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 V2.2 (R2007b+)	Yes Details	Yes Summary	Bug Reports	Printable Release Notes: PDF Current product documentation
V2.1.2 (R2007b)	No	No	Bug Reports	No
V2.1.1 (R2007a)	No	No	Bug Reports	No
V2.1 (R2006b+)	Yes Details	Yes Summary	Bug Reports Includes fixes	No
V2.0.1 (R2006b)	No	No	Bug Reports Includes fixes	No
V2.0 (R2006a+)	Yes Details	Yes Summary	Bug Reports Includes fixes	No
V1.0.1 (R2006a)	Yes Details	No	Bug Reports	No
V1.0 (R14SP3+)	Yes Details	No	Bug Reports	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 reported 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 reported compatibility impact, see the "Compatibility Summary for SimBiology" on page 35.

Compatibility issues that are reported 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.

About Functions Being Removed

This section lists functions removed or in the process of being removed. Functions typically go through several stages across multiple releases before being completely removed. This provides time for you to make adjustments to your code.

- Announcement – the Release Notes announce the planned removal, but there are no functional changes; the function runs as it did before.

- Warning – when you run the function, it displays a warning message indicating it will be removed in a future release; otherwise the function runs as it did before.

- Error – when you run the function, it produces an error. The error message indicates the function was removed and suggests a replacement function, if one is available.

- Removal – when you run the function, it fails. The error message is the standard message when MATLAB does not recognize an entry.

Functions might be in a stage for one or more releases before moving to another stage. Functions are listed in the Functions Being Removed section only when they enter a new stage and their behavior changes. For example, if a function displayed a warning in the previous release and errors in this release, it appears on the list. If it continues to display a warning, it does not appear on the list because there was no change between the releases.

Not all functions go through all stages. For example, a function's impending removal might not be announced, but instead the first notification might be that the function displays a warning.

The Release Notes include actions you can take to mitigate the effects of a function's removal, such as adapting your code to use a replacement function.

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 2.2 (Release 2007b+) SimBiology

This table summarizes what's new in Version 2.2 (Release 2007b+):

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 Summary.	Bug Reports Includes fixes	Printable Release Notes: PDF Current product documentation

New features and changes introduced in this version are

- "Changes to the Model Structure" on page 5

- "Events" on page 7

- "Variants" on page 7

- "Support for Analysis Tasks in the Desktop" on page 8

- "Changes to the Library Structure in the Root" on page 11

- "New Features for Simulation and Solvers" on page 12

- "New Plot Functions" on page 14

- "New Sensitivity Analysis Property for Species Outputs" on page 14

- "New Way to Add Units and Unit Prefixes" on page 14

- "Functions and Properties Being Removed" on page 15

Changes to the Model Structure

The following new features and changes are for a model's structure:

- "Compartments Now Supported " on page 6

- "Submodel Support Will Be Removed" on page 6

Compartments Now Supported

SimBiology models now let you add compartments to a model, specify compartment size, simulate, and do analysis with multiple compartments. Any model containing species must have a compartment, and the species must belong to a compartment. You can also perform dimensional analysis and unit conversion accounting for the specified compartment size. For more information on compartments, refer to the following sources in the documentation:

- "Compartment" — Introduction to compartments in Getting Started with SimBiology.

- Compartment object — Reference for compartment objects

Submodel Support Will Be Removed

Support for submodels will be removed in a future version. You can still open models containing submodels and create submodels, but you cannot simulate or perform any analysis tasks on the model. Therefore, you should transition to using compartments where applicable.

Compatibility Considerations. If you have submodels in your previously created model, you can still open your model, but you must convert the submodels into top-level SimBiology models to be able to perform any tasks.

To convert submodels, use sbioupdate.

If you open a model that contains submodels in the SimBiology desktop, the submodels model are automatically converted to models and placed in separate model sessions. See sbioupdate for more information

As a result of removing submodels, the addmodel method and Models property of the model object are no longer relevant. You can still access the addmodel method and the Models property for this version of the software, though it may be removed in a future release.

