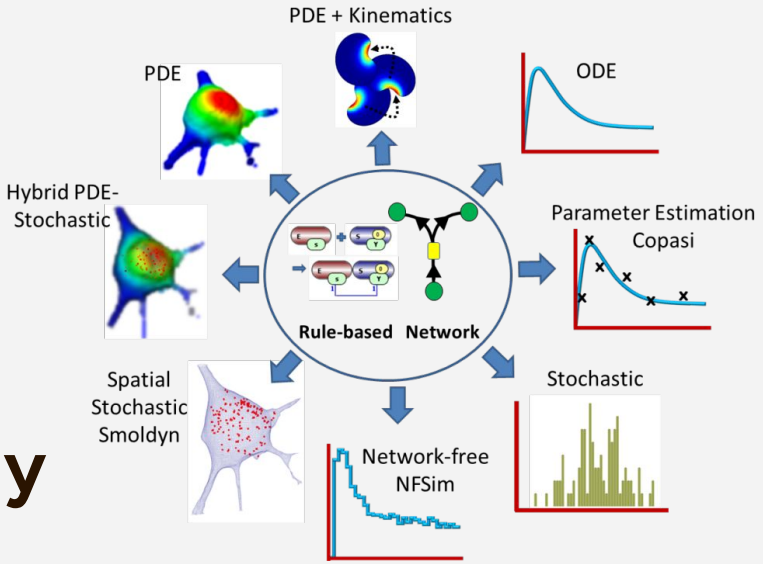
VCell

The Virtual Cell

A modeling environment for the simulation of cellular events. Download at vcell.org
Version 7.7 July 2025



Defining Model Physiology

Virtual Cell is developed by the Center for Cell Analysis and Modeling at the University of Connecticut Health Center. It is funded by the National Institute of General Medical Sciences (NIGMS)

NIH National Institute of General Medical Sciences

VCell is funded by the NIGMS

CCAM VCell is developed at CCAM

Center for Cell Analysis & Modeling

Defining Model Physiology

Objective:

Create a single Biomodel of Ran nuclear transport using Virtual Cell modeling and analysis software.

Goals:

- ➔ Understand the basic functions of VCell software as it pertains to this tutorial.
- ➔ Create a Biomodel Physiology with species, reactions, and fluxes.

General familiarity with VCell software is recommended. Although this tutorial can be followed by a VCell novice, it is recommended that novice users first look through the VCell tutorials available at http://vcell.org/support

Model building can be matched to the BioModel **Tutorial_MultiApp** in the Tutorial folder in the **VCell Database.**

How to Save Your Model

- **To save your model, go to the top left corner and click:**
  - **File → Save**

- If your model cannot be saved, check your errors in the bottom panel titled “Problems.” Clicking on an error will lead you to the part of the model that may not let you save.

- If you can’t save your model because of errors, you can save as local in the VCML format and reload into VCell later.

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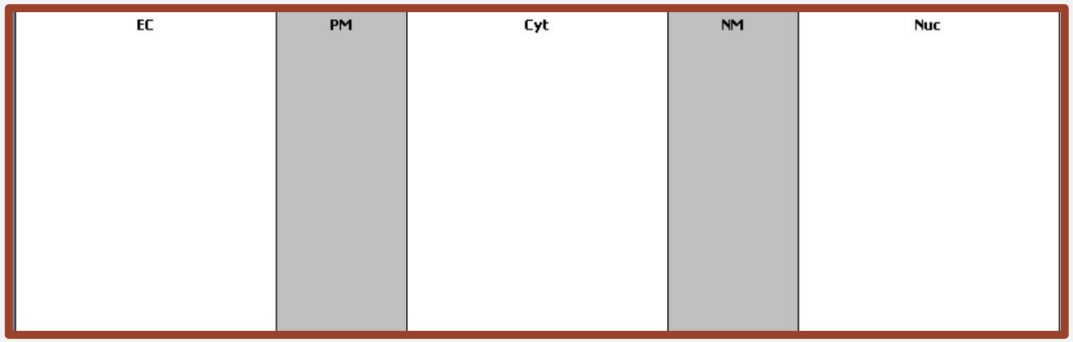
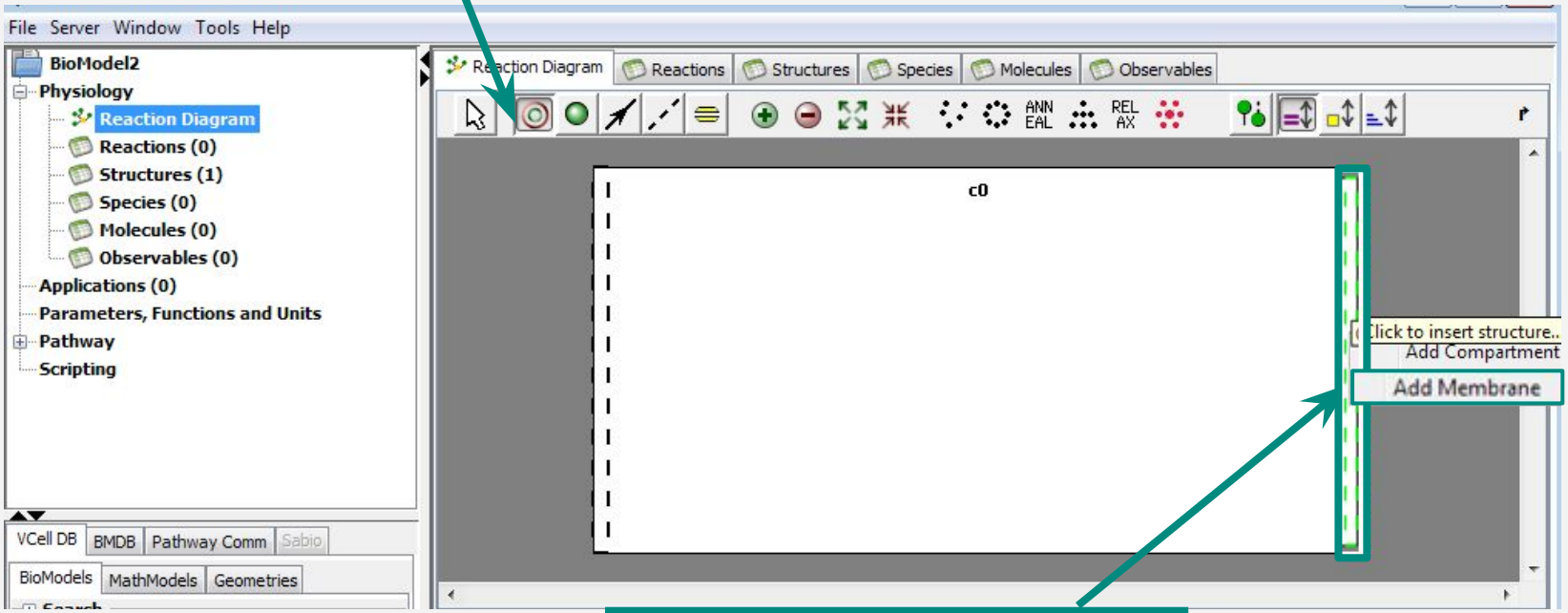
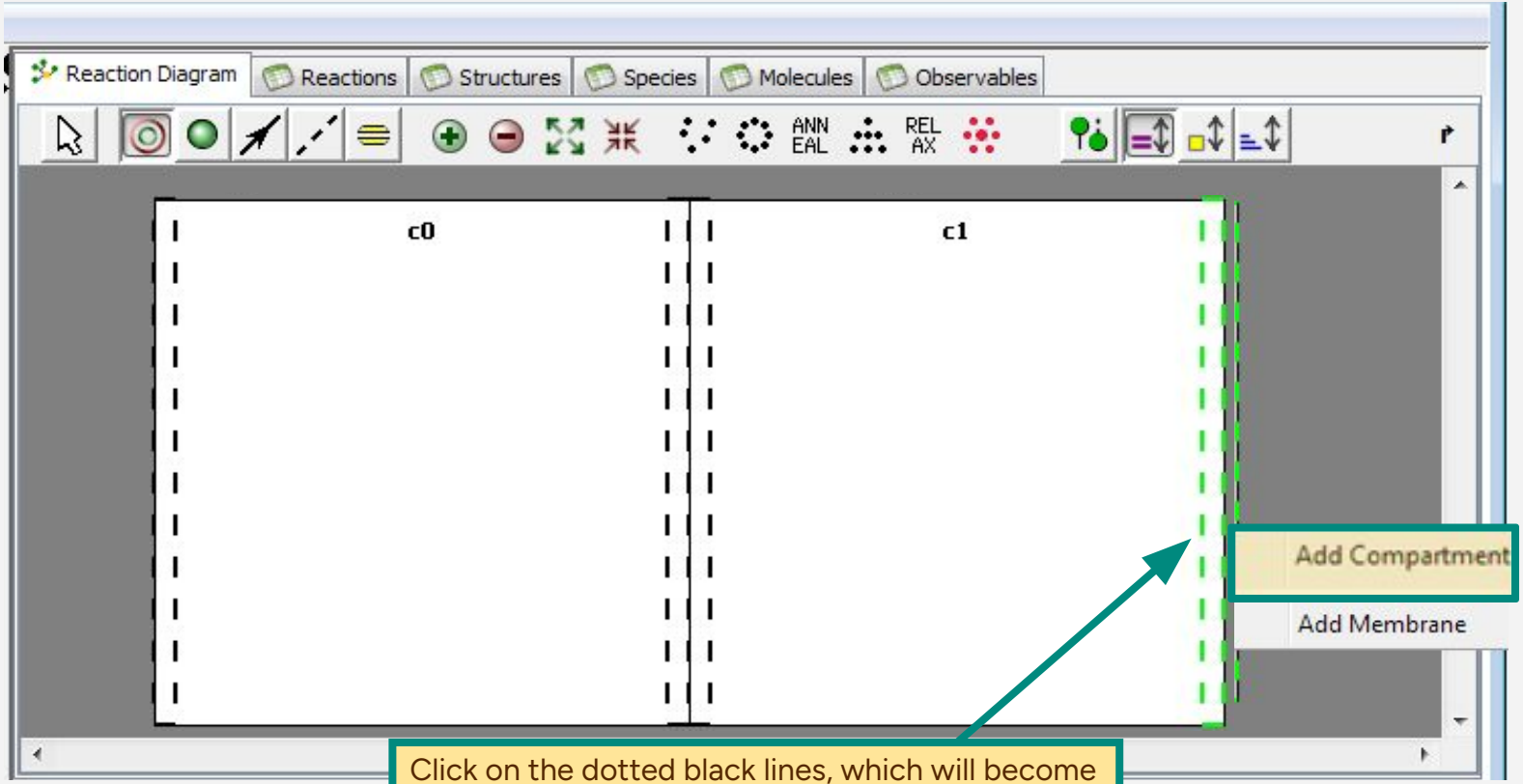


