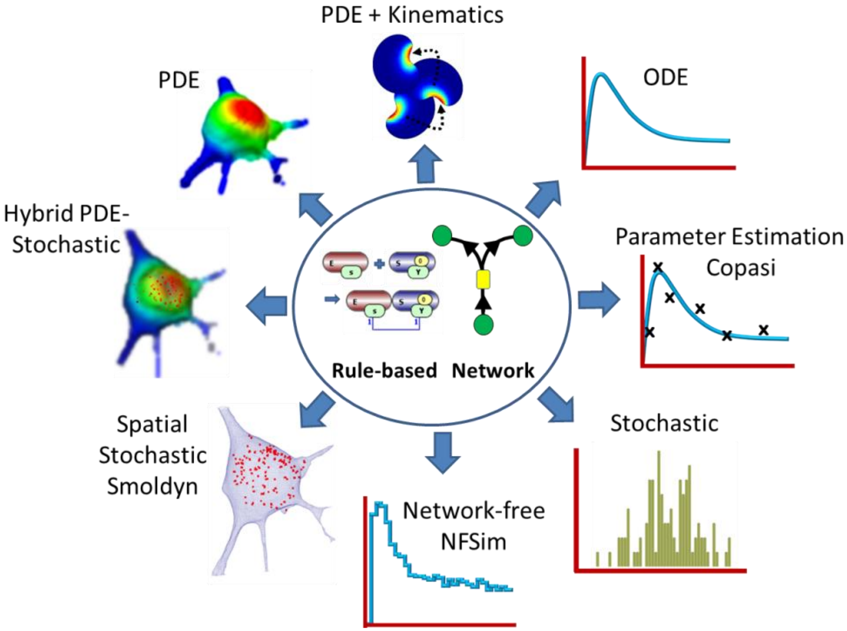
VCell

modeling environment for mathematical simulation of cellular events.

To run VCell go to:

vcell.org


PDE + Kinematics
PDE
ODE
Hybrid PDE-Stochastic
Parameter Estimation
Copasi
Rule-based
Network
Spatial
Stochastic
Smoldyn
Stochastic
Network-free
NFSim

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

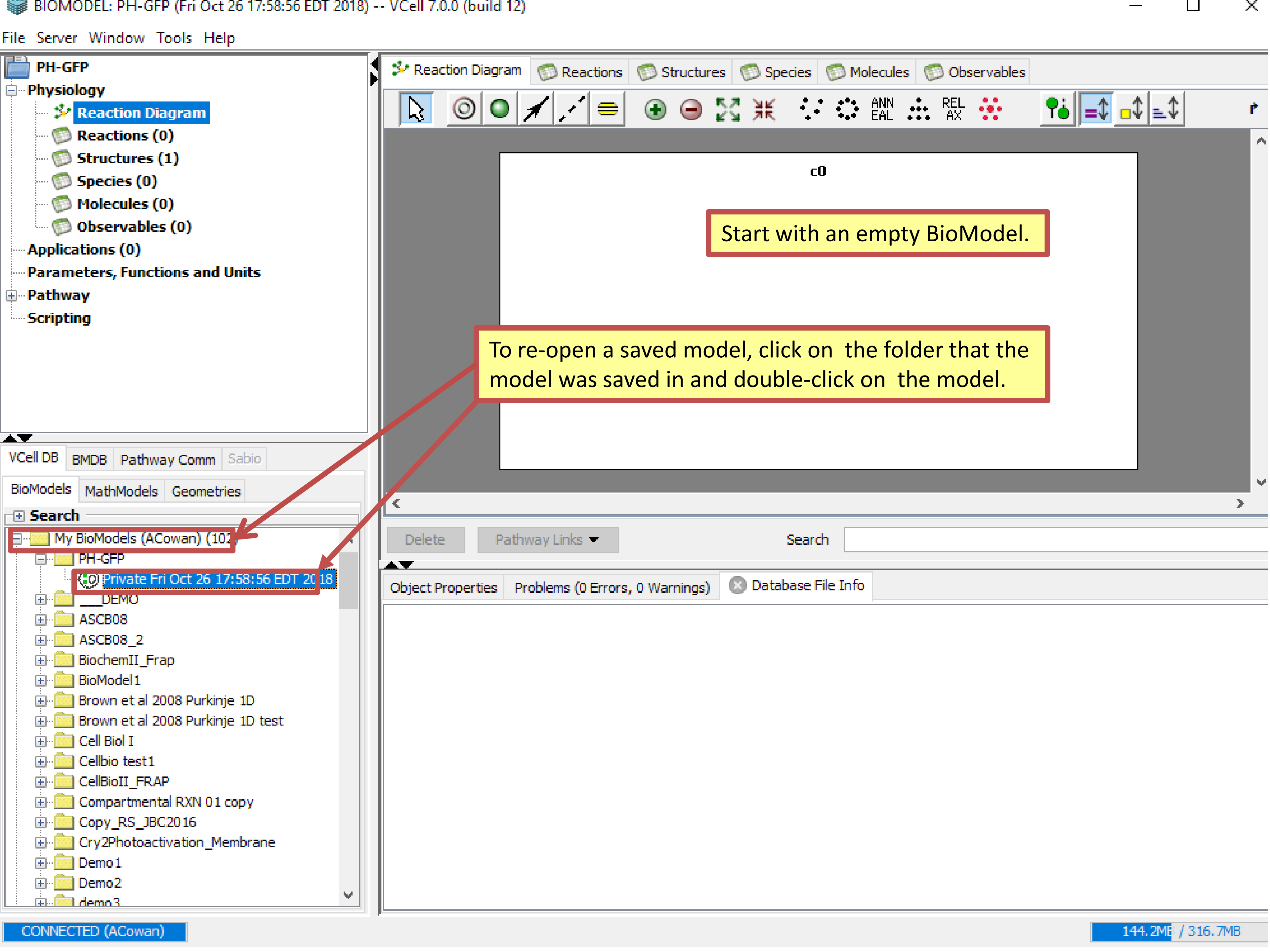
VCell Tutorial

PH-GFP binding to PIP2 and IP3

Create a biomodel and 3D spatial (PDE) application to simulate pleckstrin homology domain (PH-GFP) reporter for conversion of PIP_2 *to* IP_3*.*

In this tutorial…

- Create a BioModel with reactions involving membrane and volume species.
- Create a compartmental (ODE) application that uses events to include time-dependent triggers.
- Create a spatial deterministic (PDE) application of a model using analytic equations to create a 3D geometry
- Define initial concentrations that are non-uniform in space and create timed events in spatial models using Boolean expressions
- Create output functions for more complex analysis of simulation results, e.g. to sum all fluorescent species in a compartment.


BIOMODEL: PH-GFP (Fri Oct 26 17:58:56 EDT 2018) -- VCell 7.0.0 (build 12)
File Server Window Tools Help
PH-GFP
Physiology
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Reactions (0)
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ASCB08
ASCB08_2
BiochemII_Frap
BioModel1
Brown et al 2008 Purkinje 1D
Brown et al 2008 Purkinje 1D test
Cell Biol I
Cellbio test1
CellBioII_FRAP
Compartmental RXN 01 copy
Copy_RS_JBC2016
Cry2Photoactivation_Membrane
Demo1
Demo2
demo3
Delete
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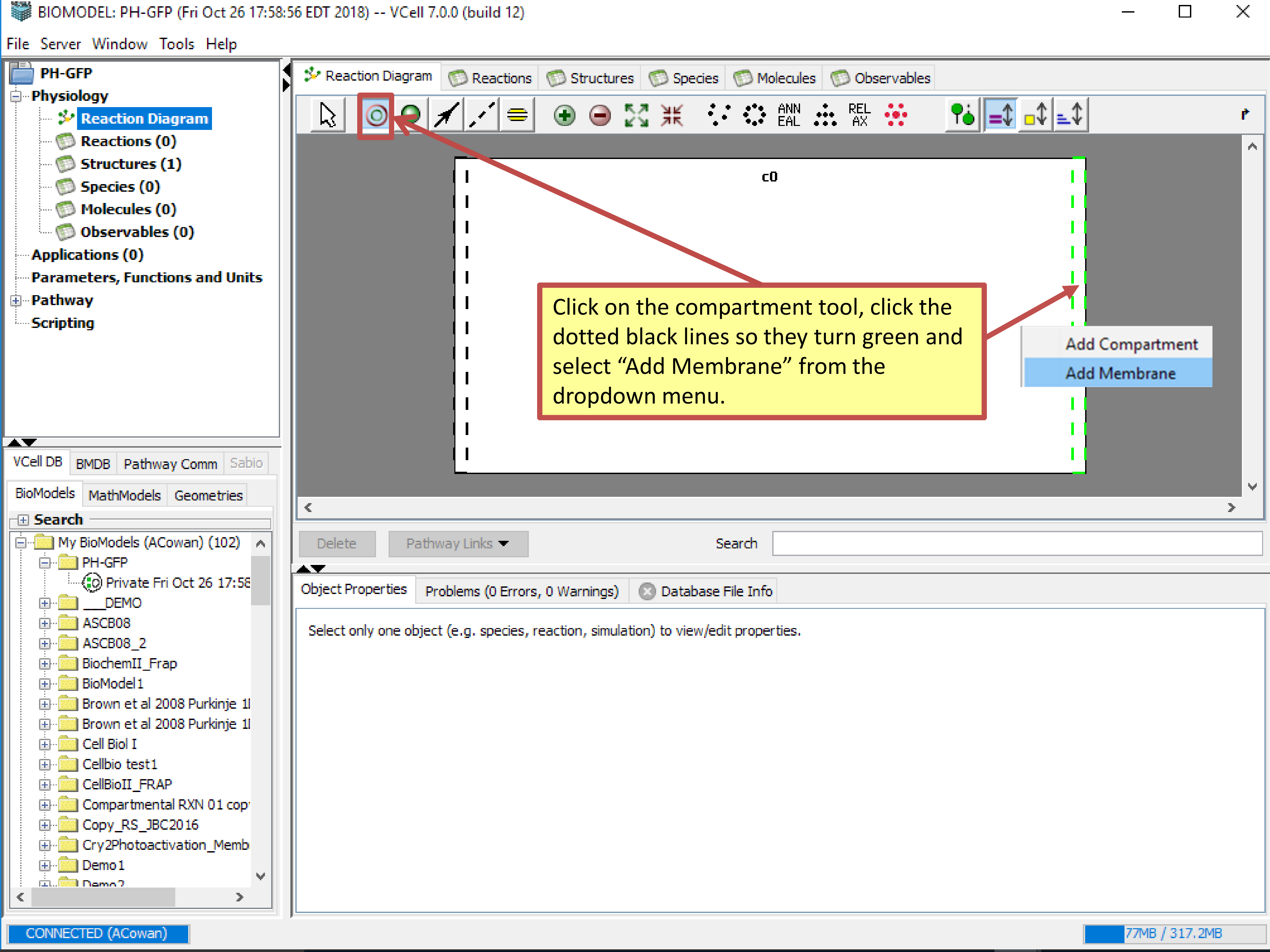
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
CONNECTED (ACowan)
144.2MB / 316.7MB

Start with an empty BioModel.

To re-open a saved model, click on the folder that the model was saved in and double-click on the model.


BIOMODEL: PH-GFP (Fri Oct 26 17:58:56 EDT 2018) -- VCell 7.0.0 (build 12)
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Add Compartment
Add Membrane
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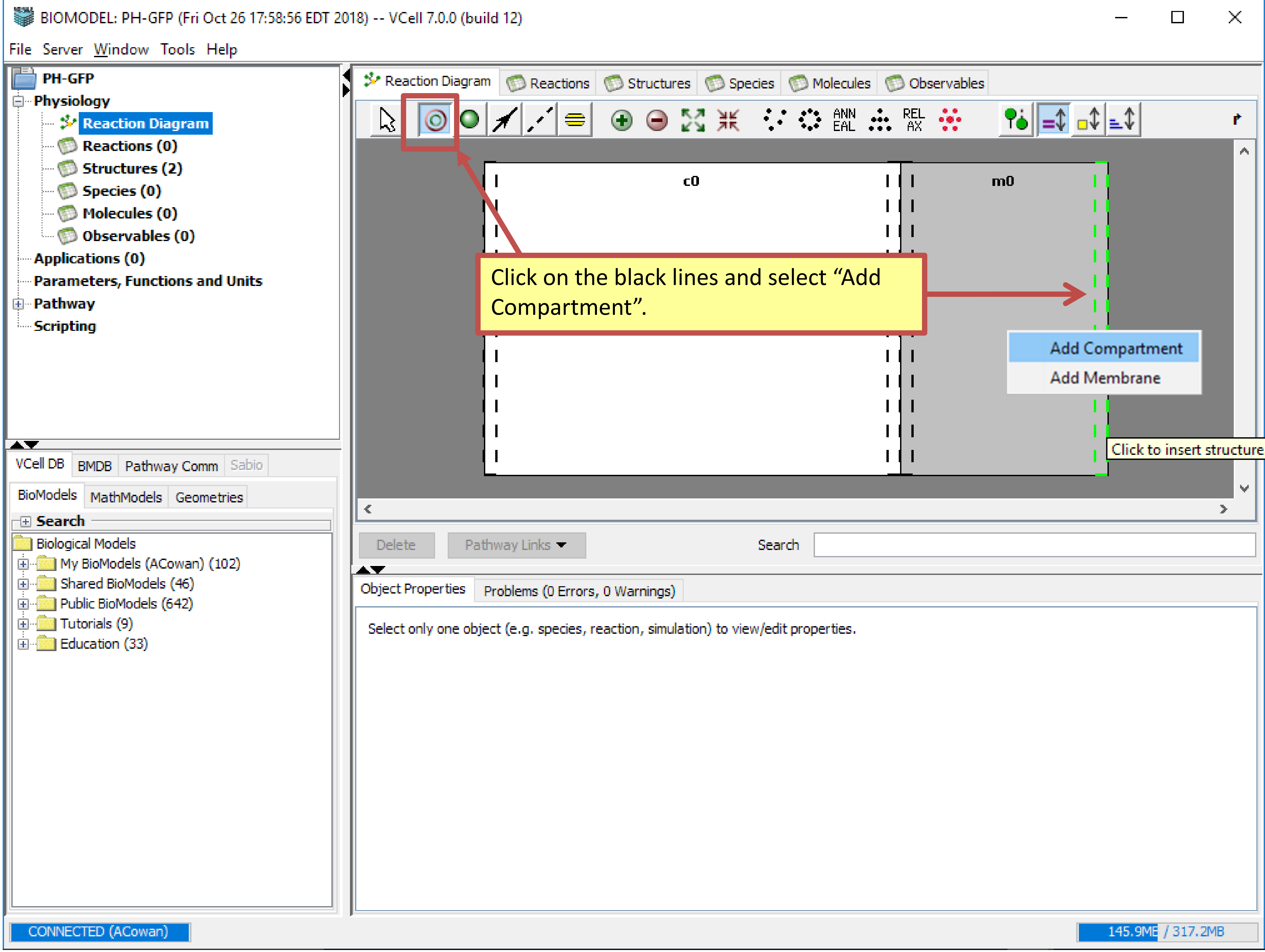
77MB / 317.2MB

Click on the compartment tool, click the dotted black lines so they turn green and select “Add Membrane” from the dropdown menu.

Select only one object (e.g. species, reaction, simulation) to view/edit properties.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Add Compartment
Add Membrane
Click to insert structure
Delete
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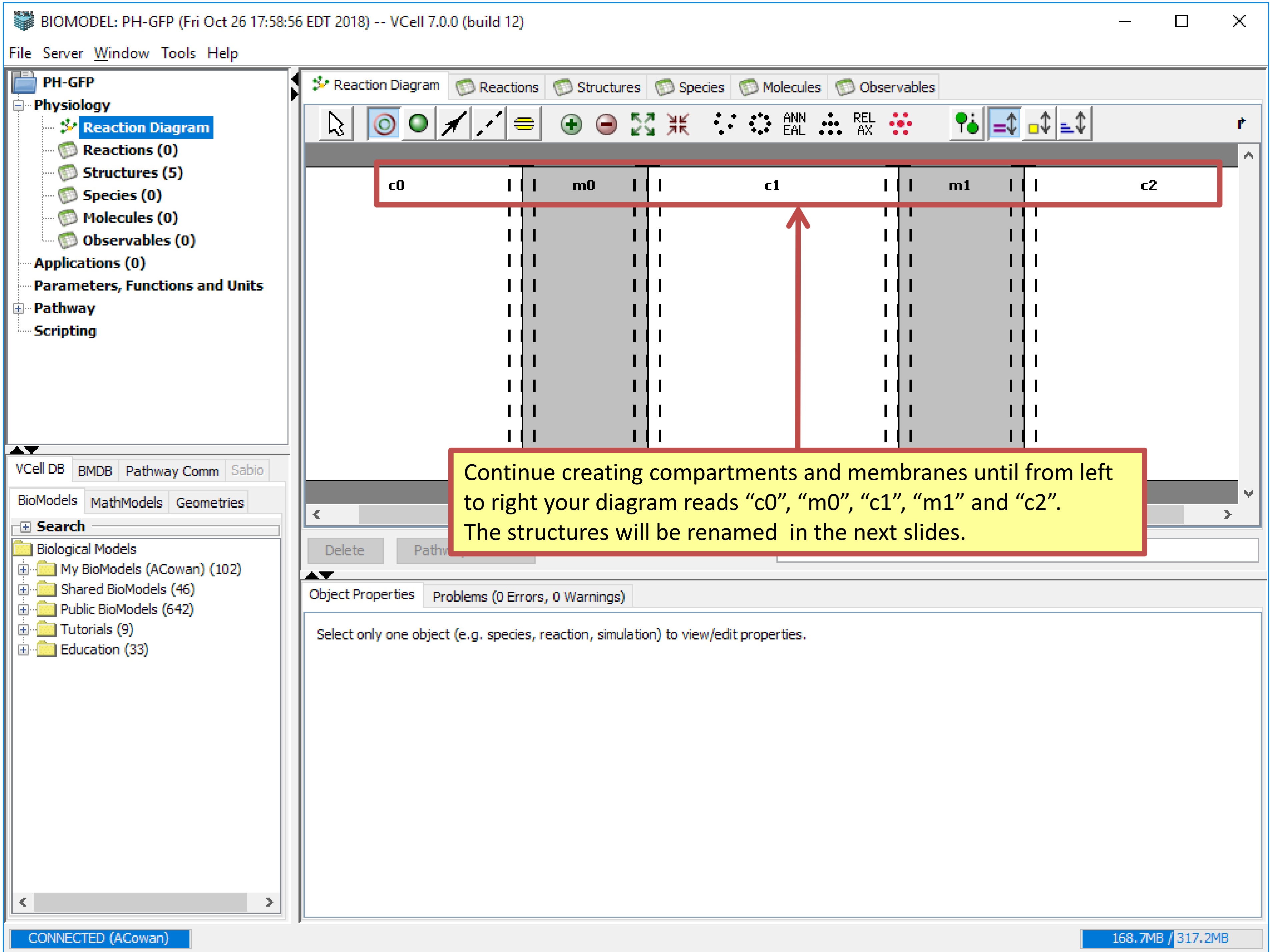
145.9MB / 317.2MB

Click on the black lines and select “Add Compartment”.

Select only one object (e.g. species, reaction, simulation) to view/edit properties.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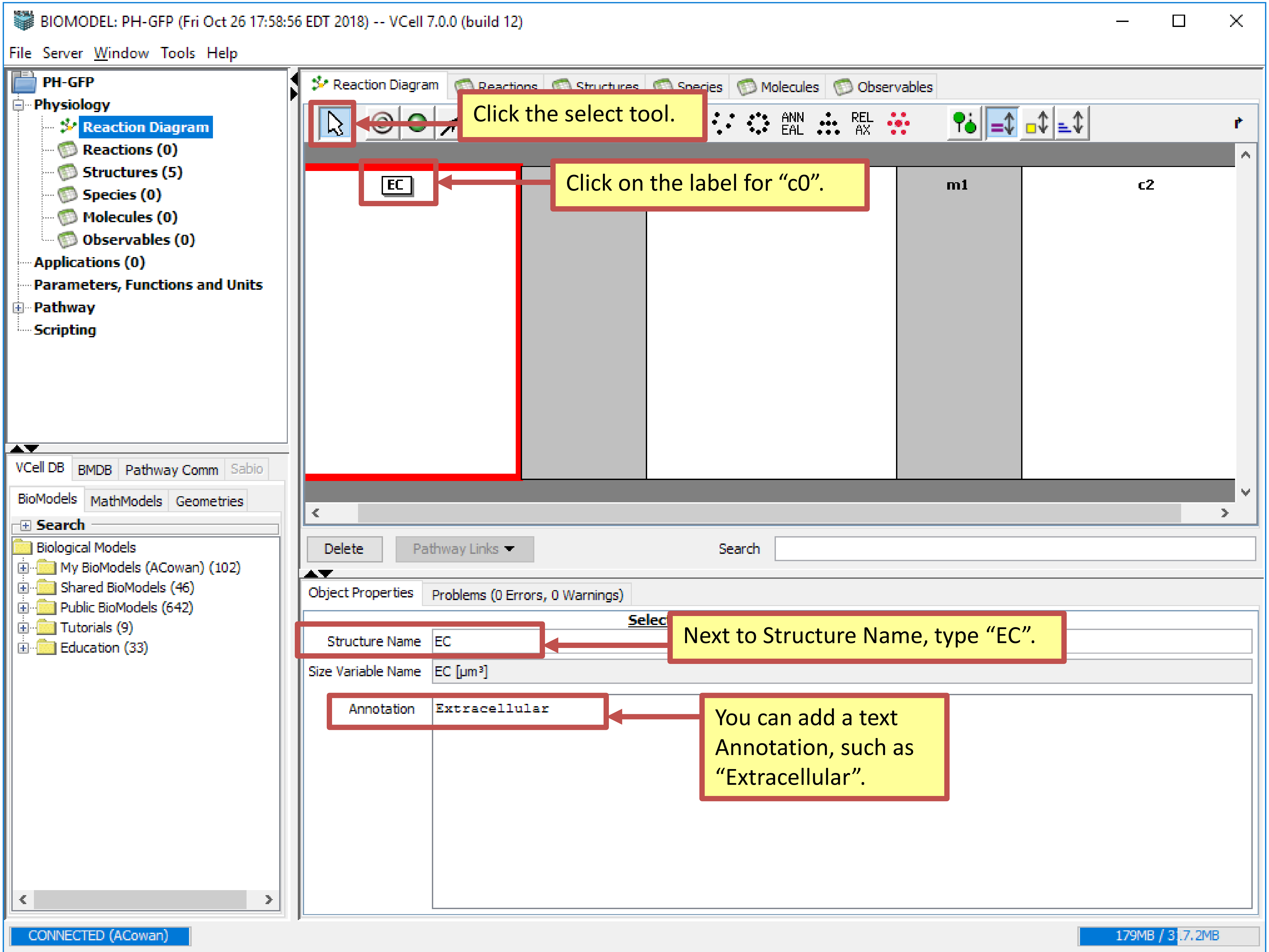
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (ACowan)
168.7MB / 317.2MB

Continue creating compartments and membranes until from left to right your diagram reads “c0”, “m0”, “c1”, “m1” and “c2”. The structures will be renamed in the next slides.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179MB / 317.2MB

Click the select tool.

Click on the label for “c0”.

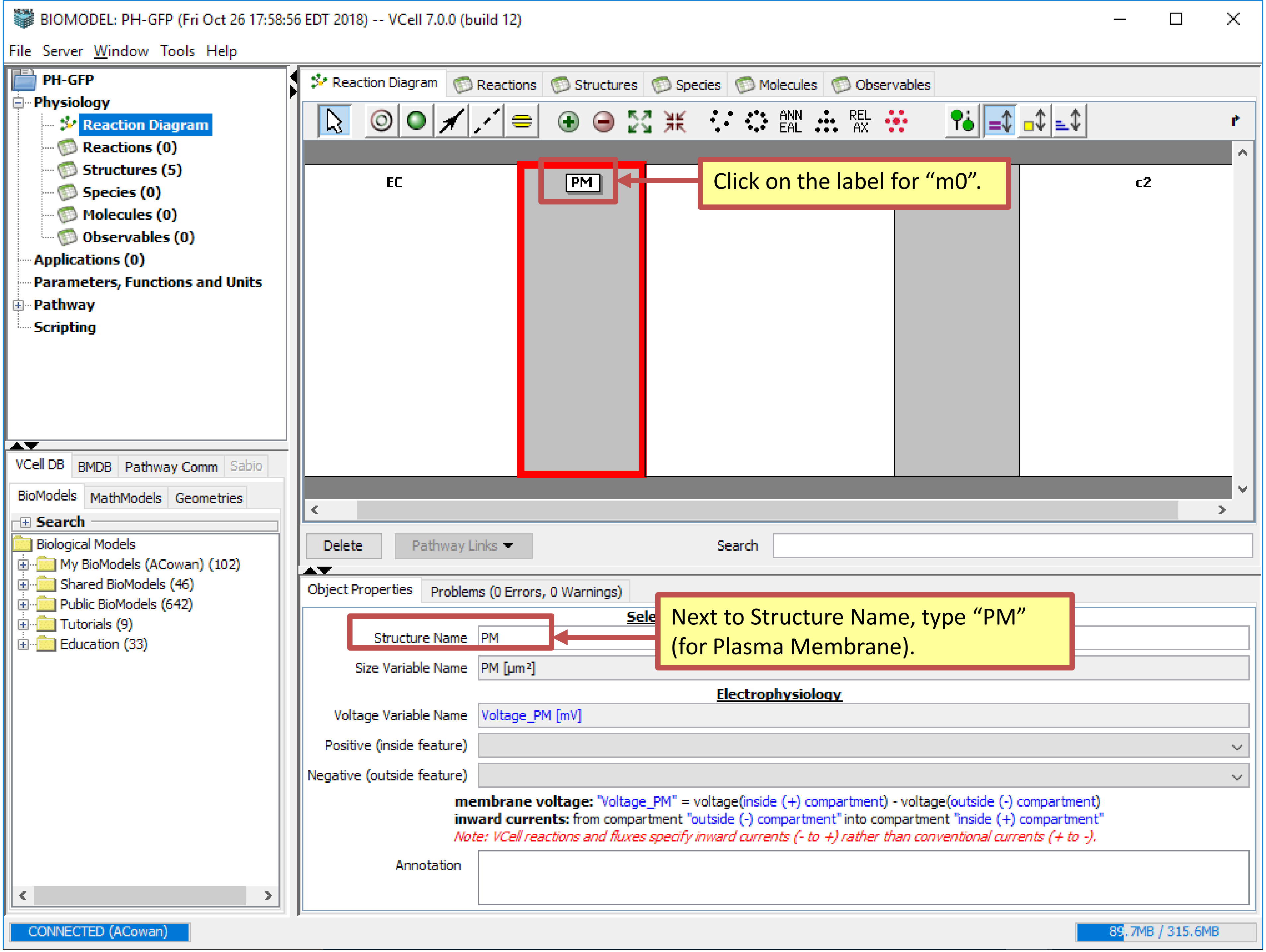
Next to Structure Name, type “EC”.

You can add a text Annotation, such as “Extracellular”.

Structure Name: EC

Size Variable Name: EC [µm³]

Annotation: Extracellular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Electrophysiology
Positive (inside feature)
Negative (outside feature)
Annotation
CONNECTED (ACowan)
89.7MB / 315.6MB

Click on the label for “m0”.

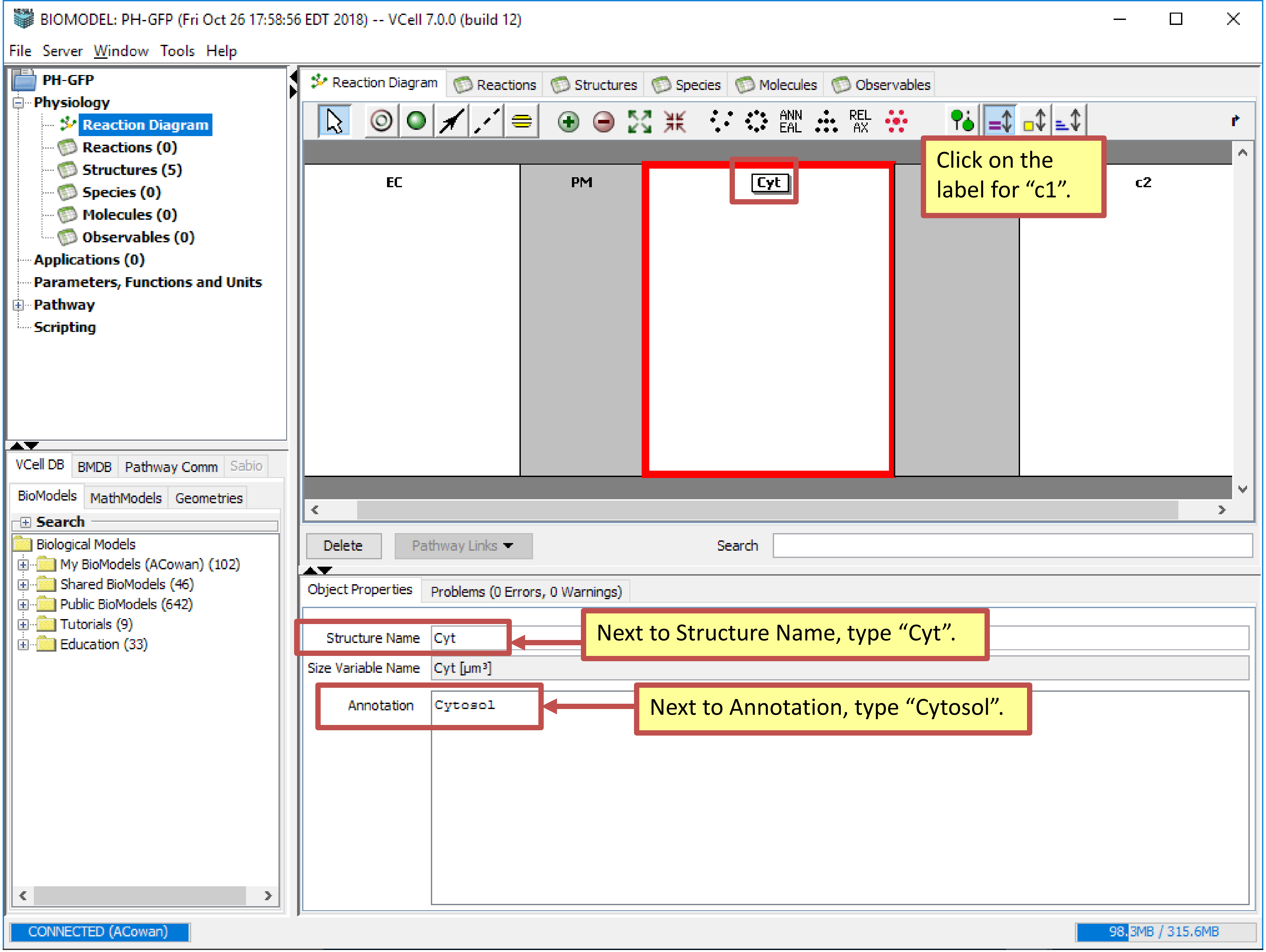
Next to Structure Name, type “PM” (for Plasma Membrane).

