JigCell Model Connector

User Manual

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1 Introduction

The ever-growing size and complexity of molecular network models makes them difficult to construct and understand. Our approach to modeling is to build large models by combining together smaller models, making them easier to comprehend. At the base, the smaller models (called modules) are defined by small collections of reactions. Modules connect together to form larger modules through clearly defined interfaces called ports, as shown in Figure 1. We present the JigCell Model Connector, a software tool that supports large-scale molecular network modeling.
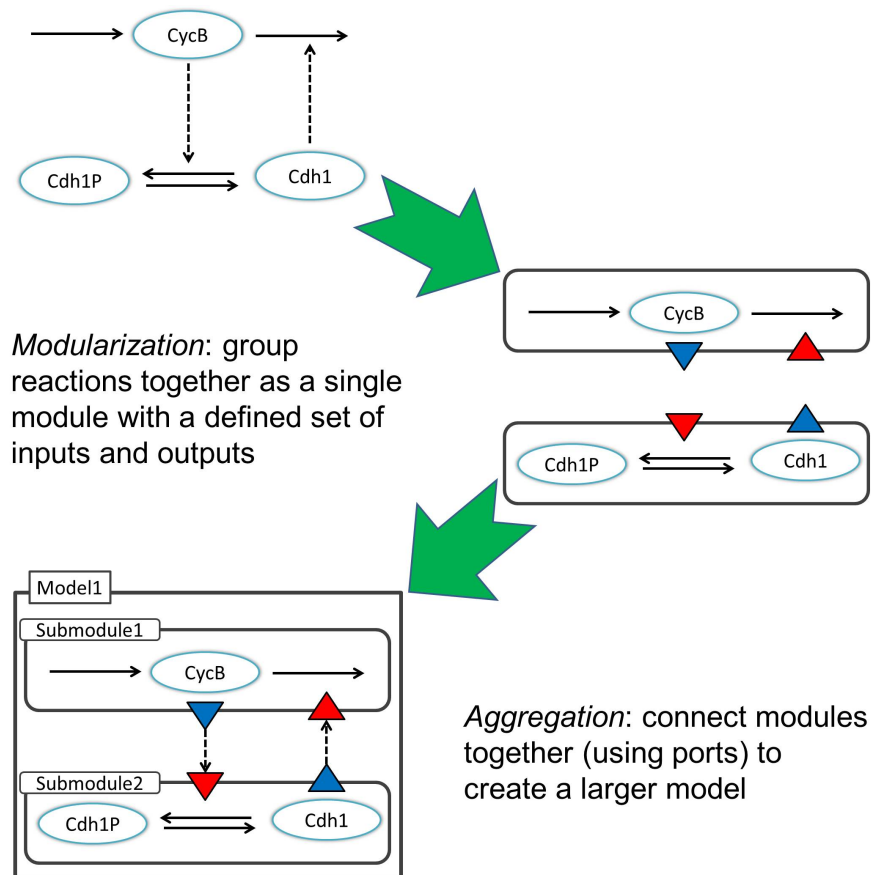

Figure 1: The Process

2 Interface

This section describes the interface of the tool, shown in Figure 2.
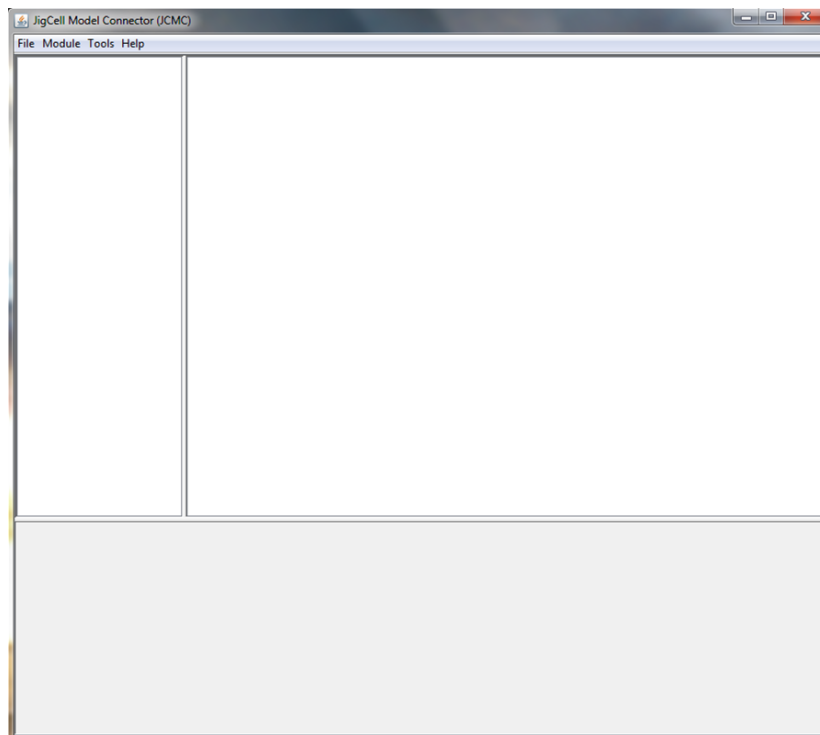

