstract="true">
  <xsd:annotation>
    <xsd:documentation>The SBase type is the base type of all main
         components in SBML.  It supports attaching notes and annotations
         to components.
    </xsd:documentation>
  </xsd:annotation>
  <xsd:sequence>
    <xsd:element name="notes" minOccurs="0">
```

</xsd:restriction></xsd:simpleType><!--The definition of Unit follows.--><xsd:complexType name="Unit"><xsd:comp

```
  </xsd:restriction>
</xsd:simpleType>
<xsd:complexType name="Rule" abstract="true">
  <xsd:complexContent>
    <xsd:extension base="SBase">
     <xsd:attribute name="formula" type="xsd:string" use="required"/>
    </xsd:extension>
  </xsd:complexContent>
</xsd:complexType>
```

```
        </xsd:complexType>
      </xsd:element>
      <xsd:element name="listOfReactions" minOccurs="0">
        <xsd:complexType>
          <xsd:sequence>
            <xsd:element name="reaction" type="Reaction" maxOccurs="unbounded"/>
          </xsd:sequence>
        </xsd:complexType>
      </xsd:element>
     </xsd:sequence>
     <xsd:attribute name="name" type="SName" use="optional"/>
    </xsd:extension>
  </xsd:complexContent>
</xsd:complexType>
<!-- The following is the type definition for the top-level element in an SBML document.-->
<xsd:complexType name="sbmlDocument">
  <xsd:sequence>
```

Name	Arguments	Meaning	Formula
massi	S_i, k	Irreversible Mass Action Kinetics	$v = k^i$

Name	Arguments	Meaning	Formula
usii	S, V, K_m, K_i	Substrate Inhibition Kinetics (Irreversible)	$b = V \dfrac{S/K_m}{1 + S/K_m + S^2/K_i}$
usir	S, P, V_f, V_r, K_{mS}, K_{mP}, K_i	Substrate Inhibition Kinetics (Reversible)	$b = \dfrac{V_f S/K_{mS} + V_r P/K_{mP}}{1 + S/K_{mS} + P/K_{mP} + S^2/K_i}$
uai	S, V, K_{sa}, K_{sc}	Substrate Activation	$b = \dfrac{V\,(S/K_{sa})^2}{1 + S/K_{sc} + (S/K_{sa})^2 + S/K_{sa}}$

ucii=1T100121.3020cm0g0G10012.2140cmBT/F89.963Tf00I.963Tf7.9540TTf21.716cm00.890.940.28k00.890.940.28KBT/F1

Name	Arguments	Meaning	Formula
uctr	S, P, A_c, V_f, V_r, K_{mS}, K_{mP}, K_a	Catalytic Activation (Reversiblguments	Catalytic Acti1539[]0837Tf6.0880Td[(P)]TJ/F89.963vTf7.472-1.495Td[95489.963=9.963Tf4.4 mP

Symbol	Meaning
α	E□ect of S and P on binding of M (if $M < 1$, M is inhibitor; if $M > 1$, M is activator)
A	First substrate in two substrate reaction
A_c	Activator
B	Second substrate in two substrate reaction
I	Inhibitor
K_1	Forward Rate Constant
K_2	Reverse Rate Constant
K_a	Activation Constant
K_{ac}	Catalytic Activation Constant
K_{as}	Specific Activation Constant
K_d	Dissociation constant of the elementary step $E + M = EM$
K_{eq}	Equilibrium Constant
K_{ii}	

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