Creating Compartments

Start with creating a volumetric compartment by selecting the **Structure Tool.**

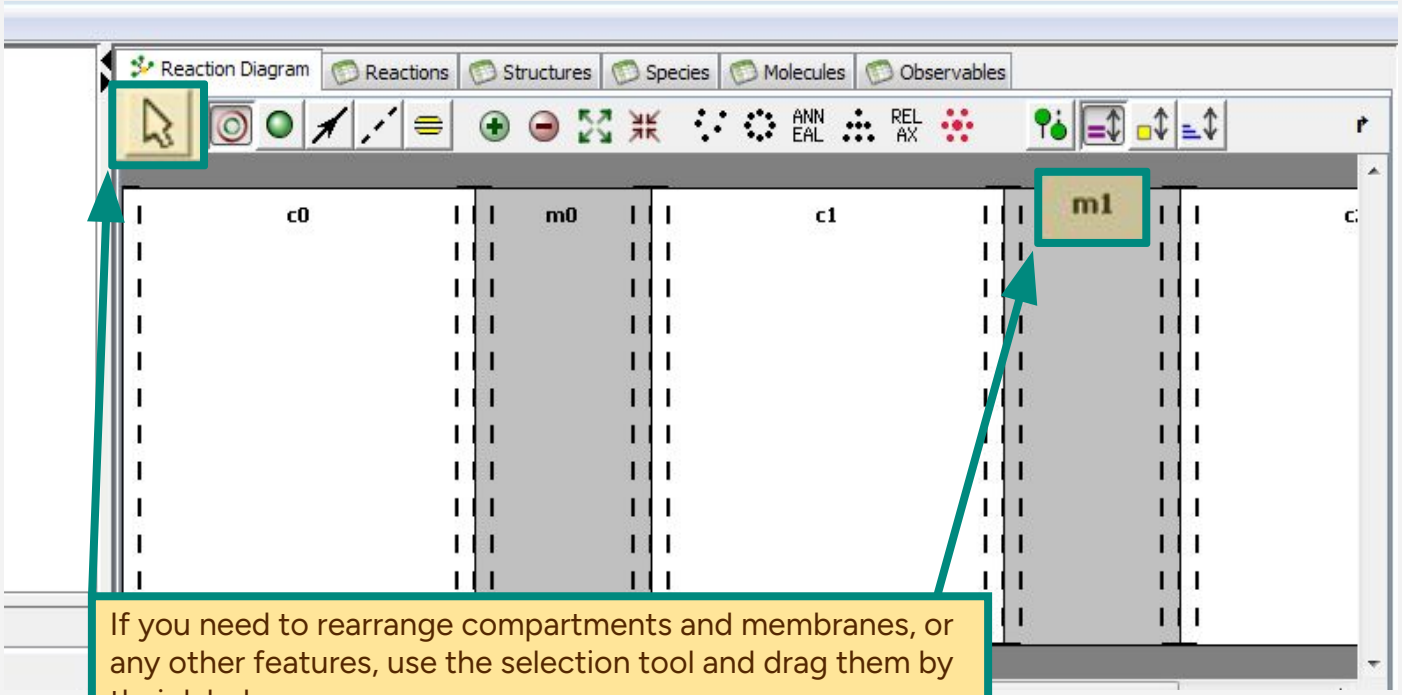


Click on one of the black lines so they turn green, and select **Add Membrane** to make a new membrane.



Click on the dotted black lines, which will become green, and select **"Add Compartment"** to create a new compartment.

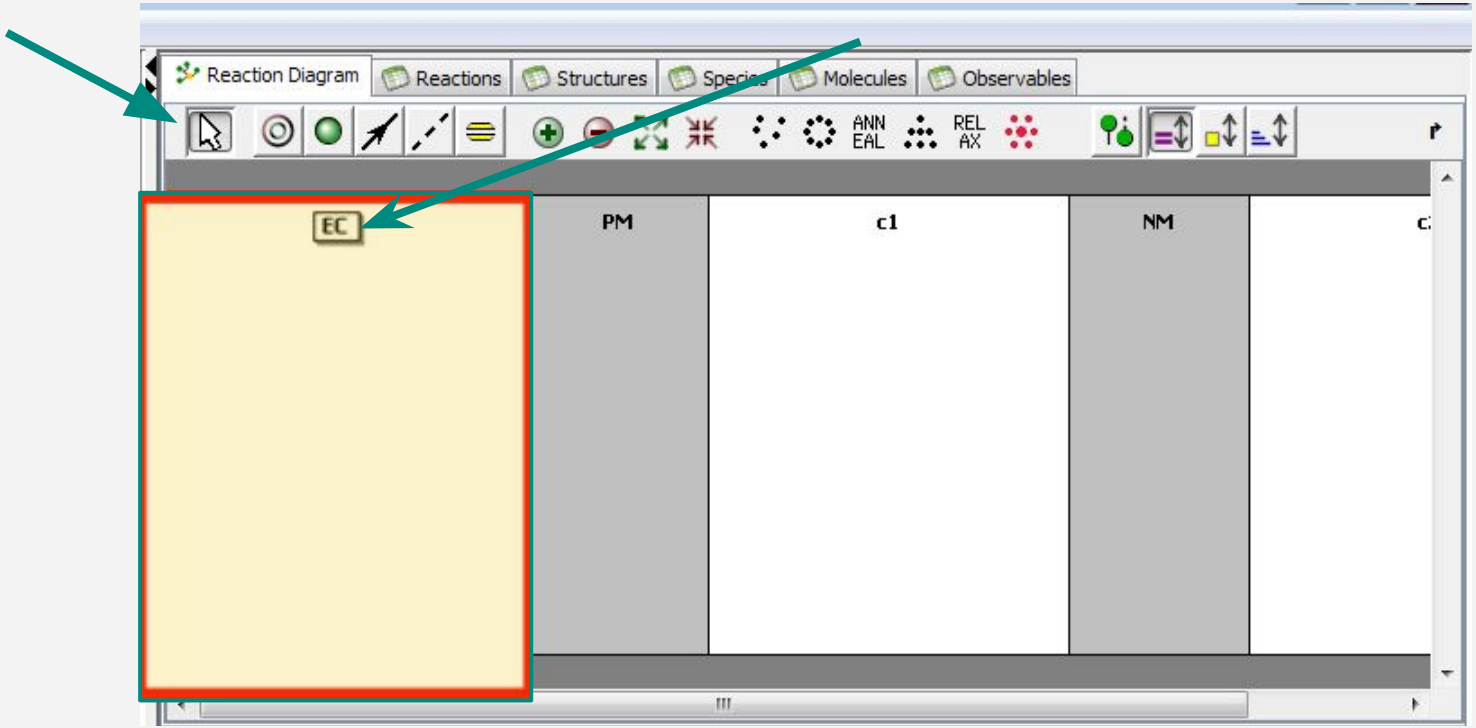
This model requires 3 compartments separated by 2 membranes. Continue creating two additional compartments that are separated by a membrane.