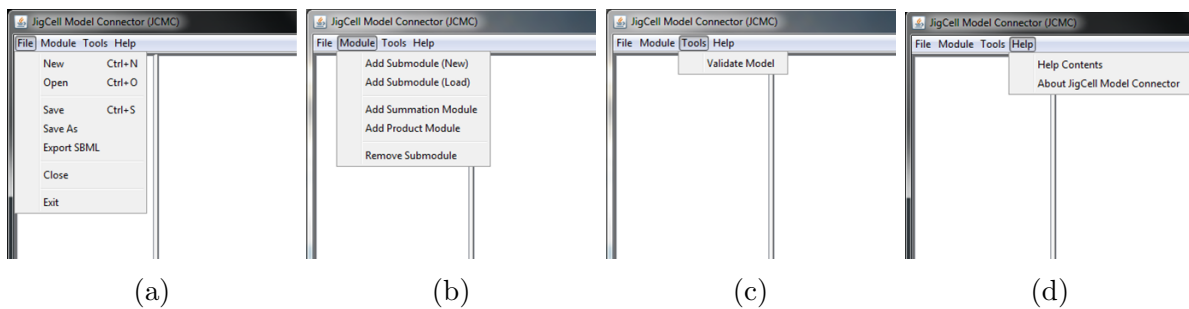Figure 2: Three panels and the menubar

2.1 Top Menu

Figure 3: Menu items

2.1.1 File Menu

Figure 3a shows the file menu items.

New create an empty model. TreeView will show the root model, DrawingBoard will show the root model, and the user may enter information in ModelBuilder.

Open open an existing model from a file and load the three panels accordingly.

- – TreeView will show the hierarchical structure of the root model and submodules.
- – DrawingBoard will show the root model, submodules, ports, and connections.
- – ModelBuilder will load the reactions/species/parameters defined in the root model.

Save/Save As save the entire model in one JCMC file. The entire model implies the complete definition of the root model, each submodule, and any connections between the modules. The layout (positions on the graph) of the modules will be saved in the same file.

Export SBML export the entire model into a SBML formatted (level 3 version 1) file.

Close give the option to save the model, unload/clear all three panels, and go back to an empty screen.

Exit exit the program after completing the steps described under the Close menu item.

2.1.2   Module Menu

Figure 3b shows the module menu items.

Add Submodule (New) add an empty submodule under the module selected in the TreeView.

Add Submodule (Load) open a file selection dialog box to select an already saved template module and will add that as a submodule under the selected module.

Add Summation Module create a module with a user specified number of input ports. The module will add each of the input values and output them into one single output port.

Add Product Module create a module with a user specified number of input ports. The module will multiply each of the input values and output them into one single output port.

Remove Module remove the currently selected module and all its submodules from the model. All of the connections with other modules will be lost.

2.1.3   Tools

Figure 3c shows the tools menu items.

Validate Model check if each module in the model is valid. A dialog box will display the results.

2.1.4   Help

Figure 3d shows the help menu items.

Help Contents where to find JCMC help documentation.

About JigCell Model Connector information about JCMC.

2.2 Three Panels

2.2.1 TreeView

The left panel is the TreeView. It displays the hierarchical structure of the model. Some features/properties of this panel:

- A node can be selected using the left mouse click (1 click), it will be highlighted.

- Double clicks (using left mouse button) will be use to expand/collapse selected node.

- Right mouse click will show the pop-up menu for the selected node, shown in Figure 4.