Events

You can now add events to SimBiology models. Use events to describe sudden changes in a model system. Events are supported only by the `sundials` solver and the stochastic solver `ssa`.

For more information on events, refer to the following:

- "Events" — Introduction to events in Getting Started with SimBiology.

- "Events" — Discussion about events including how events are evaluated.

- `Event object` — Reference for event objects.

- "Sundials Solvers" — Deterministic solver for simulating models with events.

Models containing events do not support sensitivity analysis.

Variants

Variants let you store the names and values of model components and use the values stored in a variant as the alternate value to apply during a simulation. You can store values for species `InitialAmount`, parameter `Value`, and compartment `Capacity` in a variant.

For more information on events refer to the following sources in the documentation:

- "Variants" — Introduction to events in Getting Started with SimBiology.

- `Variant object` — Reference for variant objects.

- "Applying Alternate Values Using Variants" — Example in a tutorial.

For more information, see .

In the SimBiology desktop, expand **Model Variable Settings** and double-click **Variants** to open the **Variants** pane. The **SimBiology Desktop Help** updates with more information on adding and setting variants. If the help is not open in the SimBiology desktop, select **Help > SimBiology Desktop Help**.
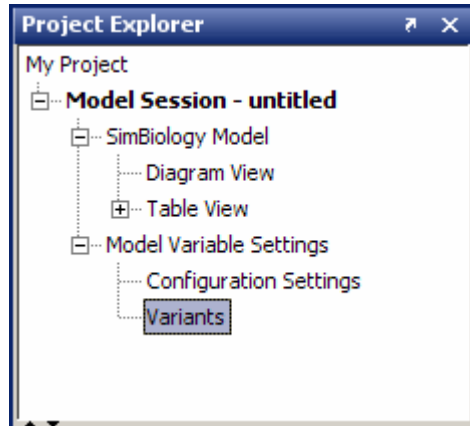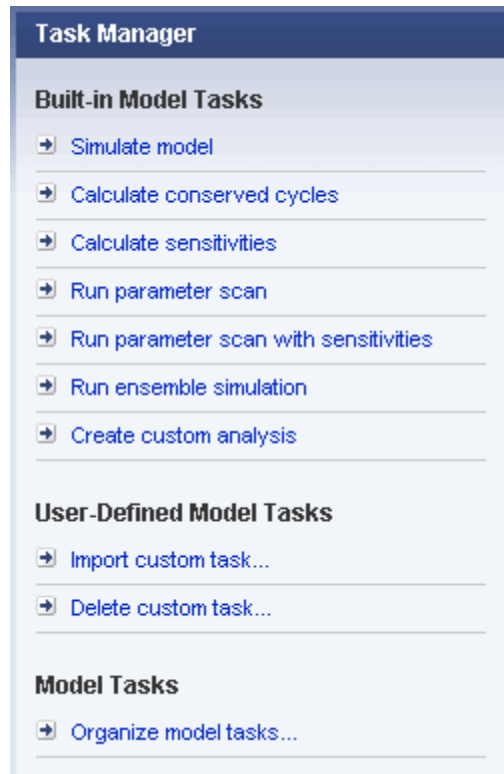
Support for Analysis Tasks in the Desktop

The SimBiology desktop now supports adding and managing analysis tasks through the following features:

- "Task Manager" on page 8
- "Sensitivity Analysis in the Desktop" on page 9
- "Scanning and Scanning with Sensitivities in the Desktop" on page 10
- "Ensemble Simulation Runs in the Desktop" on page 10
- "Conserved Cycle Calculations in the Desktop" on page 10
- "Create Custom Analyses Tasks" on page 11
- "Generate Reports for Projects" on page 11

Task Manager

The **Task Manager** lets you add and manage simulation and analysis tasks. In the **Project Explorer** double-click **Model Session**. The **Model Session** pane opens with the **Task Manager** listed on the right.

