

SimBiology Release Notes

The Chapter 1, “SimBiology 1.0 Release Notes” describe the changes introduced in the latest version of SimBiology. The following topics are discussed in these Release Notes:

- “Introduction” on page 1-2
- “Features” on page 1-2
- “Major Bug Fixes” on page 1-3
- “Known Software Problems” on page 1-4
- “Upgrading from a Beta Release” on page 1-8

Printing the Release Notes

If you would like to print the Release Notes, you can link to a PDF version.

SimBiology 1.0 Release Notes

1

| | |
|---|------------|
| Introduction | 1-2 |
| Features | 1-2 |
| Major Bug Fixes | 1-3 |
| Known Software Problems | 1-4 |
| Unsupported SBML Level 2 Version 1 Features | 1-4 |
| Functional Limitations | 1-5 |
| Tips | 1-6 |
| Upgrading from a Beta Release | 1-8 |

SimBiology 1.0 Release Notes

Introduction

SimBiology Version 1.0 (Release R14SP3+) is an integrated environment for modeling biological processes, simulating the dynamic behavior of these processes, and analyzing simulation and experimental data. Biological processes include metabolic, genetic, and signaling pathways with transform, binding, and transport reactions. You can use SimBiology as a tool in three major areas:

- **Model** — Design and build models by entering model components with a graphical desktop interface, or use the MATLAB Command Window.
- **Simulate** — Select deterministic or stochastic solvers and observe the changes in species amounts and variable parameter values over time.
- **Analyze** — Log data from a simulation and export the data to the MATLAB workspace. Compare simulation with experimental data, for parameter estimation and model validation.

Features

This section introduces the features for SimBiology Version 1.0.

- **Graphical User Interface** — SimBiology provides access to the command-line functionality through a graphical user interface (GUI).
- **Command Line Interface** — All the features in SimBiology are accessible and executable from the MATLAB Command Window.
- **Data Formats and Projects** — Organize and save related models, simulation data, and analysis results in project files. Save user-defined kinetic laws and units. Share models by exporting SBML level 2 files.
- **Modeling** — Create biological models by adding components that include reactions, species, parameters, kinetic laws, rules, and submodels.
- **Simulation** — Select either deterministic or stochastic solvers with dimensional analysis and unit conversion.
- **Analysis** — SimBiology is fully integrated with MATLAB. Log data during a simulation and analyze results in MATLAB.

Major Bug Fixes

To view major bug fixes made in R14SP3 for SimBiology Version 1.0, use the Bug Reports interface on the MathWorks Web site.

Note If you are not already logged in to Access Login, when you link to the Bug Reports interface (see below), you will be prompted to log in or create an Access Login account.

After you are logged in, use this [Bug Reports](#) link. You will see the bug report for SimBiology. The report is sorted with fixed bugs listed first, and then open bugs.

If you are viewing these release notes in PDF form on the MathWorks Web site, you can refer to the [HTML](#) form of the release notes on the MathWorks Web site and use the link provided.

Known Software Problems

To view important open bugs in R14SP3 for SimBiology Version 1.0, use the Bug Reports interface on the MathWorks Web site.

Note If you are not already logged in to Access Login, when you link to the Bug Reports interface (see below), you will be prompted to log in or create an Access Login account.

After you are logged in, use this Bug Reports link. You will see the bug report for SimBiology. The report is sorted with fixed bugs listed first, and then open bugs. You can select the Status column to list the open bugs first.

If you are viewing these release notes in PDF form on the MathWorks Web site, you can refer to the HTML form of the release notes on the MathWorks Web site and use the link provided.

Software problems include unsupported SBML features and current feature and function limitations.

Unsupported SBML Level 2 Version 1 Features

SimBiology supports a subset of the SBML Level 2 Version 1 specification. Unsupported features include

- Compartments — Model compartments are not supported. If an imported SBML model has a single compartment, the model is loaded as a top-level model. If the model has multiple compartments, SimBiology returns a warning and does not load the SBML file.
- Volume — Volume is not supported and cannot be specified.
- Events — Events in an SBML file are ignored when you are importing into a project.
- Piecewise kinetics — Models with piecewise kinetics are loaded in, but SimBiology ignores the definitions for piecewise kinetics..
- Function definitions — Models containing functional definitions are loaded, but SimBiology generates a warning and ignores the function definitions.

- MATLAB incompatible variable names in UnitDefinitions — Models with UnitDefinitions that have variable names are incompatible with MATLAB not loaded, and you see an error message.