    – Edit Name: edit the module name

    – Load Module: load the selected module in DrawingBoard and ModelBuilder. Previously loaded module will be saved first in internal data structure.

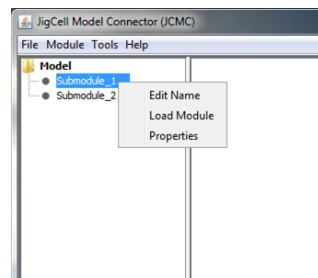   – Properties: show a message box containing some basic information about the module, for example, list of ports.

Figure 4: TreeView popup menu

- After selecting a module, the user can add submodules (from Module menu) or can delete it (from Module menu).

2.2.2 DrawingBoard

The right panel is the DrawingBoard. It displays the graphical view of the modules and connections among them. An example is shown in Figure 5. Some features/properties of this panel:

- The current loaded module is the container module. In Figure 5 the container module is named "Model".

- Submodules can be moved inside of the container module. In Figure 5, "Submodule_1" and "Submodule_2" are submodules.

- Ports are displayed on both the container module and submodules.

- Connections between ports, visible variables, and equivalence nodes are shown.
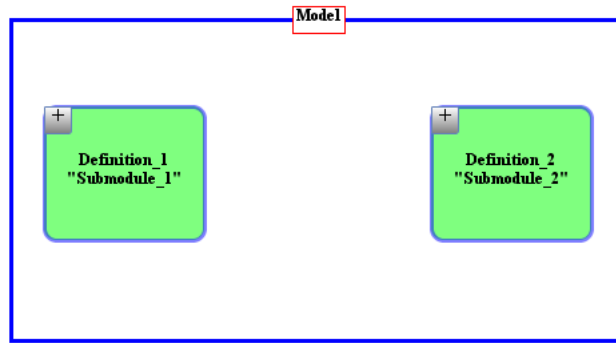
Figure 5: DrawingBoard

2.2.3 ModelBuilder

The bottom panel is the ModelBuilder, shown in Figure 6. This is where the details of a module are displayed. Attributes such as reactions, species, parameters, and events can be modified.
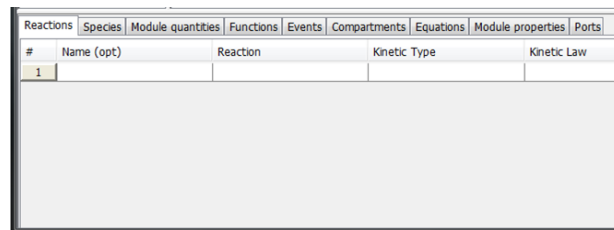

Figure 6: ModelBuilder

3 Components

3.1 Active Module

The active module is the current loaded module. The TreeView panel shows the active module's name in bold font. The ModelBuilder panel displays the reactions, species, parameters, events, etc. of the active module. The DrawingBoard displays the active module and any submodules, ports, or connections contained in the module. When selected by a right click, the module will show the following popup menu options:

- Edit Name: edit the module name.

- Add Port: add a port to reference an existing species or global quantity in the module (see details in the Add Ports subsection).

- Show Variable: display a visible variable node to reference an existing species or global quantity in the module (see details in the Visible Variable Nodes subsection).

There can only be one active module loaded at a time.

3.2 Submodules

A submodule is simply a module contained within another module. The TreeView panels lists a submodule under its container module. In the DrawingBoard, a submodule can be moved and resized within the bounds of its container module. A submodule's detailed information (reactions, species, parameters, events, etc) is not listed in the ModelBuilder panel because the active module's information is displayed. However, a submodule's information can be previewed in the ModelBuilder panel. Each submodule has a button in the top left-hand corner. When this button is pressed, the information for that submodule will be displayed in the ModelBuilder. An example is shown in Figure 7. After the button for Submodule_1 is pressed, the template information for Submodule_1 will be displayed in the ModelBuilder. This is shown in Figure 7b. Notice the tables are grayed-out. This is because the information is preview only and cannot be modified. To modify the information, load the submodule as the active module. Figure 7c shows when the button for Submodule_2 has been pressed.
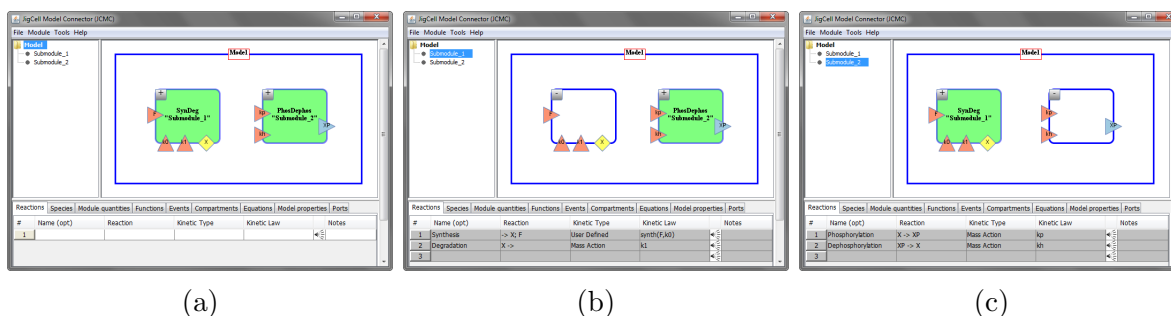