Task Manager

Built-in Model Tasks

→ Simulate model

→ Calculate conserved cycles

→ Calculate sensitivities

→ Run parameter scan

→ Run parameter scan with sensitivities

→ Run ensemble simulation

→ Create custom analysis

User-Defined Model Tasks

→ Import custom task...

→ Delete custom task...

Model Tasks

→ Organize model tasks...

Click a task to add it to your model. The desktop adds the task to the **Project Explorer** and opens the task pane. For more information on setting up and running a task in the desktop, open the task pane and select **Help > SimBiology Desktop Help** to see the context-sensitive help.

Sensitivity Analysis in the Desktop

Sensitivity analysis is now supported in the desktop. Sensitivity analysis was previously available only through command line. Sensitivity analysis lets you calculate the time-dependent sensitivities of a species specified in **SpeciesOutputs** with respect to species initial conditions and parameter values.

See "Performing Sensitivity Analysis Using the Desktop" in the SimBiology documentation for more information. You must have a model in the desktop for this feature to be enabled.

For more information on sensitivity analysis, see "Sensitivity Analysis" in the SimBiology User's Guide.

Scanning and Scanning with Sensitivities in the Desktop

You can perform species and parameter scanning analysis alone or in combination with sensitivity analysis in the desktop. Scan a parameter value or a species initial amount to determine the effect of a range of values of the parameter or species.

Combine the scan with sensitivity analysis to explore the sensitivity of a species with respect to a range of values of a parameter or a species.

For information on how to add the task to a model, see "Task Manager" on page 8. For more information on setting up and running the task in the desktop, open the task pane and select **Help > SimBiology Desktop Help** to see the context-sensitive help. You need a model in the desktop for this feature to be enabled.

Ensemble Simulation Runs in the Desktop

The SimBiology desktop now supports ensemble simulations. You can perform ensemble simulations using the stochastic solvers to gather data from multiple stochastic runs of the model.

See "Running Ensemble Simulations in the Desktop" in the SimBiology documentation for more information. You must have a model in the desktop for this feature to be enabled.

Conserved Cycle Calculations in the Desktop

The SimBiology desktop now supports conserved cycle calculations. This feature lets you calculate a complete set of linear conservation relations for the species in a SimBiology model object. For an introduction, see "Moiety Conservation" in the SimBiology documentation.

For information on how to add the task to a model, see "Task Manager" on page 8. For more information on setting up and running the task in the desktop, open the task pane and select **Help > SimBiology Desktop Help** to see the context-sensitive help. You need a model in the desktop for this feature to be enabled.

Create Custom Analyses Tasks

The SimBiology desktop lets you create custom tasks that are associated with a project. You can either write new code or copy and modify task code from built-in tasks in the desktop. For more information about creating custom tasks see "Performing Custom Analysis in the Desktop".

For information on how to add the task to a model, see "Task Manager" on page 8. For more information on setting up and running the task in the desktop, open the task pane and select **Help > SimBiology Desktop Help** to see the context-sensitive help. You need a model in the desktop for this feature to be enabled.

Generate Reports for Projects

You can now generate reports for your projects. Report templates let you generate a report with specified information about a model. To generate a template. In the **Project Explorer**, click **Report Templates** to open the **Report Templates** pane. Select **Help > SimBiology Desktop Help** to see the context-sensitive help for information on how to generate reports.

Changes to the Library Structure in the Root

Built-in and user-defined libraries for units, unit-prefixes, and abstract kinetic laws are now organized under two root object properties, `BuiltInLibrary` and `UserDefinedLibrary`, with subcategories for units, unit-prefixes, and abstract kinetic laws. See `Root object`, `BuiltInLibrary`, and `UserDefinedLibrary` for more information.

Compatibility Considerations

In previous versions, the libraries were organized under six properties,

- `UserDefinedKineticLaws`.