Structure Name: PM

Size Variable Name: PM [µm²]

Voltage Variable Name: Voltage_PM [mV]

membrane voltage: "Voltage_PM" = voltage(inside (+) compartment) - voltage(outside (-) compartment)
inward currents: from compartment "outside (-) compartment" into compartment "inside (+) compartment"
Note: VCell reactions and fluxes specify inward currents (- to +) rather than conventional currents (+ to -).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CONNECTED (ACowan)
98.3MB / 315.6MB

Structure Name: Cyt

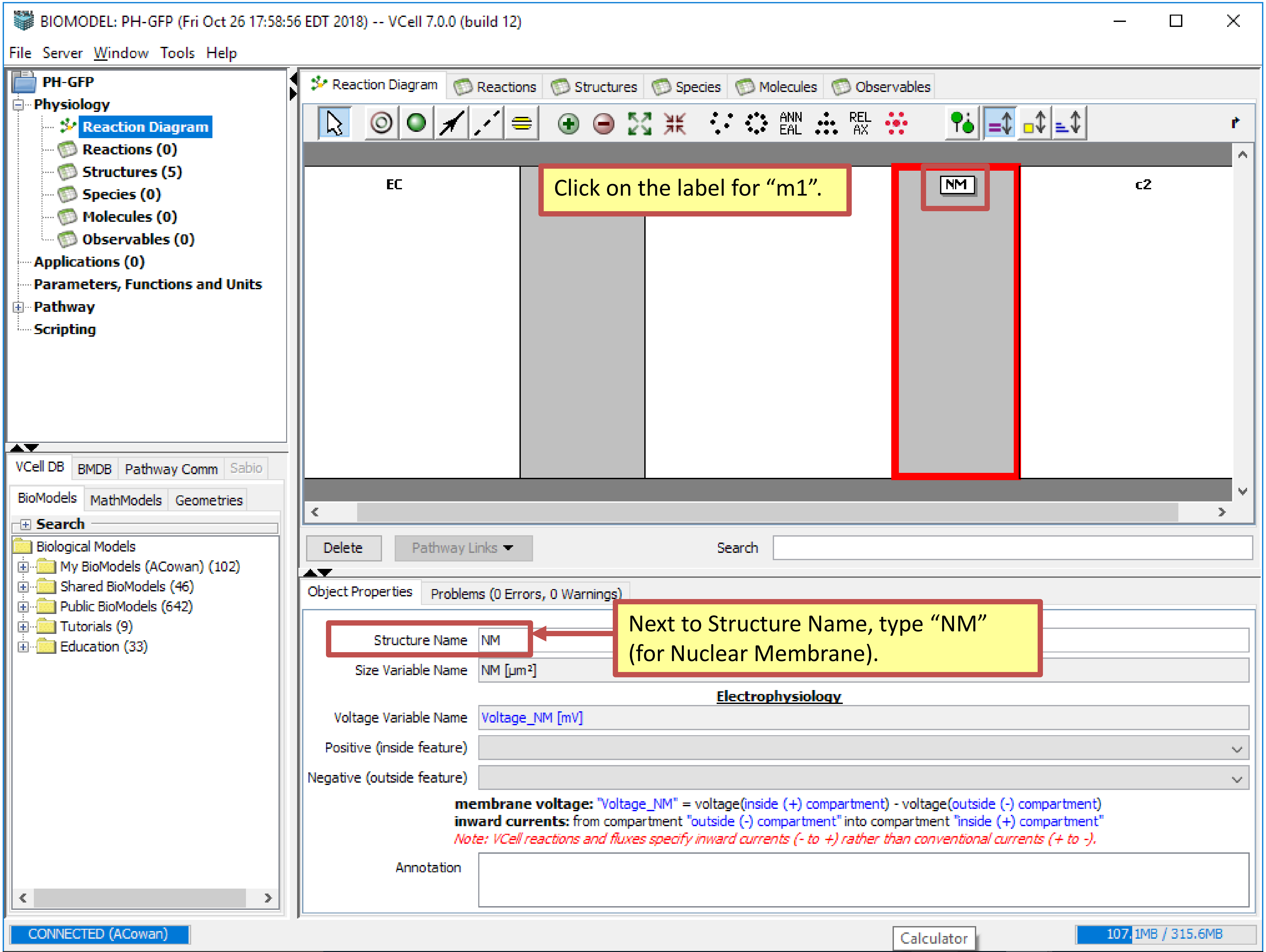
Size Variable Name: Cyt [µm³]

Annotation: Cytosol

Click on the label for “c1”.

Next to Structure Name, type “Cyt”.

Next to Annotation, type “Cytosol”.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CONNECTED (ACowan)
Calculator
107.1MB / 315.6MB

Click on the label for “m1”.

Next to Structure Name, type “NM” (for Nuclear Membrane).

Structure Name: NM

Size Variable Name: NM [µm²]

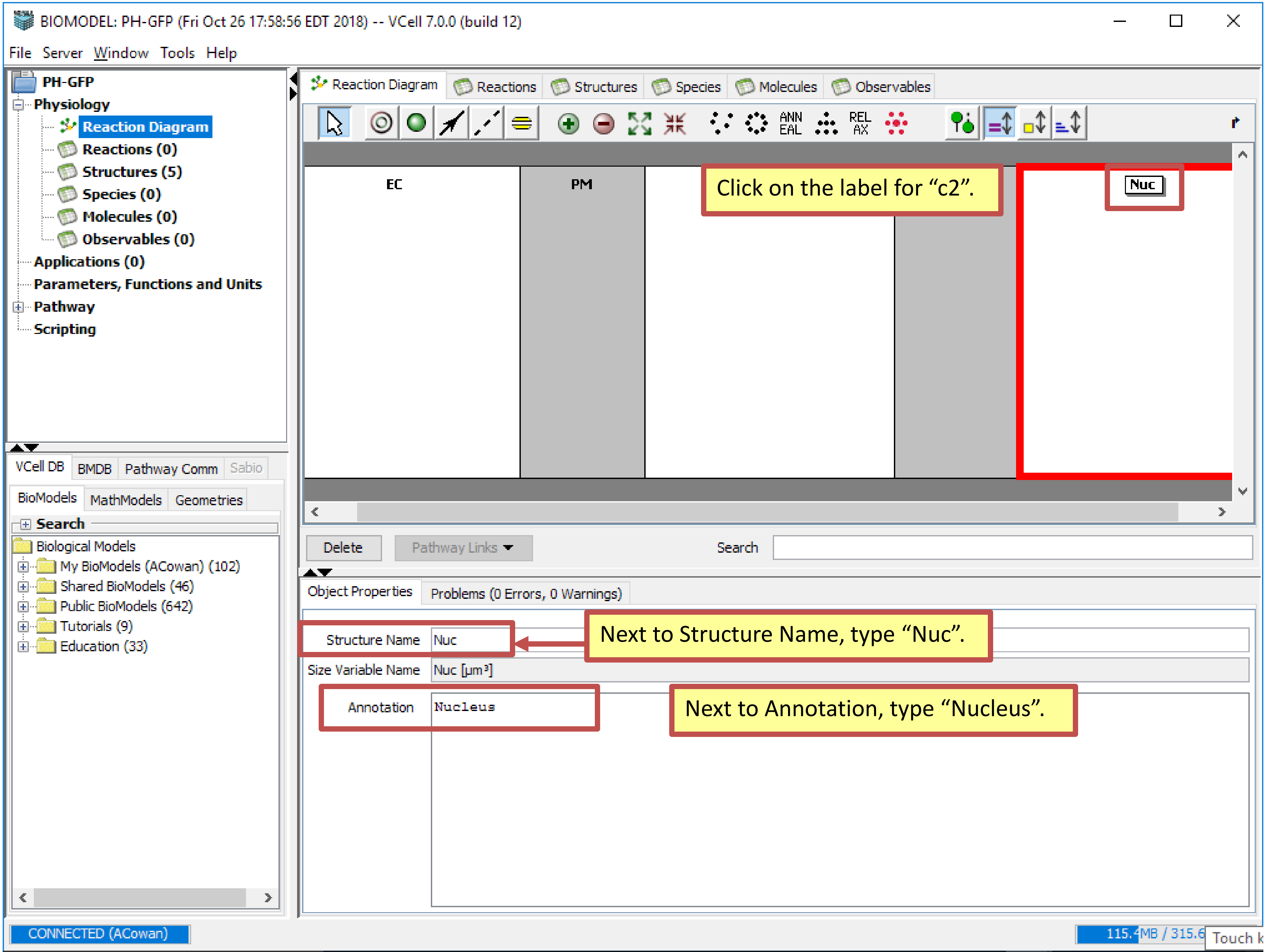
Electrophysiology

Voltage Variable Name: Voltage_NM [mV]

Positive (inside feature):

Negative (outside feature):

membrane voltage: "Voltage_NM" = voltage(inside (+) compartment) - voltage(outside (-) compartment)
inward currents: from compartment "outside (-) compartment" into compartment "inside (+) compartment"
Note: VCell reactions and fluxes specify inward currents (- to +) rather than conventional currents (+ to -).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115.4MB / 315.6
Touch k

Click on the label for “c2”.

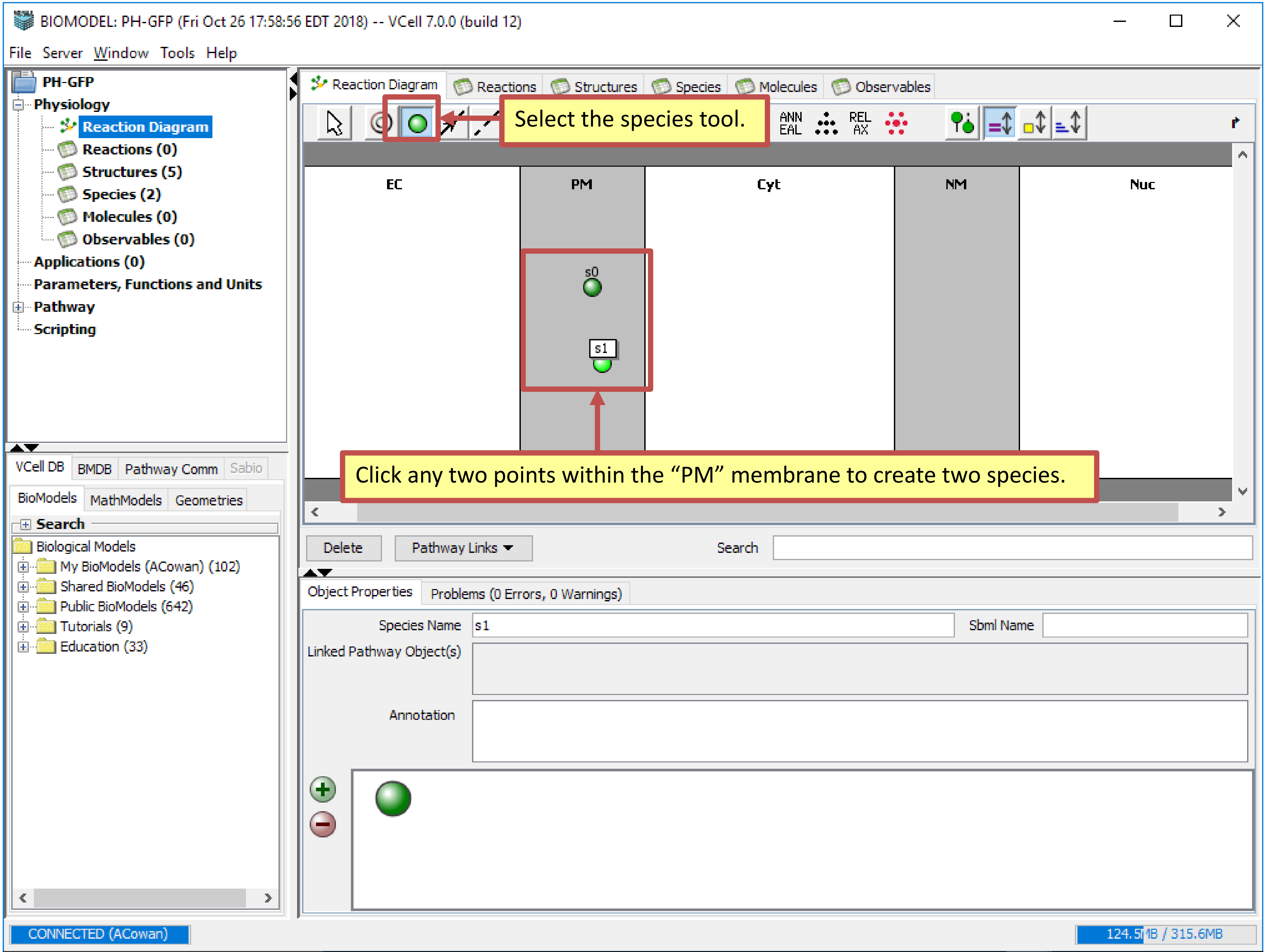
Structure Name: Nuc

Size Variable Name: Nuc [µm³]

Annotation: Nucleus

Next to Structure Name, type “Nuc”.

Next to Annotation, type “Nucleus”.



BIOMODEL: PH-GFP (Fri Oct 26 17:58:56 EDT 2018) -- VCell 7.0.0 (build 12)

Select the species tool.

Click any two points within the “PM” membrane to create two species.

Species Name: s1

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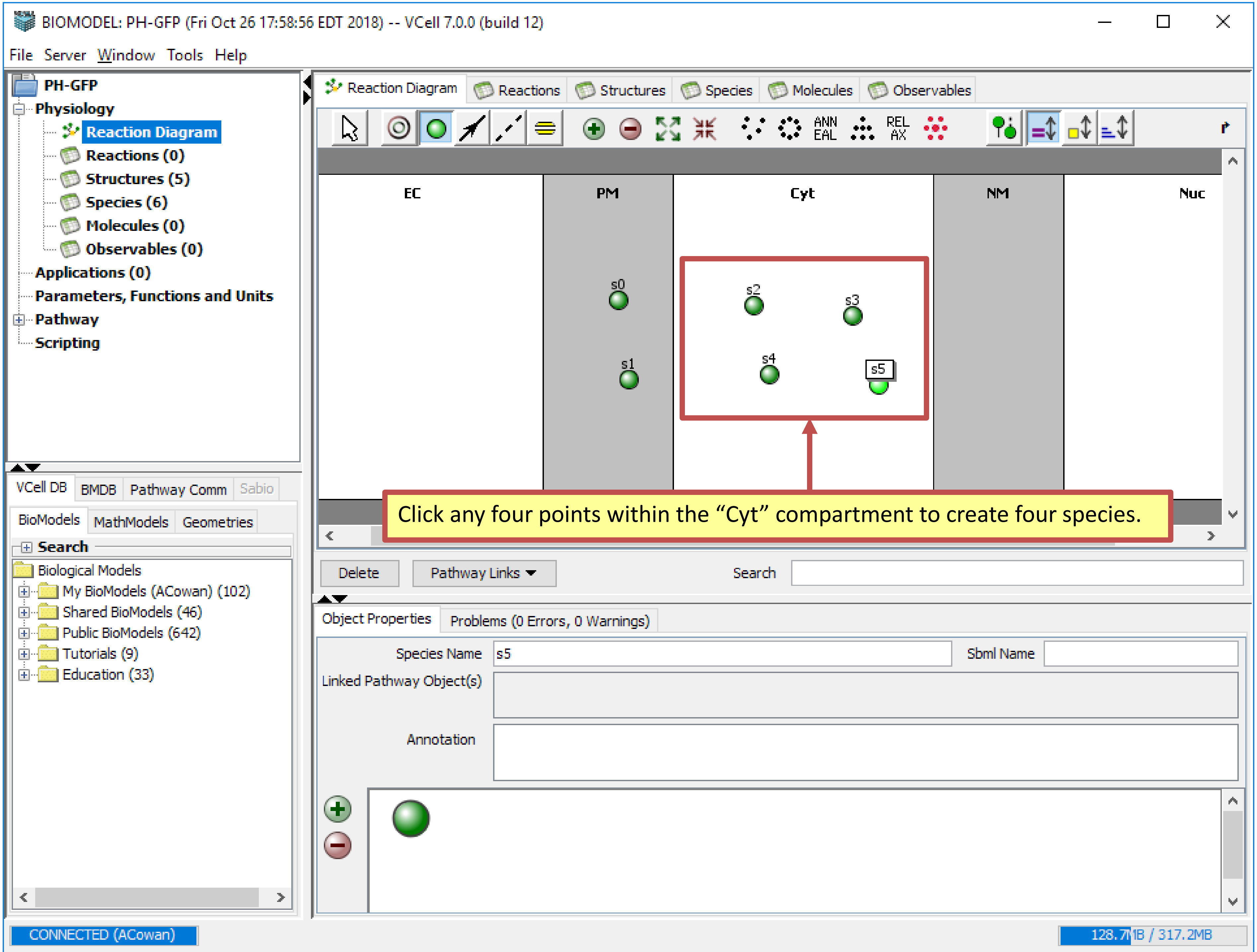
124.5MB / 315.6MB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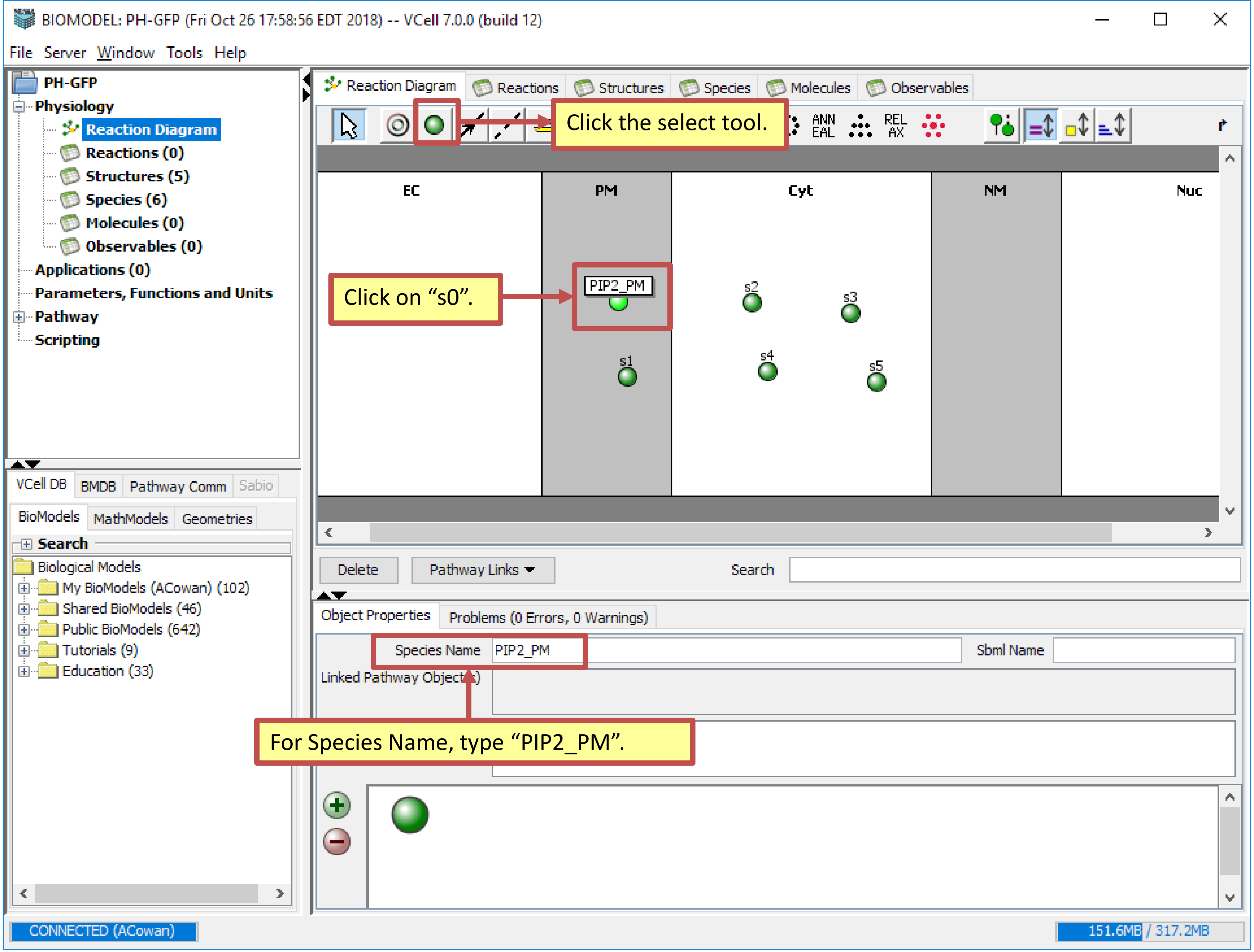
CONNECTED (ACowan)
128.7MB / 317.2MB

Species Name: s5

Click any four points within the “Cyt” compartment to create four species.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Sbml Name
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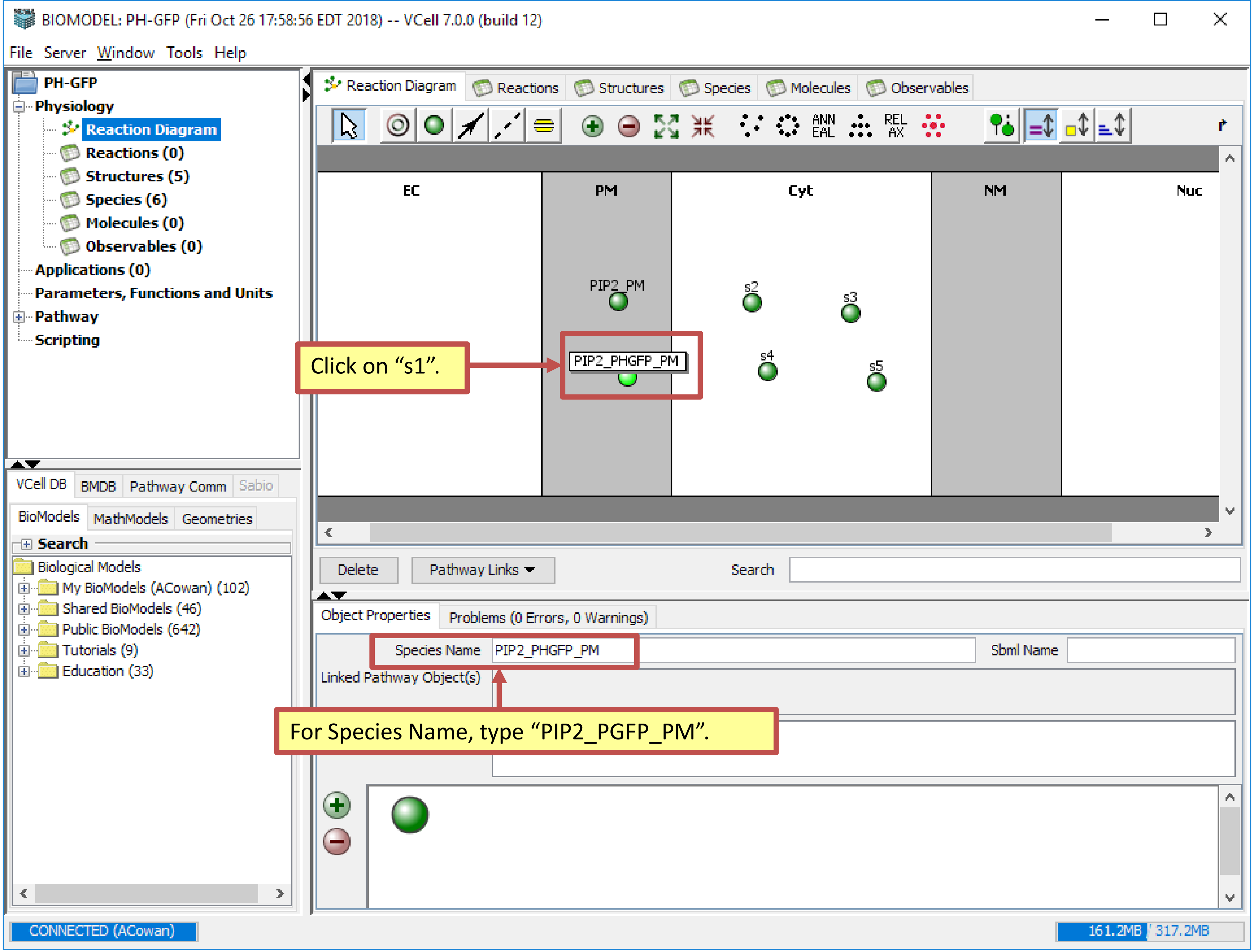
151.6MB / 317.2MB

Click the select tool.

Click on “s0”.

For Species Name, type “PIP2_PM”.

Species Name PIP2_PM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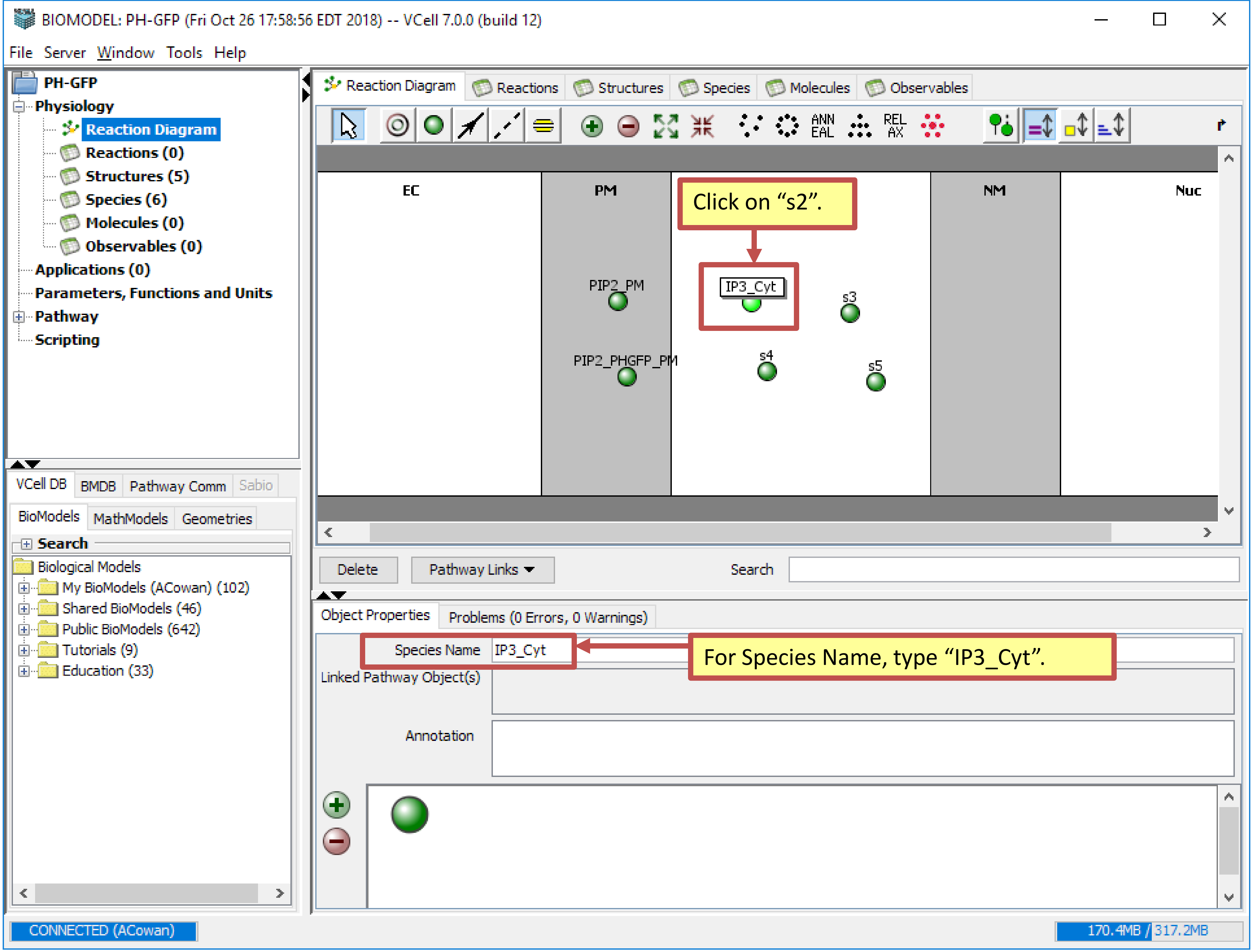
161.2MB 317.2MB

Species Name PIP2_PHGFP_PM

Click on “s1”.

For Species Name, type “PIP2_PGFP_PM”.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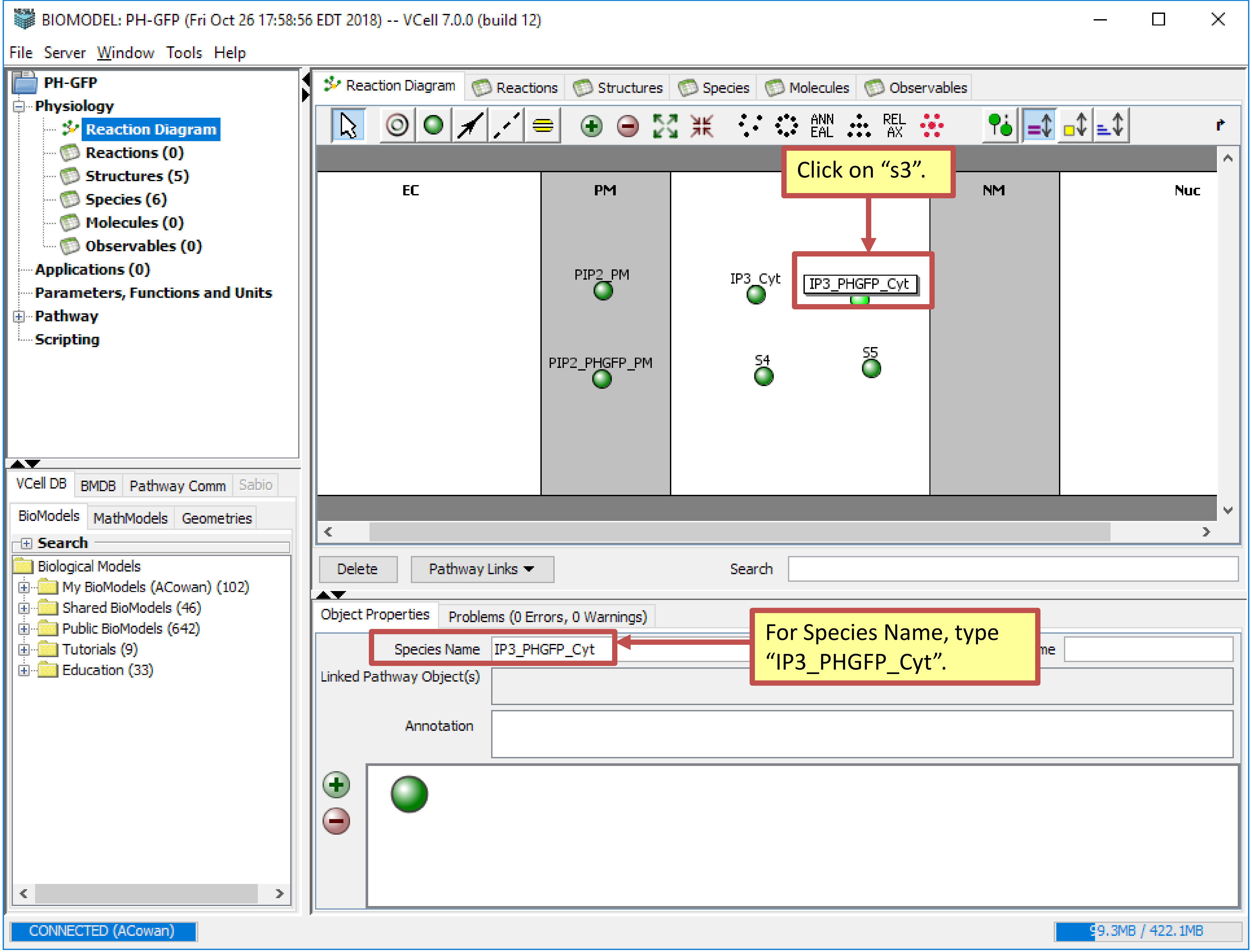
170.4MB / 317.2MB

Click on “s2”.

Species Name IP3_Cyt

For Species Name, type “IP3_Cyt”.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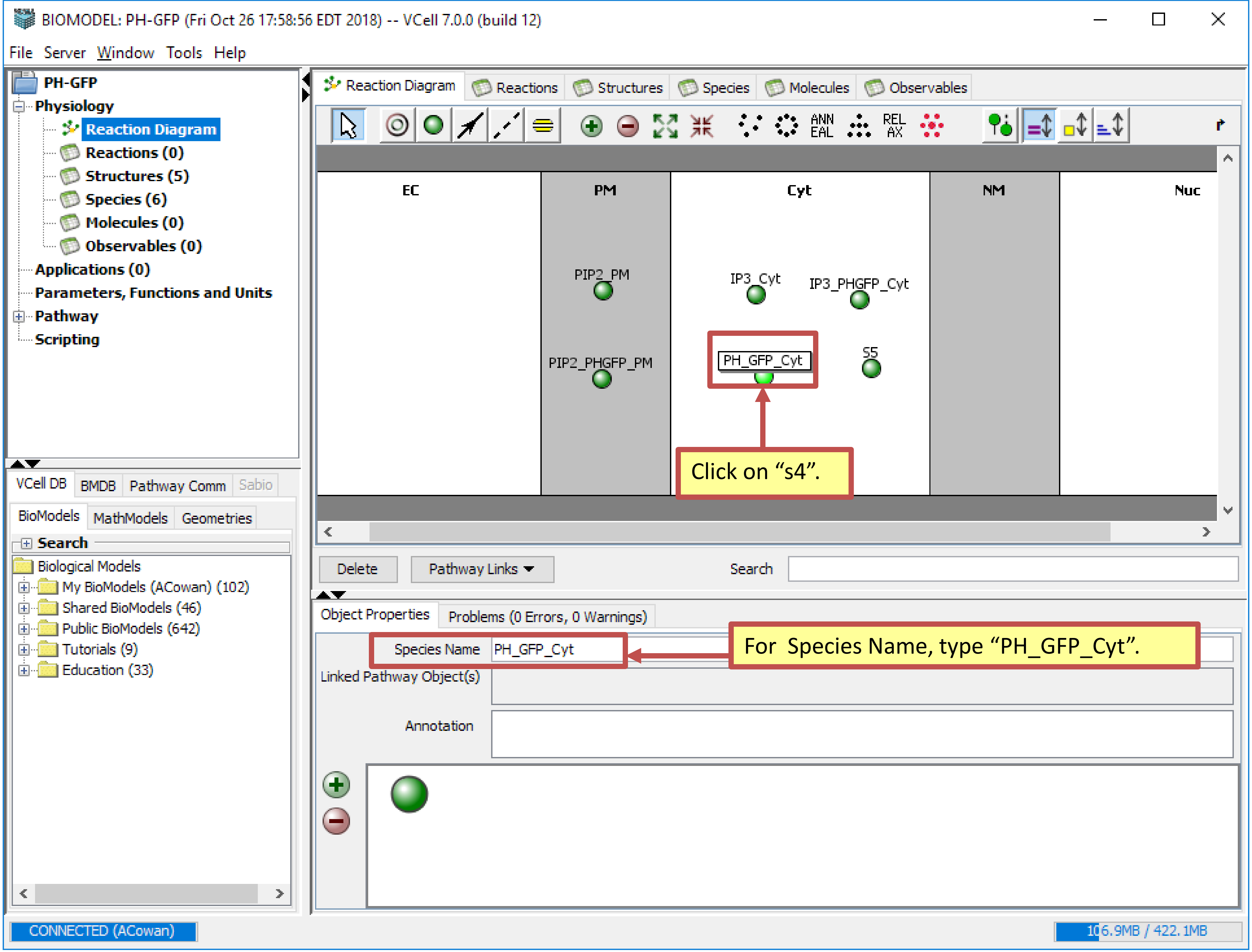
99.3MB / 422.1MB

Species Name IP3_PHGFP_Cyt

Click on “s3”.