(a)   (b)   (c)

Figure 7: Submodule information preview

The submodule name is listed as:

<center>

<Definition Name>
"*<Submodule Name>*"

</center>

Definition Name corresponds to the name of the module definition. A module definition contains detailed information, such as reactions, species, parameters, and events. *Submodule Name* corresponds to the name of a specific instantiation of the template.

When selected by a right click, the submodule will show the following popup menu option:

- Edit Name: edit the submodule name.

Add

A submodule can be added using the Module Menu.

Remove

A submodule can be removed using the Module Menu. First, select the submodule to be removed. Next, under the Module Menu select Remove Module.

Note: this operation will remove the selected module, all of its submodules, and any connections associated with other modules.

3.3   Ports

Ports allow internal components of a module to be referenced outside of that module. A port can be linked to either a species or module quantity. Once created, the ports combine to form an interface. External access to a module's internal components is regulated by the interface. Modules can be connected together by their interfaces to build larger models.

An output port is linked to an internal component that will send a value to an external reference. The component linked to the port may be modified inside the module but the component is not meant to be modified outside the module. Consider the scenario where a species is synthesized in a module and then used as a transcription factor outside of the module. An output port is appropriate because the species is not modified outside of the module. Output ports are represented as triangles on the edge of modules. They are oriented so the arrowhead points out of the module.

An input port is linked to an internal component that will receive a value from an external reference. The component linked to the port is not meant to be modified within the module. Consider the scenario where a rate constant for a reaction within a module has a value determined outside of the module. An input port is appropriate because the rate constant is only used in calculations for the reaction and not modified inside the module. Input ports are represented as triangles on the edge of modules. They are oriented so the arrowhead points into the module.

An equivalence port is linked to an internal component that will both receive and send values from an external reference. The component linked to the port may be modified inside and outside the module. Consider the scenario where a species is synthesized in one module and phosphorylated in another module. An equivalence port is appropriate because the species is modified in both modules. Equivalence ports are represented as diamonds on the edge of modules.

When a port on the active module is selected by a right click (shown in Figure 8), the port will show the following popup menu options:

- Remove: remove the port and all associated connections.
- Properties: show the basic port properties.

In the ModelBuilder panel, ports are listed under the "Ports" tab (also shown in Figure 8). The list is populated with ports from the active module and ports from any submodules contained in the active module. When a port is selected in the DrawingBoard panel, the "Ports" tab is displayed and the corresponding port is highlighted in the ModelBuilder panel. Each port has three properties:

- Ref Name: the species or global quantity referenced by the port.
- Port Type: the type of port.
- Port Name: the name of the port.

Add

To add a port, right click the active module in the DrawingBoard and select "Add Port" from the module popup menu.