- `BuiltInKineticLaws`

- `UserDefinedUnits`

- `BuiltInUnits`

- `UserDefinedUnitPrefixes`

- `BuiltInUnitPrefixes`

The changes to the library structure improve the organization of root object properties.

To illustrate the change using an example, previously you would access a user-defined kinetic law using the following syntax:

```
rootObj = sbioroot;
get(rootObj, 'UserDefinedKineticLaws')
```

You must now use the following syntax:

```
rootObj = sbioroot;
get(rootObj.UserDefinedLibrary, 'KineticLaws')
```

New Features for Simulation and Solvers

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

- "Support for Sundials Solvers" on page 12

- "New Property in Configuration Sets to Specify Species Dimensions" on page 13

- "SimData Object Holds All Simulation Data" on page 13

Support for Sundials Solvers

Sundials – The Sundials package of solvers has been added in this release. The Sundials solvers are part of a freely available third-party package developed at Lawrence Livermore National Laboratory. Models that contain events are supported by the Sundials solvers and by the stochastic solver `ssa`. For more information, see "Sundials Solvers".

New Property in Configuration Sets to Specify Species Dimensions

There is a new property called `DefaultSpeciesDimension` that lets you specify whether the default species dimensions should be `concentration` (default) or `substance`. This property thus lets you specify whether the solver should account for compartment capacity. If however, you specify the species units in the `InitialAmountUnits` property, these units define the species dimension regardless of the value in `DefaultSpeciesDimension`.

SimData Object Holds All Simulation Data

The SimBiology `SimData` object now stores the data returned from any simulation. For example, the output from the `sbiosimulate` function is now stored in a `SimData` object which holds time and state data as well as metadata, such as the types and names for the logged states or the configuration set used during simulation.

You can also store data from multiple simulation runs as an array of SimData objects. Thus, the output of `sbioensemblerun` is an array of SimData objects. See `SimData object` for more information and a list of methods and properties.

Compatibility Considerations. The SimData object is now the preferred container for simulation and analysis task data. Previously, simulation and analysis data were stored as time series objects. Functions that used to return time series objects now return SimData objects. If you have time series objects in your projects, you can convert them using `sbioupdate`. Functions that used to take time series object as input argument now take SimData object. You can use time series objects in an input argument, but you see a warning. Support for time series objects in SimBiology functions may be removed in a future version.

The `sbiogetsensmatrix`, and `sbiogetnamedstate` functions are being replaced by the SimData object methods `getsensmatrix` and `selectbyname` respectively.

New Plot Functions

There are two new plot functions — `sbioplot` and `sbiosubplot`. Both functions let you plot data directly from the SimData object (see "SimData Object Holds All Simulation Data" on page 13).

`sbioplot` plots each simulation run for a SimData object or array of SimData objects from a model, in the same figure. The plot is a time plot of each state in the object. The figure also shows a hierarchical display of all the runs in a tree, where you can choose which trajectories to show.

`sbiosubplot` plots each simulation run for a SimData object or array of objects, into its own subplot. The subplot is a time plot of each state in the object. You can navigate through the plots in the figure window and select a subset of the plots to view.

New Sensitivity Analysis Property for Species Outputs

To set up sensitivity analysis, you must now specify an additional property called `SpeciesOutputs`. In `SpeciesOutputs`, specify the species for which you want to compute sensitivities.

Compatibility Considerations

Previously, sensitivity analysis used the species specified in `StatesToLog` as the species for which sensitivities should be calculated. `SpeciesOutputs` improves the functionality by separating the use of the properties.

If you have models from a previous version configured for sensitivity analysis, you must specify species for which you want to compute sensitivities in the `SpeciesOutputs` property. Until this property is specified, sensitivity analysis gives a warning that the `SpeciesOutputs` property is not set, and continues to use the species specified in `StatesToLog`. The use of `StatesToLog` in this context may not be available in a future version, so you should set the `SpeciesOutputs` property for your models, if applicable.