For Species Name, type “IP3_PHGFP_Cyt”.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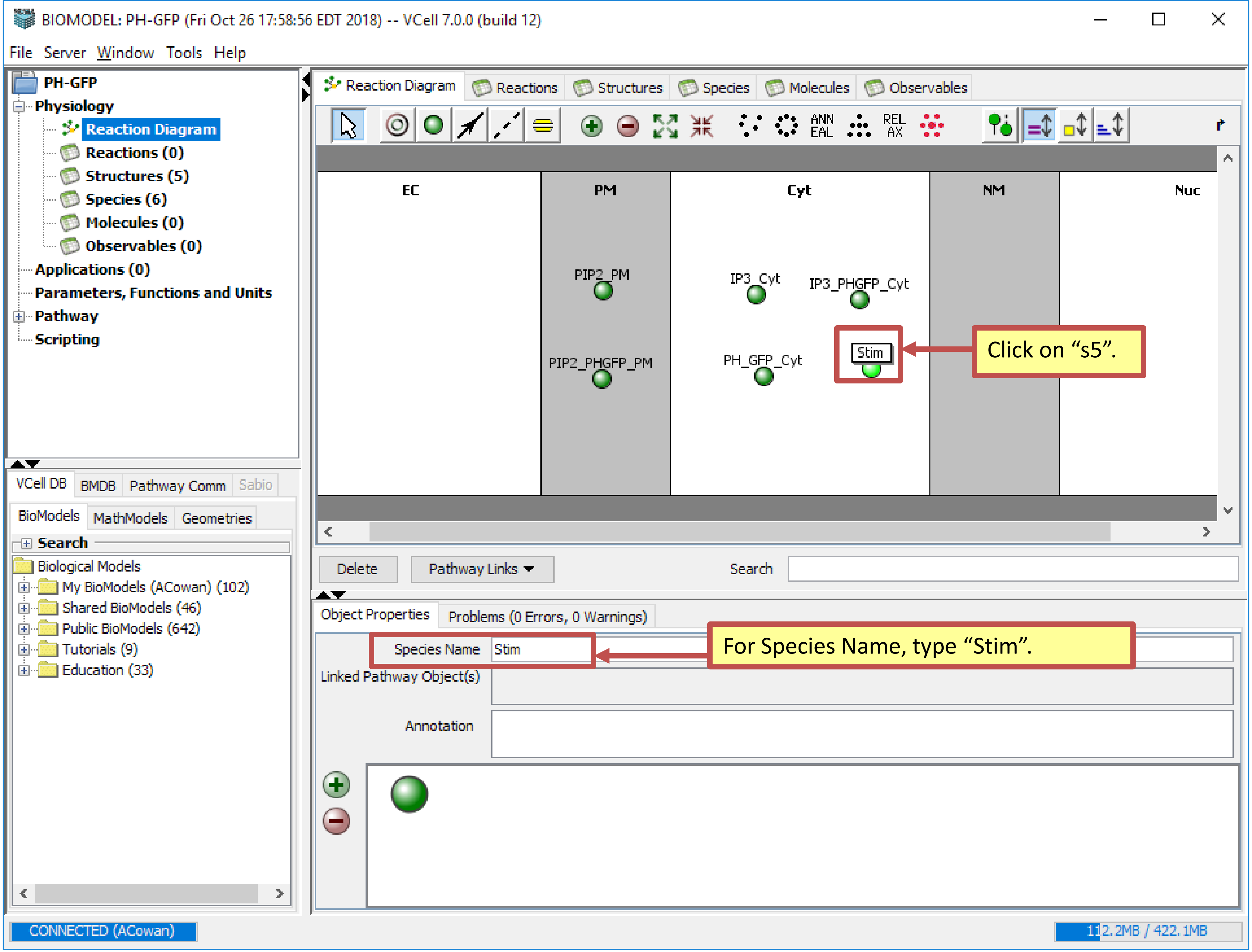
106.9MB / 422.1MB

Click on “s4”.

For Species Name, type “PH_GFP_Cyt”.

Species Name: PH_GFP_Cyt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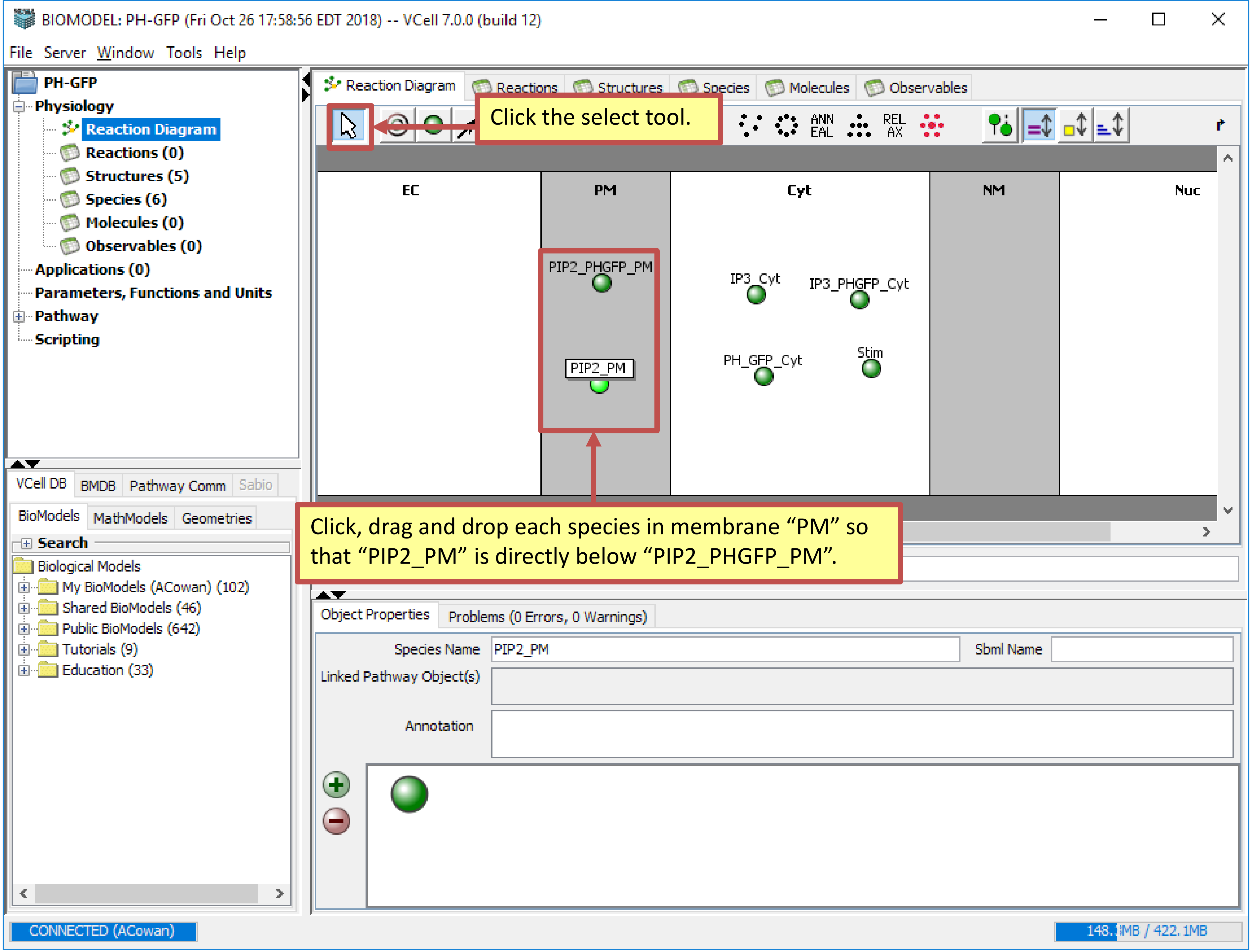
CONNECTED (ACowan)
112.2MB / 422.1MB

Click on “s5”.

Species Name: Stim

For Species Name, type “Stim”.


BIOMODEL: PH-GFP (Fri Oct 26 17:58:56 EDT 2018) -- VCell 7.0.0 (build 12)
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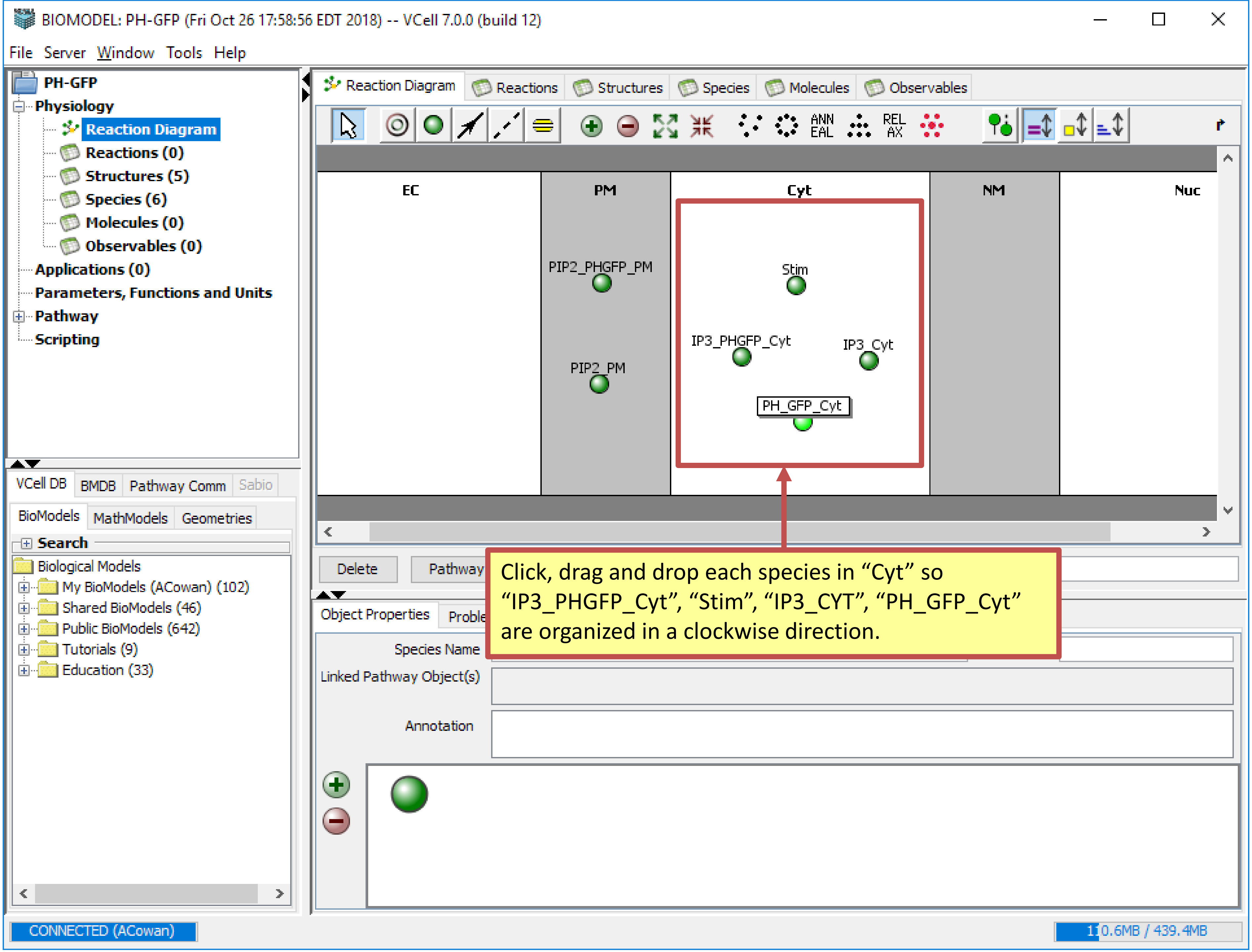
CONNECTED (ACowan)
148.1MB / 422.1MB

Click the select tool.

Click, drag and drop each species in membrane “PM” so that “PIP2_PM” is directly below “PIP2_PHGFP_PM”.

Species Name: PIP2_PM

Sbml Name: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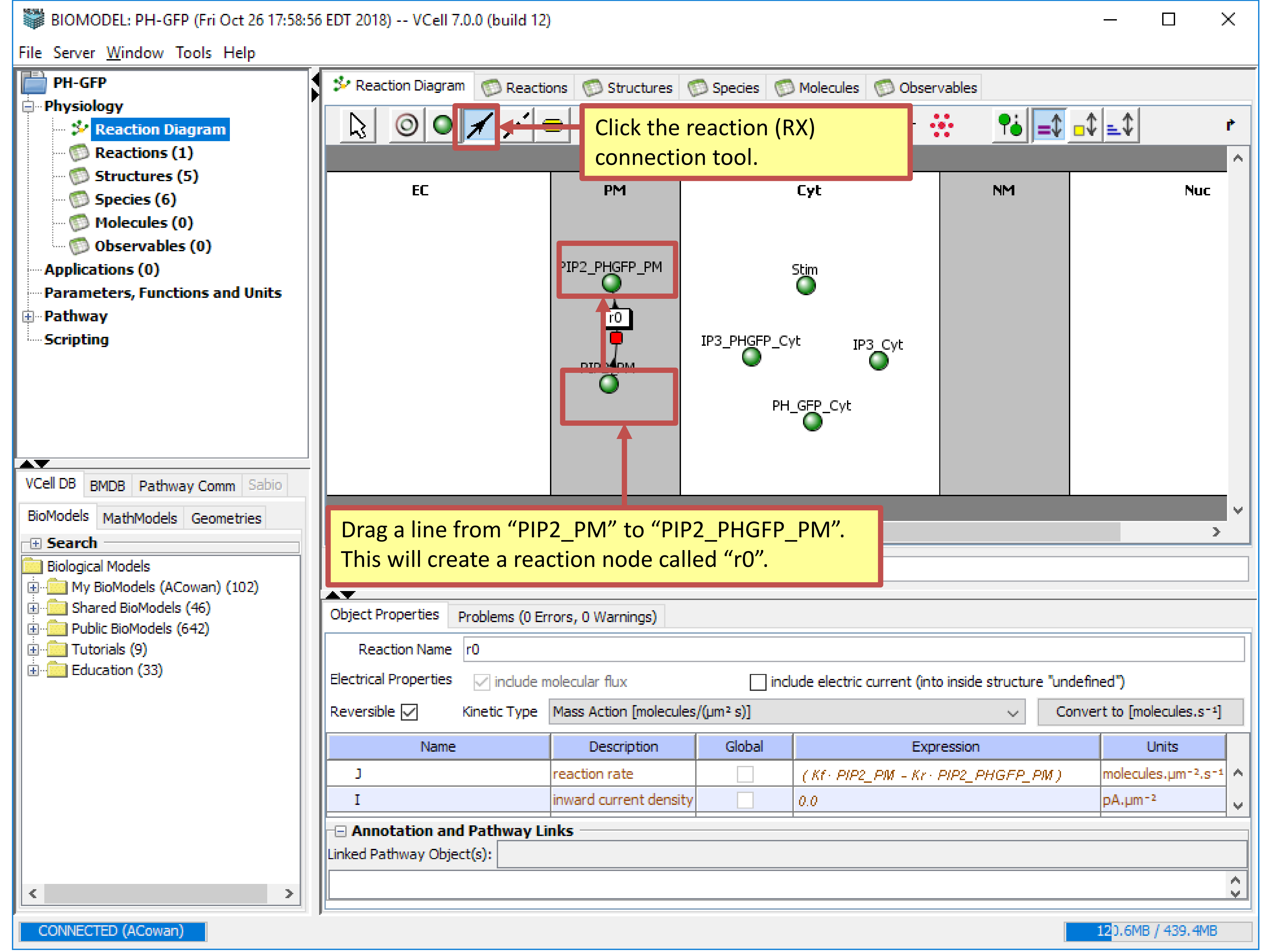
110.6MB / 439.4MB

Click, drag and drop each species in “Cyt” so “IP3_PHGFP_Cyt”, “Stim”, “IP3_CYT”, “PH_GFP_Cyt” are organized in a clockwise direction.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Annotation and Pathway Links
Linked Pathway Object(s):
CONNECTED (ACowan)
120.6MB / 439.4MB

Click the reaction (RX) connection tool.

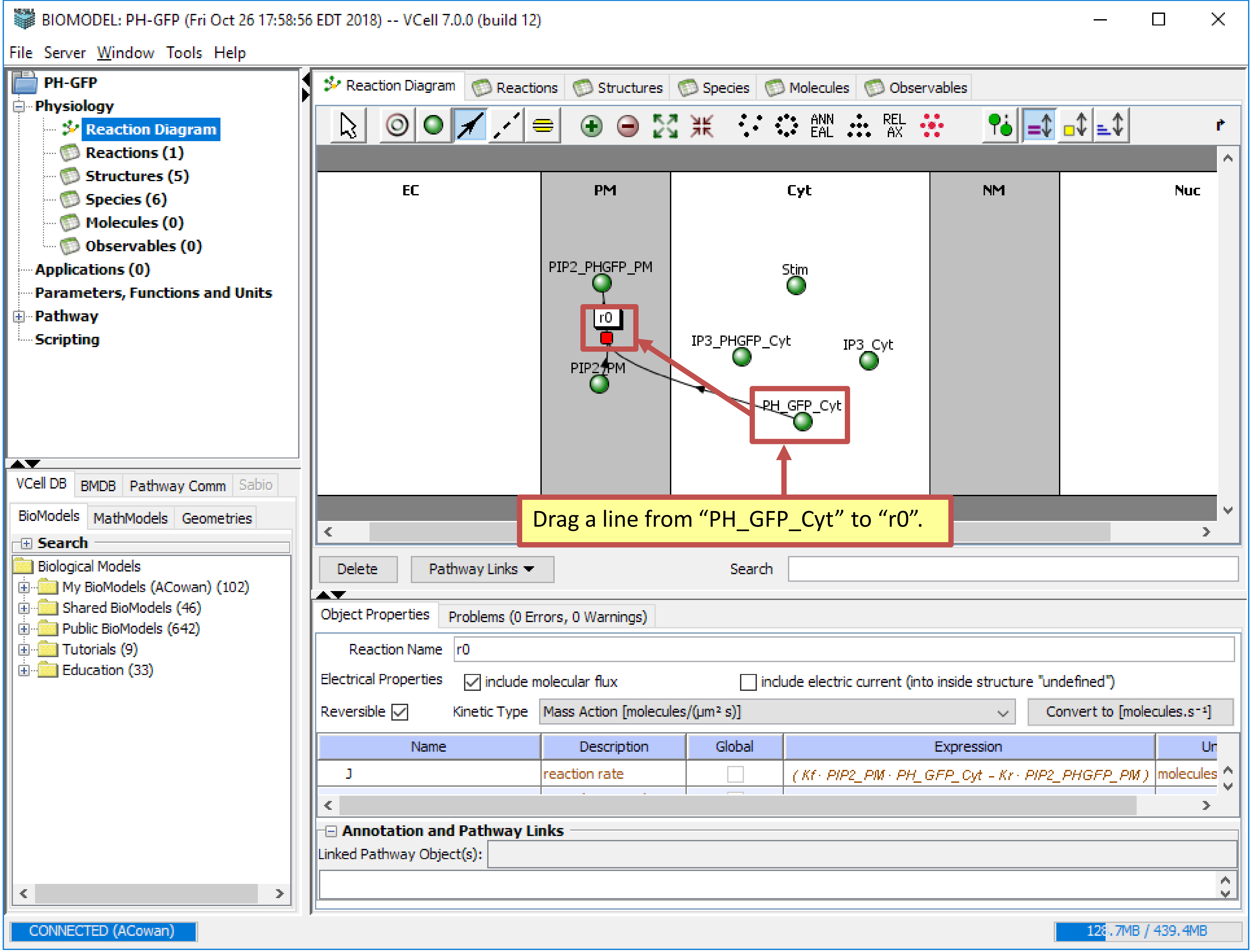
Drag a line from “PIP2_PM” to “PIP2_PHGFP_PM”. This will create a reaction node called “r0”.

Reaction Name: r0

Electrical Properties ☑ include molecular flux ☐ include electric current (into inside structure "undefined")

Reversible ☑ Kinetic Type: Mass Action [molecules/(μm² s)] Convert to [molecules.s^{-1}]

Name	Description	Global	Expression	Units
J	reaction rate	☐	(Kf · PIP2_PM - Kr · PIP2_PHGFP_PM)	molecules.μm^{-2}.s^{-1}
I	inward current density	☐	0.0	pA.μm^{-2}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128.7MB / 439.4MB

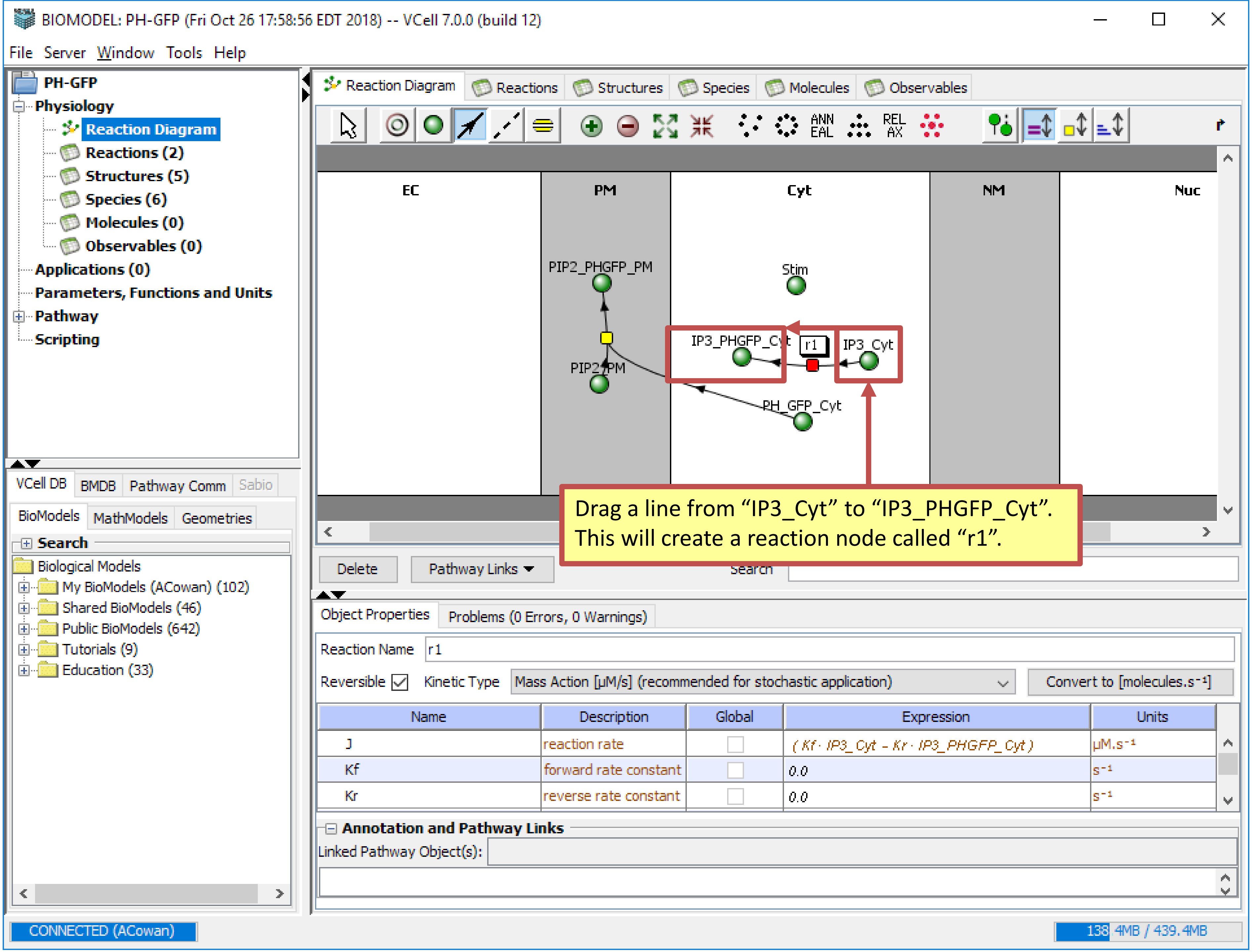
Drag a line from “PH_GFP_Cyt” to “r0”.

Reaction Name: r0

Electrical Properties: ☑ include molecular flux ☐ include electric current (into inside structure "undefined")

Reversible ☑ Kinetic Type: Mass Action [molecules/(µm² s)] Convert to [molecules.s⁻¹]

Name	Description	Global	Expression	Ur
J	reaction rate	☐	(Kf · PIP2_PM · PH_GFP_Cyt − Kr · PIP2_PHGFP_PM)	molecules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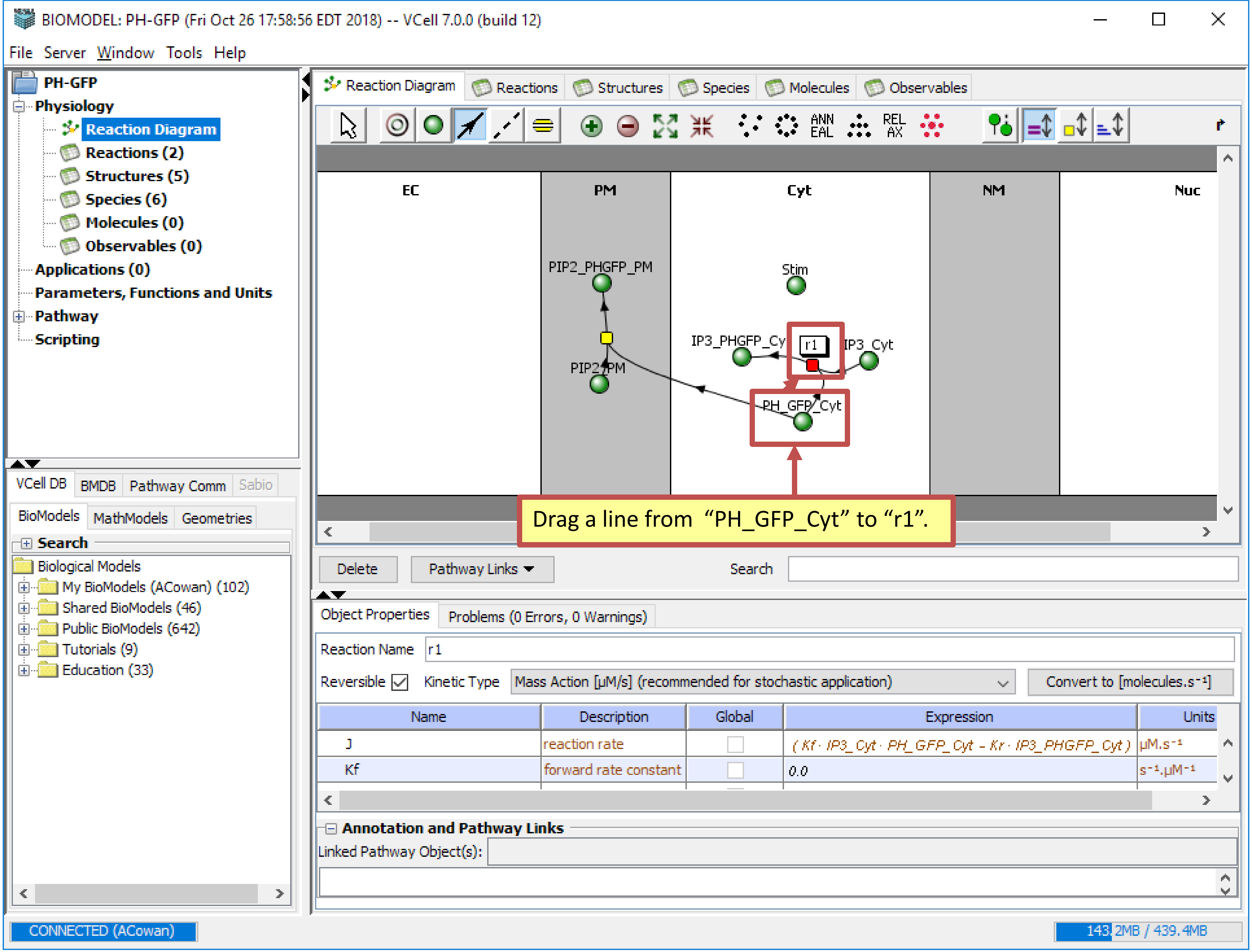
Linked Pathway Object(s):
CONNECTED (ACowan)
138.4MB / 439.4MB

Drag a line from “IP3_Cyt” to “IP3_PHGFP_Cyt”. This will create a reaction node called “r1”.

Reaction Name: r1

Reversible ☑ Kinetic Type: Mass Action [µM/s] (recommended for stochastic application) Convert to [molecules.s⁻¹]

Name	Description	Global	Expression	Units
J	reaction rate	☐	(Kf · IP3_Cyt - Kr · IP3_PHGFP_Cyt)	$\mu M.s^{-1}$
Kf	forward rate constant	☐	0.0	s^{-1}
Kr	reverse rate constant	☐	0.0	s^{-1}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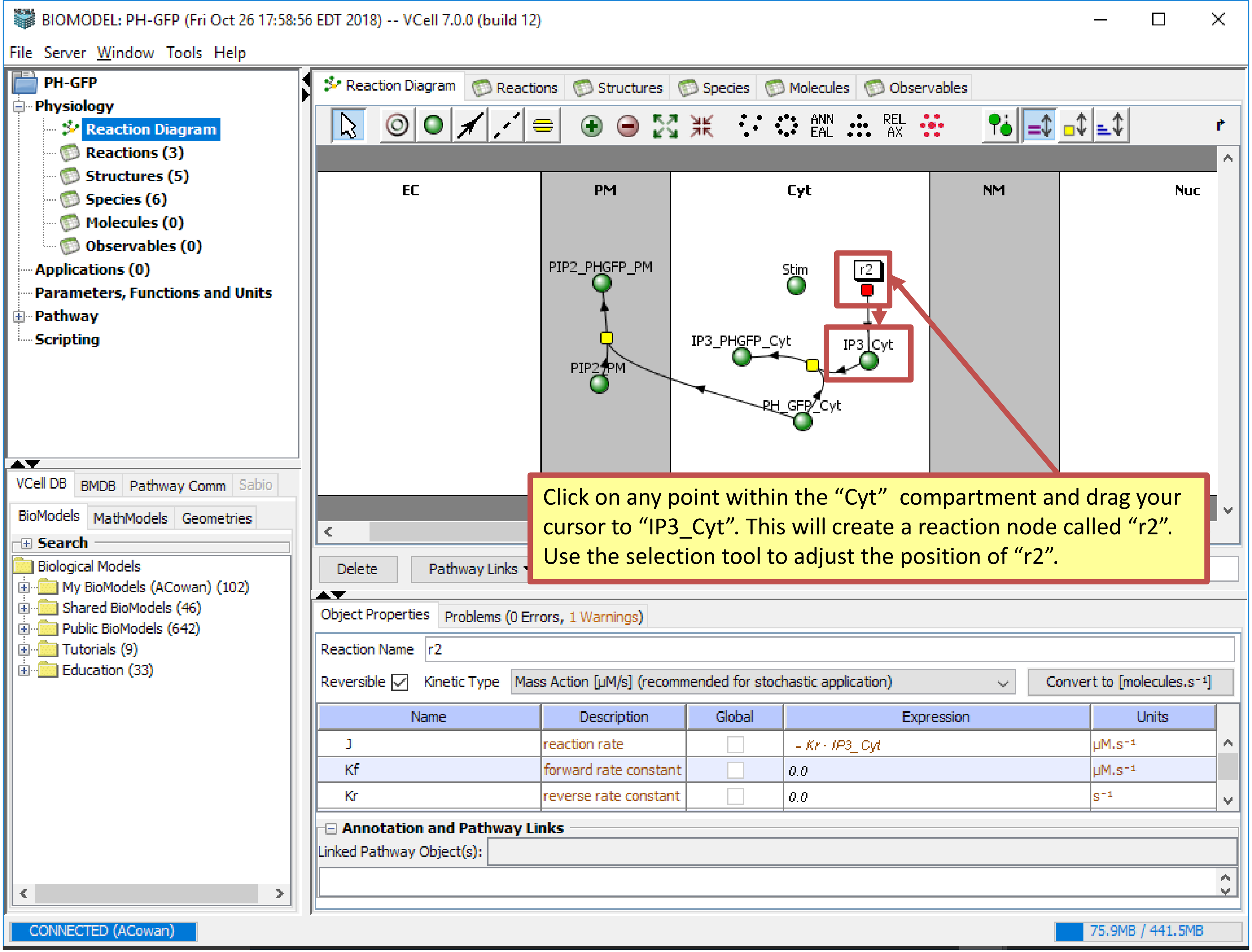
Problems (0 Errors, 0 Warnings)
Convert to [molecules.s⁻¹]
Annotation and Pathway Links
Linked Pathway Object(s):
CONNECTED (ACowan)
143.2MB / 439.4MB

Drag a line from “PH_GFP_Cyt” to “r1”.