Below is a description of the fields:

- Ref Name: A drop-down box listing all of the species and global quantities in the module.
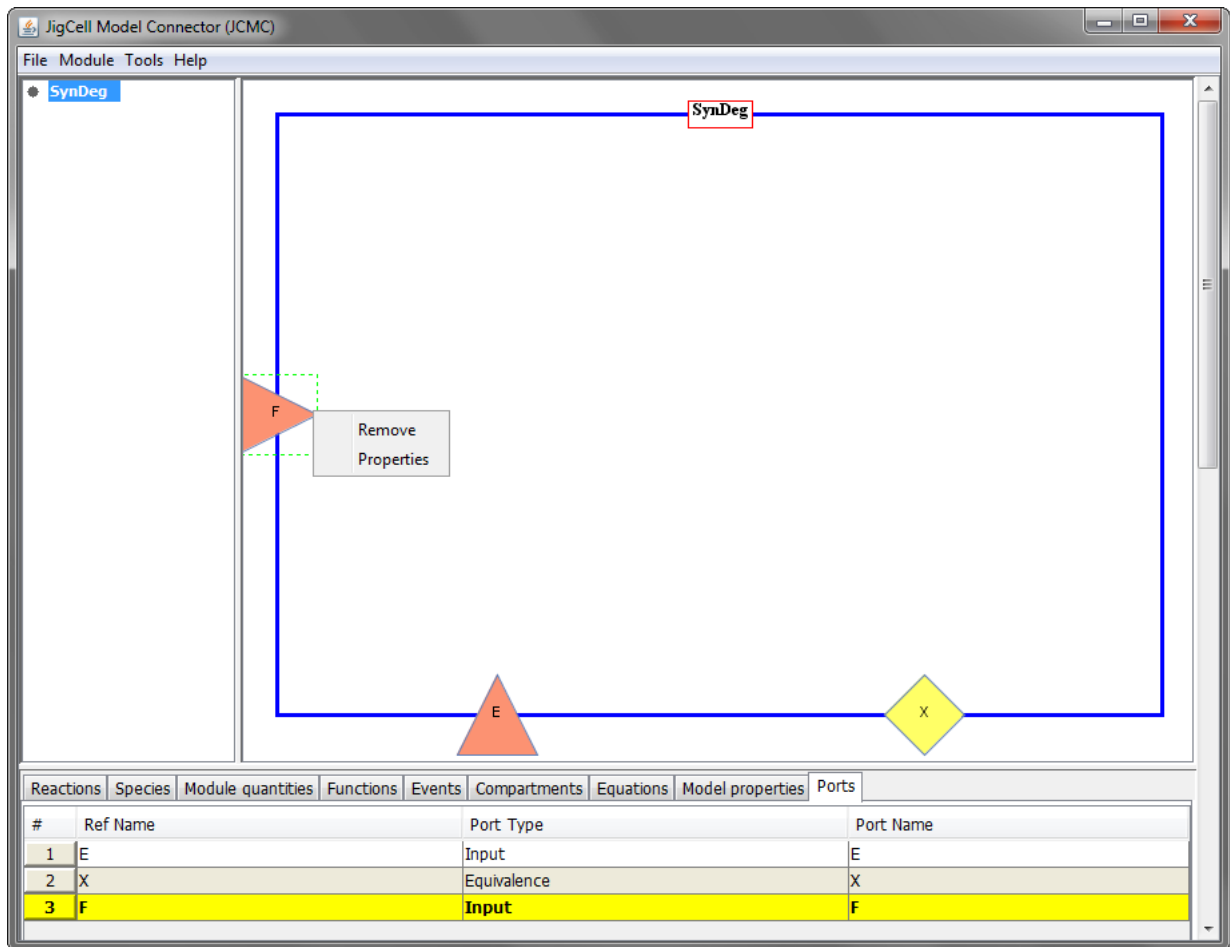
Figure 8: Port menu and tab

- Port Type: A drop-down box listing the three port types.
- Port Name: A text box for the user to input a name for the port.

Note: a port can only be added to the active module. To add a port to a submodule, load the submodule as the active module then add the port.

Remove

To remove a port, right click a port on the active module and select "Remove" from the popup menu.

Note: this will remove the port and any connections associated with the port. This will not remove the variable (species or global quantity) referenced by the port from the module.

3.4   Connections

A set of connections can link modules together. Connections can occur between the ports of different modules, visible variable nodes, and equivalence nodes. The rules for connections are listed in Tables 1, 2, and 3.