Functional Limitations

Simulation and Solvers

- Stochastic solvers only support mass action kinetics, while ODE solvers support all built-in and user-defined kinetic laws.
- ODE solvers support algebraic, rate, and assignment rules, but stochastic solvers do not.
- If you have DimensionalAnalysis and UnitConversion on for the stochastic solvers, note that SimBiology assumes that volume is unity during simulation. The stochastic solvers perform calculations using species units in molecules. Therefore, if you specify the species units in molecules per unit volume or moles per unit volume, SimBiology assumes volume to be unity and converts species amounts to molecules for simulation. The results are finally plotted in the units you specified for the species.

In addition, if you have reactions with stoichiometric coefficients greater than or equal to 2, you need to convert the deterministic rate constants to stochastic rate constants. For example, $2 R \rightarrow P$ has a reaction rate of $v=k[R]^2$. If R is moles/liter, the deterministic rate constant k has units of liter/mole-second. If the unit of species concentration is molecule, then the stochastic rate constant c has units of 1/molecule-second, and $c = 2k/NV$ where N is Avogadro's Number, $6.022e23$ molecules/mole, and V is the volume of the model in liters.

- When you select the Implicit Tau solver, SimBiology ignores any changes to AbsoluteTolerance and RelativeTolerance options within a configuration set. SimBiology uses the default values that are set internally.
- By default, StatesToLog is set to 'all' and all variable parameters are logged. Variable parameters are those that have ConstantValue unchecked or false. If you choose the species to log, however, you cannot log the variable parameters.
- The characters \backslash , \wedge , and $*$ in species and parameter names are not supported in rules.

Units

- Stochastic solvers support dimensional analysis and unit conversion. ODE solvers support dimensional analysis but not unit conversion.
- Dimensional analysis cannot evaluate rules or rate equations that contain MATLAB functions.
- You can delete a unit that is being used in a model; however, you will see an error when you try to simulate the model or export to SBML.

Submodels

- The context menus (right-click options) for the **Species**, **Reaction**, **Parameter** and **Rule** nodes that appear beneath a submodel node all act on the corresponding parent model node, and not on the submodel node. For example, if you select **Delete All Species** in the submodel **Species** node, this selection deletes the species in the parent model.
- Rules are not supported in submodels.

SBML Export Limitations

There are features in SimBiology that are not supported in SBML. When you export a model to an SBML file, you might lose some of these features.

- Submodels are not supported by SBML export.
- The abstract kinetic law name and corresponding expression are not supported by SBML, but the associated reaction rate equation is exported to SBML.
- The properties Tag, UserData, and Active are not supported by SBML export.

Tips

Naming SimBiology Variables

- If you are using a species or parameter name that is not a valid MATLAB variable name, do the following:

- Enclose the name in square brackets when writing a reaction rate equation or a rule.
- Enter the name without brackets when you are creating the species or parameter, or when you add a reaction.

For example, enclose [DNA polymerase+] and [K_DNA polymerase+] within brackets in reaction rates and rules, but, enter DNA polymerase+ or K_DNA polymerase+ when creating a species, adding a reaction, or creating a parameter.

- The names *i* and *j* are reserved MATLAB characters. Because expressions in abstract kinetic laws, reaction rates, and rules are considered to be MATLAB code, SimBiology evaluates *i* or *j* as an imaginary number and not as the value of species *i* or *j*. For example, an expression $V*S^i/K$ is interpreted to have three names, *V*, *S*, and *K*, instead of four. Use brackets to protect such variables.

If a variable in a reaction rate equation or rule has the same name as a MATLAB function, SimBiology evaluates the expression as a call to the MATLAB function. In general, when creating variable names, you should avoid using MATLAB function names or variable names that are invalid in MATLAB.

Changing SimBiology Variable Names

- If you change the Name of a parameter you must configure all applicable elements, such as rules that use the parameter, any user-specified ReactionRate, or the kinetic law object property ParameterVariableNames. Use the method setparameter to configure ParameterVariableNames.

To update parameter names in the SimBiology graphical user interface, access each appropriate pane through the **Project Explorer**.

- If you change the Name of a species you must configure all applicable elements, such as rules that use the parameter, any user-specified ReactionRate, or the kinetic law object property SpeciesVariableNames. Use the method setspecies to configure SpeciesVariableNames.

To update species names in the SimBiology graphical user interface, access each appropriate pane through the **Project Explorer**. SimBiology automatically updates species names for reactions that use MassAction kinetic law.

Upgrading from a Beta Release

Any projects that you created and saved with a beta release of SimBiology will not load in Version 1.0.

As a workaround, before upgrading to version 1.0, save your models to SBML, upgrade to Version 1.0, and then import the SBML models into Version 1.0 projects. Alternatively, contact The MathWorks for help with your conversion.