Reaction Name: r1

Reversible ☑ Kinetic Type: Mass Action [μM/s] (recommended for stochastic application)

Name	Description	Global	Expression	Units
J	reaction rate	☐	$(Kf \cdot IP3\_Cyt \cdot PH\_GFP\_Cyt - Kr \cdot IP3\_PHGFP\_Cyt)$	$\mu M.s^{-1}$
Kf	forward rate constant	☐	0.0	$s^{-1}.\mu M^{-1}$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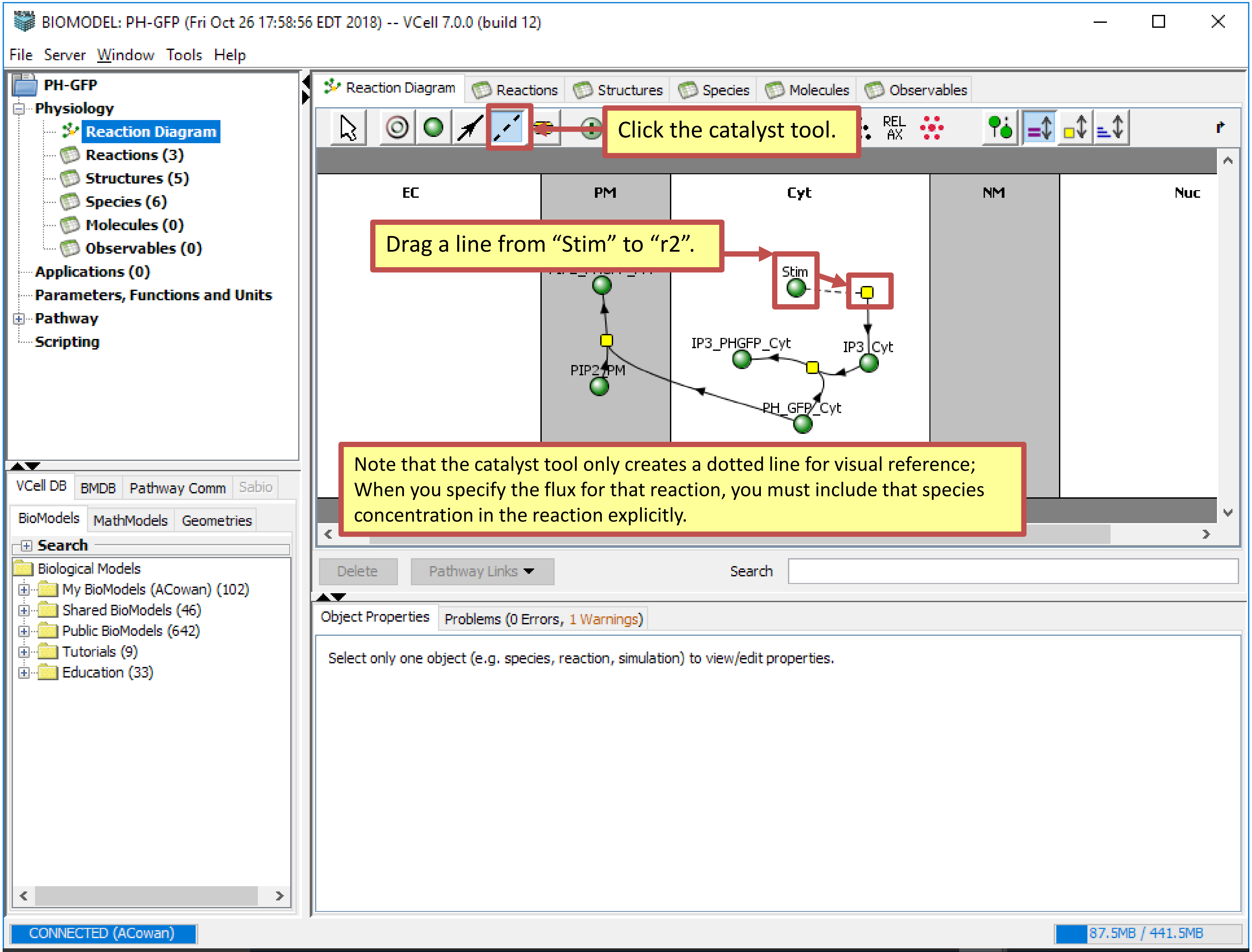
Convert to [molecules.s-1]
Annotation and Pathway Links
Linked Pathway Object(s):
CONNECTED (ACowan)
75.9MB / 441.5MB

Click on any point within the “Cyt” compartment and drag your cursor to “IP3_Cyt”. This will create a reaction node called “r2”. Use the selection tool to adjust the position of “r2”.

Reaction Name: r2

Reversible ☑ Kinetic Type: Mass Action [μM/s] (recommended for stochastic application)

Name	Description	Global	Expression	Units
J	reaction rate	☐	- Kr · IP3_Cyt	$\mu M.s^{-1}$
Kf	forward rate constant	☐	0.0	$\mu M.s^{-1}$
Kr	reverse rate constant	☐	0.0	s^{-1}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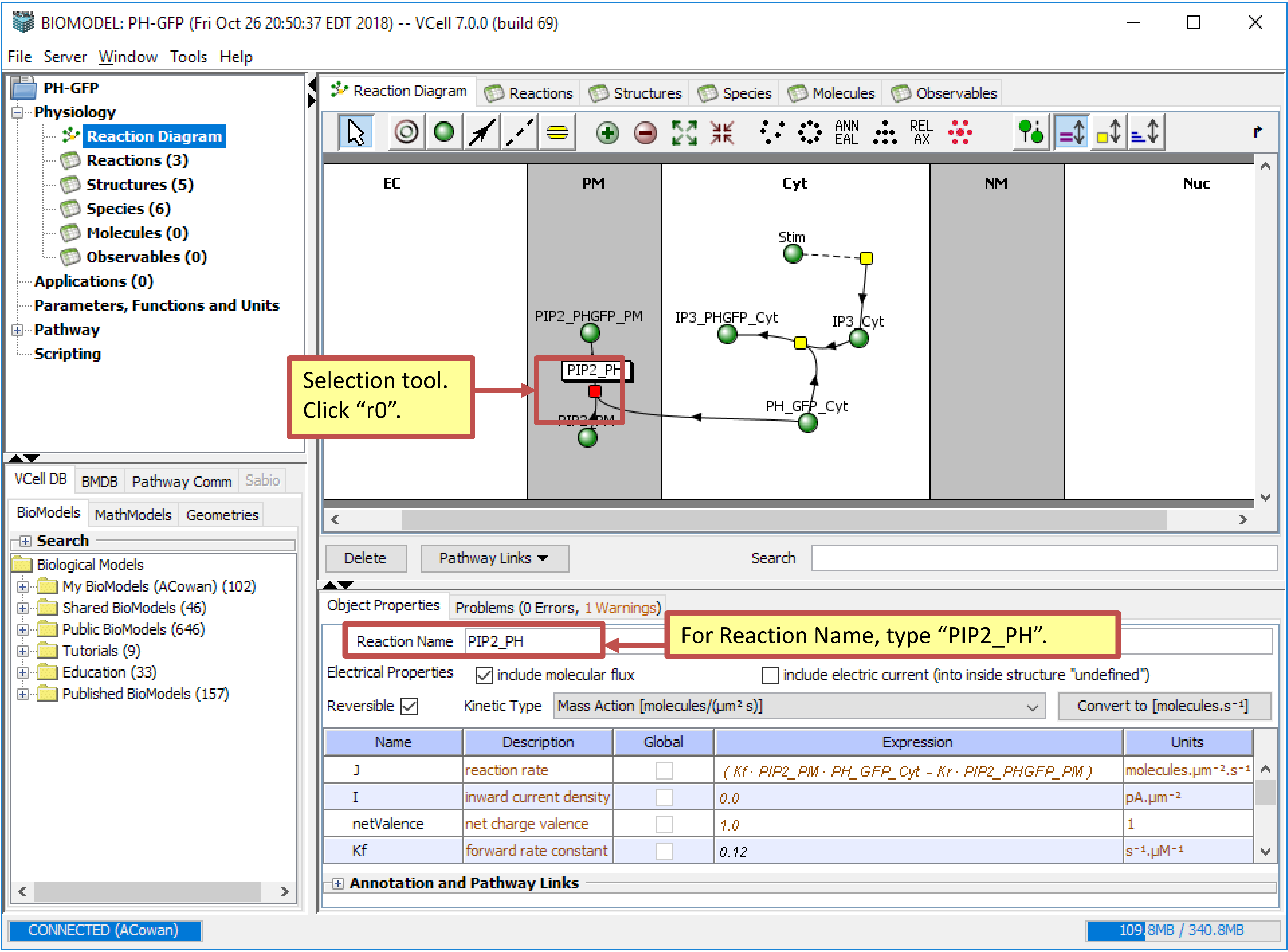
Object Properties
Problems (0 Errors, 1 Warnings)
CONNECTED (ACowan)
87.5MB / 441.5MB

Click the catalyst tool.

Drag a line from “Stim” to “r2”.

Note that the catalyst tool only creates a dotted line for visual reference; When you specify the flux for that reaction, you must include that species concentration in the reaction explicitly.

Select only one object (e.g. species, reaction, simulation) to view/edit properties.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Annotation and Pathway Links
CONNECTED (ACowan)
109.8MB / 340.8MB

Selection tool. Click “r0”.

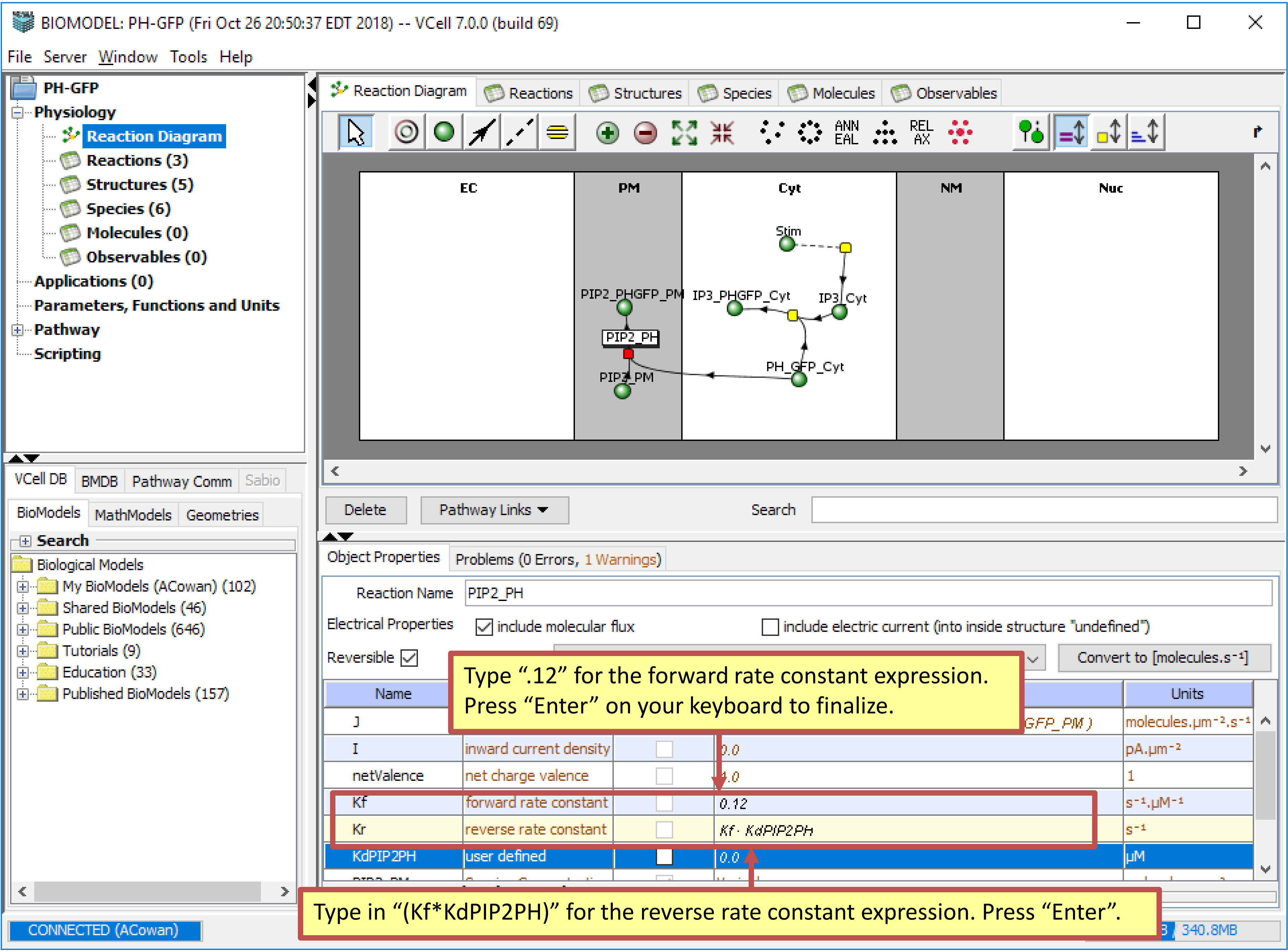
For Reaction Name, type “PIP2_PH”.

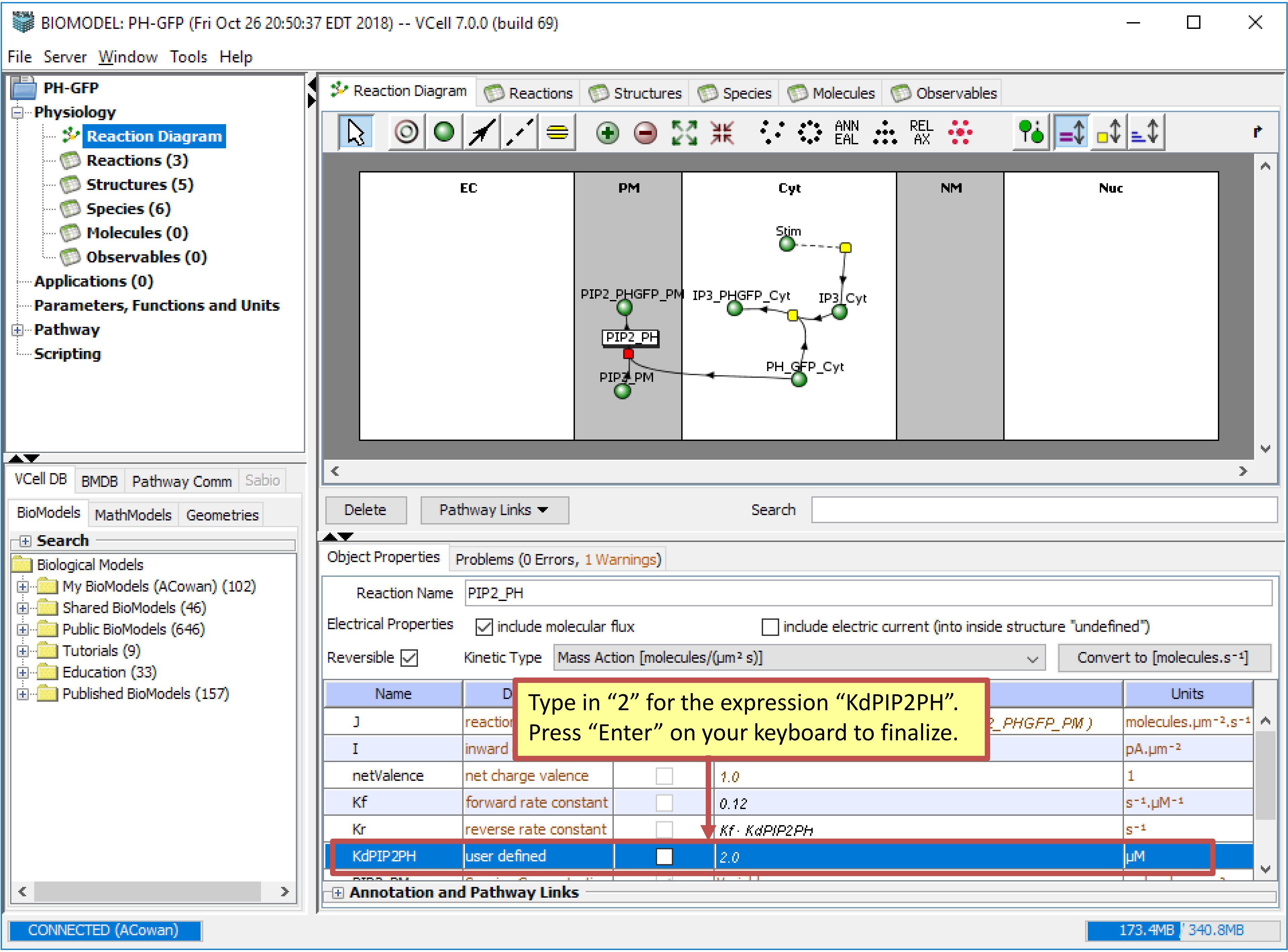
Reaction Name PIP2_PH

Electrical Properties ☑ include molecular flux ☐ include electric current (into inside structure "undefined")

Reversible ☑ Kinetic Type Mass Action [molecules/(µm² s)] Convert to [molecules.s⁻¹]

Name	Description	Global	Expression	Units
J	reaction rate	☐	(Kf · PIP2_PM · PH_GFP_Cyt - Kr · PIP2_PHGFP_PM)	molecules.µm⁻².s⁻¹
I	inward current density	☐	0.0	pA.µm⁻²
netValence	net charge valence	☐	1.0	1
Kf	forward rate constant	☐	0.12	s⁻¹.µM⁻¹





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173.4MB / 340.8MB

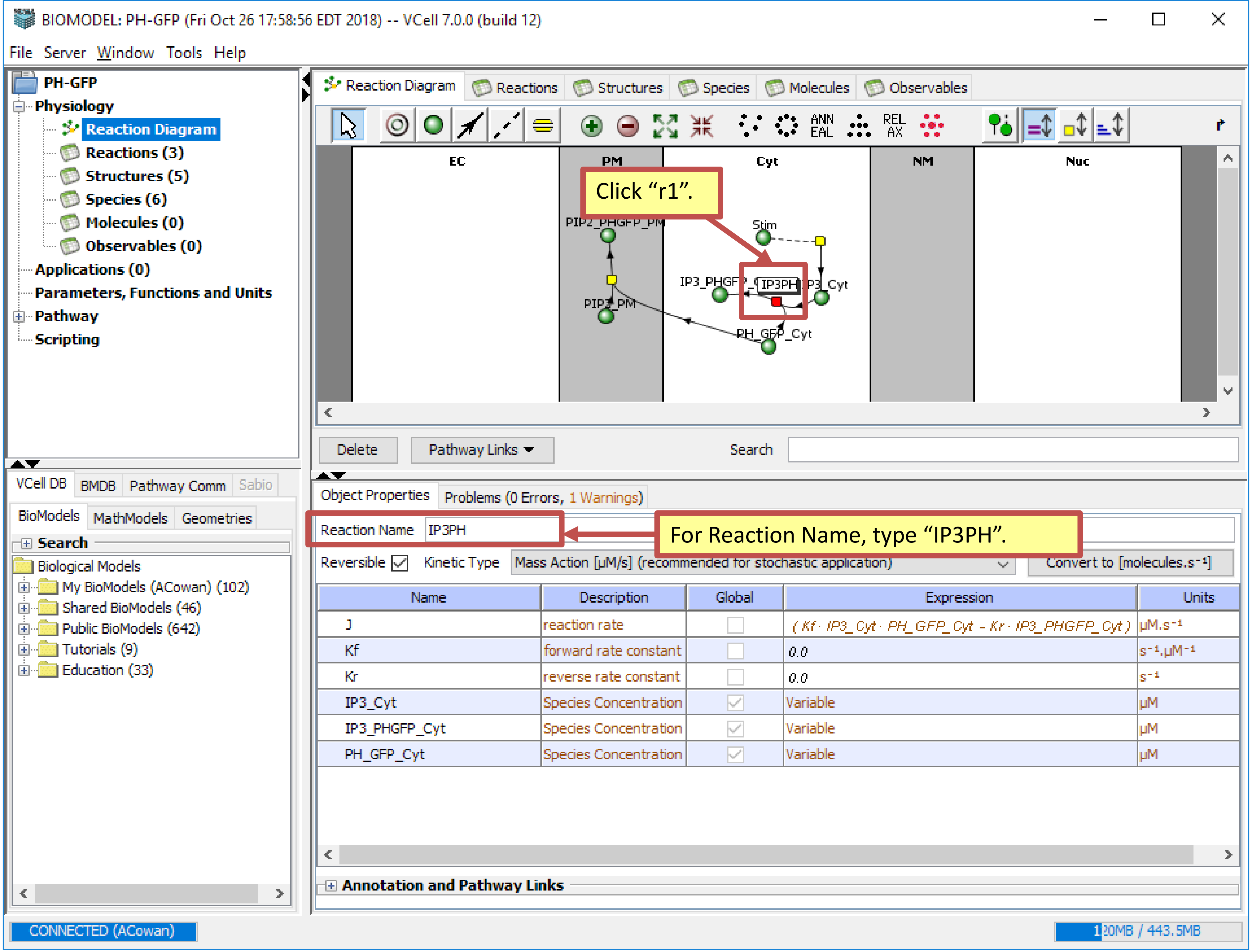
Reaction Name: PIP2_PH

Electrical Properties: ☑ include molecular flux ☐ include electric current (into inside structure "undefined")

Reversible ☑ Kinetic Type: Mass Action [molecules/(µm² s)] Convert to [molecules.s⁻¹]

Name	D…		…Expression	Units
J	reaction…		…2_PHGFP_PM)	molecules.µm⁻².s⁻¹
I	inward…			pA.µm⁻²
netValence	net charge valence	☐	1.0	1
Kf	forward rate constant	☐	0.12	s⁻¹.µM⁻¹
Kr	reverse rate constant	☐	Kf · KdPIP2PH	s⁻¹
KdPIP2PH	user defined	☐	2.0	µM

Type in “2” for the expression “KdPIP2PH”. Press “Enter” on your keyboard to finalize.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Convert to [molecules.s⁻¹]
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120MB / 443.5MB

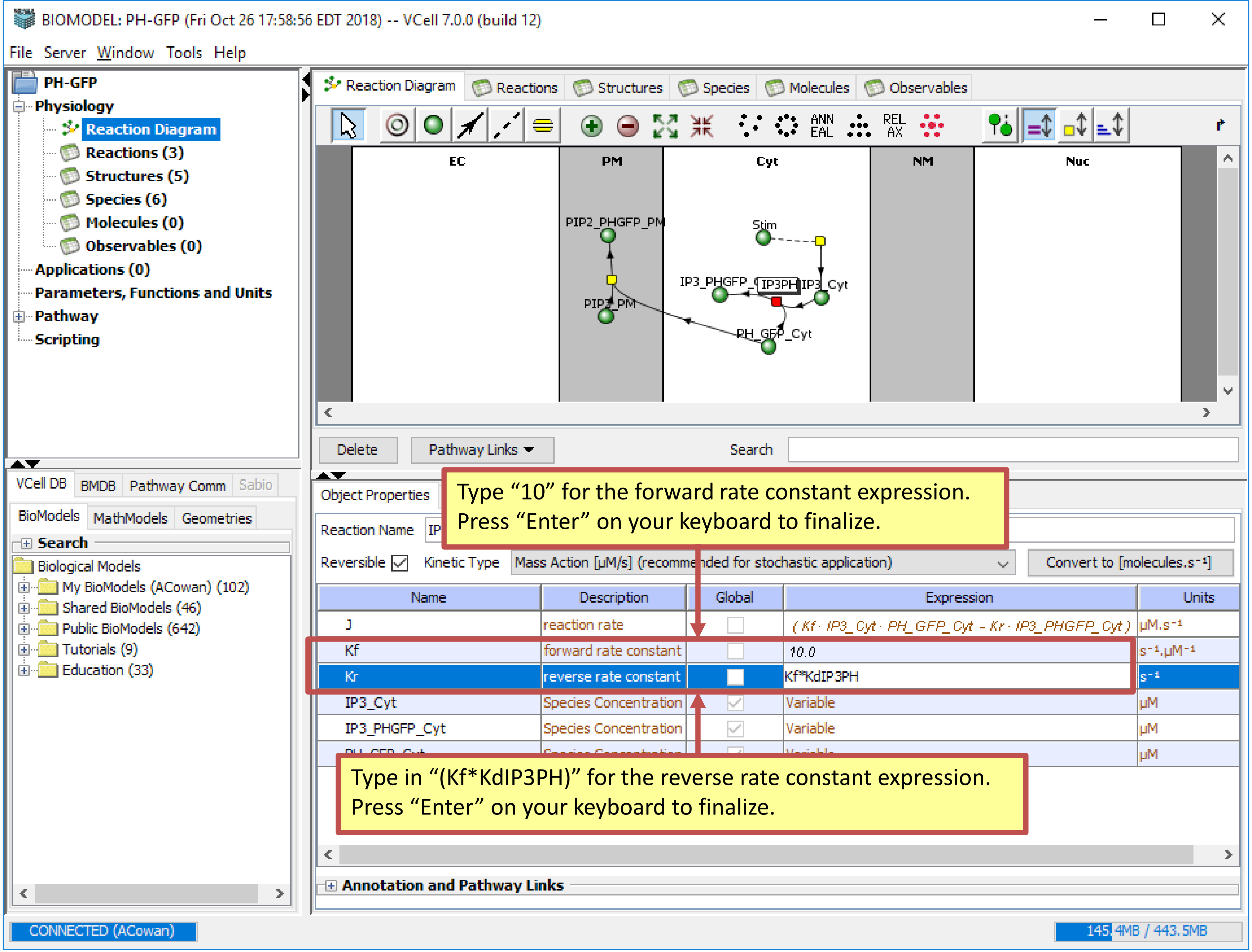
Click “r1”.

For Reaction Name, type “IP3PH”.

Reaction Name: IP3PH

Reversible ☑ Kinetic Type: Mass Action [µM/s] (recommended for stochastic application)

Name	Description	Global	Expression	Units
J	reaction rate	☐	(Kf · IP3_Cyt · PH_GFP_Cyt – Kr · IP3_PHGFP_Cyt)	µM.s⁻¹
Kf	forward rate constant	☐	0.0	s⁻¹.µM⁻¹
Kr	reverse rate constant	☐	0.0	s⁻¹
IP3_Cyt	Species Concentration	☑	Variable	µM
IP3_PHGFP_Cyt	Species Concentration	☑	Variable	µM
PH_GFP_Cyt	Species Concentration	☑	Variable	µM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145.4MB / 443.5MB

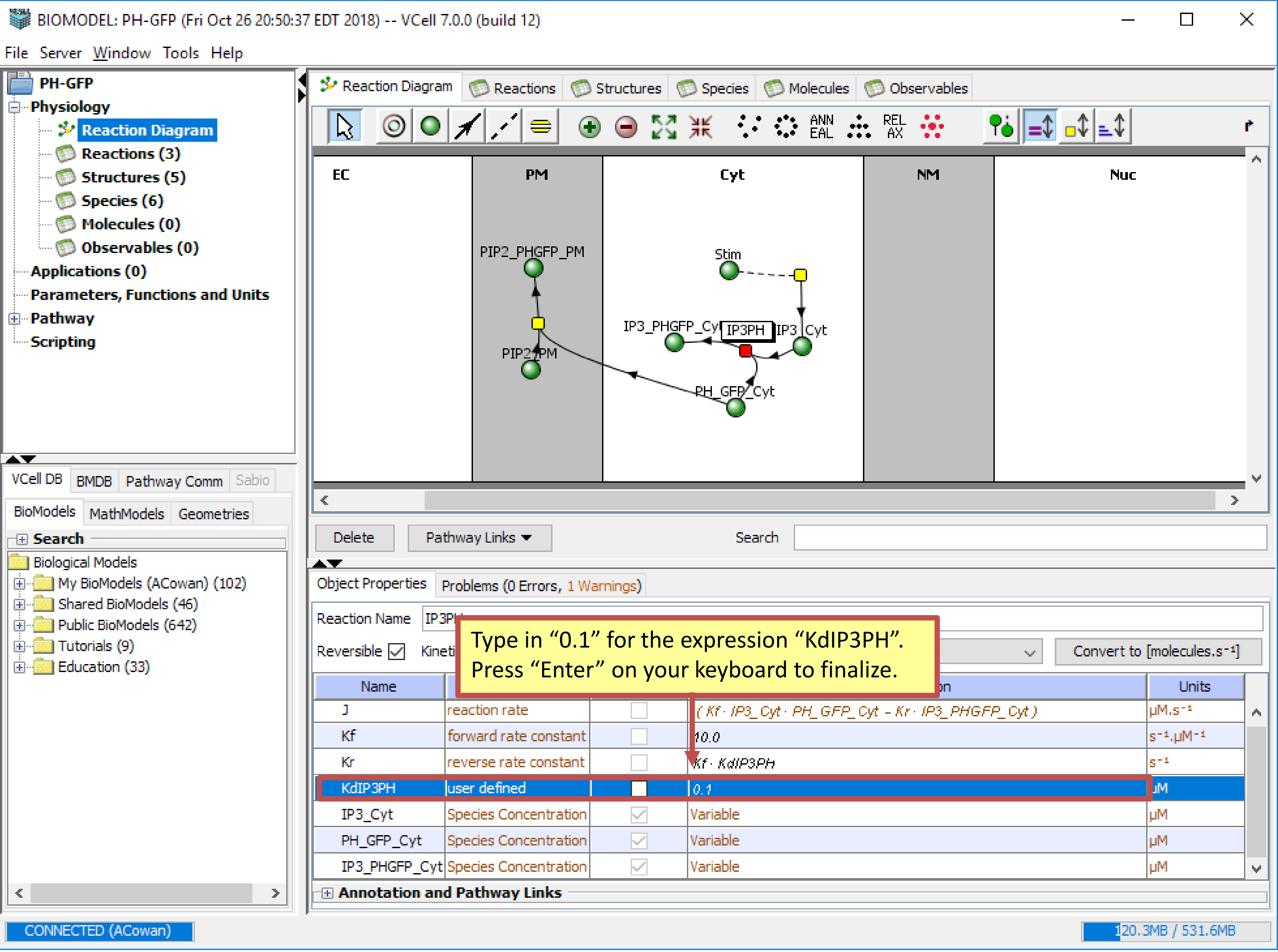
Type “10” for the forward rate constant expression. Press “Enter” on your keyboard to finalize.

Reaction Name IP

Reversible ☑ Kinetic Type Mass Action [µM/s] (recommended for stochastic application) Convert to [molecules.s⁻¹]

Name	Description	Global	Expression	Units
J	reaction rate	☐	(Kf · IP3_Cyt · PH_GFP_Cyt − Kr · IP3_PHGFP_Cyt)	$\mu M.s^{-1}$
Kf	forward rate constant	☐	10.0	$s^{-1}.\mu M^{-1}$
Kr	reverse rate constant	☐	Kf*KdIP3PH	s^{-1}
IP3_Cyt	Species Concentration	☑	Variable	µM
IP3_PHGFP_Cyt	Species Concentration	☑	Variable	µM
PH_GFP_Cyt	Species Concentration	☑	Variable	µM

Type in “(Kf*KdIP3PH)” for the reverse rate constant expression. Press “Enter” on your keyboard to finalize.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ANN EAL
REL AX
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PIP2_PHGFP_PM
Stim
IP3_PHGFP_Cyt
IP3PH
IP3_Cyt
PIP2_PM
PH_GFP_Cyt
Delete
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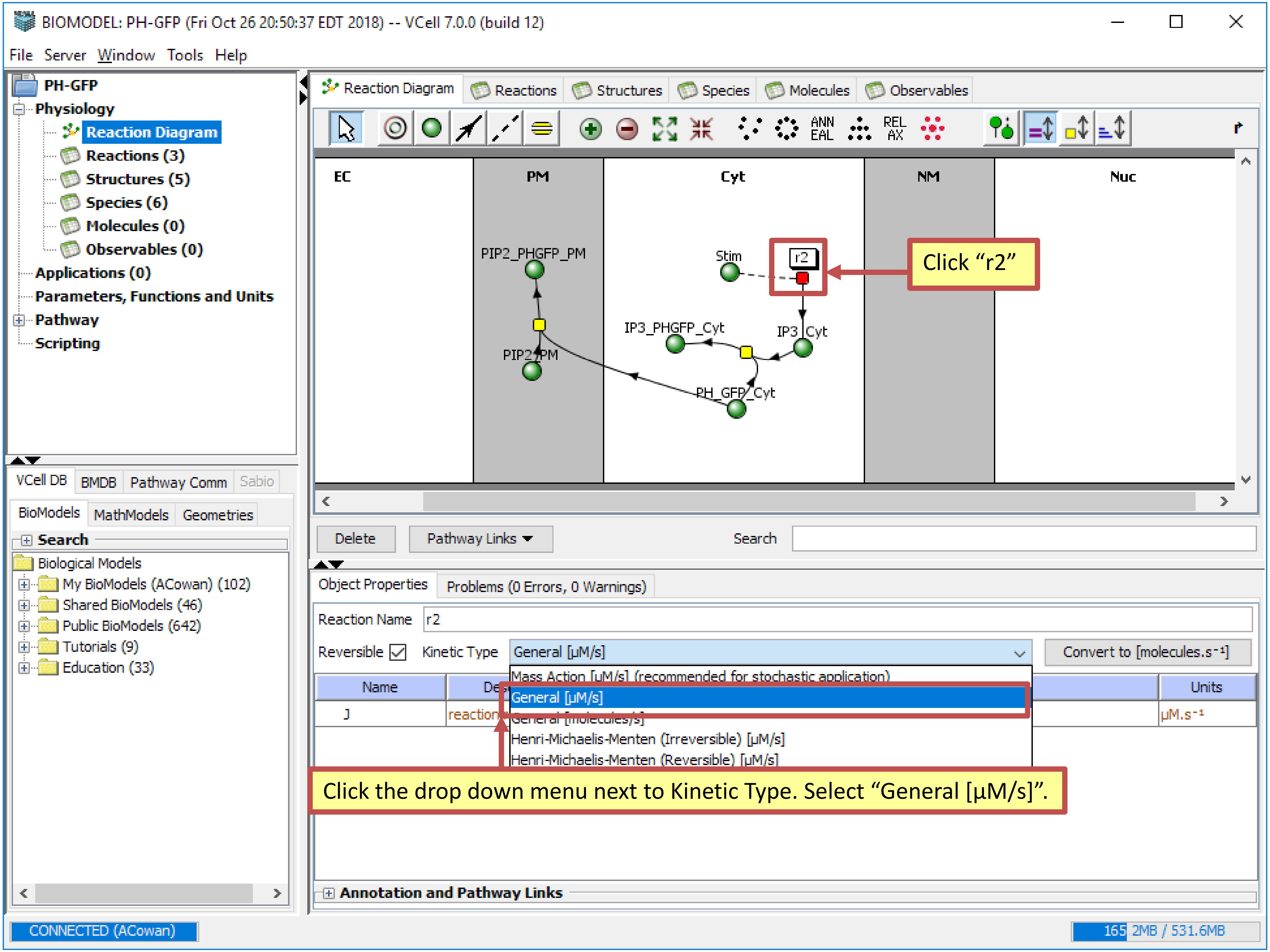
Search
Object Properties
Problems (0 Errors, 1 Warnings)
Reaction Name IP3PH
Reversible ☑ Kineti
Convert to [molecules.s⁻¹]
Annotation and Pathway Links
CONNECTED (ACowan)
120.3MB / 531.6MB

Type in “0.1” for the expression “KdIP3PH”. Press “Enter” on your keyboard to finalize.