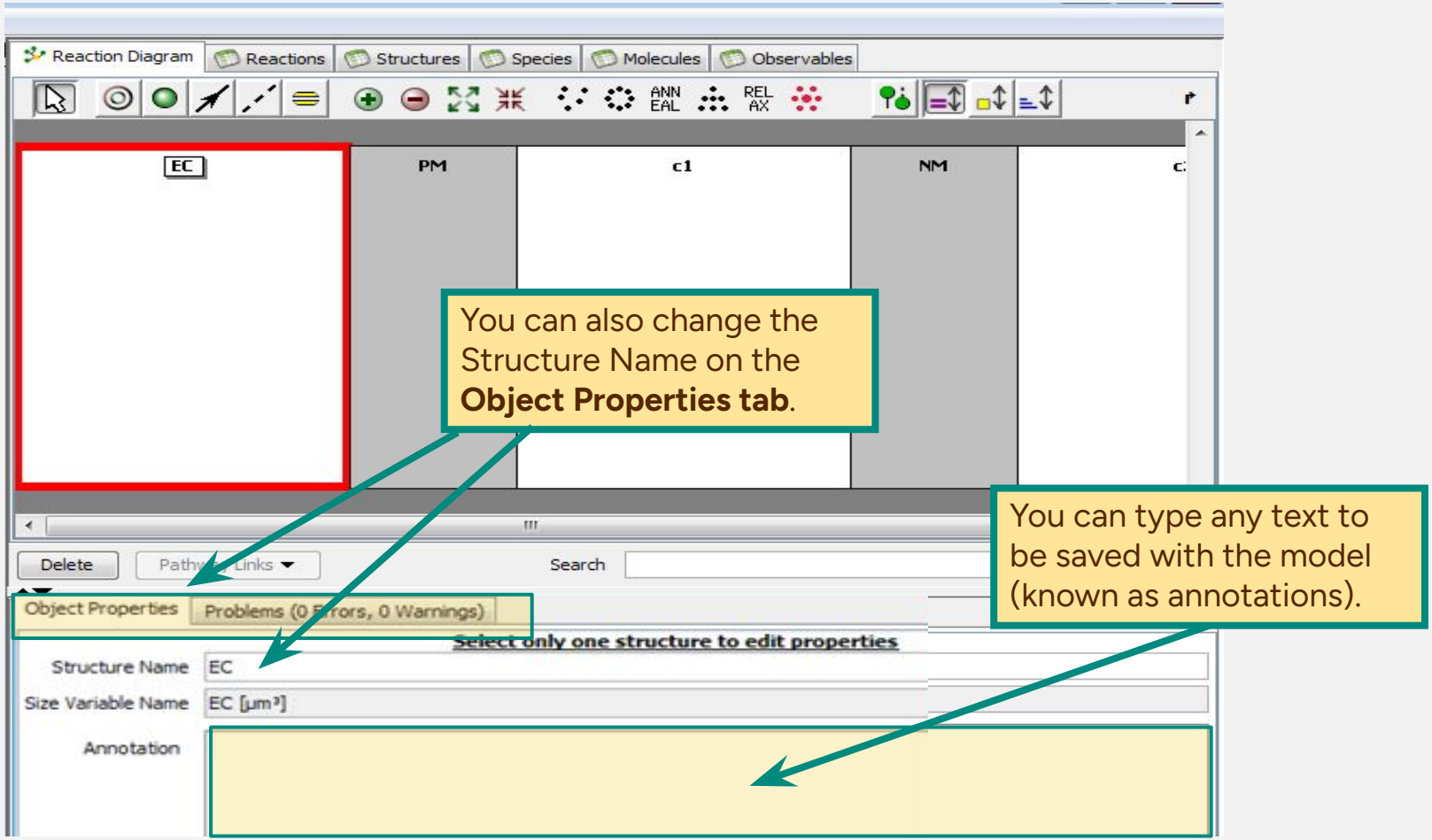


If you need to rearrange compartments and membranes, or any other features, use the selection tool and drag them by their label.

TIP: add compartments and membranes in numerical order (e.g. c0, c1, c2).

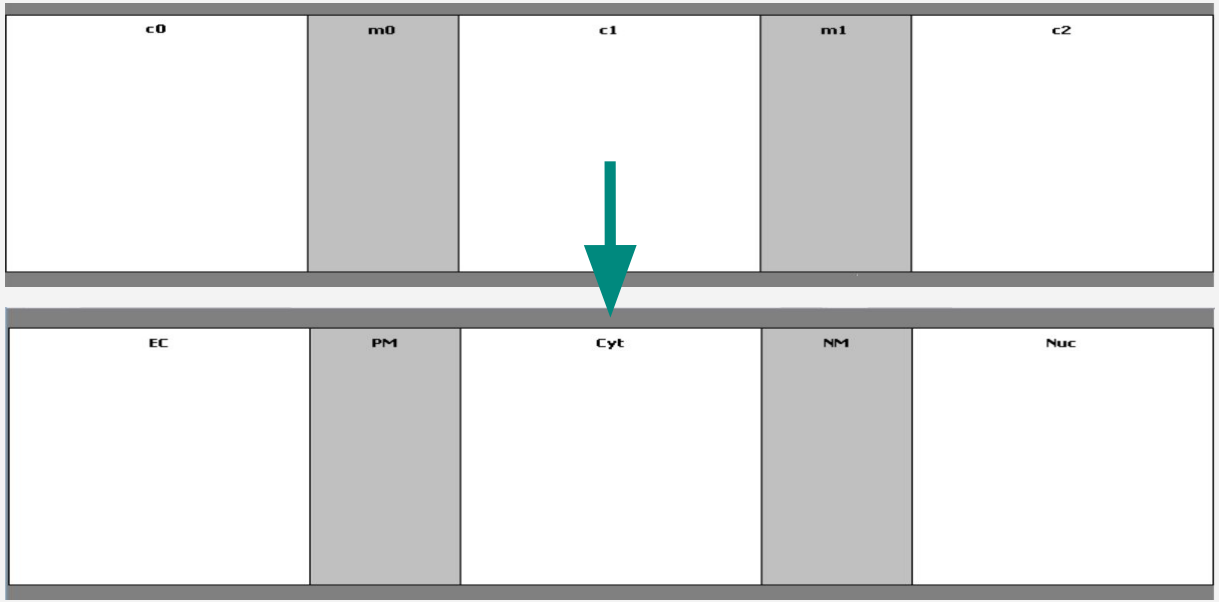
Use the **selection tool** to name compartments and membranes. The area will turn red upon selection. Double click the structure name you wish to change and enter the new name.




Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
EC
PM
c1
NM
Delete
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one structure to edit properties
Structure Name
EC
Size Variable Name
EC [μm³]
Annotation
You can also change the Structure Name on the **Object Properties tab**.
You can type any text to be saved with the model (known as annotations).

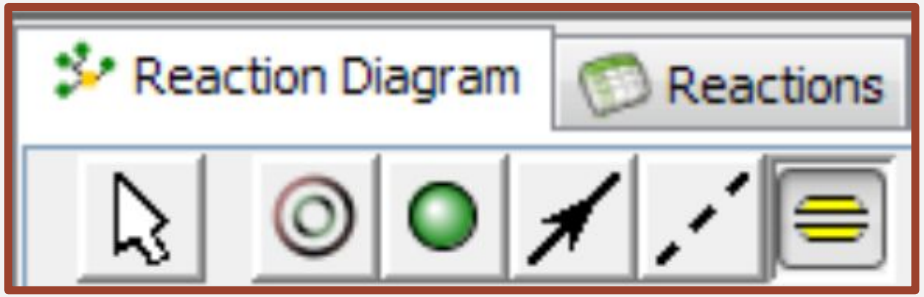
To be consistent with the next tutorials and the MultiApp_Tutorial model, please rename the compartments and membranes to the following:

- C0 -> EC (Extracellular)
- M0 -> PM (Plasma Membrane)
- C1 -> Cyt (Cytosol)
- M1 -> NM (Nuclear Membrane)
- C2 -> Nuc (Nucleus)



