

SimBiology Release Notes

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Summary by Version

This table provides quick access to what's new in each version. For clarification, see “About Release Notes” on page 1.

Version (Release)	New Features and Changes	Version Compatibility Considerations	Fixed Bugs and Known Problems	Related Documentation at Web Site
Latest Version V2.0 (R2006a+)	Yes Details	Yes Summary	Bug Reports at Web site	Printable Release Notes: PDF Full product documentation:V2.0 product documentation
V1.0.1 (R2006a)	Yes Details	No	Bug Reports at Web site	No
V1.0 (R14SP3+)	Yes Details	No	Bug Reports at Web site	No

About Release Notes

Use release notes when upgrading to a newer version to learn about new features and changes, and the potential impact on your existing files and practices. Release notes are also beneficial if you use or support multiple versions.

If you are not upgrading from the most recent previous version, review release notes for all interim versions, not just for the version you are installing. For example, when upgrading from V1.0 to V1.2, review the New Features and Changes, Version Compatibility Considerations, and Bug Reports for V1.1 and V1.2.

New Features and Changes

These include

- New functionality

- Changes to existing functionality
- Changes to system requirements (complete system requirements for the current version are at the MathWorks Web site)
- Any version compatibility considerations associated with each new feature or change

Version Compatibility Considerations

When a new feature or change introduces a known incompatibility between versions, its description includes a **Compatibility Considerations** subsection that details the impact. For a list of all new features and changes that have compatibility impact, see the “Compatibility Summary for SimBiology” on page 16.

Compatibility issues that become known after the product has been released are added to Bug Reports at the MathWorks Web site. Because bug fixes can sometimes result in incompatibilities, also review fixed bugs in Bug Reports for any compatibility impact.

Fixed Bugs and Known Problems

MathWorks Bug Reports is a user-searchable database of known problems, workarounds, and fixes. The MathWorks updates the Bug Reports database as new problems and resolutions become known, so check it as needed for the latest information.

Access Bug Reports at the MathWorks Web site using your MathWorks Account. If you are not logged in to your MathWorks Account when you link to Bug Reports, you are prompted to log in or create an account. You then can view bug fixes and known problems for R14SP2 and more recent releases.

Related Documentation at Web Site

Printable Release Notes (PDF). You can print release notes from the PDF version, located at the MathWorks Web site. The PDF version does not support links to other documents or to the Web site, such as to Bug Reports. Use the browser-based version of release notes for access to all information.

Product Documentation. At the MathWorks Web site, you can access complete product documentation for the current version and some previous versions, as noted in the summary table.

Version 2.0 (Release 2006a+) SimBiology

This table summarizes what's new in Version 2.0 (Release 2006a+):

New Features and Changes	Version Compatibility Considerations	Fixed Bugs and Known Problems	Related Documentation at Web Site
Yes Details below	Yes. Details labeled as Compatibility Considerations , below. See also "Compatibility Summary for SimBiology" on page 16.	Bug Reports at Web site	Printable Release Notes: PDF V2.0 product documentation

New features and changes introduced in this version are

- "Diagram Interface" on page 4
- "Find and Bookmarks in Projects" on page 5
- "Sensitivity Analysis" on page 5
- "Parameter Estimation" on page 6
- "Ensemble Simulation Runs" on page 6
- "Moiety Conservation" on page 7
- "Model Verification and Validation" on page 7
- "Simulation and Solvers" on page 7
- "New Demos for SimBiology Version 2.0" on page 8

Diagram Interface

The Diagram is a graphical user interface you can use to enter model pathways using block representations for species, reactions, and submodels. Use the Plot block to visualize simulation data during a simulation. For a tutorial in the documentation, see Modeling Using the SimBiology Diagram

in Getting Started with SimBiology. You can also access video demos from a list of SimBiology Demos.

Find and Bookmarks in Projects

- **Find** – Type a string in the **Find** box to quickly find matching model components in the project and in abstract kinetic laws.
- **Bookmarks** – Use complex rules to identify objects from the project, and create a custom and persistent set of desktop and project objects.

Compatibility Considerations

In Versions 1.0 and 1.0.1, SimBiology projects saved searches. In Version 2.0, the project saves bookmarks. SimBiology converts a previous version's saved search into a bookmark. After you save a project in Version 2.0, a bookmark is saved and the old search is no longer available. If a project contains a search, SimBiology warns that the project file will contain a bookmark rather than a search after saving.

All functionality available in Version 1.0 searches are present in Version 2.0 bookmarks except for the ability to mix and match and and or between the search rows. If you have a multiple-row search saved with a mixture of and and or, when you load this project into Version 2.0, it is converted to either all or any based on whether SimBiology first encounters and or or.

Sensitivity Analysis

You can perform sensitivity analysis in SimBiology by using the following properties:

- **SensitivityAnalysis** – Configuration set property that lets you calculate the time-dependent sensitivities of all the species states defined by the StatesToLog property with respect to species initial conditions, and parameter values.
- **SensitivityAnalysisOptions** – An object that holds the sensitivity analysis options in the configuration set object. Properties of **SensitivityAnalysisOptions** are summarized below:

- `SpeciesInputFactors` – Specify the species with respect to which you want to compute the sensitivities of the species states in your model.
- `ParameterInputFactors` – Specify the parameters with respect to which you want to compute the sensitivities of the species states in your model.
- `Normalization` – Specify the normalization for the calculated sensitivities.

For an introduction and an example in the documentation, see [Sensitivity Analysis](#) in the SimBiology User's Guide.

Parameter Estimation

The `sbioparamestim` function lets you estimate any or all parameters in your model using the experimental data you provide. SimBiology uses the optimization functions in MATLAB®, the Optimization Toolbox, and the Genetic Algorithm and Direct Search Toolbox to enable parameter estimation.