New Way to Add Units and Unit Prefixes

Units and unit prefixes are now represented by objects. You can create units and prefixes and add them to the user-defined library using the function

sbioaddtolibrary. See `Unit object` and `UnitPrefix object`, for more information.

Compatibility Considerations

Previously, `sbioregisterunit` and `sbiounregisterunit` created and removed units respectively. These functions now produce warnings and will be removed in a future version. Use unit objects and `sbioremovefromlibrary` instead.

Similarly, `sbioregisterunitprefix` and `sbiounregisterunitprefix` created and removed unit prefixes respectively. These functions now produce warnings and will be removed in a future version. Use unit prefix objects and `sbioremovefromlibrary` instead.

Functions and Properties Being Removed

For more information about the process of removing functions, see "About Functions Being Removed" on page 2 in the documentation.

Function or Property Name	What Happens When You Use Function or Property?	Use This Instead	Compatibility Considerations
addmodel	Warns	addcompartment, where applicable	See "Submodel Support Will Be Removed" on page 6.
Models	Still runs	Compartments, where applicable	See "Submodel Support Will Be Removed" on page 6.

Function or Property Name	What Happens When You Use Function or Property?	Use This Instead	Compatibility Considerations
sbioregisterunit	Warns	Unit object and sbioaddtolibrary	See "New Way to Add Units and Unit Prefixes" on page 14.
sbiounregisterunit	Warns	sbioremovefromlibrary	See "New Way to Add Units and Unit Prefixes" on page 14.
sbioregisterunitprefix	Warns	Unit object and sbioaddtolibrary	See "New Way to Add Units and Unit Prefixes" on page 14.
sbiounregisterunitprefix	Warns	sbioremovefromlibrary	See "New Way to Add Units and Unit Prefixes" on page 14
sbiogetsensmatrix	Warns	getsensmatrix	See "SimData Object Holds All Simulation Data" on page 13
sbiogetnamedstate	Warns	selectbyname	See "SimData Object Holds All Simulation Data" on page 13

Version 2.1.2 (Release 2007b) SimBiology

This table summarizes what's new in Version 2.1.2 (Release 2007b):

New Features and	Version	Fixed Bugs and	Related
No	No	Bug Reports	No

Version 2.1.1 (Release 2007a) SimBiology

This table summarizes what's new in Version 2.1.1 (Release 2007a):

New Features and	Version	Fixed Bugs and	Related
No	No	Bug Reports	No

Version 2.1 (Release 2006b+) SimBiology

This table summarizes what's new in Version 2.1 (Release 2006b+):

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 Summary.	Bug Reports Includes fixes	No

New features and changes introduced in this version are

- "Printing and Exporting the Diagram" on page 19

- "Diagram Menu" on page 19

- "Block Overview Tool" on page 20

- "Miscellaneous Desktop Enhancements" on page 20

Printing and Exporting the Diagram

You can annotate and print your pathway's block diagram in SimBiology™, or export the diagram using .svg, .jpeg, or .pdf file formats. For example, you can annotate the diagram with the name of the author, the date, notes, and name of the organization. You can choose to place this content as a header or footer on the diagram page.

Diagram Menu

The SimBiology desktop supports multiple diagram features and actions through the **Diagram** menu. Use the options in the **Diagram** menu to do the following:

- Copy, paste, and delete blocks.

- Select model or diagram components by category (for example, select all lines or all Species blocks).

- Filter selected portions of a model diagram to include only model or diagram components by category.

- Edit multiple blocks or lines.

- Add selected blocks to a Block Library.

- Annotate and print, or export your model diagram.

- Perform layout tasks, for example, hide and show blocks, move blocks to the front or back of a diagram, rotate a block, and pin or unpin selected blocks.

- Copy the style of a block and apply the style to a group of selected blocks.

- Reload a graphic used for a block in the Block Properties dialog box.