02

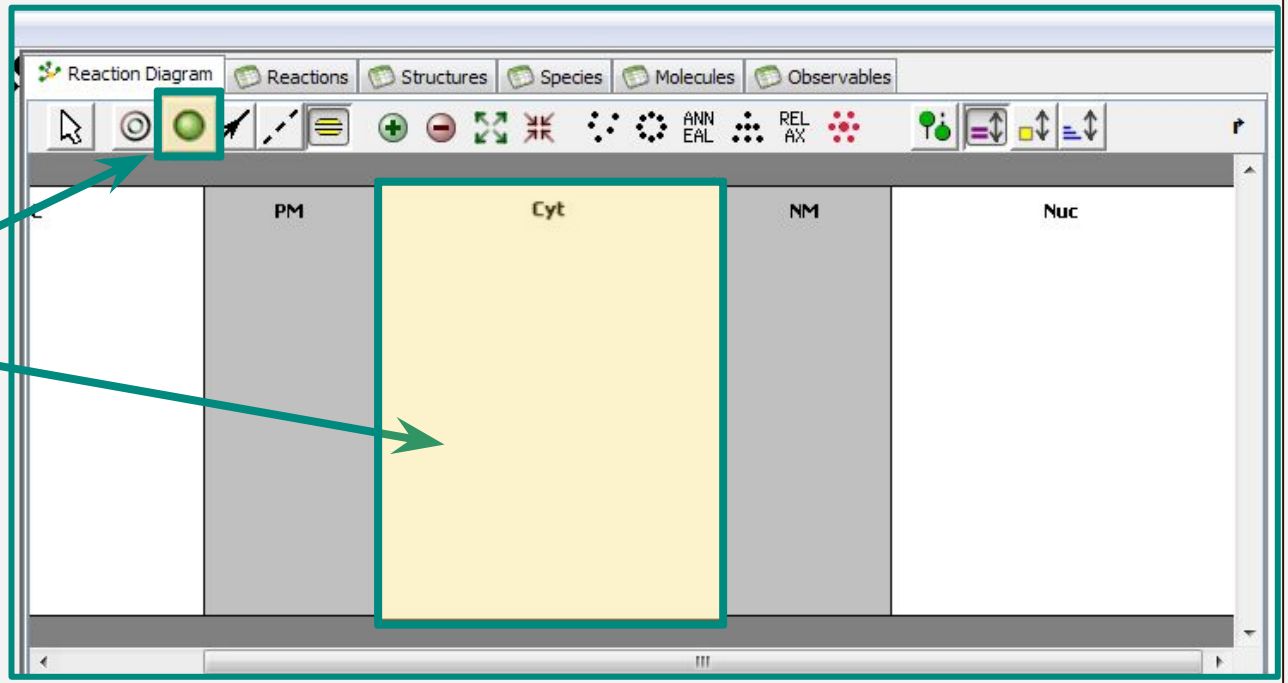
Defining a Species



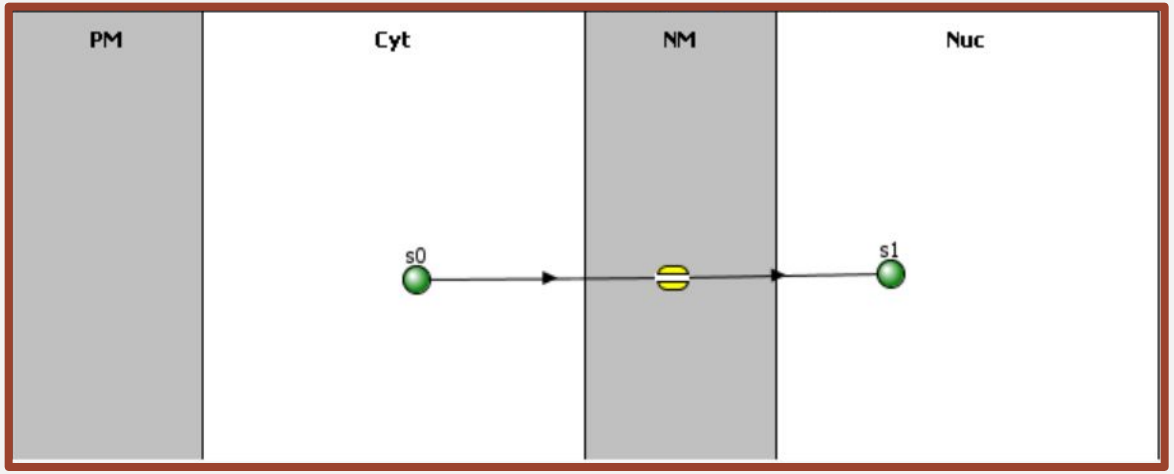
Chemical Species - A pool of chemically identical molecular entities that serve as variables in the model.

TIP: Always save your model as soon as possible; begin saving after adding your first species and structures.

To create a species, click on the **species** tool and click in the area you want to place the species.

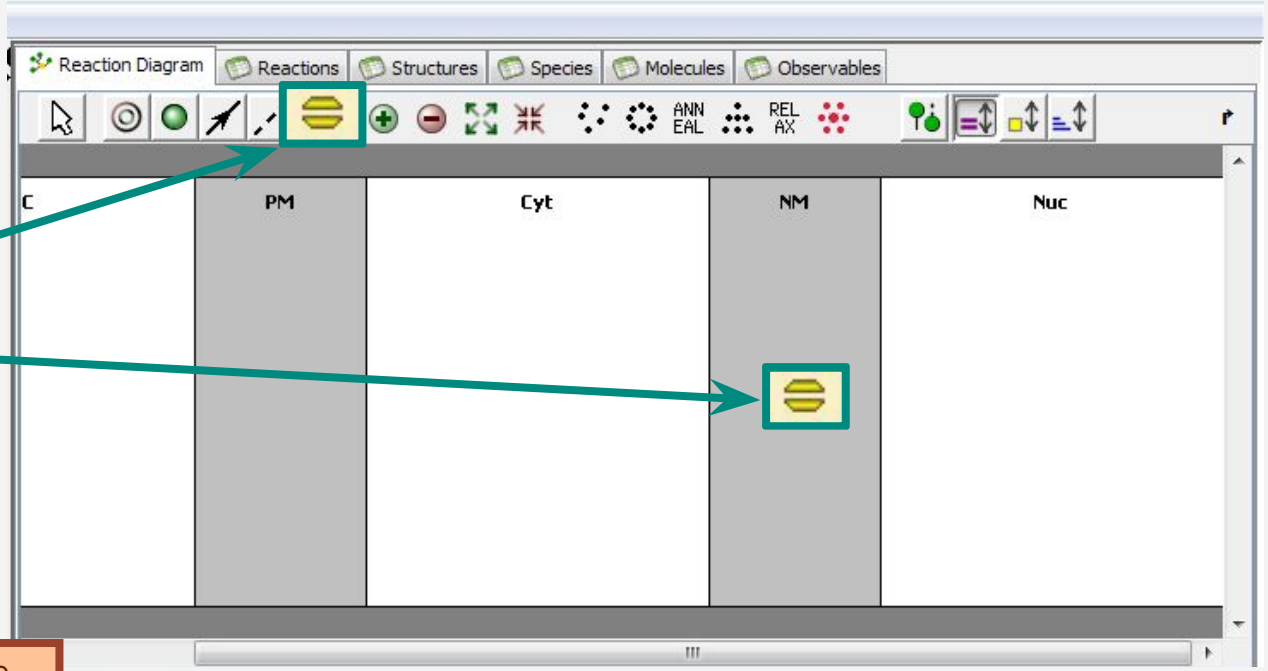


03

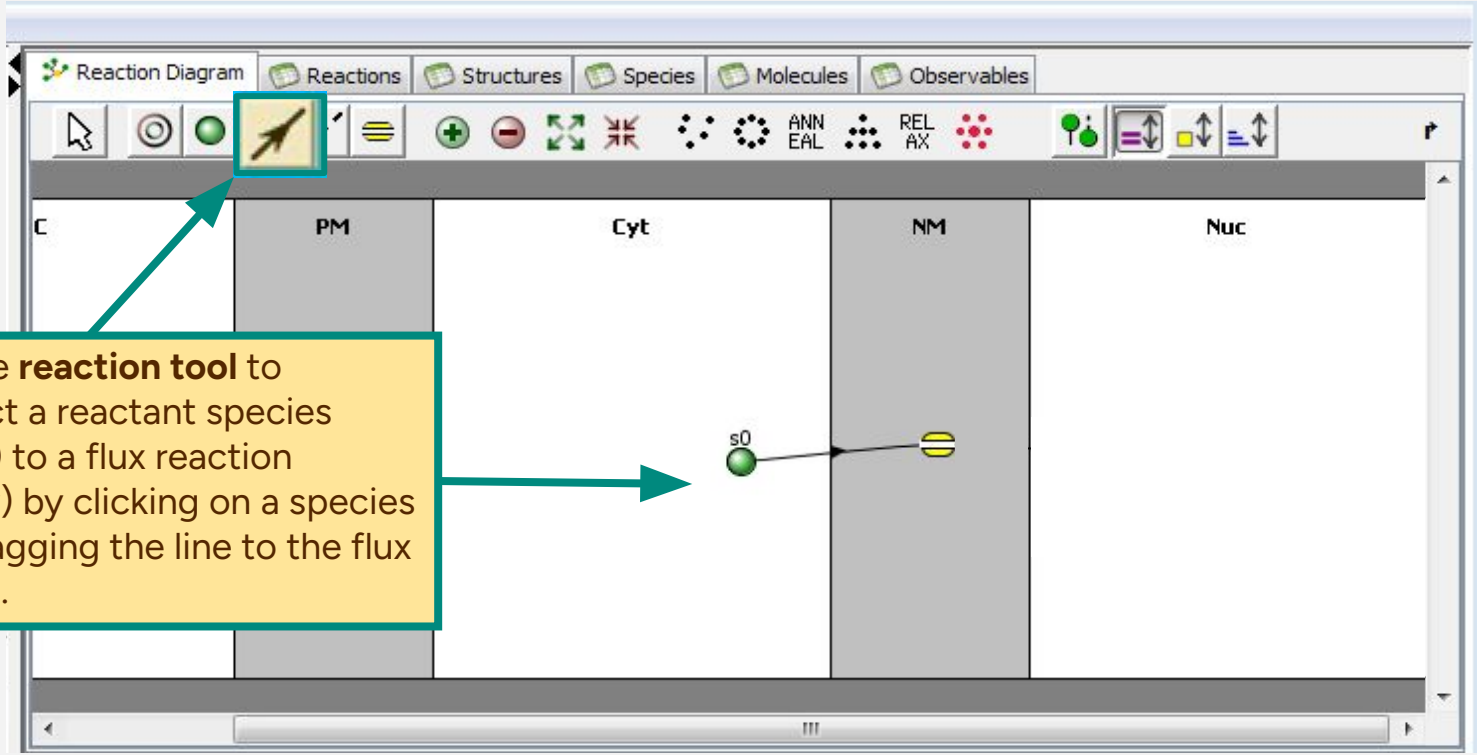


Making a Reaction Across a Membrane

Click on the **FluxReaction** tool, then click in the area where you want to place the flux (NM). Fluxes can be placed in membranes only.