The Optimization Toolbox and the Genetic Algorithm and Direct Search Toolbox are not required for you to use `sbioparamestim`. If you do not have these products installed, `sbioparamestim` uses the MATLAB function `fminsearch` by default.

For an introduction and an example in the documentation, see [Parameter Estimation](#) in the SimBiology User's Guide.

Ensemble Simulation Runs

You can perform ensemble simulations using the stochastic solvers to gather data from multiple stochastic runs of the model. The following functions let you perform ensemble runs:

- `sbioensamplerun` – Performs multiple stochastic ensemble runs of the SimBiology model object.
- `sbioensembleplot` – Shows a 2-D distribution plot or a 3-D shaded plot of the time varying distribution of one or more specified species in the ensemble data generated by `sbioensamplerun`.
- `sbioensemblestats` – Gets mean and variance as a function of time for all the species in the ensemble data generated by `sbioensamplerun`.

Moiety Conservation

The `sbioconsmoiety` function lets you calculate a complete set of linear conservation relations for the species in a SimBiology model object.

For an introduction and an example in the documentation, see *Moiety Conservation* in the SimBiology User's Guide.

Model Verification and Validation

SimBiology performs model verification and validation either during simulation, or when you explicitly execute the commands for verification before simulation.

Verification at the Command Line

The following new functions lets you verify and validate at the command line, that your model is ready for simulation:

- `verify` – Performs checks on a model to verify that you can simulate the model. SimBiology generates stacked errors and warnings if any problems are found. To see the entire list of errors and warnings, use `sbiolasterror` and `sbiolastwarning`.
- `sbiolasterror` – Returns a SimBiology diagnostic structure array containing the last errors generated by SimBiology.
- `sbiolastwarning` – Returns a SimBiology diagnostic structure array containing the last warnings generated by SimBiology.

Verification on the SimBiology Desktop

Click the **Verify** button on the SimBiology desktop toolbar to perform verification and validation of your model. SimBiology opens the **Output** pane containing the errors and warnings. You can double-click a result row to go to the location of the error or warning.

Simulation and Solvers

The following new features and changes apply to simulation settings and solvers:

- **MaxStep** – Lets you specify the upper bound on solver step size for a deterministic solver. MaxStep is a property of the SolverOptions object.
- **Implicit Tau Solver Settings** – For impltau, AbsoluteTolerance holds the value for convergence tolerance for the nonlinear solver that is used internally by the Implicit Tau solver. You can now specify AbsoluteTolerance for impltau in SimBiology. Previously, if you selected the Implicit Tau solver, SimBiology ignored any changes to the AbsoluteTolerance and RelativeTolerance options within a configuration set. SimBiology used the default values set internally.
- **UnitConversion** – Supported by both deterministic solvers and stochastic solvers. Previously UnitConversion was supported only by the stochastic solvers.

Implicit Tau Solver Settings Compatibility Considerations

The RelativeTolerance property is no longer valid for the Implicit Tau (impltau) solver.

When you load a file created in a previous version of SimBiology, the project loads the RelativeTolerance property. But when you save the file, SimBiology updates the change.

Unit Conversion Compatibility Considerations

The UnitConversion property default is now 'false'. If you load a SimBiology project created in a previous version into the SimBiology desktop, the UnitConversion setting in each model in the project remains as the saved setting. If however, you are running an M-file, you must now remember to set the UnitConversion property to true if you want SimBiology to perform unit conversions

New Demos for SimBiology Version 2.0

There are 14 new demos for SimBiology Version 2.0. Click SimBiology Demos or type demo('MATLAB', 'SimBiology') at the command prompt.

Version 1.0.1 (Release 2006a) SimBiology

This table summarizes what's new in Version 1.0.1 (Release 2006a):

New Features and Changes	Version Compatibility Considerations	Fixed Bugs and Known Problems	Related Documentation at Web Site
Yes Details below	No	Bug Reports at Web site	No

The changes introduced in this version are

- The characters \, ^, and * in species and parameter names are now supported in rules.
- Rules are now supported in submodels.

Version 1.0 (Release 14SP3+) SimBiology

This table summarizes what's new in Version 1.0 (Release 14SP3):

New Features and Changes	Version Compatibility Considerations	Fixed Bugs and Known Problems	Related Documentation at Web Site
Yes Details below	No	No bug fixes	No

The features introduced are described below:

- “Introduction” on page 10
- “Features” on page 11
- “Known Software Problems” on page 11
- “Upgrading from a Beta Release” on page 15

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

The features in SimBiology Version 1.0 are the following:

- **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.

Known Software Problems

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

Note If you are not already logged in to your MathWorks Account, when you link to the Bug Reports interface (see below), you will be prompted to log in or create an 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 `UnitDefinition` — Models that have variable names incompatible with MATLAB in `UnitDefinition`, are 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.
- If you use a stochastic solver to simulate a model, SimBiology ignores any rate, assignment, or algebraic rules if present in the model.
- 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 cleared or false. If you choose the species to log, however, you cannot log the variable parameters.
- The characters \, ^, 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.
- 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.

Compatibility Summary for SimBiology

This table summarizes new features and changes that might cause incompatibilities when you upgrade from an earlier version, or when you use files on multiple versions. Details are provided in the description of the new feature or change.

Version (Release)	New Features and Changes with Version Compatibility Impact
Latest Version V2.0 (R2006a+)	See the Compatibility Considerations subheading for each of these new features or changes: <ul style="list-style-type: none">• “Find and Bookmarks in Projects” on page 5• Implicit Tau Solver Settings• Unit Conversion
V1.0.1 (R2006a)	None
V1.0 (R14SP3+)	None