- Access diagram tools such as the Diagram Table View, Block Library Browser, Diagram Overview, and Block Overview tool.

Compatibility Considerations

There is a compatibility consideration regarding the support for editing multiple blocks or lines. In SimBiology Versions 2.0 and 2.0.1, if you selected multiple blocks and/or lines and applied an editing action such as **Hide**, **Pin**, or **Hide Name**, the action applied only to the block on which you selected the right-click (context) menu. Starting in Version 2.1, applicable editing actions are propagated to all selected blocks.

Block Overview Tool

The Block Overview tool provides a summary of key information about a particular block. Hover the mouse over a block to find information in the **Block Overview** pane. Each block includes information pertinent to that type of block, for example, a species block overview shows **Name**, **InitialAmount**, **InitialAmountUnits**, the number and list of reactions the species is involved in, and a description of any indicators shown in the diagram.

Miscellaneous Desktop Enhancements

The enhancements for the SimBiology desktop let you do the following:

- Set your preference to open a SimBiology pane with a single-click in the Project Explorer. Select **File > Preferences** to open the Preferences dialog box.

- Interrupt and stop model verification by clicking **Stop** when **Verify** is running.

- Sort the available plot arguments in the **Simulation** and **Data** panes. The X and Y argument lists are now tabulated.

- View a species and any of its cloned blocks from the search results for the species.

- Select and view multiple results for **Find** and **Bookmarks** in either the **Diagram** or the table form.

Version 2.0.1 (Release 2006b) SimBiology

This table summarizes what's new in Version 2.0.1 (Release 2006b):

New Features and	Version	Fixed Bugs and	Related
No	No	Bug Reports Includes fixes	No

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 Summary.	Bug Reports Includes fixes	No

New features and changes introduced in this version are

- "Diagram Interface" on page 23

- "Find and Bookmarks in Projects" on page 24

- "Sensitivity Analysis" on page 24

- "Parameter Estimation" on page 25

- "Ensemble Simulation Runs" on page 25

- "Moiety Conservation" on page 25

- "Model Verification and Validation" on page 26

- "Simulation and Solvers" on page 26

- "New Demos for SimBiology Version 2.0" on page 27

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 the Getting Started with SimBiology documentation. 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 documentation.

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®, Optimization Toolbox, and Genetic Algorithm and Direct Search Toolbox to enable parameter estimation.

Optimization Toolbox and 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 documentation.

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:

- sbioensemblerun – 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 sbioensemblerun.

- sbioensemblestats – Gets mean and variance as a function of time for all the species in the ensemble data generated by sbioensemblerun.

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 documentation.

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 let 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	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	Bug Reports	No

The features introduced in this version are

- "Introduction" on page 29
- "Features" on page 30
- "Known Software Problems" on page 30
- "Upgrading from a Beta Release" on page 34

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 -> 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 a 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 V2.2 (R2007b+)	See the **Compatibility Considerations** subheadings for • "Submodel Support Will Be Removed" on page 6 • "Changes to the Library Structure in the Root" on page 11 • "SimData Object Holds All Simulation Data" on page 13 • "New Sensitivity Analysis Property for Species Outputs" on page 14 • "New Way to Add Units and Unit Prefixes" on page 14 • "Functions and Properties Being Removed" on page 15
V2.1.2 (R2007b)	None
V2.1.1 (R2007a)	None
V2.1 (R2006b+)	See the **Compatibility Considerations** subheading for "Diagram Menu" on page 19.
V2.0.1 (R2006b)	None

Version (Release)	New Features and Changes with Version Compatibility Impact
V2.0 (R2006a+)	See the **Compatibility Considerations** subheading for "Find and Bookmarks in Projects" on page 24 and the following: • "Implicit Tau Solver Settings Compatibility Considerations" on page 27 • "Unit Conversion Compatibility Considerations" on page 27
V1.0.1 (R2006a)	None
V1.0 (R14SP3+)	None