Flux: The rate at which a substance, energy, or property passes through a surface.


Reaction Diagram
Reactions
Structures
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ANN EAL
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PM
Cyt
NM
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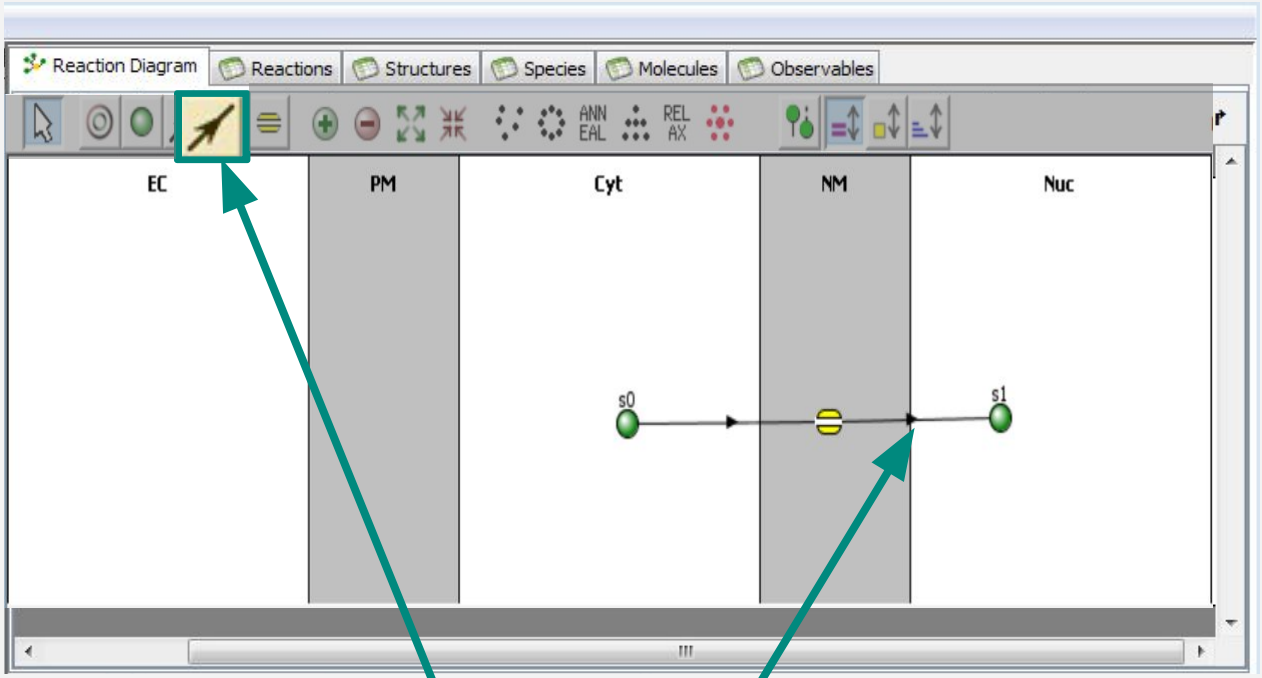
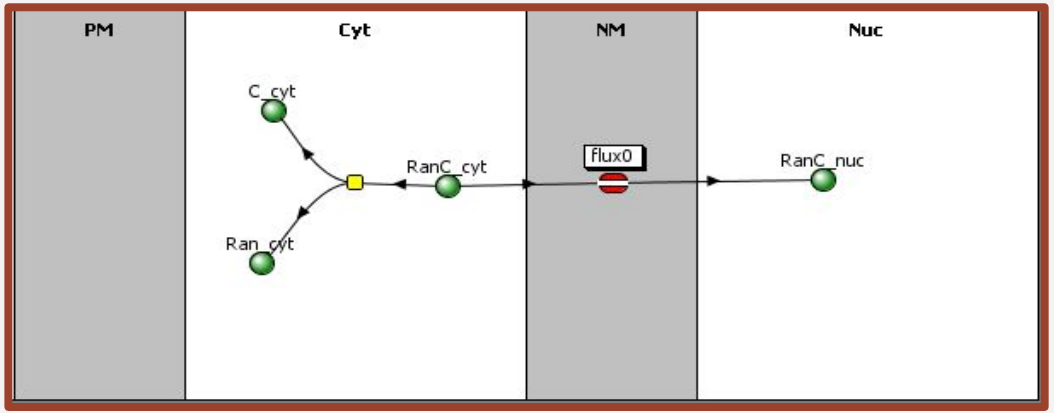
Use the **reaction tool** to connect a reactant species (green) to a flux reaction (yellow) by clicking on a species and dragging the line to the flux symbol.

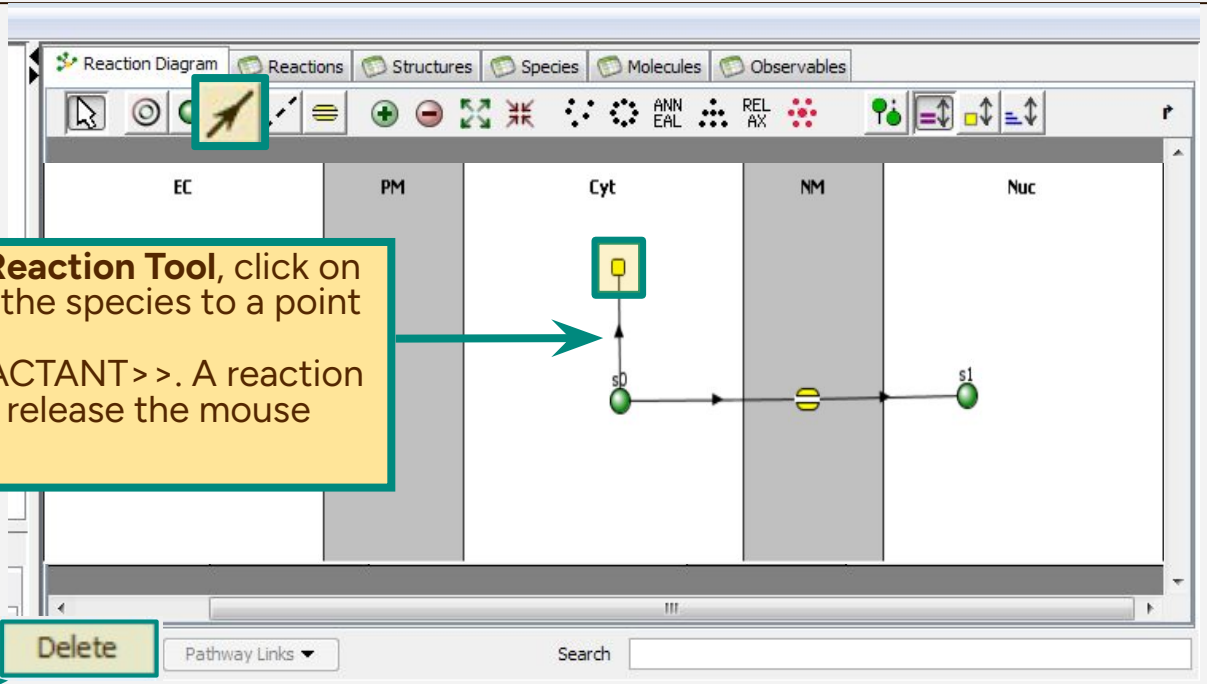


To create a product of a flux reaction, use the **reaction tool** to drag a line from the flux to a point inside the compartment where a product species will be made.