Name			n	Units
J	reaction rate	☐	(Kf · IP3_Cyt · PH_GFP_Cyt - Kr · IP3_PHGFP_Cyt)	µM.s⁻¹
Kf	forward rate constant	☐	10.0	s⁻¹.µM⁻¹
Kr	reverse rate constant	☐	Kf · KdIP3PH	s⁻¹
KdIP3PH	user defined	☐	0.1	µM
IP3_Cyt	Species Concentration	☑	Variable	µM
PH_GFP_Cyt	Species Concentration	☑	Variable	µM
IP3_PHGFP_Cyt	Species Concentration	☑	Variable	µM


File Server Window Tools Help
PH-GFP
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Reaction Diagram
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Structures (5)
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Molecules (0)
Observables (0)
Applications (0)
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PIP2_PM
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IP3_PHGFP_Cyt
IP3_Cyt
PH_GFP_Cyt
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Convert to [molecules.s⁻¹]
Annotation and Pathway Links
CONNECTED (ACowan)
165.2MB / 531.6MB

BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 12)

Reaction Name r2

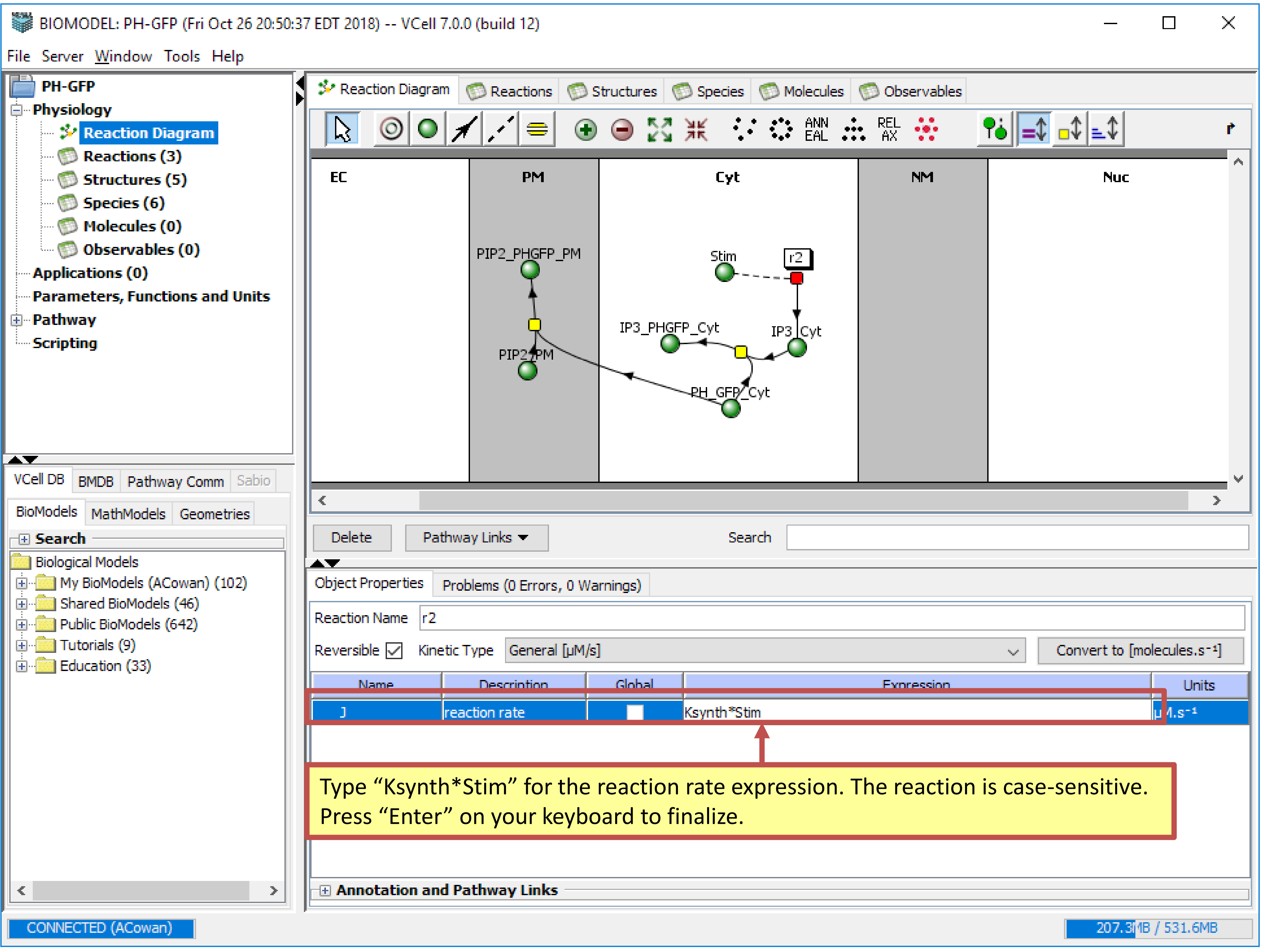
Reversible ☑ Kinetic Type General [µM/s]

- Mass Action [µM/s] (recommended for stochastic application)
- General [µM/s]
- General [molecules/s]
- Henri-Michaelis-Menten (Irreversible) [µM/s]
- Henri-Michaelis-Menten (Reversible) [µM/s]

Name	De	Units
J	reaction	µM.s⁻¹

Click “r2”

Click the drop down menu next to Kinetic Type. Select “General [µM/s]”.



BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 12)
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Applications (0)
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Reaction Diagram Reactions Structures Species Molecules Observables
EC PM Cyt NM Nuc
PIP2_PHGFP_PM
PIP2_PM
Stim
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IP3_PHGFP_Cyt
IP3_Cyt
PH_GFP_Cyt
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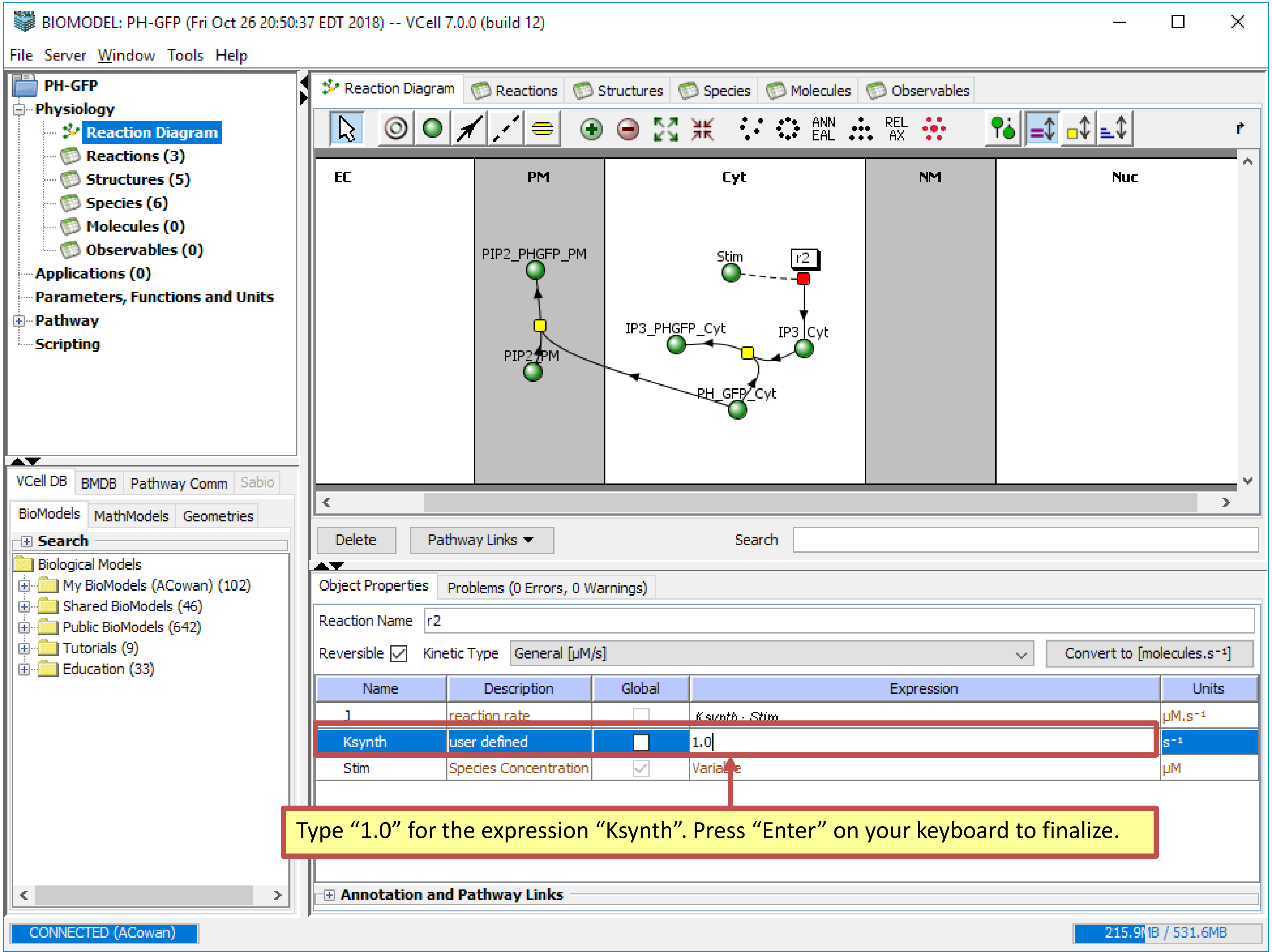
Object Properties Problems (0 Errors, 0 Warnings)
Convert to [molecules.s⁻¹]
Annotation and Pathway Links
CONNECTED (ACowan)
207.3MB / 531.6MB

Reaction Name: r2

Reversible ☑ Kinetic Type: General [µM/s]

Name	Description	Global	Expression	Units
J	reaction rate	☐	Ksynth*Stim	µM.s⁻¹

Type "Ksynth*Stim" for the reaction rate expression. The reaction is case-sensitive. Press "Enter" on your keyboard to finalize.


BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 12)
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Nuc
PIP2_PHGFP_PM
PIP2_PM
Stim
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IP3_PHGFP_Cyt
IP3_Cyt
PH_GFP_Cyt
Delete
Pathway Links
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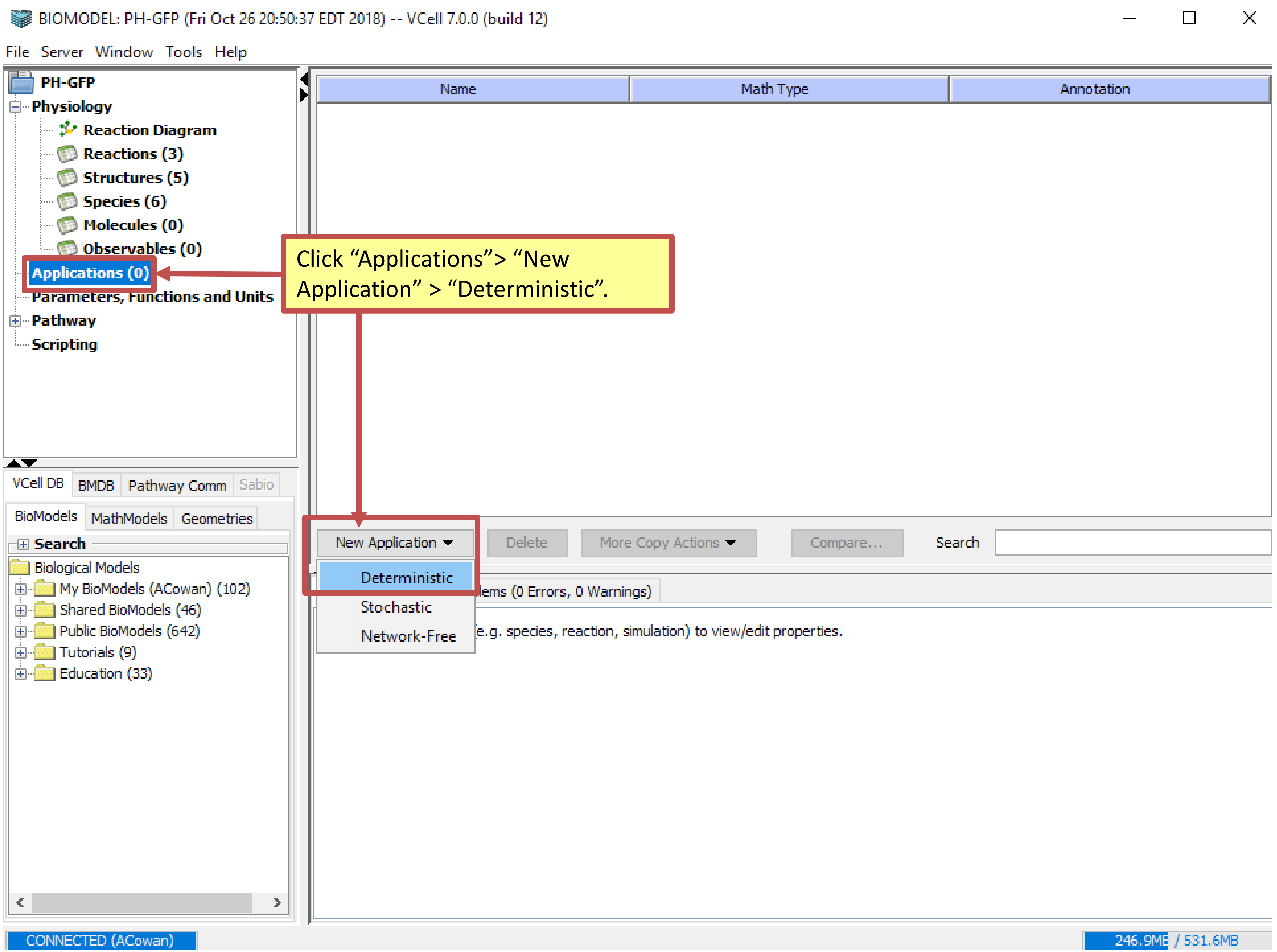
Object Properties
Problems (0 Errors, 0 Warnings)
Annotation and Pathway Links
CONNECTED (ACowan)
215.9MB / 531.6MB

Reaction Name r2

Reversible ☑ Kinetic Type General [µM/s] Convert to [molecules.s^{-1}]

Name	Description	Global	Expression	Units
J	reaction rate	☐	Ksynth · Stim	µM.s^{-1}
Ksynth	user defined	☐	1.0	s^{-1}
Stim	Species Concentration	☑	Variable	µM

Type “1.0” for the expression “Ksynth”. Press “Enter” on your keyboard to finalize.



BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 12)
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New Application
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Search
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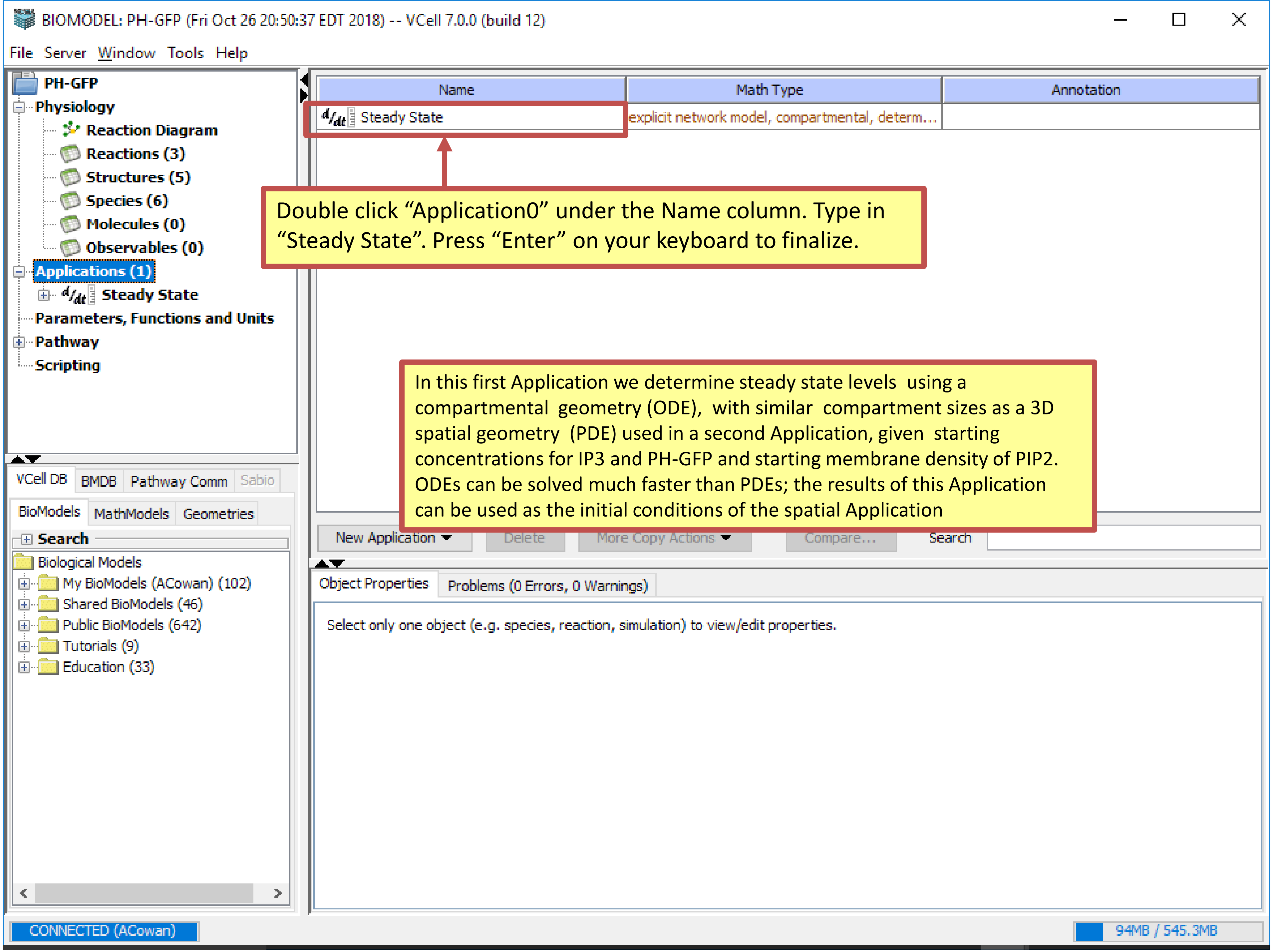
Stochastic
Network-Free
lems (0 Errors, 0 Warnings)
CONNECTED (ACowan)
246.9MB / 531.6MB

(e.g. species, reaction, simulation) to view/edit properties.

Click “Applications”> “New Application” > “Deterministic”.


BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 12)
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Name
Math Type
Annotation
New Application
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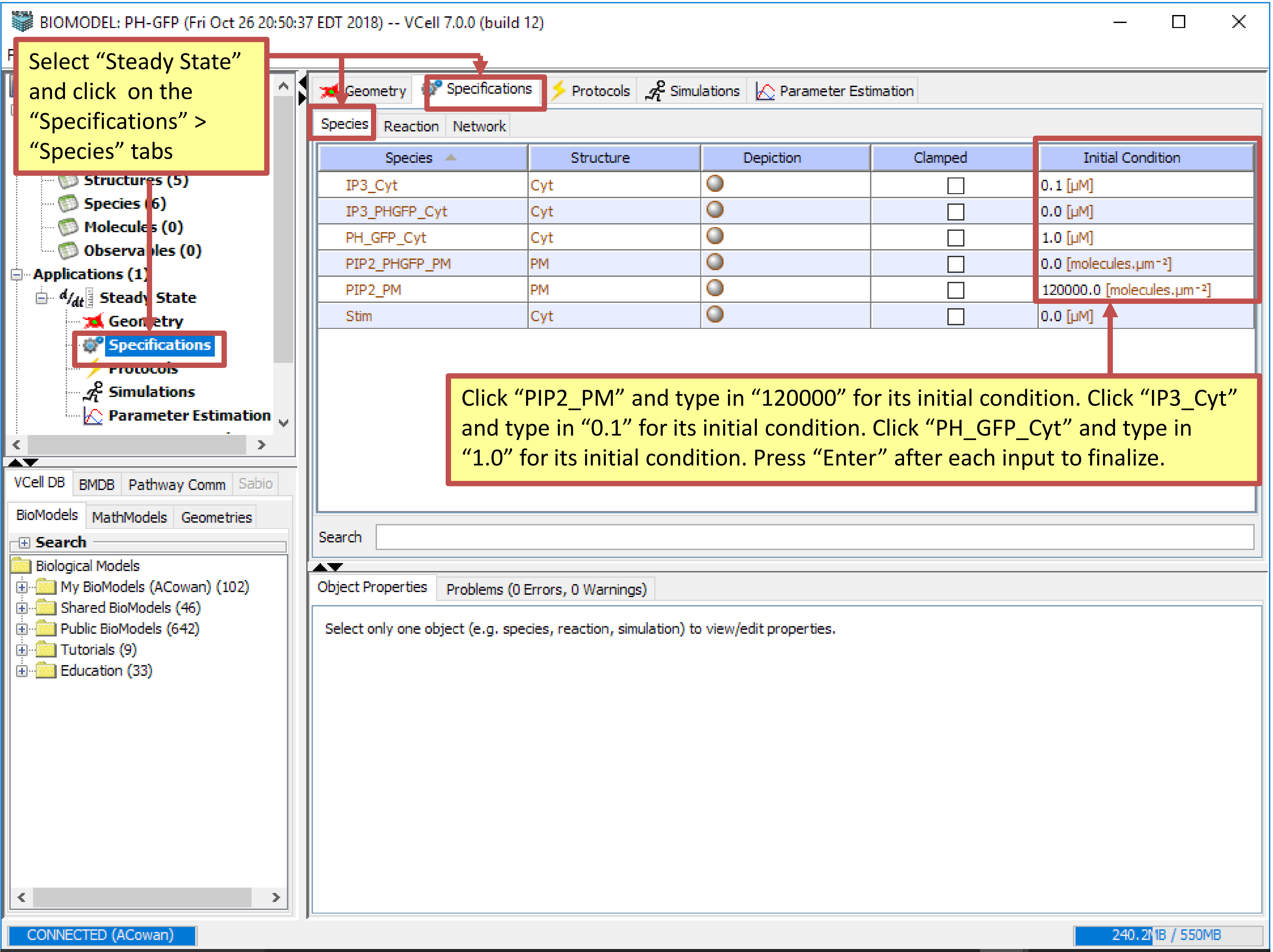
More Copy Actions
Compare...
Search
Object Properties
Problems (0 Errors, 0 Warnings)
CONNECTED (ACowan)
94MB / 545.3MB

Name	Math Type	Annotation
Steady State	explicit network model, compartmental, determ...	

Select only one object (e.g. species, reaction, simulation) to view/edit properties.

Double click "Application0" under the Name column. Type in "Steady State". Press "Enter" on your keyboard to finalize.

In this first Application we determine steady state levels using a compartmental geometry (ODE), with similar compartment sizes as a 3D spatial geometry (PDE) used in a second Application, given starting concentrations for IP3 and PH-GFP and starting membrane density of PIP2. ODEs can be solved much faster than PDEs; the results of this Application can be used as the initial conditions of the spatial Application


BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 12)
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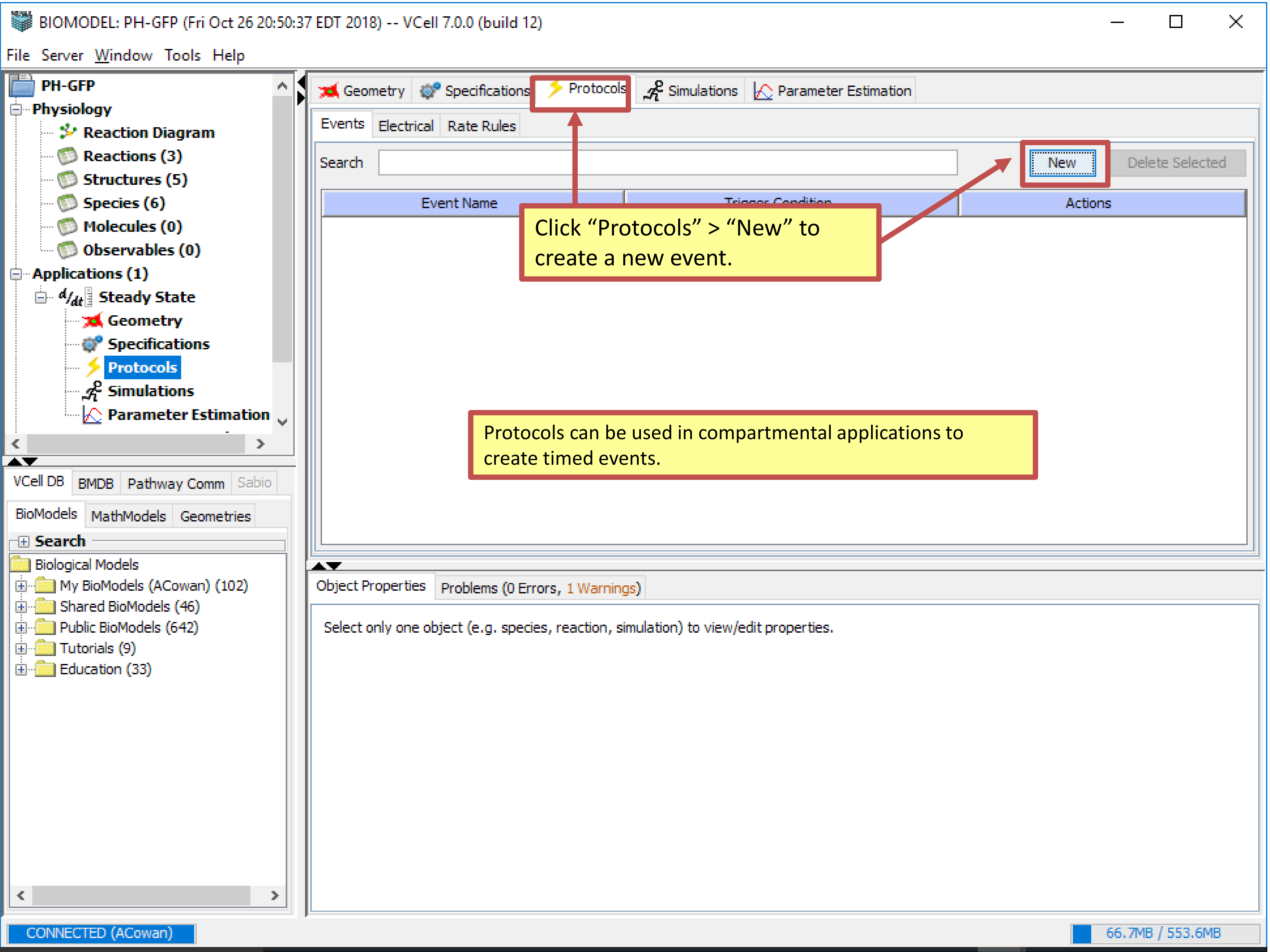
Problems (0 Errors, 0 Warnings)
CONNECTED (ACowan)
240.2MB / 550MB

Select “Steady State” and click on the “Specifications” > “Species” tabs

Species	Structure	Depiction	Clamped	Initial Condition
IP3_Cyt	Cyt	●	☐	0.1 [µM]
IP3_PHGFP_Cyt	Cyt	●	☐	0.0 [µM]
PH_GFP_Cyt	Cyt	●	☐	1.0 [µM]
PIP2_PHGFP_PM	PM	●	☐	0.0 [molecules.µm-²]
PIP2_PM	PM	●	☐	120000.0 [molecules.µm-²]
Stim	Cyt	●	☐	0.0 [µM]

Click “PIP2_PM” and type in “120000” for its initial condition. Click “IP3_Cyt” and type in “0.1” for its initial condition. Click “PH_GFP_Cyt” and type in “1.0” for its initial condition. Press “Enter” after each input to finalize.

Select only one object (e.g. species, reaction, simulation) to view/edit properties.


BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 12)
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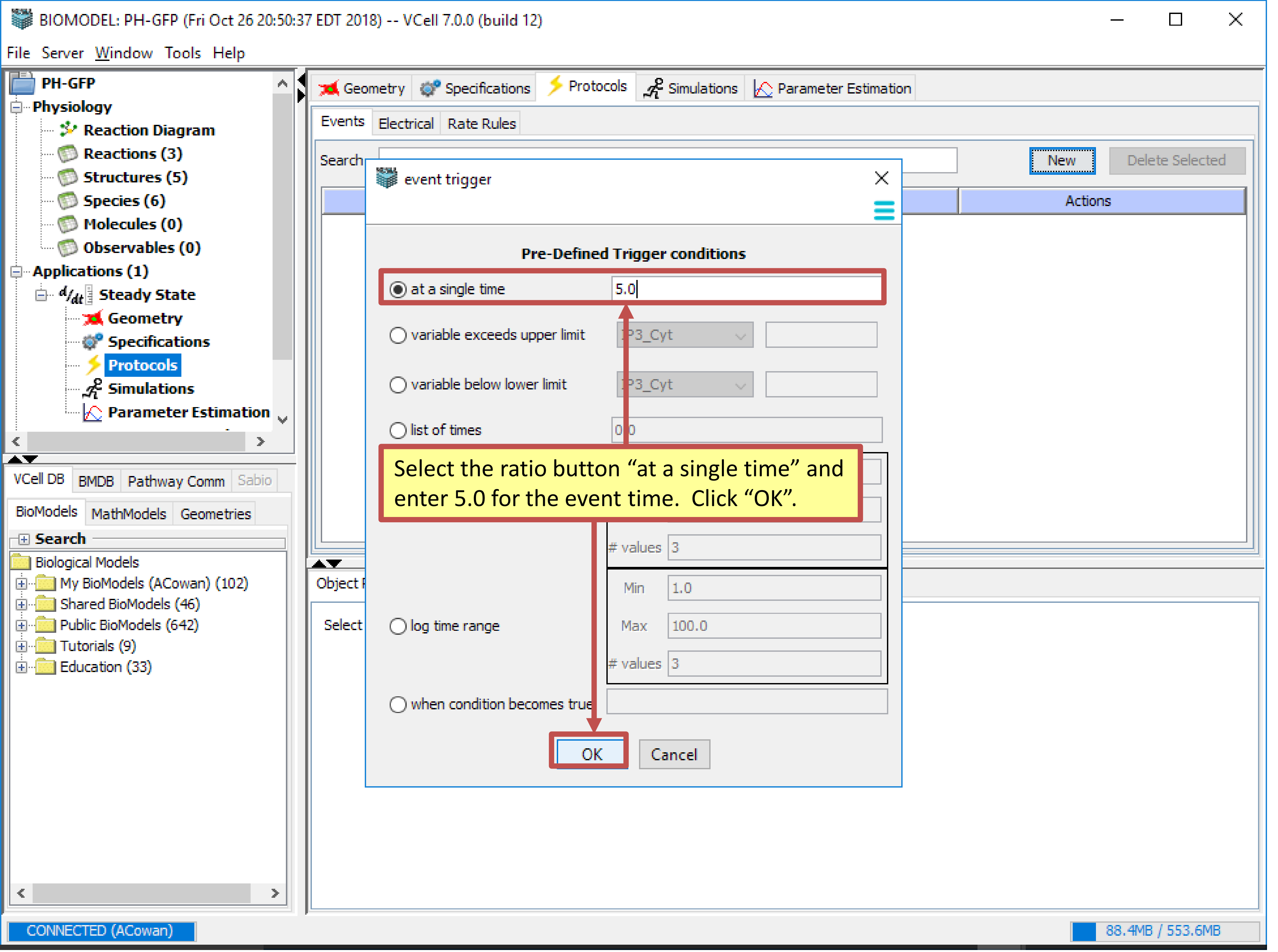
New
Delete Selected
Event Name
Trigger Condition
Actions
Object Properties
Problems (0 Errors, 1 Warnings)
CONNECTED (ACowan)
66.7MB / 553.6MB

Click “Protocols” > “New” to create a new event.