		Target Submodule Port		
		Input	Output	Equivalence
Source Submodule Port	Input	Invalid	Invalid	Invalid
	Output	Valid	Invalid	Invalid
	Equivalence	Valid	Invalid	Valid

Table 1: Rules for Submodule to Submodule connections

		Target Submodule Port		
		Input	Output	Equivalence
Source Module Port	Input	Valid	Invalid	Invalid
	Output	Invalid	Invalid	Invalid
	Equivalence	Valid	Invalid	Valid

Table 2: Rules for Module to Submodule connections

		Target Module Port		
		Input	Output	Equivalence
Source Submodule Port	Input	Invalid	Invalid	Invalid
	Output	Invalid	Valid	Invalid
	Equivalence	Invalid	Invalid	Valid

Table 3: Rules for Submodule to Module connections

Add

A connection can be created by dragging a line from a valid source to a valid target, as determined in Tables 1, 2, and 3 . When creating a possible connection, if the source and target would result in a valid connection then the target will be outlined in green (shown in Figure 9a). However, if the source and/or target would not result in a valid connection then the target will be outlined in red (shown in Figure 9b).
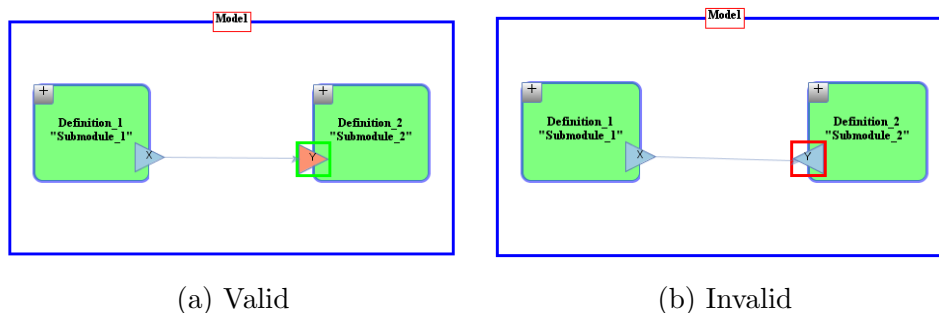

(a) Valid   (b) Invalid

Figure 9: Connections

Remove

To remove a connection, right click the edge and select "Remove Connection".

3.5   Visible Variable Nodes

A visible variable node allows connections to occur between the ports of modules and submodules.

Add

A visible variable node is automatically created when a connection is made between the ports of two modules. Figure 10a displays a module with two submodules. When a connection is made between the ports of the submodules, a visible variable is created. The new variable is added under the Species tab in the ModelBuilder panel (Figure 10b). Another way to create a visible variable node is to right click the active module and select "Show Variable". Once selected, a popup window will appear with a drop down box that contains a list of all the species and global quantities in the module. Select a variable, click Add, and a visible variable node will be created in the DrawingBoard panel.

Remove

To remove a visible variable node, right click the node and select "Remove".

Note: this will remove the visible variable node and any connections associated with the node.
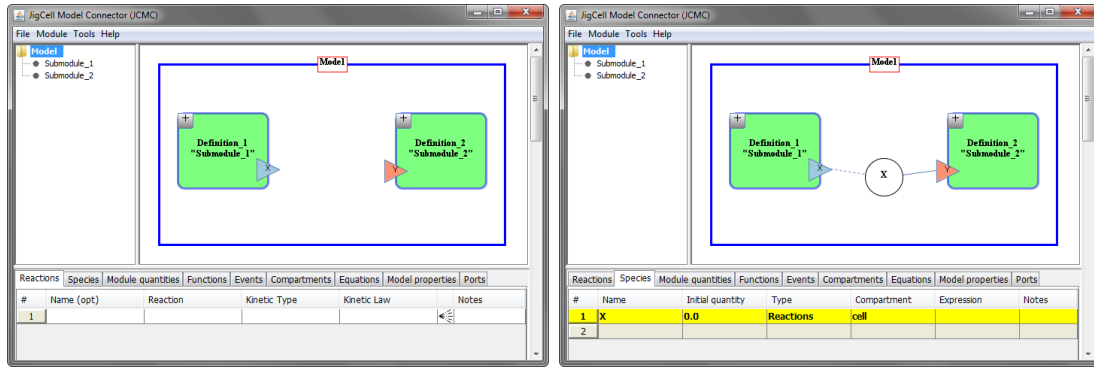
Figure 10: Visible Variable created with a connection

3.6 Equivalence Nodes

Add

An equivalence node is created automatically when a connection is made between an equivalence port and any other port in the DrawingBoard panel. When created, the new variable is added under the Species tab in the ModelBuilder panel.

Remove

To remove an equivalence node, right click the node and select "Remove".

Note: this will remove the equivalence node and any connections associated with the node.