04



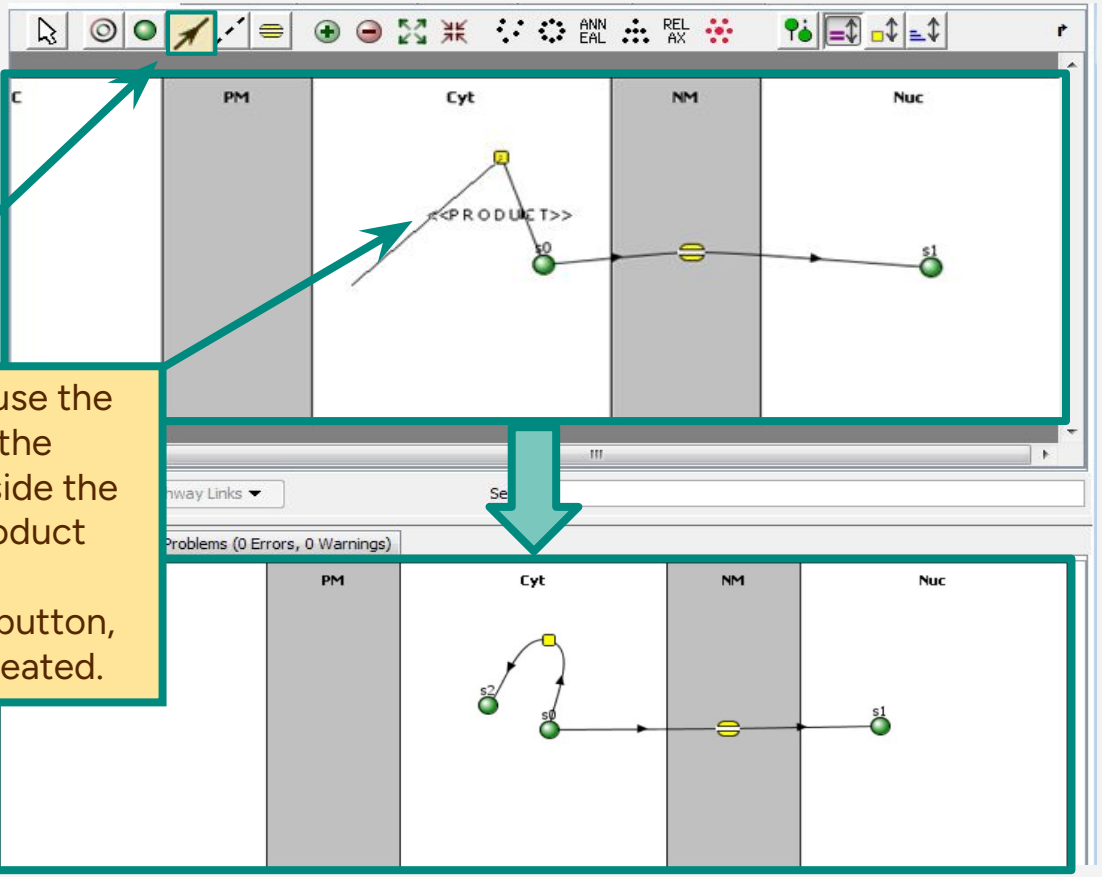
Creating a Reaction in a Compartment

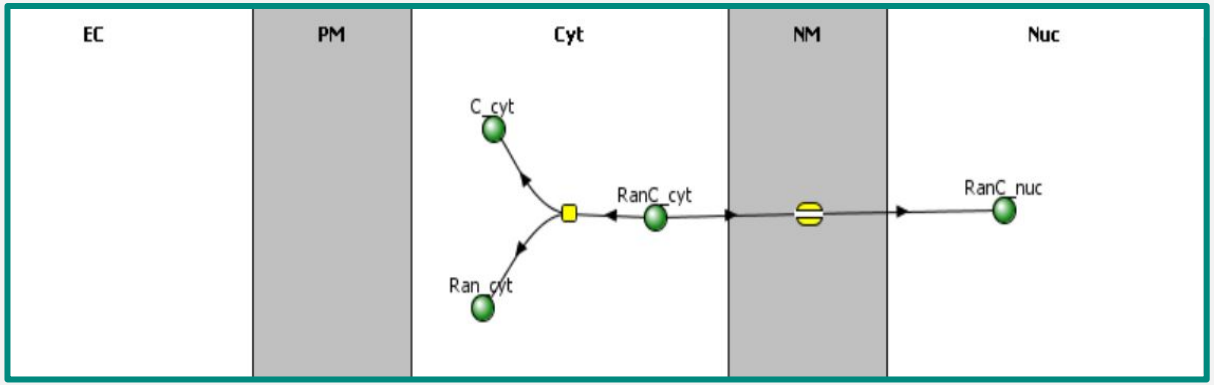


To create a reaction with the **Reaction Tool**, click on a species and drag a line from the species to a point inside the compartment.
The active line will read <<REACTANT>>. A reaction node will be created once you release the mouse button.

To remove a species or reaction from your model, select the species/reaction and click either the "**Delete**" button or backspace on your keyboard.

To create a product species, use the **Reaction Tool** and drag from the reaction symbol to a point inside the compartment where your product species will be located.
Once you release the mouse button, the product species will be created.



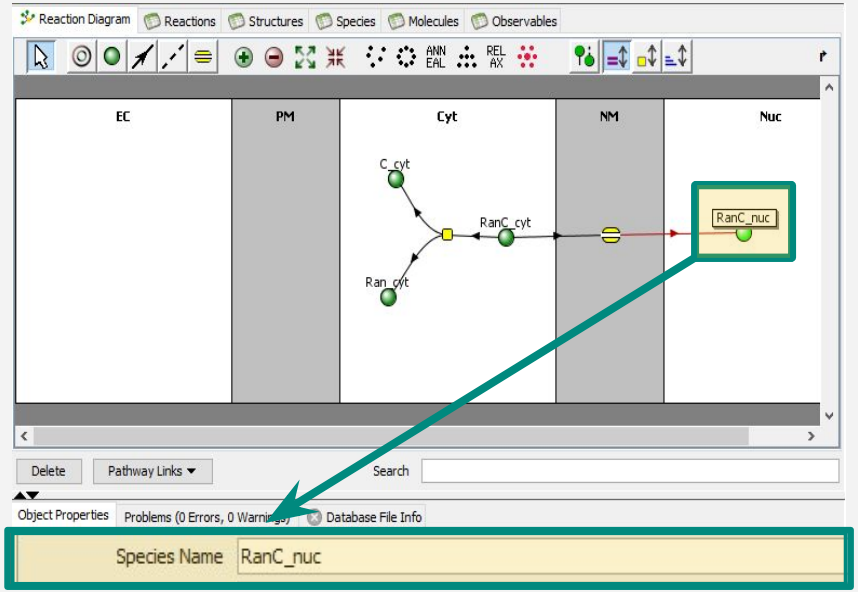


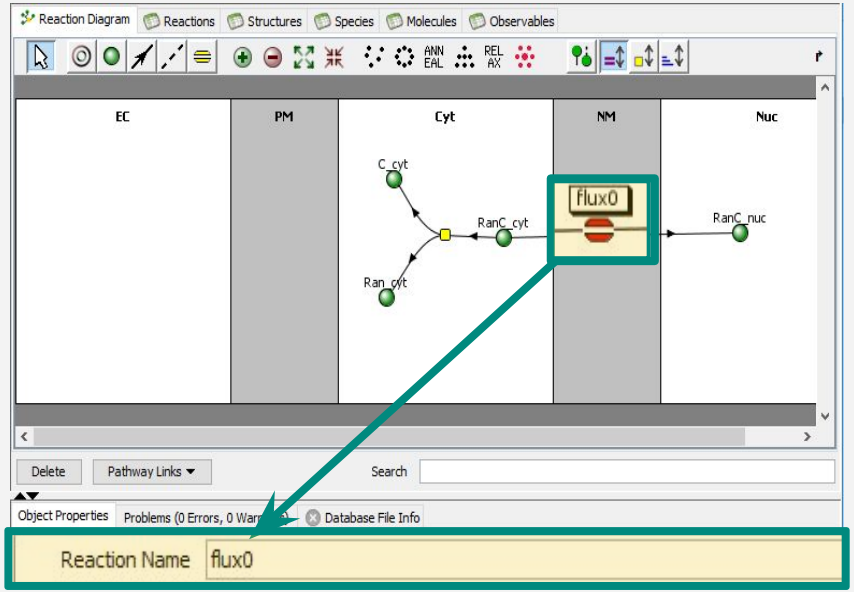
Continue adding components to your model and naming them until you have the following objects as described in the table below.

NOTE: you can't move species, reactions, or fluxes from one compartment to another. You must delete a species, flux, or reaction from one compartment and then create it in another compartment.

Name	Description	Location
RanC_nuc	Ran-Cargo Complex	Nucleus
	Flux Reaction Node	Nuclear Membrane
RanC_cyt	Ran-Cargo Complex	Cytoplasm
	Reaction Node	Cytoplasm
C-cyt	Cargo	Cytoplasm
Ran_cyt	Ran- GTPase	Cytoplasm

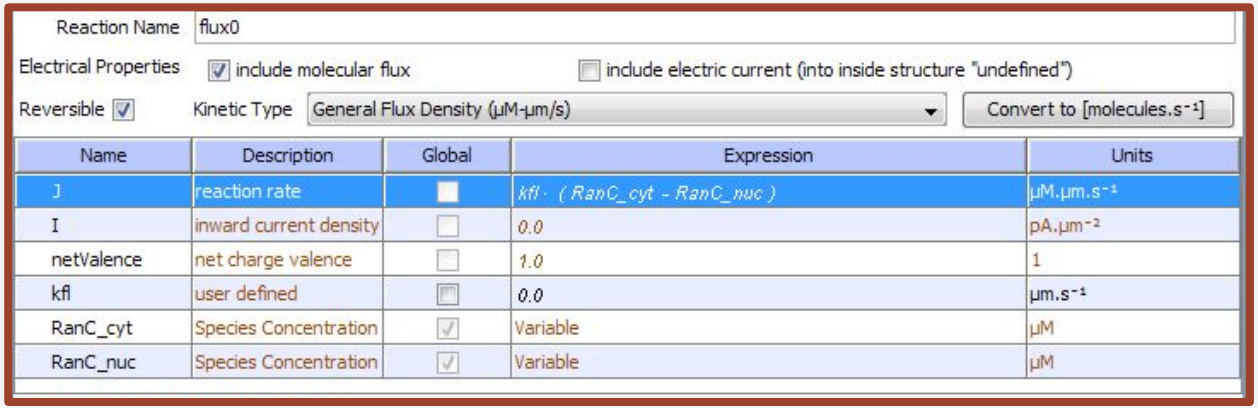
If you need to rename a component, select it, and on the **Object Properties** tab, use the component's name text field to supply the new name.