Protocols can be used in compartmental applications to create timed events.

Select only one object (e.g. species, reaction, simulation) to view/edit properties.


BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 12)
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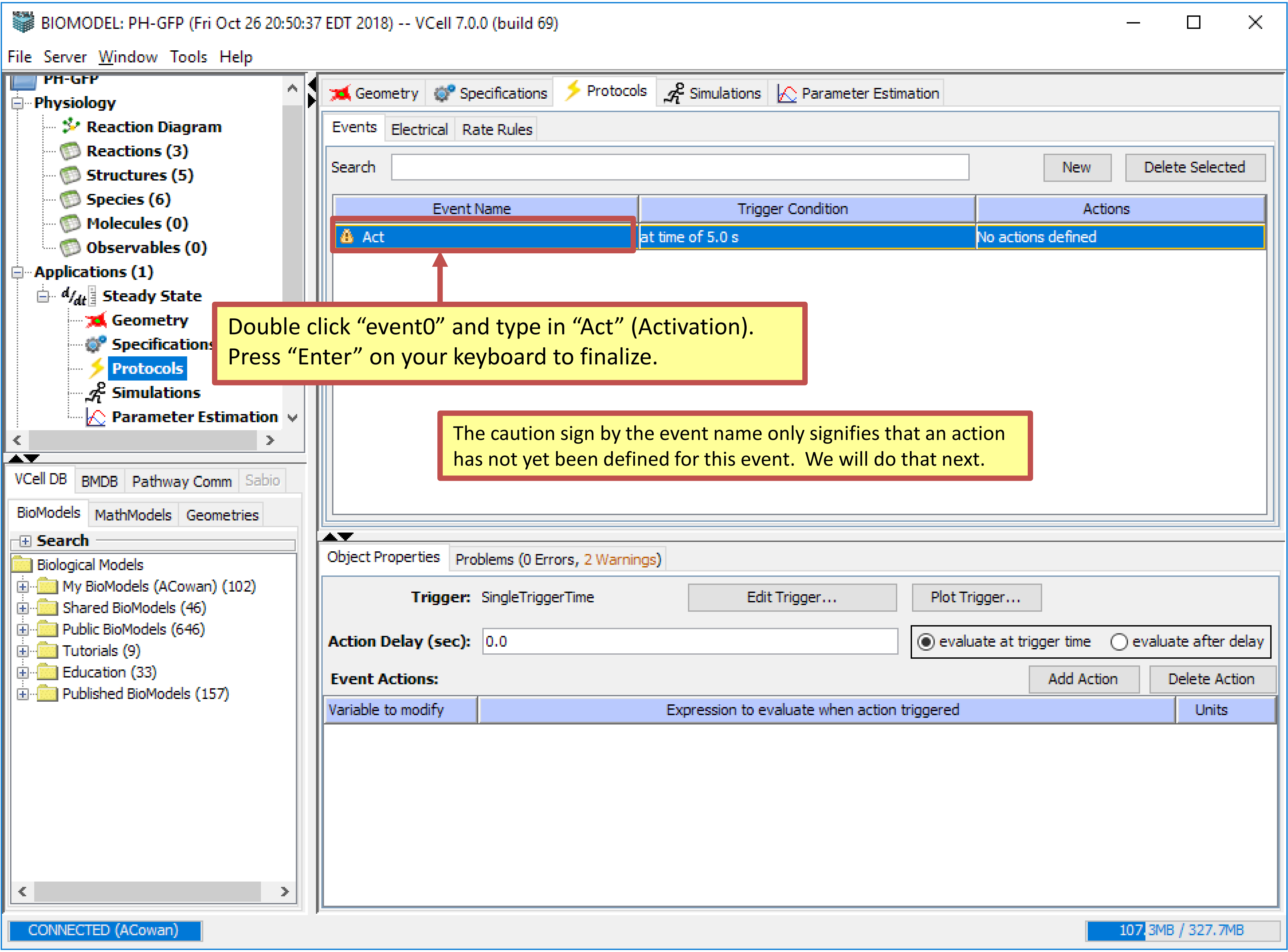
Search
New Delete Selected
Actions
Object
Select
event trigger
Pre-Defined Trigger conditions
○ variable exceeds upper limit IP3_Cyt
○ variable below lower limit IP3_Cyt
○ list of times 0.0
# values 3
Min 1.0
Max 100.0
○ log time range
# values 3
○ when condition becomes true
OK Cancel
CONNECTED (ACowan)
88.4MB / 553.6MB

● at a single time 5.0

Select the ratio button “at a single time” and enter 5.0 for the event time. Click “OK”.


BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 69)
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New
Delete Selected
Object Properties
Problems (0 Errors, 2 Warnings)
Edit Trigger...
Plot Trigger...
Add Action
Delete Action
CONNECTED (ACowan)
107.3MB / 327.7MB

Event Name	Trigger Condition	Actions
Act	at time of 5.0 s	No actions defined

Trigger: SingleTriggerTime

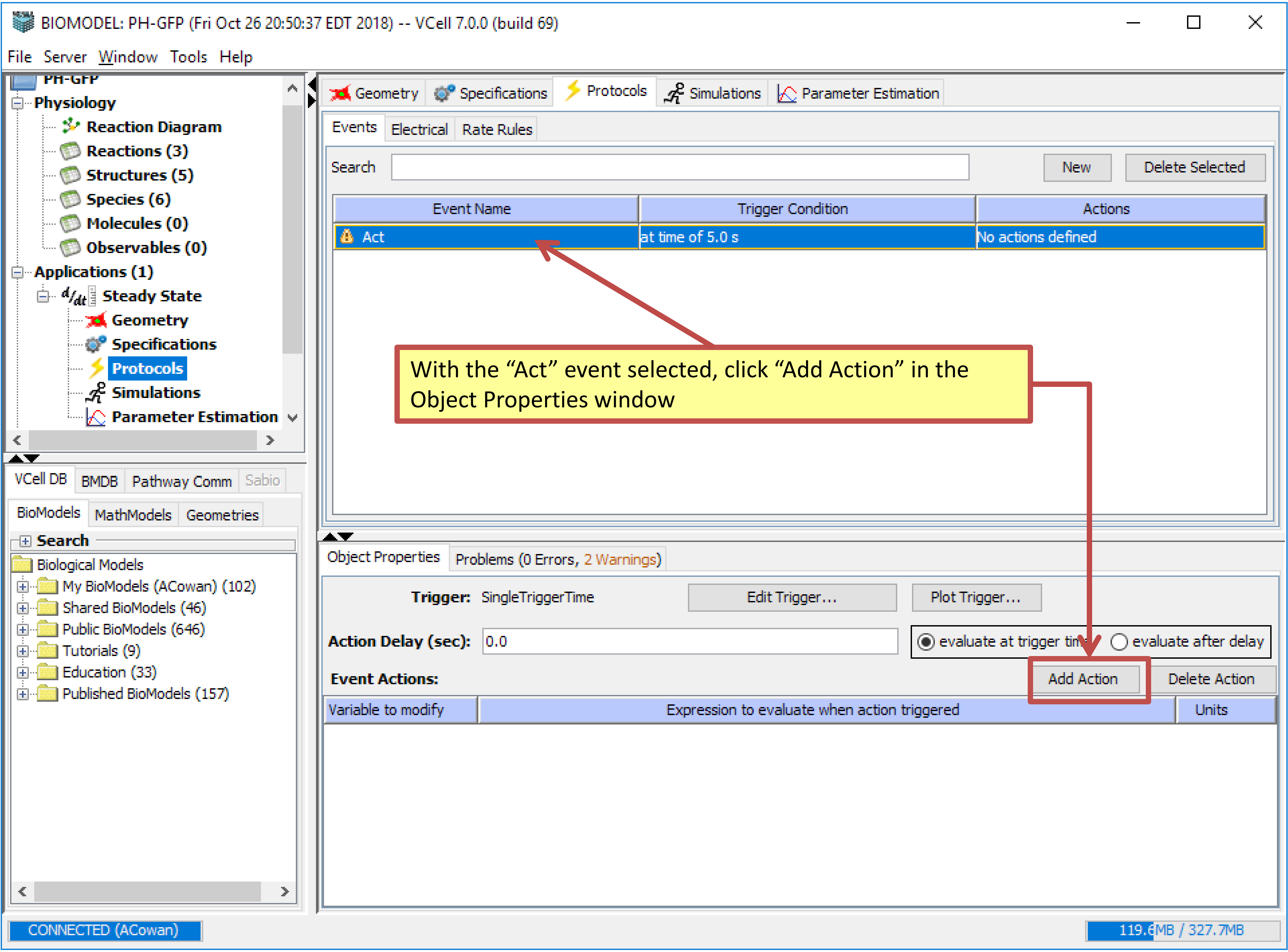
Action Delay (sec): 0.0 ● evaluate at trigger time ○ evaluate after delay

Event Actions:

Variable to modify	Expression to evaluate when action triggered	Units

Double click "event0" and type in "Act" (Activation). Press "Enter" on your keyboard to finalize.

The caution sign by the event name only signifies that an action has not yet been defined for this event. We will do that next.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New
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Object Properties
Problems (0 Errors, 2 Warnings)
Edit Trigger...
Plot Trigger...
Add Action
Delete Action

BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 69)

Event Name	Trigger Condition	Actions
Act	at time of 5.0 s	No actions defined

With the “Act” event selected, click “Add Action” in the Object Properties window

Trigger: SingleTriggerTime

Action Delay (sec): 0.0

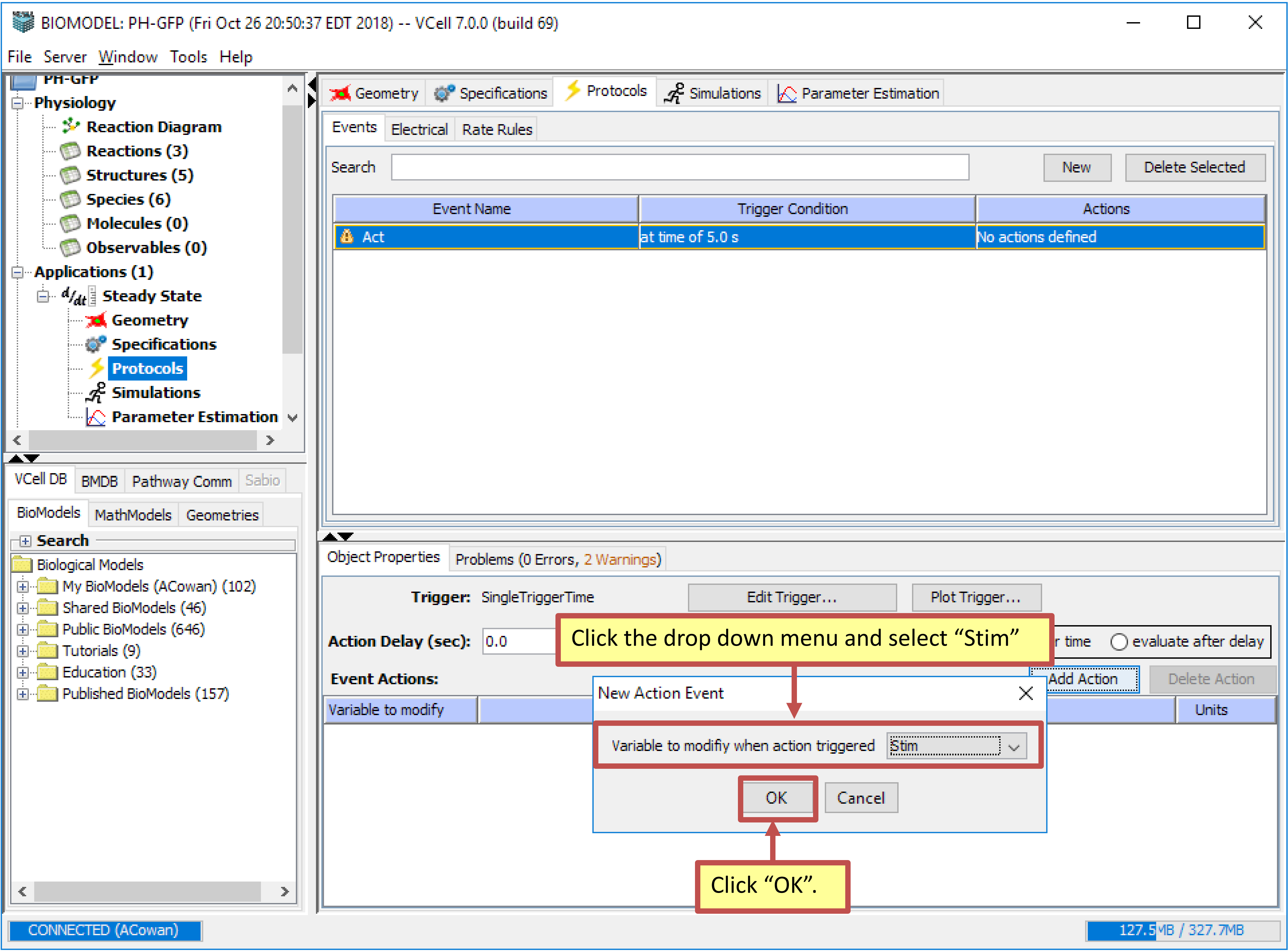
● evaluate at trigger time ○ evaluate after delay

Event Actions:

Variable to modify	Expression to evaluate when action triggered	Units

CONNECTED (ACowan)

119.6MB / 327.7MB


BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 69)
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New
Delete Selected
Object Properties
Problems (0 Errors, 2 Warnings)
Edit Trigger…
Plot Trigger…
r time
○ evaluate after delay
Add Action
Delete Action
Units
Cancel
CONNECTED (ACowan)
127.5MB / 327.7MB

Event Name	Trigger Condition	Actions
Act	at time of 5.0 s	No actions defined

Trigger: SingleTriggerTime

Action Delay (sec): 0.0

Event Actions:

Variable to modify

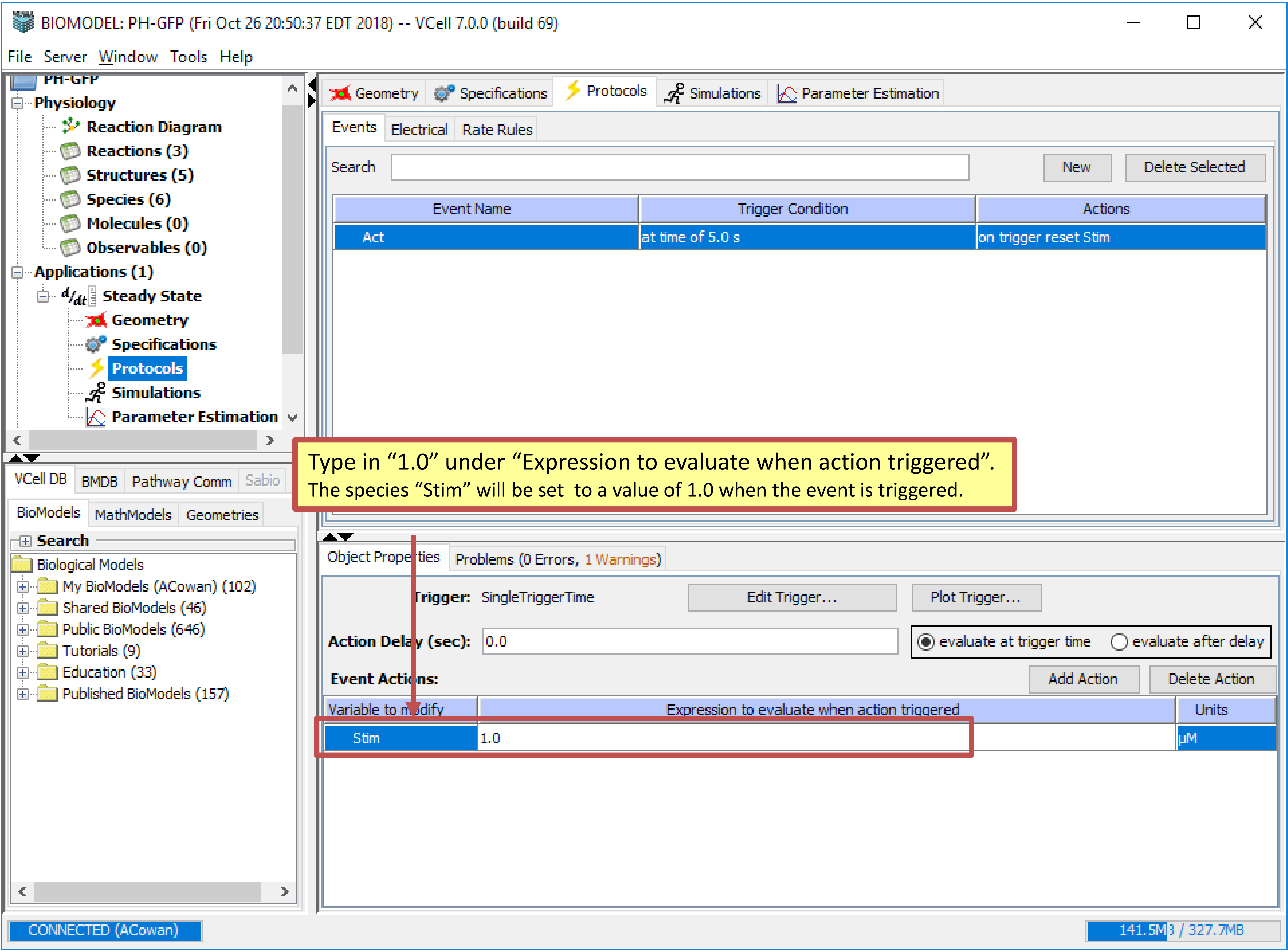
New Action Event

Variable to modify when action triggered: Stim

OK

Click the drop down menu and select “Stim”

Click “OK”.


BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 69)
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New
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Object Properties
Problems (0 Errors, 1 Warnings)
Edit Trigger…
Plot Trigger…
Add Action
Delete Action
CONNECTED (ACowan)
141.5MB / 327.7MB

Event Name	Trigger Condition	Actions
Act	at time of 5.0 s	on trigger reset Stim

Trigger: SingleTriggerTime

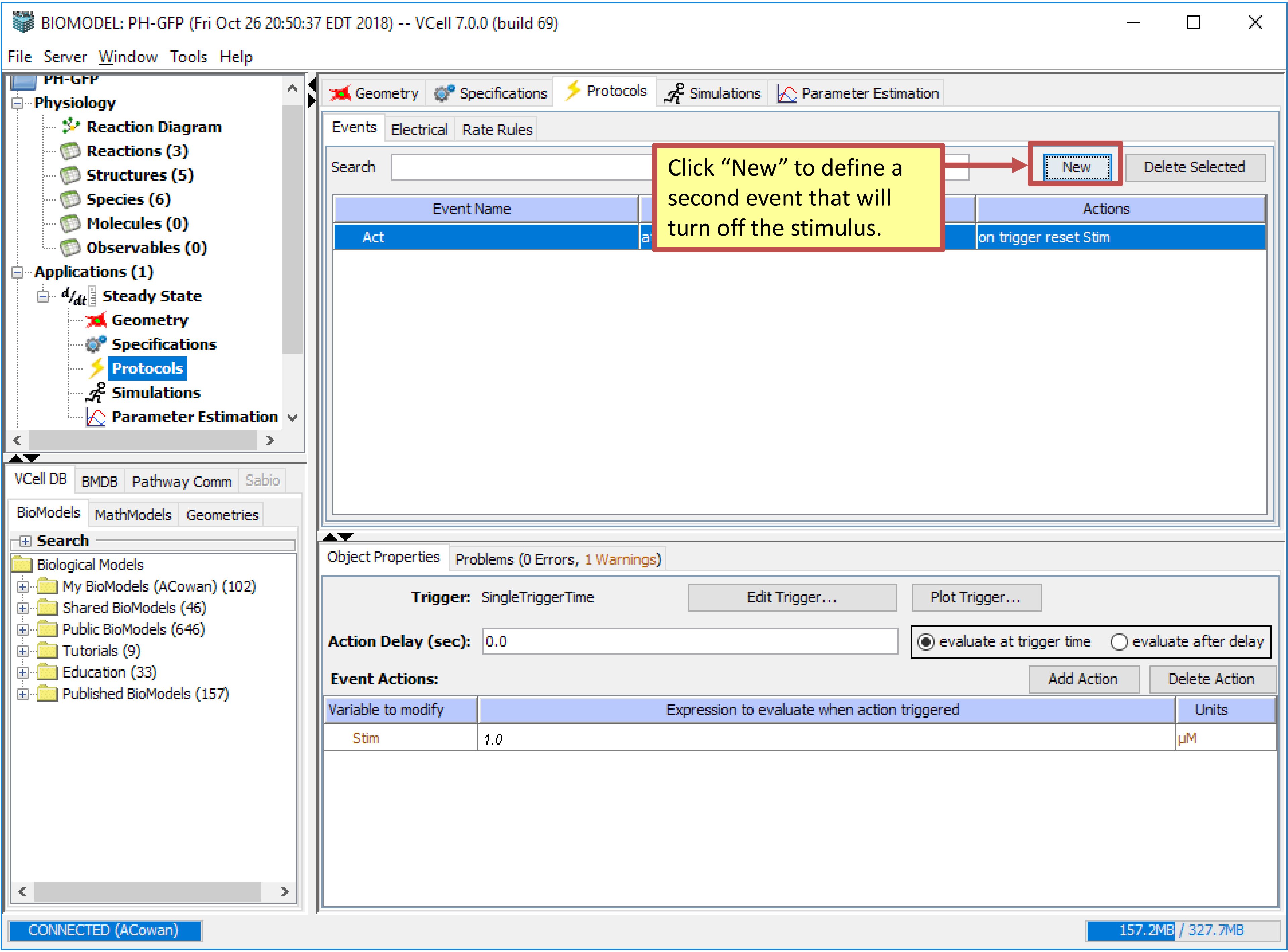
Action Delay (sec): 0.0 ● evaluate at trigger time ○ evaluate after delay

Event Actions:

Variable to modify	Expression to evaluate when action triggered	Units
Stim	1.0	µM

Type in “1.0” under “Expression to evaluate when action triggered”.

The species “Stim” will be set to a value of 1.0 when the event is triggered.


BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 69)
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New
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Problems (0 Errors, 1 Warnings)
Edit Trigger...
Plot Trigger...
Add Action
Delete Action
CONNECTED (ACowan)
157.2MB / 327.7MB

Click “New” to define a second event that will turn off the stimulus.

Event Name		Actions
Act	at	on trigger reset Stim

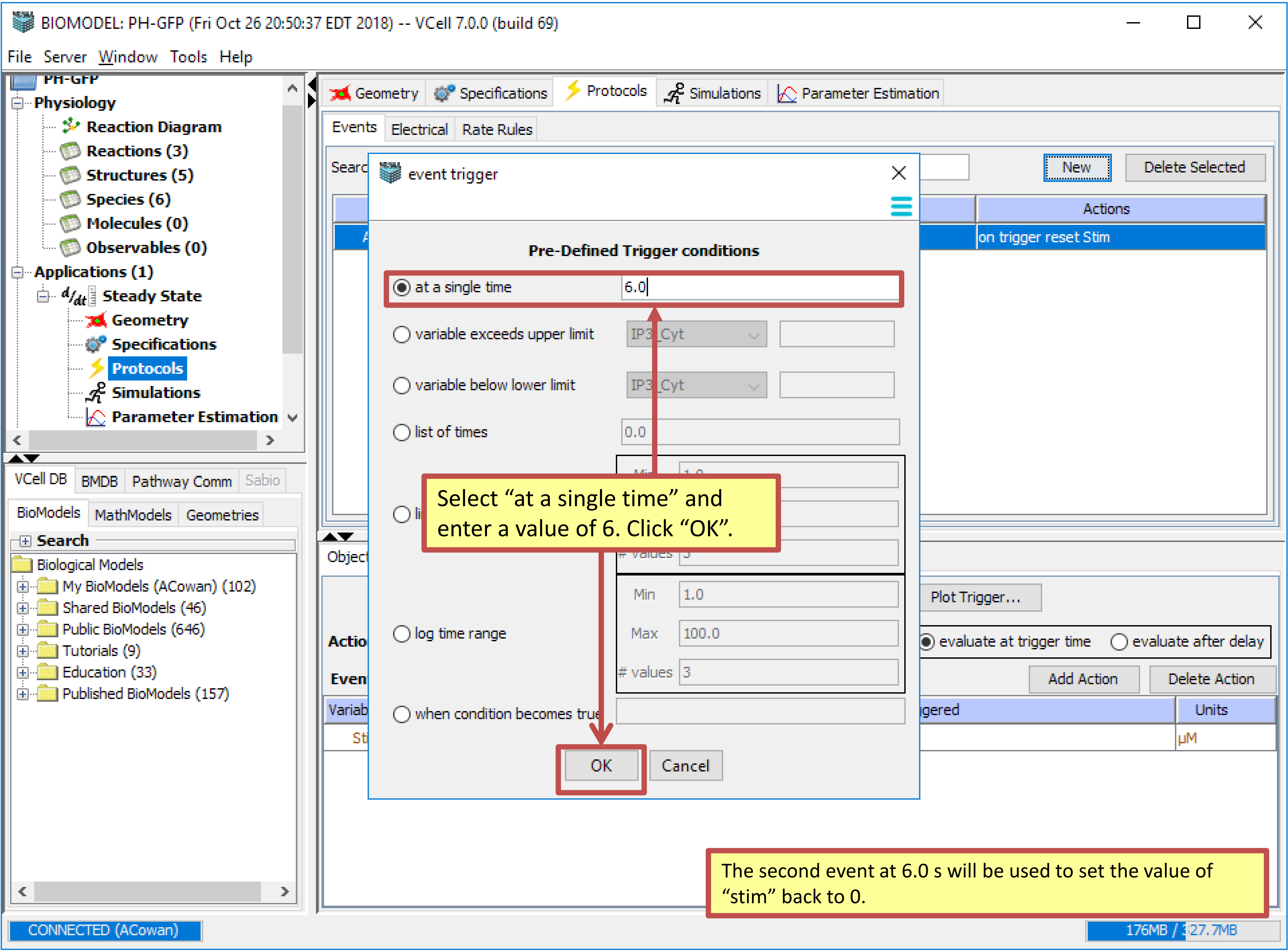
Trigger: SingleTriggerTime

Action Delay (sec): 0.0

● evaluate at trigger time ○ evaluate after delay

Event Actions:

Variable to modify	Expression to evaluate when action triggered	Units
Stim	1.0	µM


BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 69)
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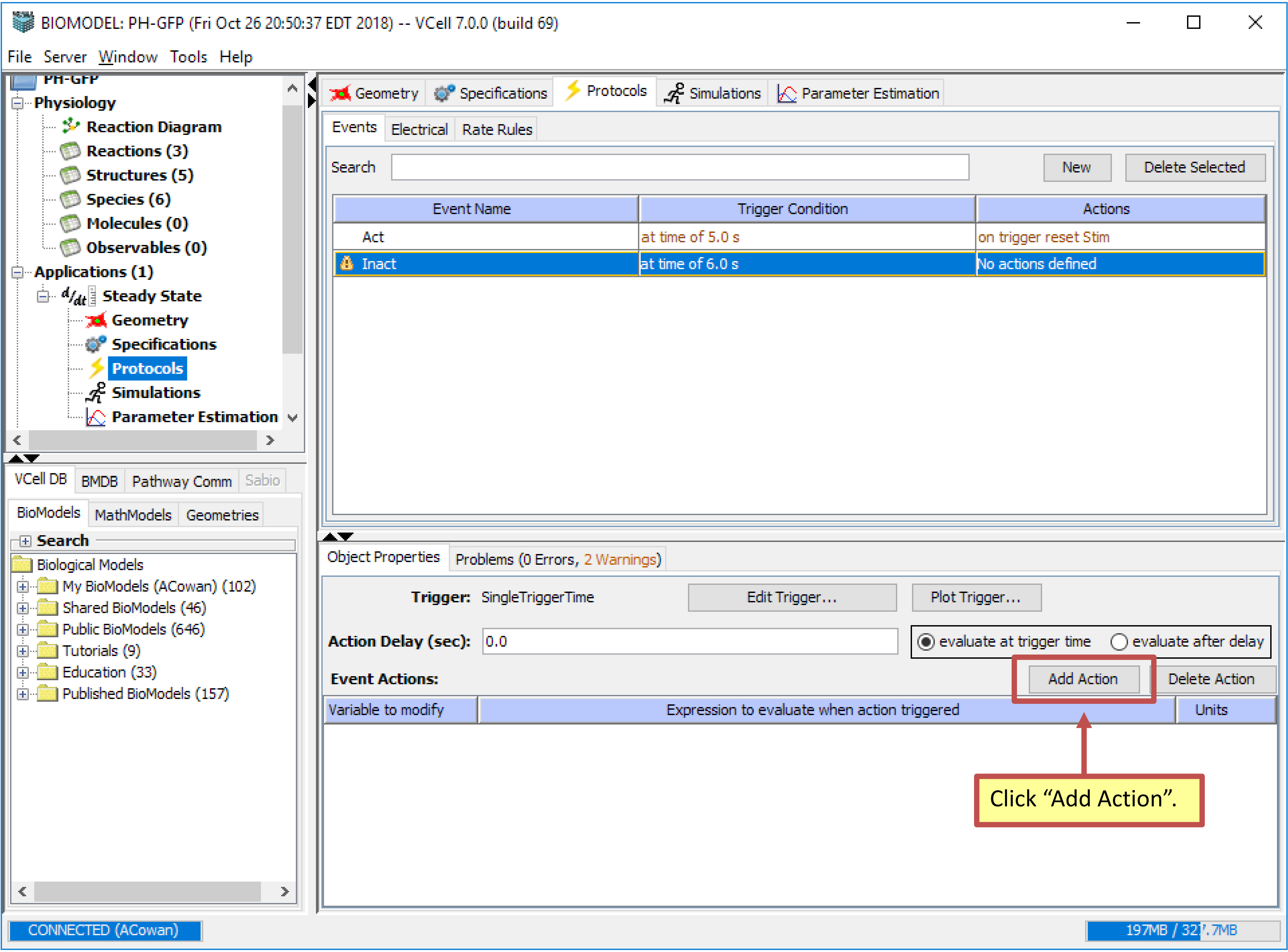
Actions
on trigger reset Stim
Plot Trigger...
evaluate at trigger time
evaluate after delay
Add Action
Delete Action
Units
μM
CONNECTED (ACowan)
176MB / 327.7MB
event trigger
Pre-Defined Trigger conditions
variable exceeds upper limit
IP3_Cyt
variable below lower limit
IP3_Cyt
list of times
0.0
Min 1.0
Max 100.0
# values 3
log time range
when condition becomes true
OK
Cancel

● at a single time 6.0

Select "at a single time" and enter a value of 6. Click "OK".

The second event at 6.0 s will be used to set the value of "stim" back to 0.



BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 69)
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Problems (0 Errors, 2 Warnings)
Edit Trigger...
Plot Trigger...
Add Action
Delete Action
CONNECTED (ACowan)
197MB / 327.7MB

Event Name	Trigger Condition	Actions
Act	at time of 5.0 s	on trigger reset Stim
Inact	at time of 6.0 s	No actions defined

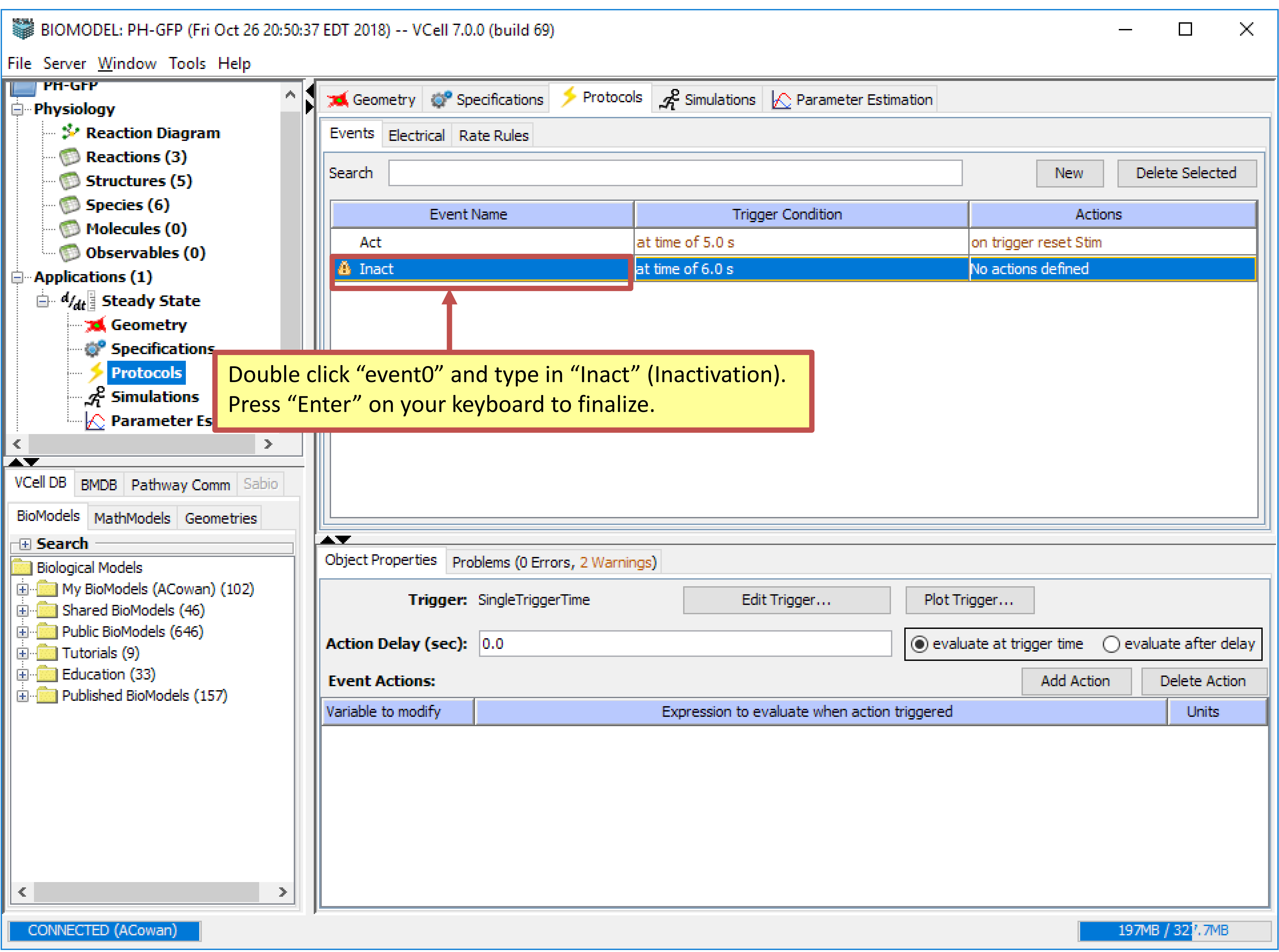
Trigger: SingleTriggerTime

Action Delay (sec): 0.0 ● evaluate at trigger time ○ evaluate after delay

Event Actions:

Variable to modify	Expression to evaluate when action triggered	Units

Click “Add Action”.


BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 69)
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Edit Trigger…
Plot Trigger…
Add Action
Delete Action
CONNECTED (ACowan)
197MB / 32?.7MB

Event Name	Trigger Condition	Actions
Act	at time of 5.0 s	on trigger reset Stim
Inact	at time of 6.0 s	No actions defined

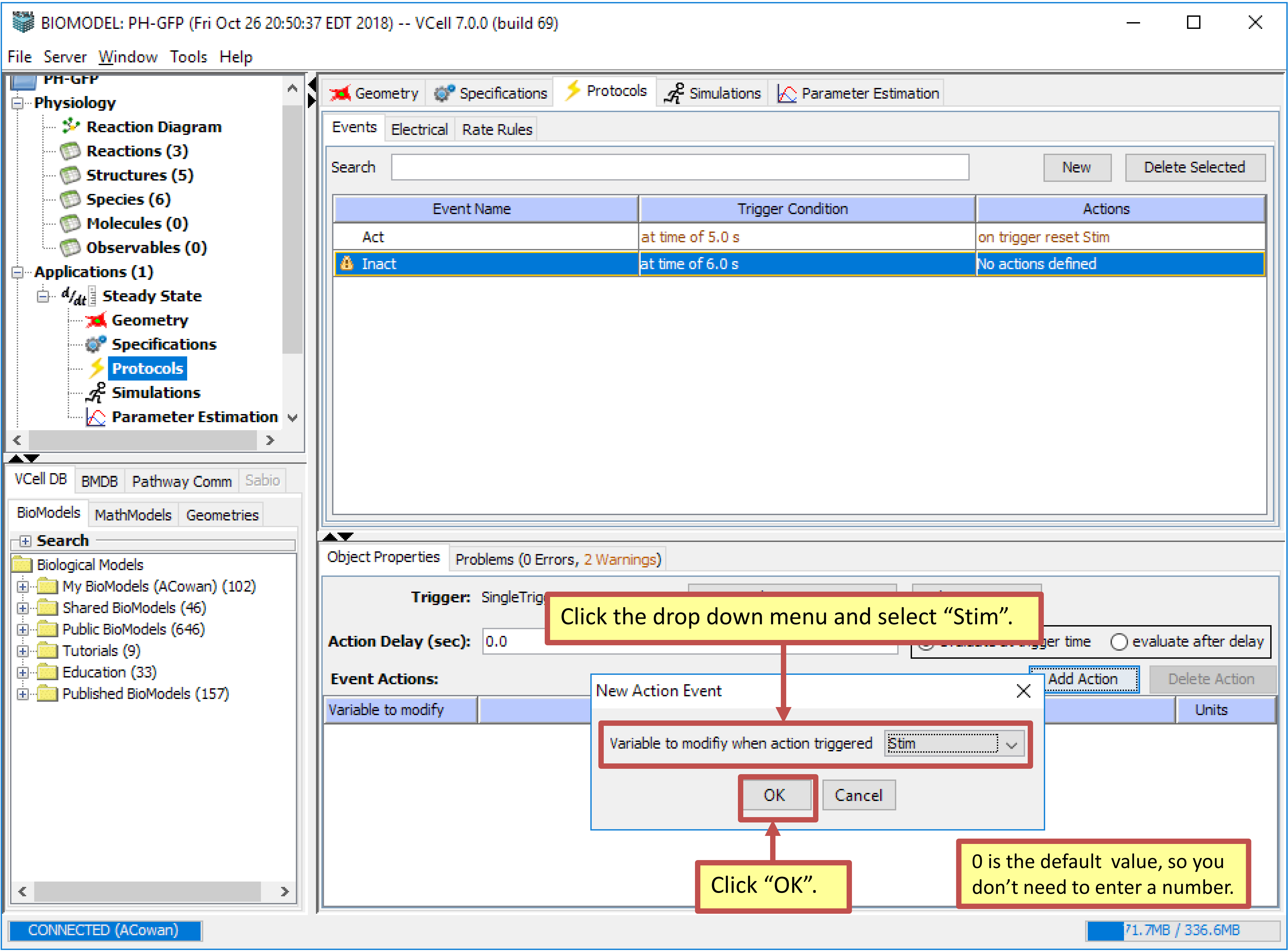
Double click “event0” and type in “Inact” (Inactivation). Press “Enter” on your keyboard to finalize.

Trigger: SingleTriggerTime

Action Delay (sec): 0.0 ● evaluate at trigger time ○ evaluate after delay

Event Actions:

Variable to modify	Expression to evaluate when action triggered	Units


BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 69)
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evaluate at trigger time
evaluate after delay
Add Action
Delete Action
Variable to modify
Units
New Action Event
OK
Cancel
CONNECTED (ACowan)
71.7MB / 336.6MB

Event Name	Trigger Condition	Actions
Act	at time of 5.0 s	on trigger reset Stim
Inact	at time of 6.0 s	No actions defined

Trigger: SingleTrig

Action Delay (sec): 0.0

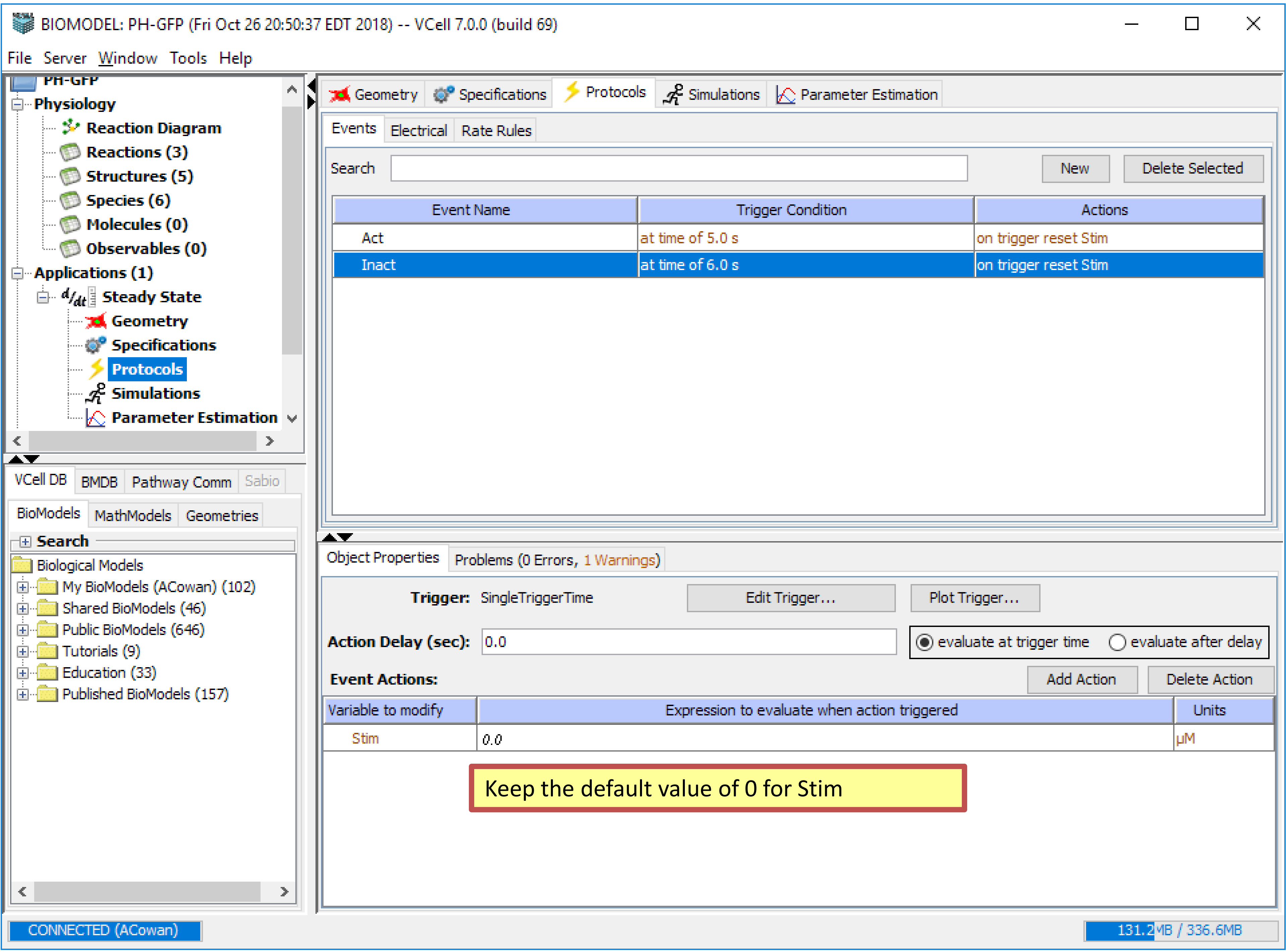
Event Actions:

Variable to modifiy when action triggered: Stim

Click the drop down menu and select “Stim”.

Click “OK”.

0 is the default value, so you don’t need to enter a number.


BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 69)
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CONNECTED (ACowan)
131.2MB / 336.6MB

Event Name	Trigger Condition	Actions
Act	at time of 5.0 s	on trigger reset Stim
Inact	at time of 6.0 s	on trigger reset Stim

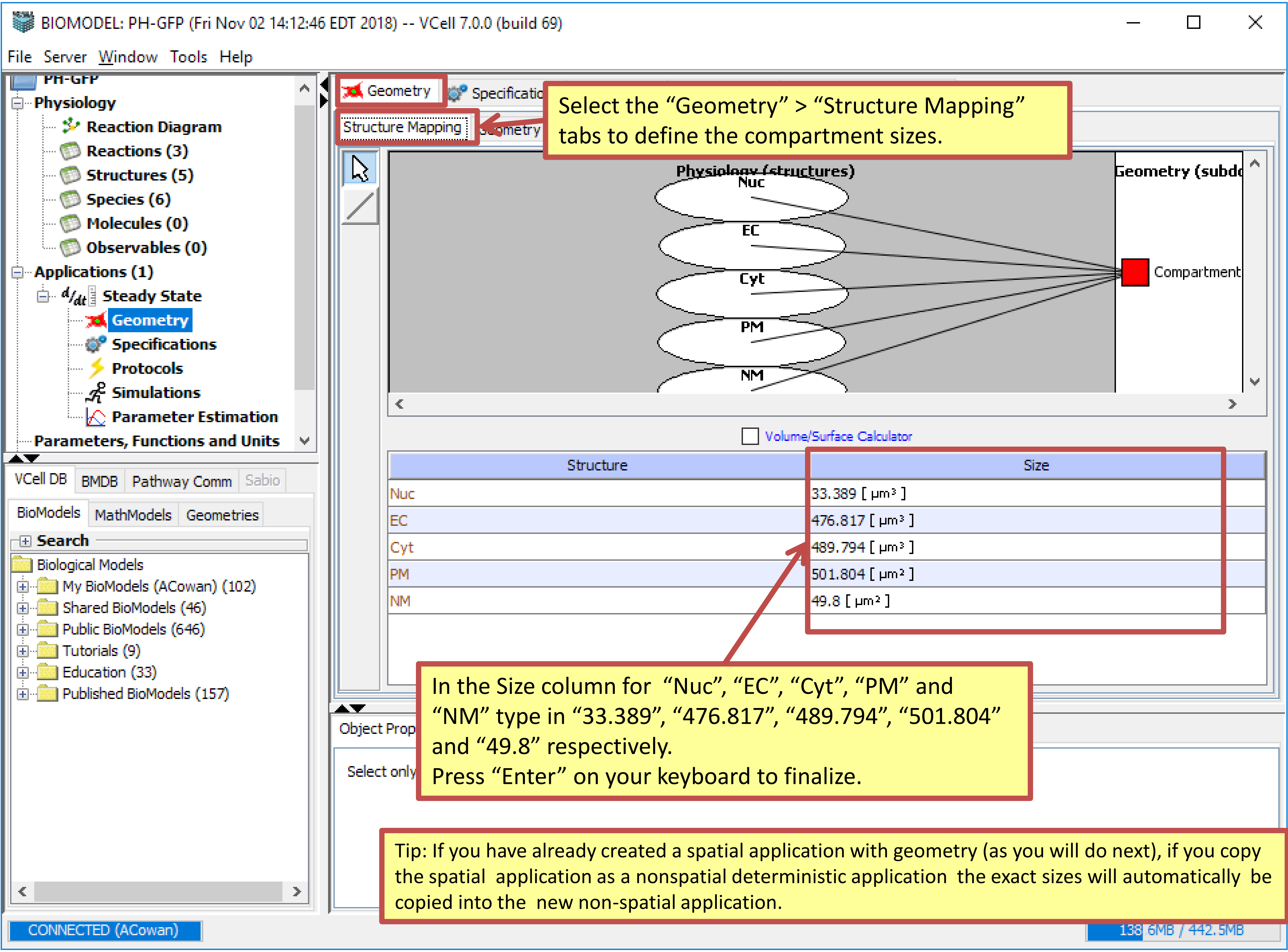
Trigger: SingleTriggerTime

Action Delay (sec): 0.0 ● evaluate at trigger time ○ evaluate after delay

Event Actions:

Variable to modify	Expression to evaluate when action triggered	Units
Stim	0.0	µM

Keep the default value of 0 for Stim


BIOMODEL: PH-GFP (Fri Nov 02 14:12:46 EDT 2018) -- VCell 7.0.0 (build 69)
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EC
Cyt
PM
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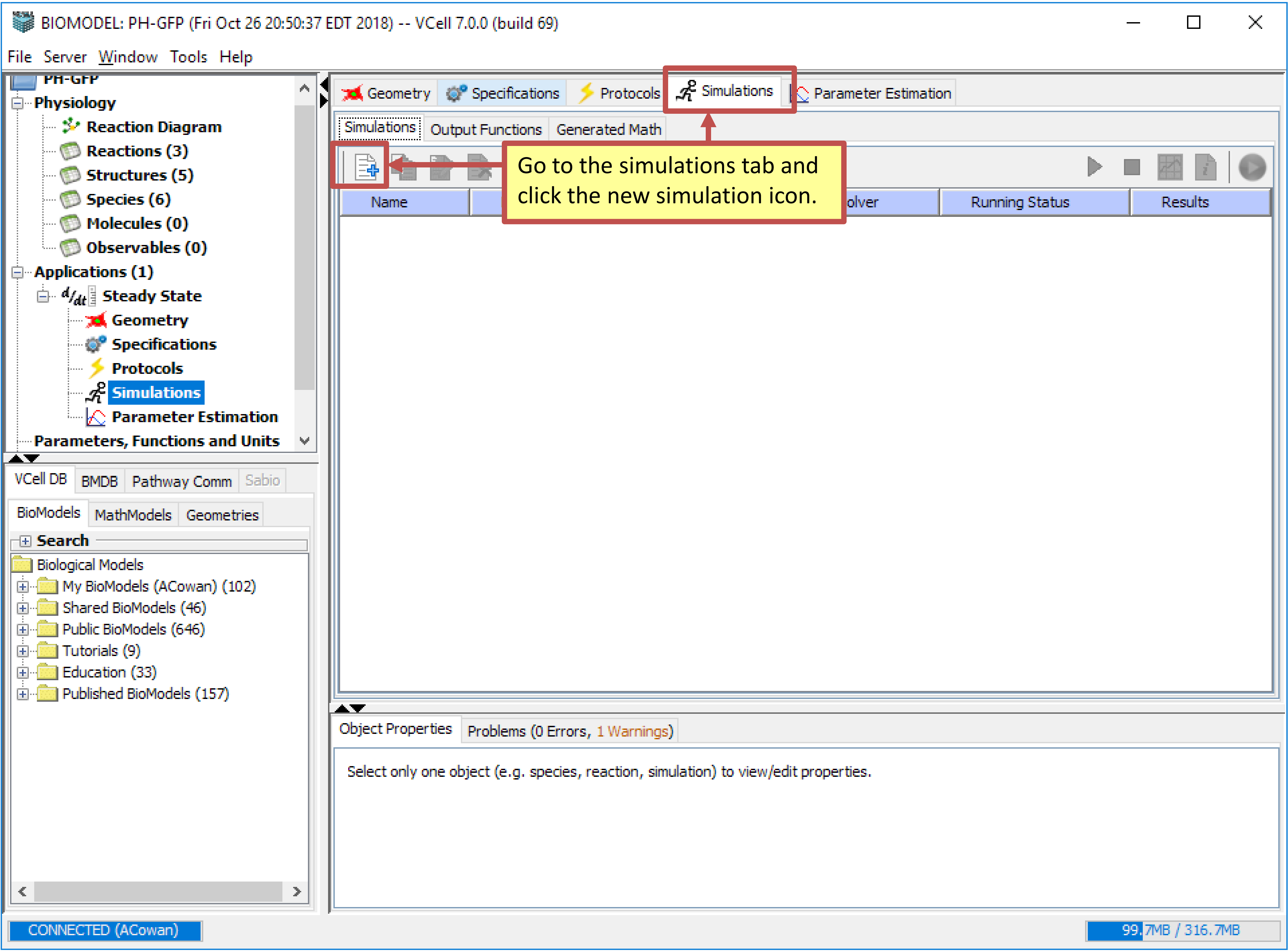
Compartment
Volume/Surface Calculator
Object Prop
Select only
138 6MB / 442.5MB

Select the "Geometry" > "Structure Mapping" tabs to define the compartment sizes.

Structure	Size
Nuc	33.389 [µm³]
EC	476.817 [µm³]
Cyt	489.794 [µm³]
PM	501.804 [µm²]
NM	49.8 [µm²]

In the Size column for "Nuc", "EC", "Cyt", "PM" and "NM" type in "33.389", "476.817", "489.794", "501.804" and "49.8" respectively.
Press "Enter" on your keyboard to finalize.

Tip: If you have already created a spatial application with geometry (as you will do next), if you copy the spatial application as a nonspatial deterministic application the exact sizes will automatically be copied into the new non-spatial application.



Go to the simulations tab and click the new simulation icon.

BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 69)

Select only one object (e.g. species, reaction, simulation) to view/edit properties.

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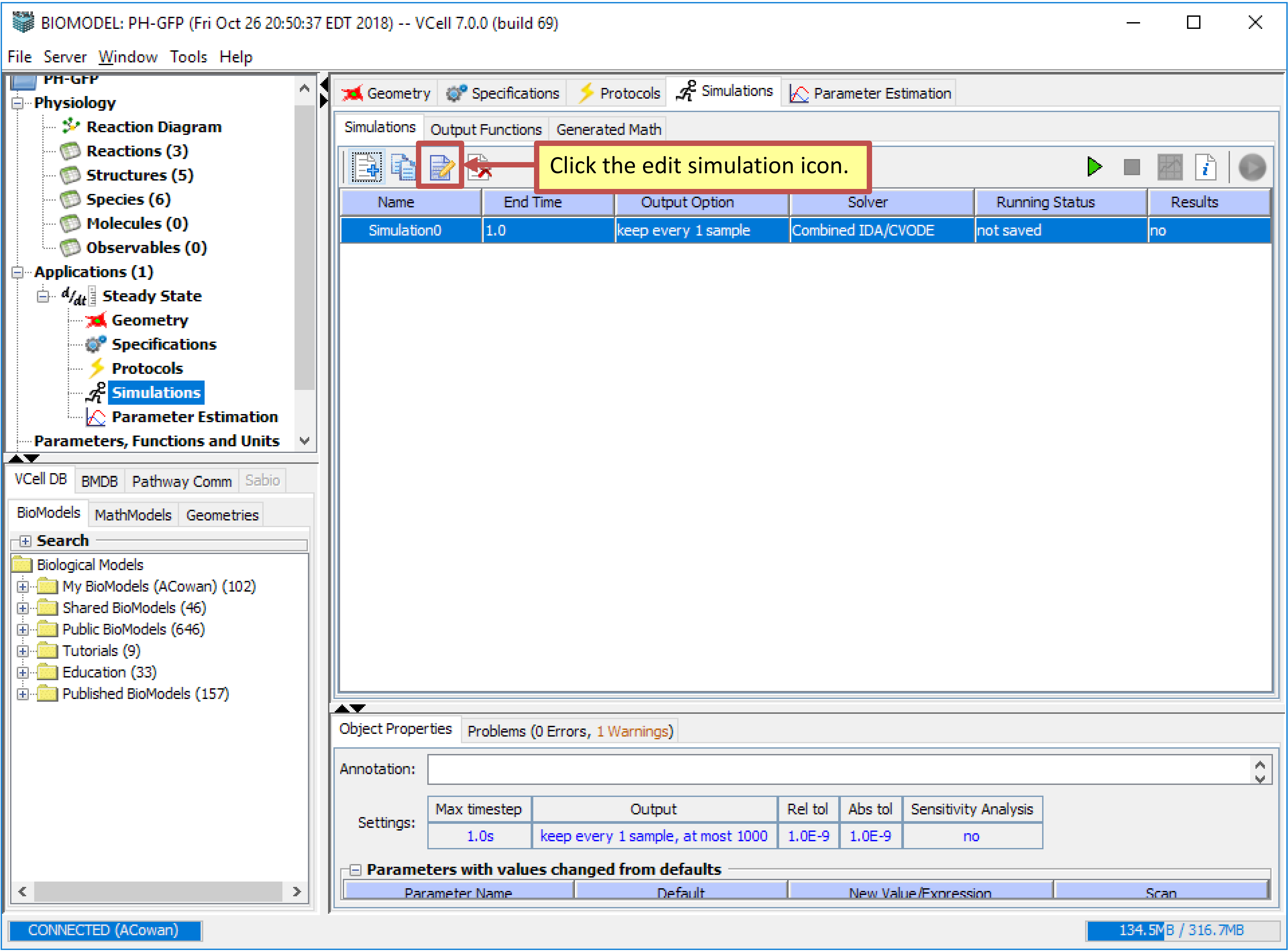
CONNECTED (ACowan)
99.7MB / 316.7MB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134.5MB / 316.7MB

Click the edit simulation icon.

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	1.0	keep every 1 sample	Combined IDA/CVODE	not saved	no

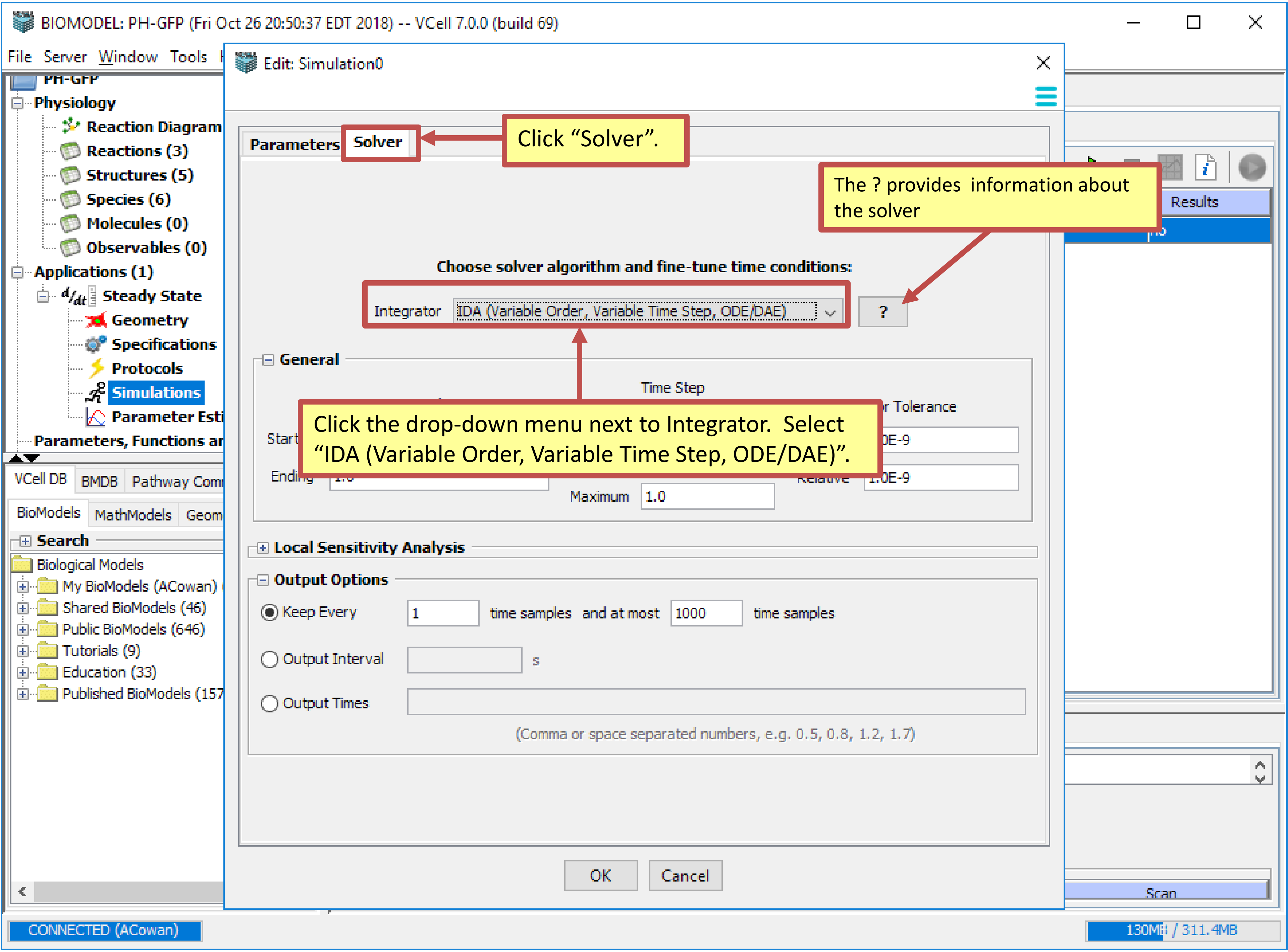
Annotation:

Settings:

Max timestep	Output	Rel tol	Abs tol	Sensitivity Analysis
1.0s	keep every 1 sample, at most 1000	1.0E-9	1.0E-9	no

Parameters with values changed from defaults

Parameter Name	Default	New Value/Expression	Scan



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Scan
CONNECTED (ACowan)
130MB / 311.4MB
Edit: Simulation0
Parameters
Solver
?
OK
Cancel

Click "Solver".

The ? provides information about the solver

Choose solver algorithm and fine-tune time conditions:

Integrator: IDA (Variable Order, Variable Time Step, ODE/DAE)

Click the drop-down menu next to Integrator. Select "IDA (Variable Order, Variable Time Step, ODE/DAE)".

General

Time Step

Start

Ending: 1.0

Maximum: 1.0

r Tolerance

0E-9

Relative: 1.0E-9

Local Sensitivity Analysis

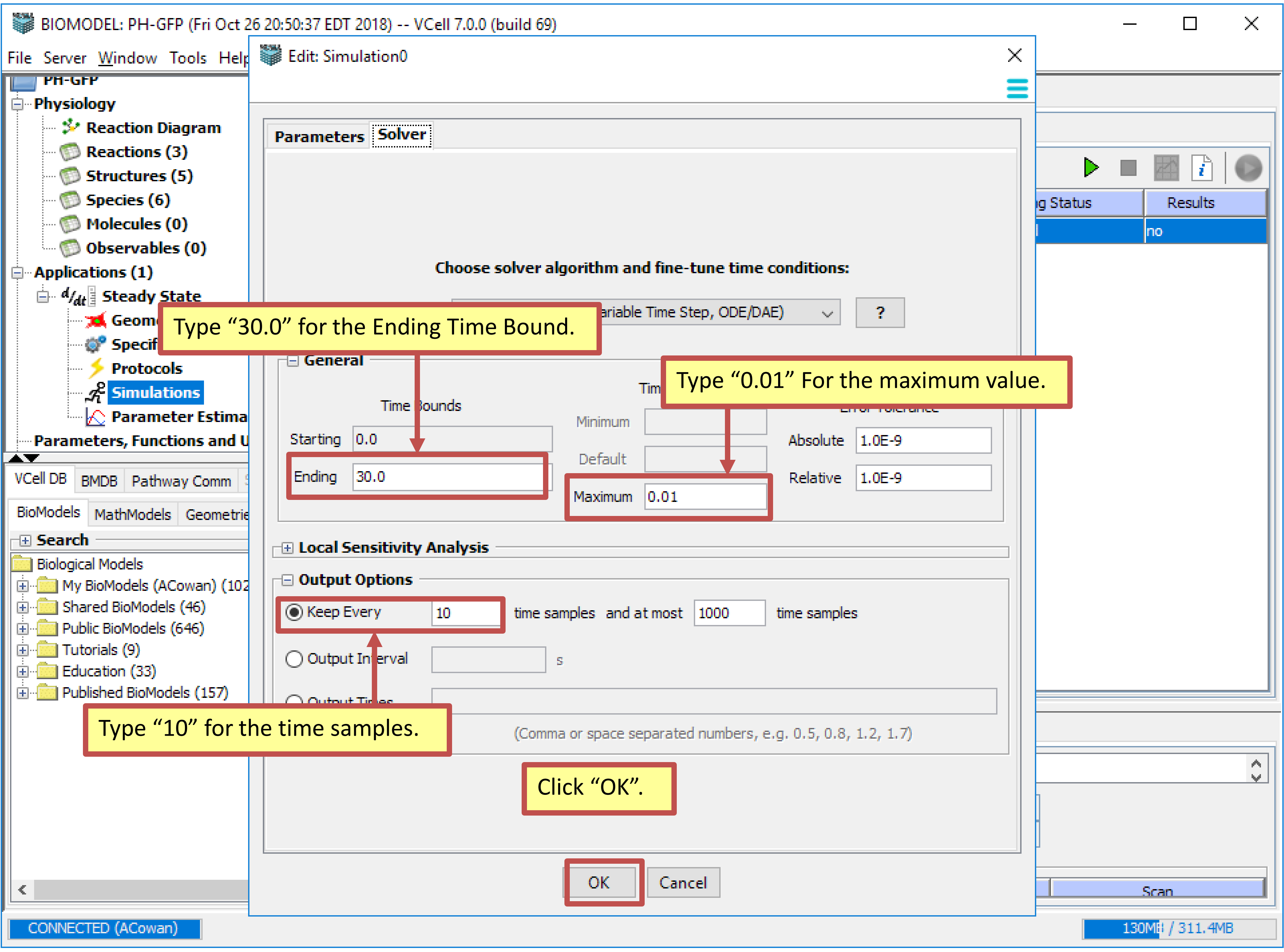
Output Options

● Keep Every 1 time samples and at most 1000 time samples

○ Output Interval s

○ Output Times

(Comma or space separated numbers, e.g. 0.5, 0.8, 1.2, 1.7)



BIOMODEL: PH-GFP (Fri Oct 26 20:50:37 EDT 2018) -- VCell 7.0.0 (build 69)
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130MB / 311.4MB
OK
Cancel
?