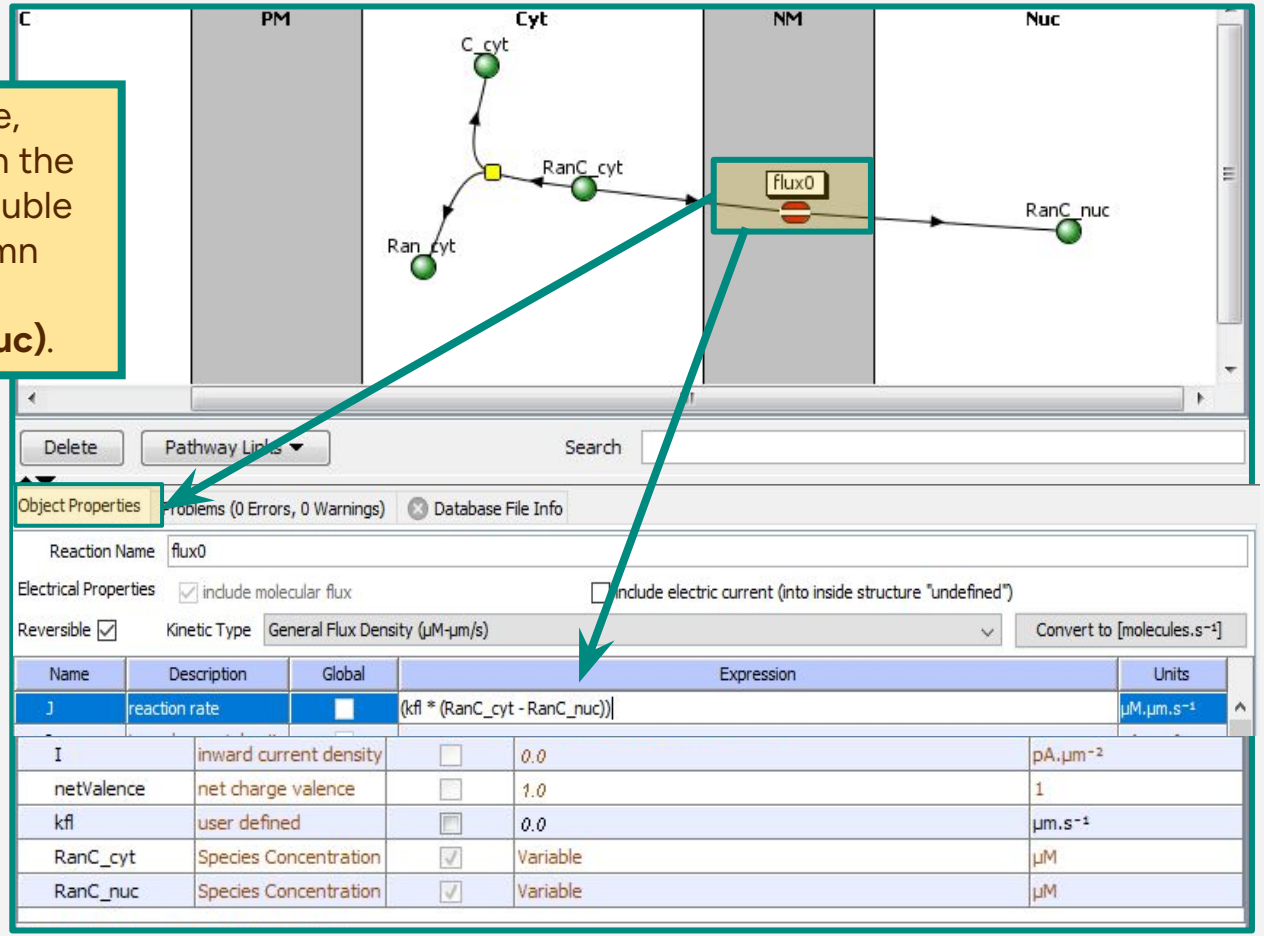


05

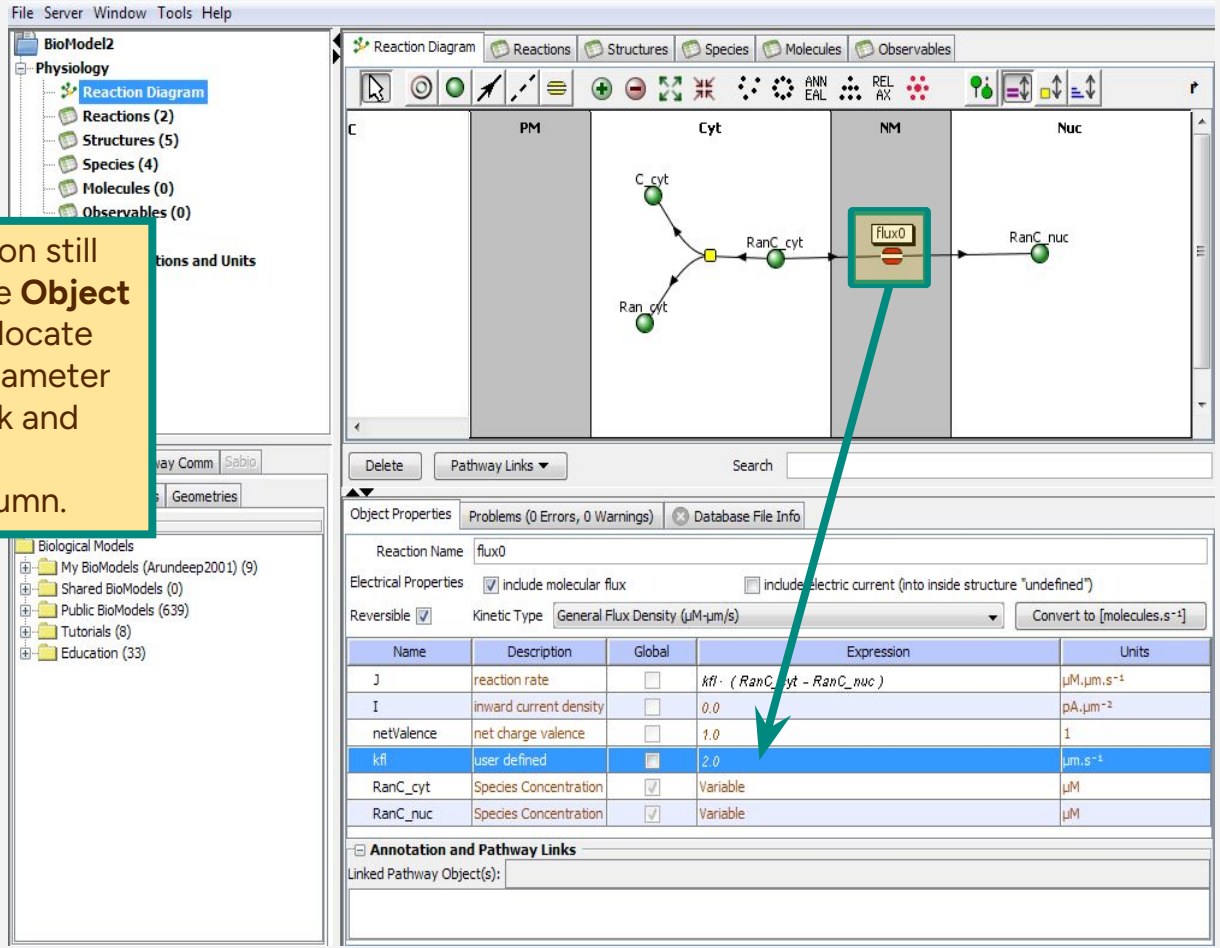
Defining Reaction Kinetics

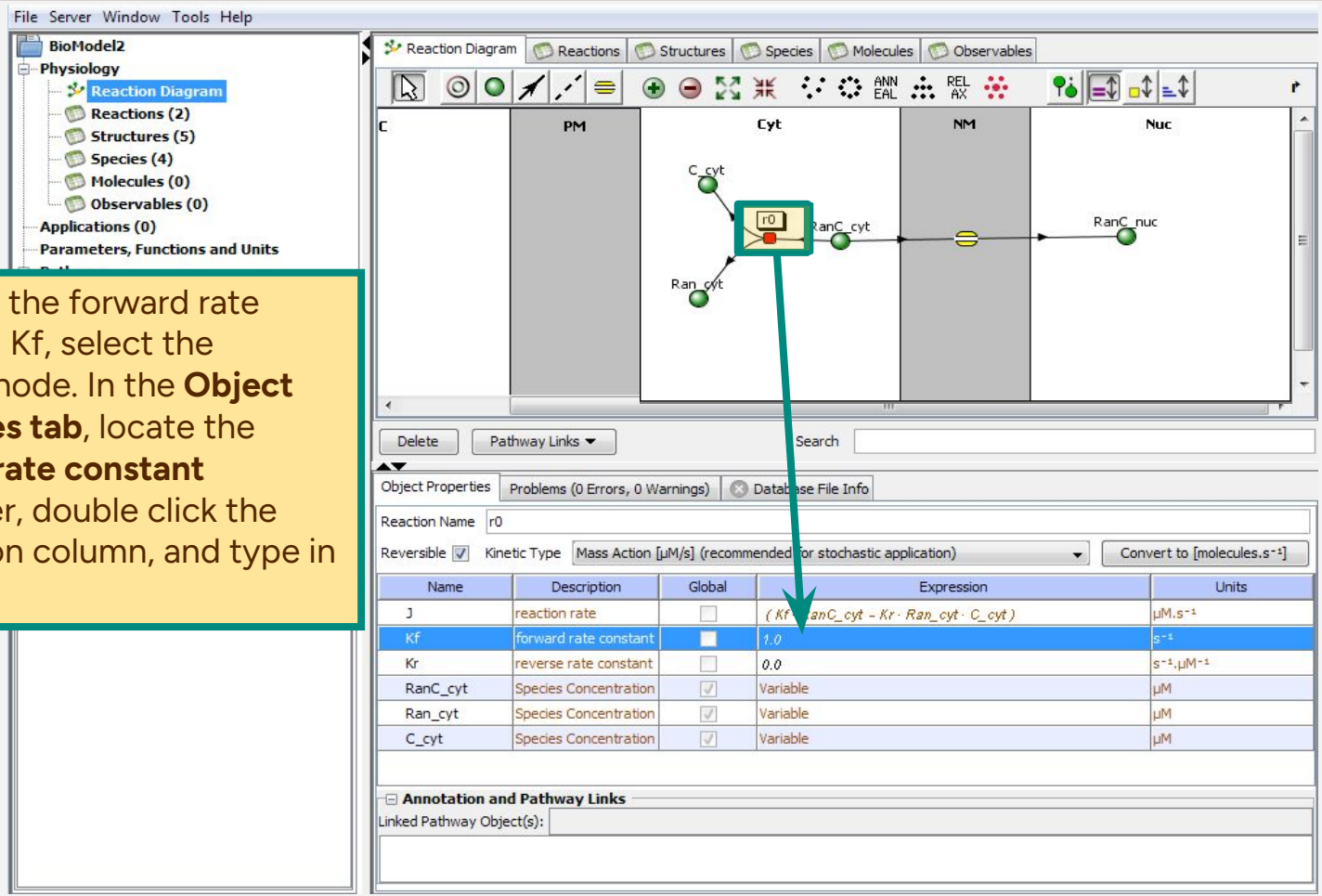


To define the reaction rate, select the **flux icon**, and in the **Object Properties** tab, double click the **Expression** column and type:
kfl * (RanC_cyt - RanC_nuc).



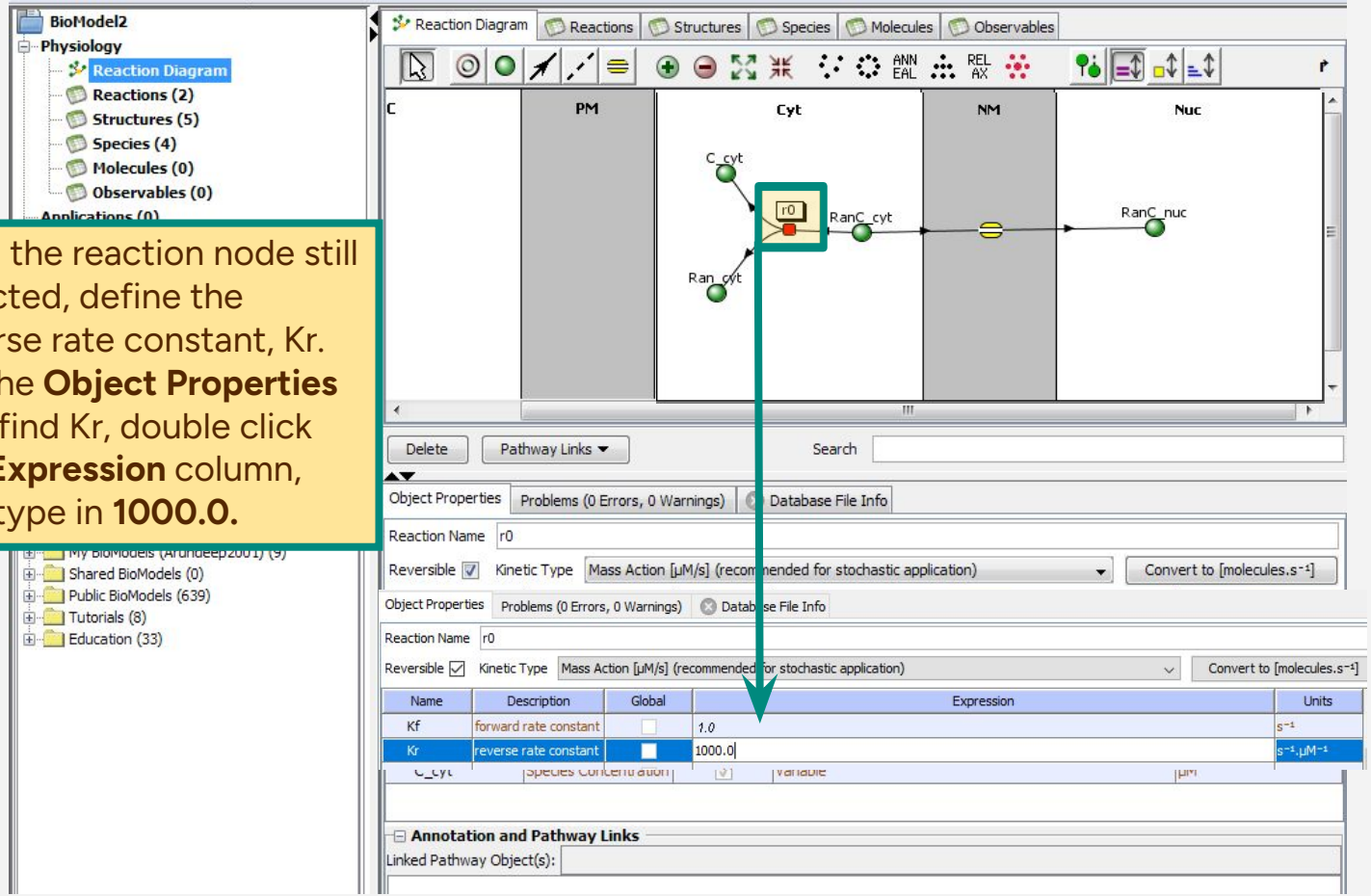
With the flux icon still selected, on the **Object Properties** tab locate the defined parameter **Kfl**. Double click and type **2.0** in the **Expression** column.

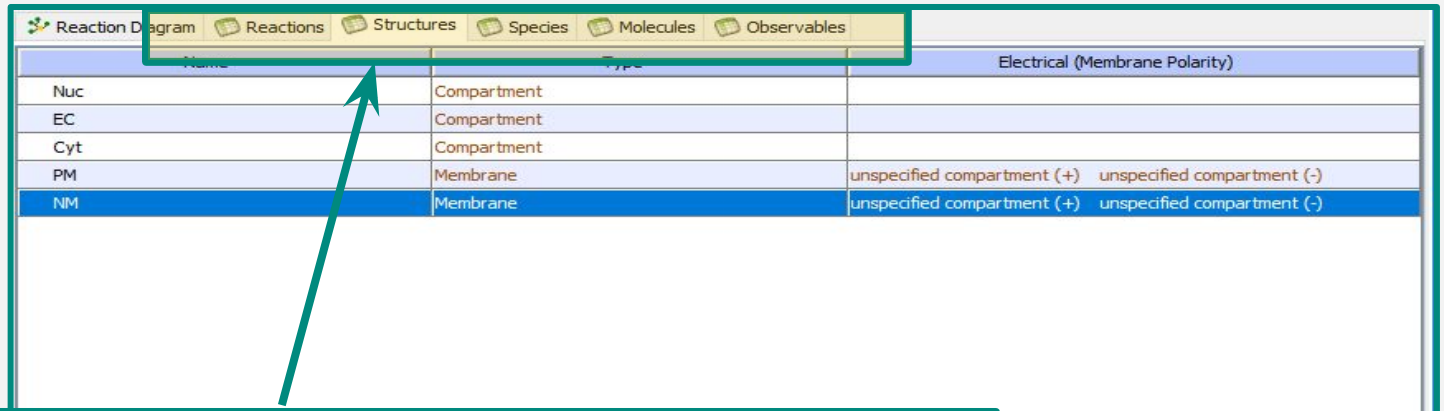




To define the forward rate constant, Kf, select the reaction node. In the **Object Properties tab**, locate the **forward rate constant** parameter, double click the Expression column, and type in **1.0.**

With the reaction node still selected, define the reverse rate constant, Kr. On the **Object Properties tab,** find Kr, double click the **Expression** column, and type in **1000.0.**





Use the **Reactions, Structures, Species, Molecules or Observables** tabs to look up specific details of the physiology shown in a table view as opposed to the Reaction Diagram. This is useful when working with large and complicated models.

Tip: If someone shares a model with you, click **Account-> Reconnect** to refresh your device's connection to the database.

Acknowledgments

This tutorial was prepared by Sreekirthana Kolla (East Granby High School) and Justine Laureano (East Hartford High School) under the guidance of Dr. Michael L. Blinov, Associate Professor, Center for Cell Analysis and Modeling. The students were funded by the Department of Health Career Opportunity Programs; the Aetna Foundation; Connecticut State Legislative Fund; John and Valerie Rowe Health Professions Scholars Program; The Hartford; the University of Connecticut Foundation; the Friends of the Department of Health Career Opportunity Programs; and UConn Health.