Choose solver algorithm and fine-tune time conditions:

ariable Time Step, ODE/DAE)

General

Time Bounds

Starting 0.0

Ending 30.0

Tim

Minimum

Default

Maximum 0.01

Error Tolerance

Absolute 1.0E-9

Relative 1.0E-9

Local Sensitivity Analysis

Output Options

● Keep Every 10 time samples and at most 1000 time samples

○ Output Interval s

○ Output Times

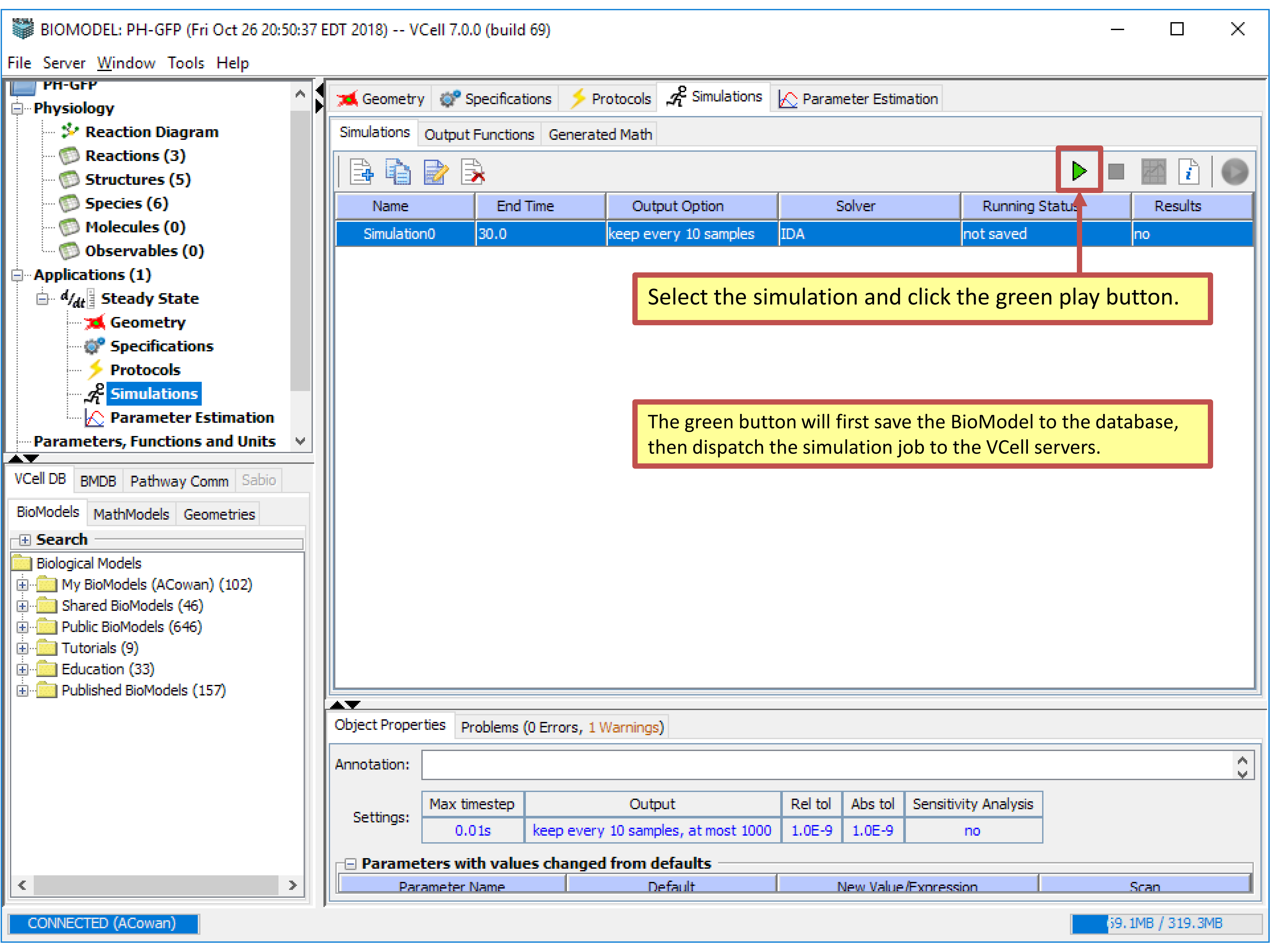
(Comma or space separated numbers, e.g. 0.5, 0.8, 1.2, 1.7)

Type “30.0” for the Ending Time Bound.

Type “0.01” For the maximum value.

Type “10” for the time samples.

Click “OK”.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Settings:
Parameters with values changed from defaults
CONNECTED (ACowan)
59.1MB / 319.3MB

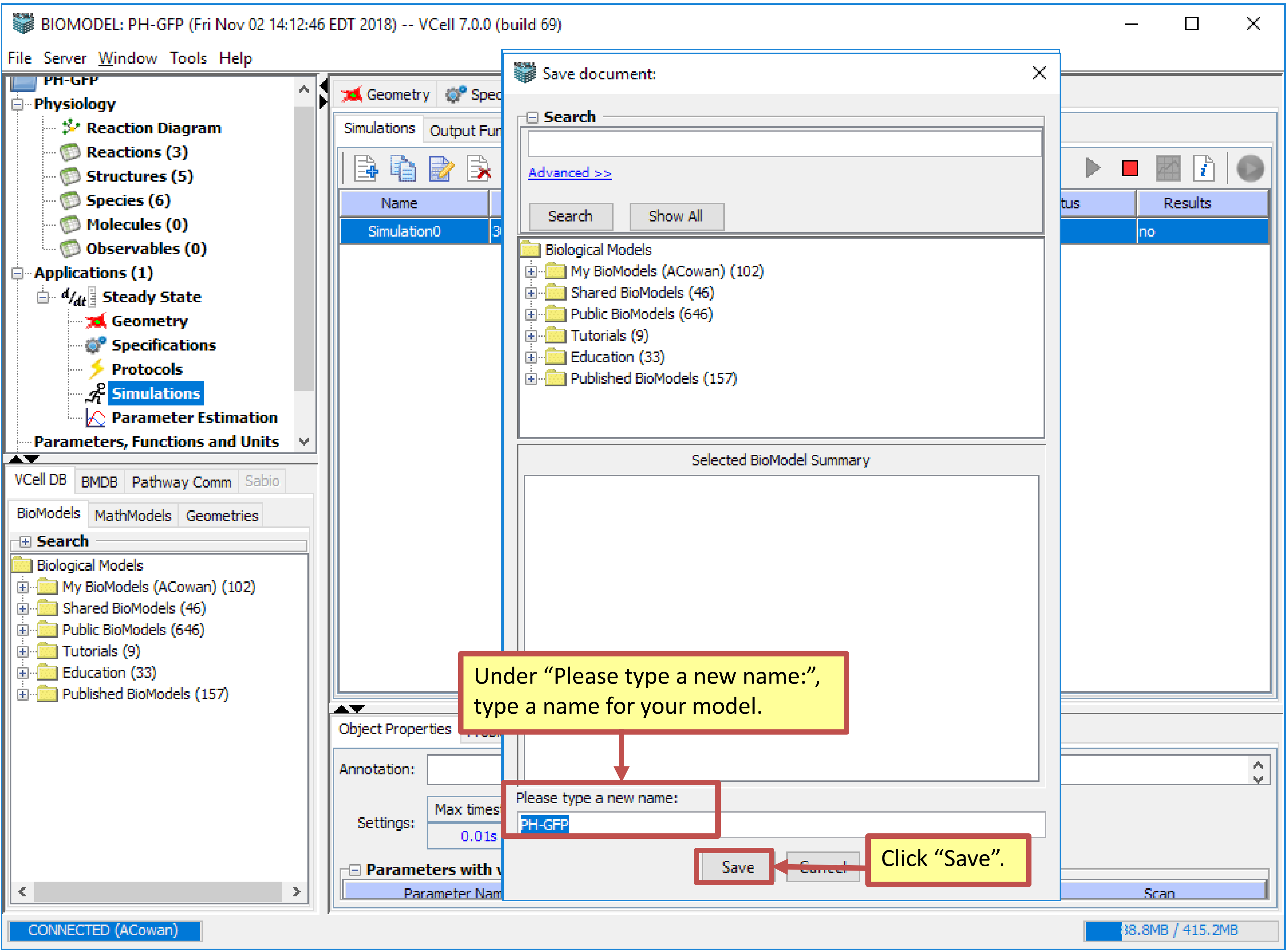
Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	30.0	keep every 10 samples	IDA	not saved	no

Select the simulation and click the green play button.

The green button will first save the BioModel to the database, then dispatch the simulation job to the VCell servers.

Max timestep	Output	Rel tol	Abs tol	Sensitivity Analysis
0.01s	keep every 10 samples, at most 1000	1.0E-9	1.0E-9	no

Parameter Name	Default	New Value/Expression	Scan



BIOMODEL: PH-GFP (Fri Nov 02 14:12:46 EDT 2018) -- VCell 7.0.0 (build 69)

Save document:

Please type a new name: PH-GFP

Under “Please type a new name:”, type a name for your model.

Click “Save”.

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Selected BioModel Summary
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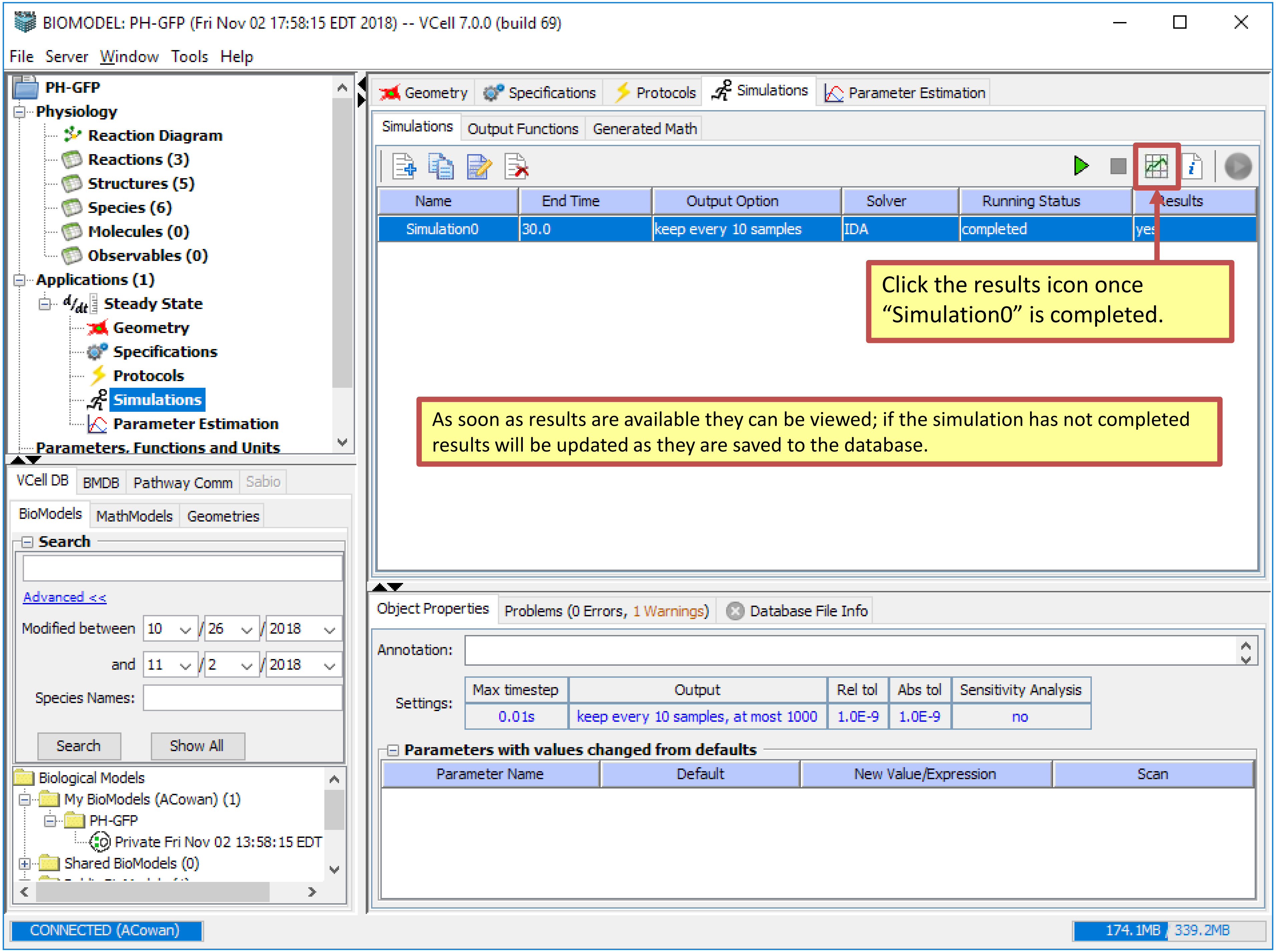
Cancel
CONNECTED (ACowan)
38.8MB / 415.2MB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Settings:
Parameters with values changed from defaults
CONNECTED (ACowan)
174.1MB / 339.2MB

Modified between 10 / 26 / 2018 and 11 / 2 / 2018

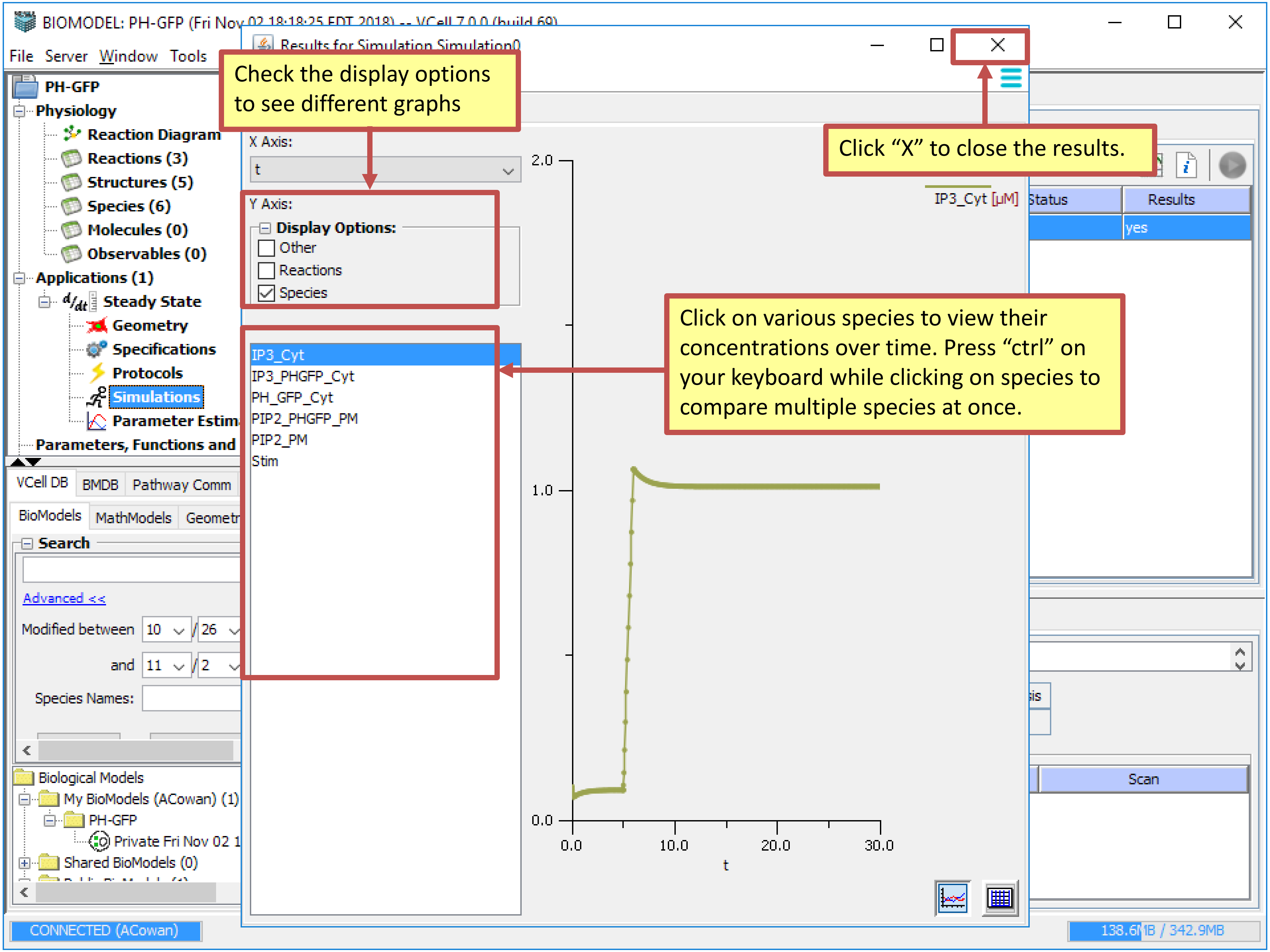
Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	30.0	keep every 10 samples	IDA	completed	yes

Click the results icon once "Simulation0" is completed.

As soon as results are available they can be viewed; if the simulation has not completed results will be updated as they are saved to the database.

Max timestep	Output	Rel tol	Abs tol	Sensitivity Analysis
0.01s	keep every 10 samples, at most 1000	1.0E-9	1.0E-9	no

Parameter Name	Default	New Value/Expression	Scan



Check the display options to see different graphs

Click “X” to close the results.

Click on various species to view their concentrations over time. Press “ctrl” on your keyboard while clicking on species to compare multiple species at once.

X Axis: t

Y Axis:

Display Options:
- ☐ Other
- ☐ Reactions
- ☑ Species

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t
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Results
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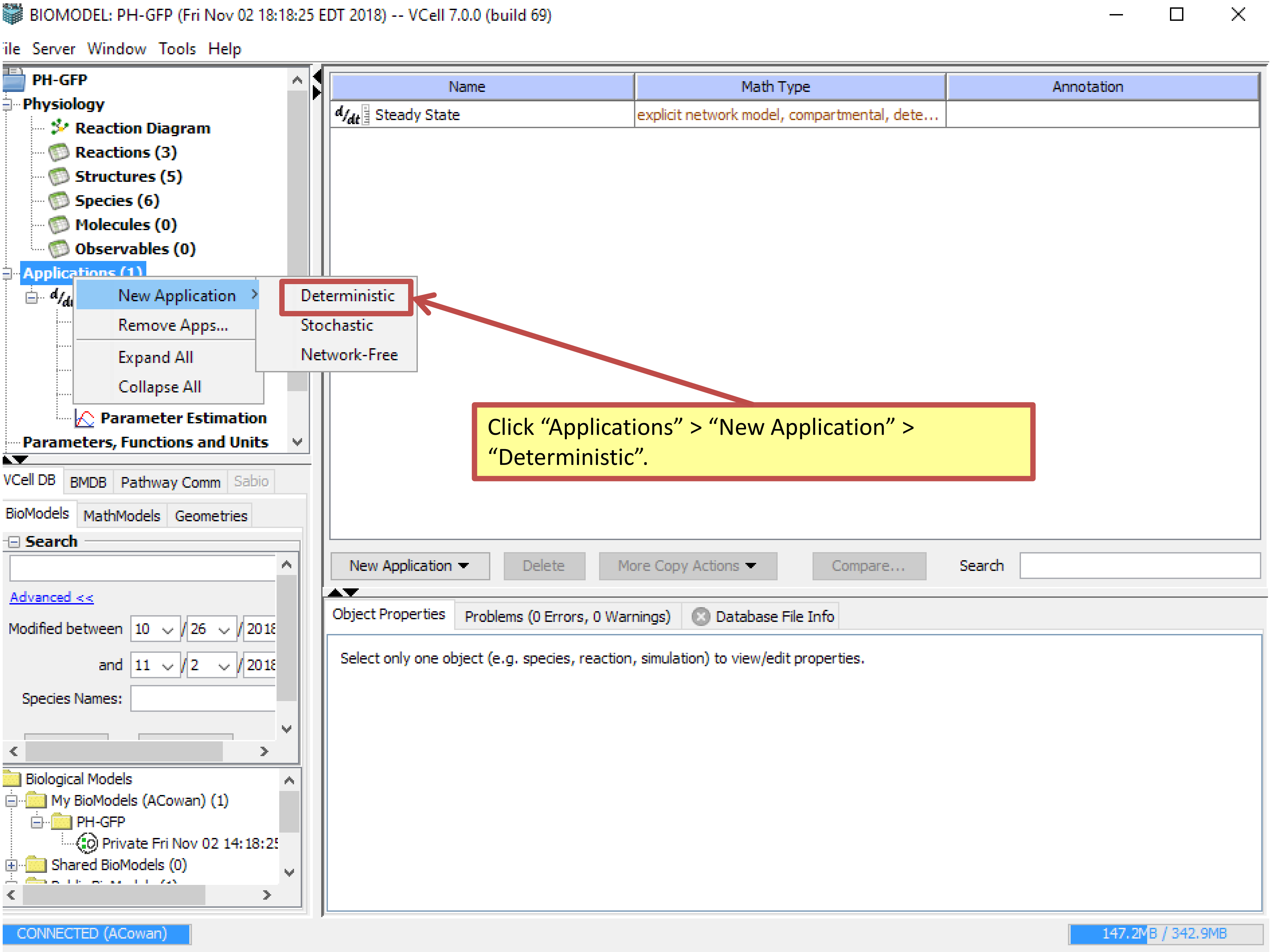
Scan
138.6MB / 342.9MB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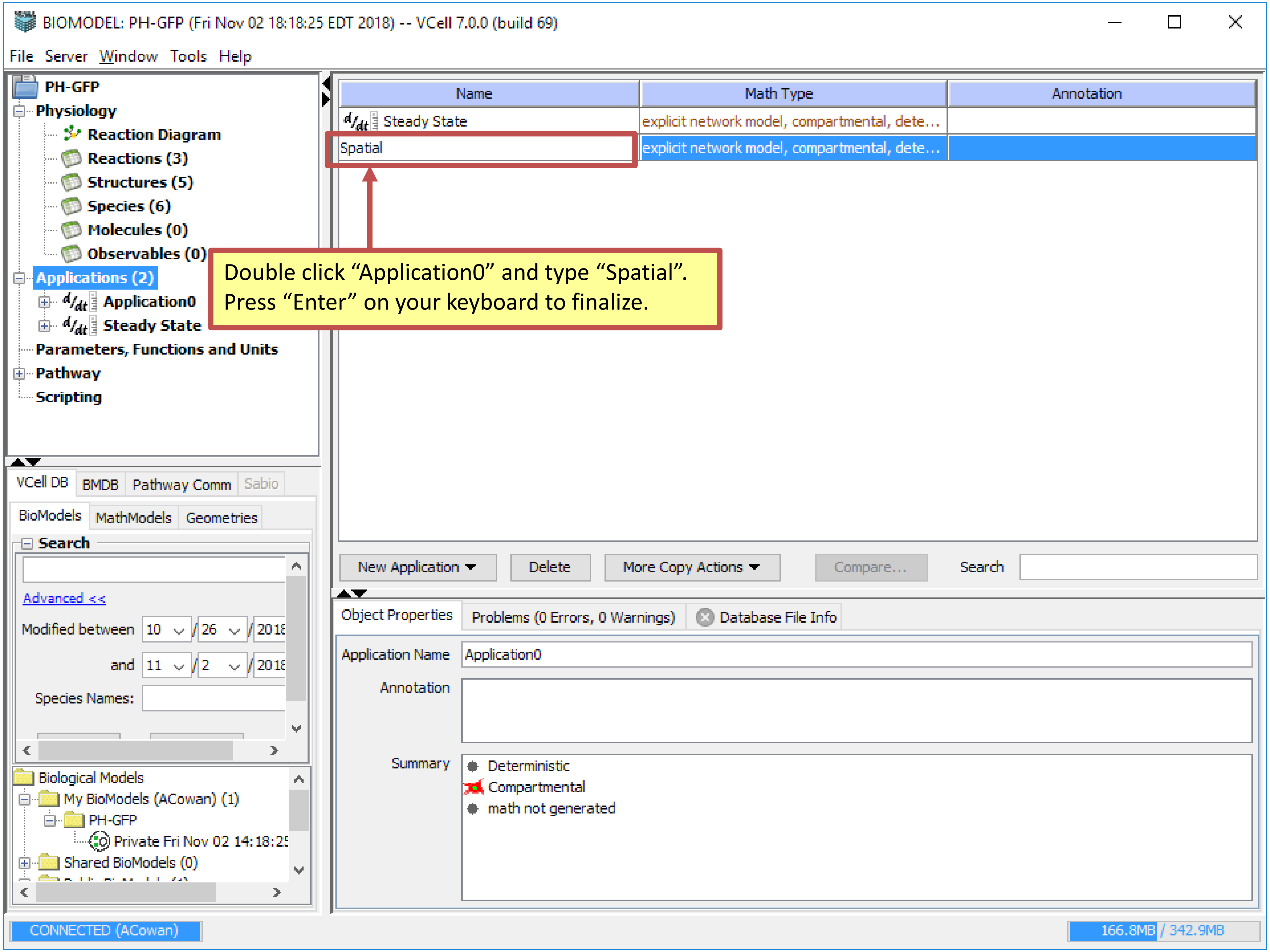
CONNECTED (ACowan)
147.2MB / 342.9MB

Select only one object (e.g. species, reaction, simulation) to view/edit properties.

Click “Applications” > “New Application” > “Deterministic”.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Problems (0 Errors, 0 Warnings)
Database File Info
CONNECTED (ACowan)
166.8MB / 342.9MB

Double click “Application0” and type “Spatial”. Press “Enter” on your keyboard to finalize.

Name	Math Type	Annotation
Steady State	explicit network model, compartmental, dete…	
Spatial	explicit network model, compartmental, dete…	

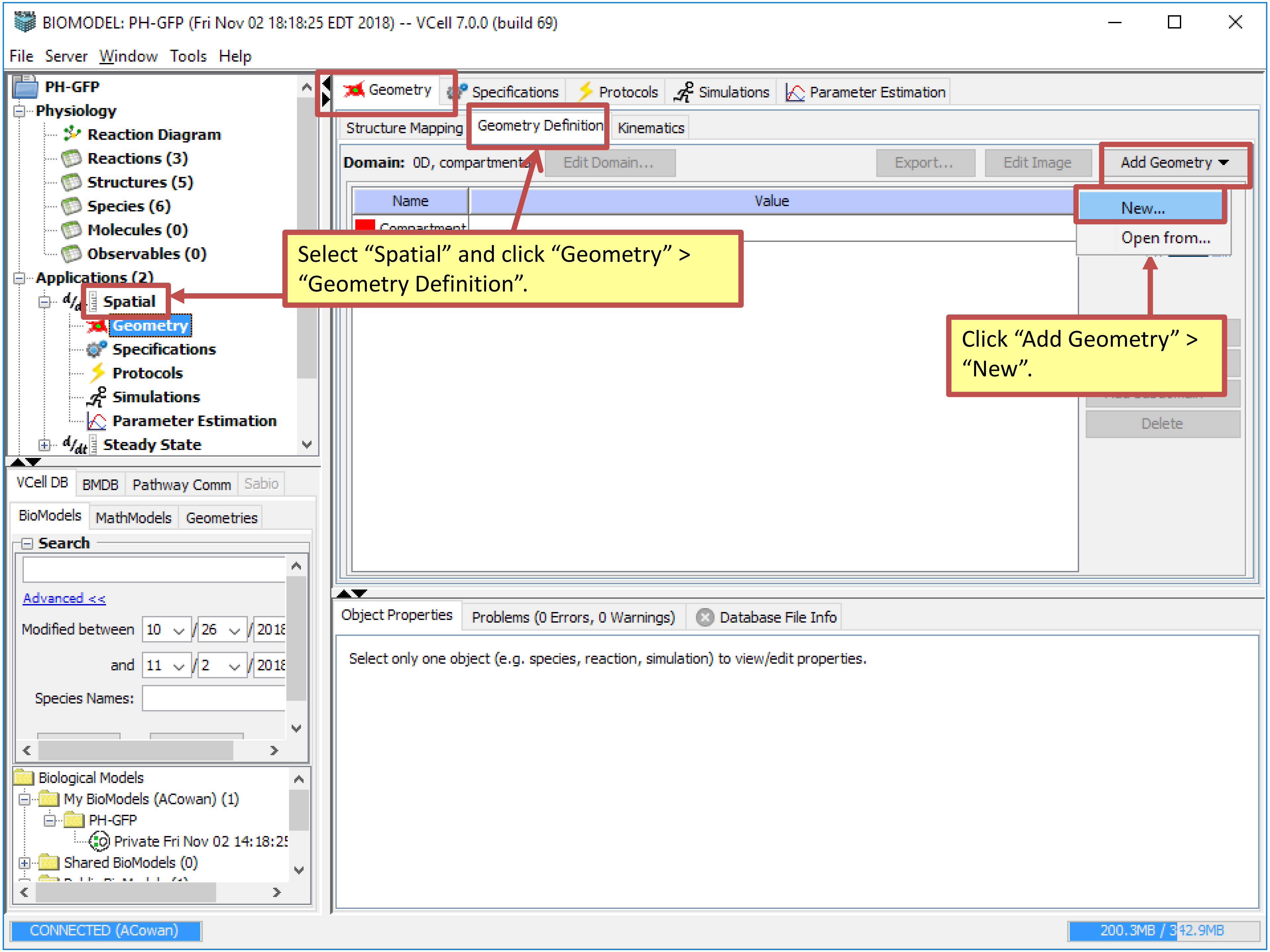
Modified between 10 / 26 / 2018 and 11 / 2 / 2018

Species Names:

Application Name: Application0

Annotation:

Summary:
- Deterministic
- Compartmental
- math not generated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Domain: 0D, compartmental

Modified between 10 / 26 / 2018 and 11 / 2 / 2018

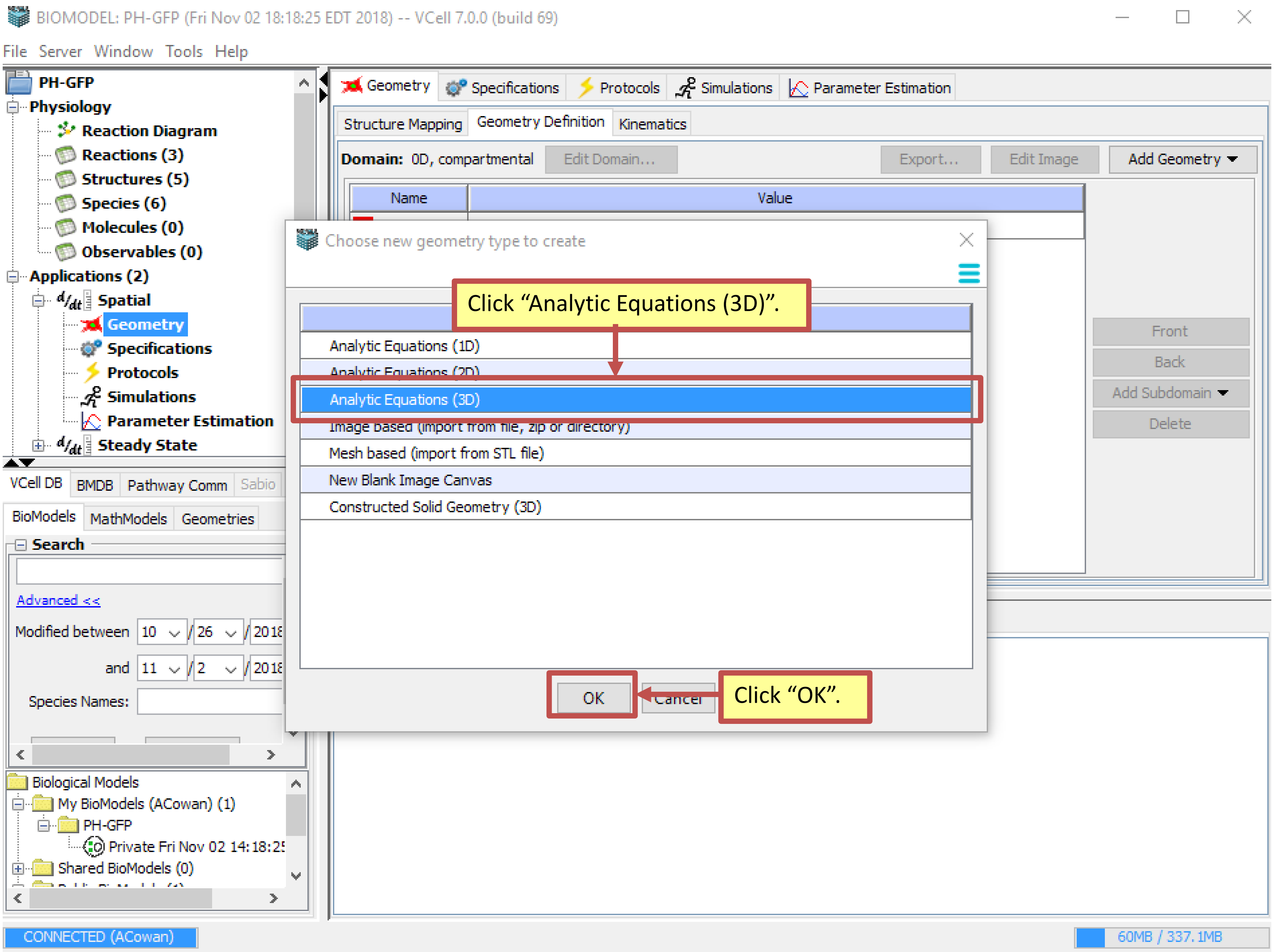
Select only one object (e.g. species, reaction, simulation) to view/edit properties.

CONNECTED (ACowan)

200.3MB / 342.9MB

Select “Spatial” and click “Geometry” > “Geometry Definition”.

Click “Add Geometry” > “New”.



Click “Analytic Equations (3D)”.

Click “OK”.

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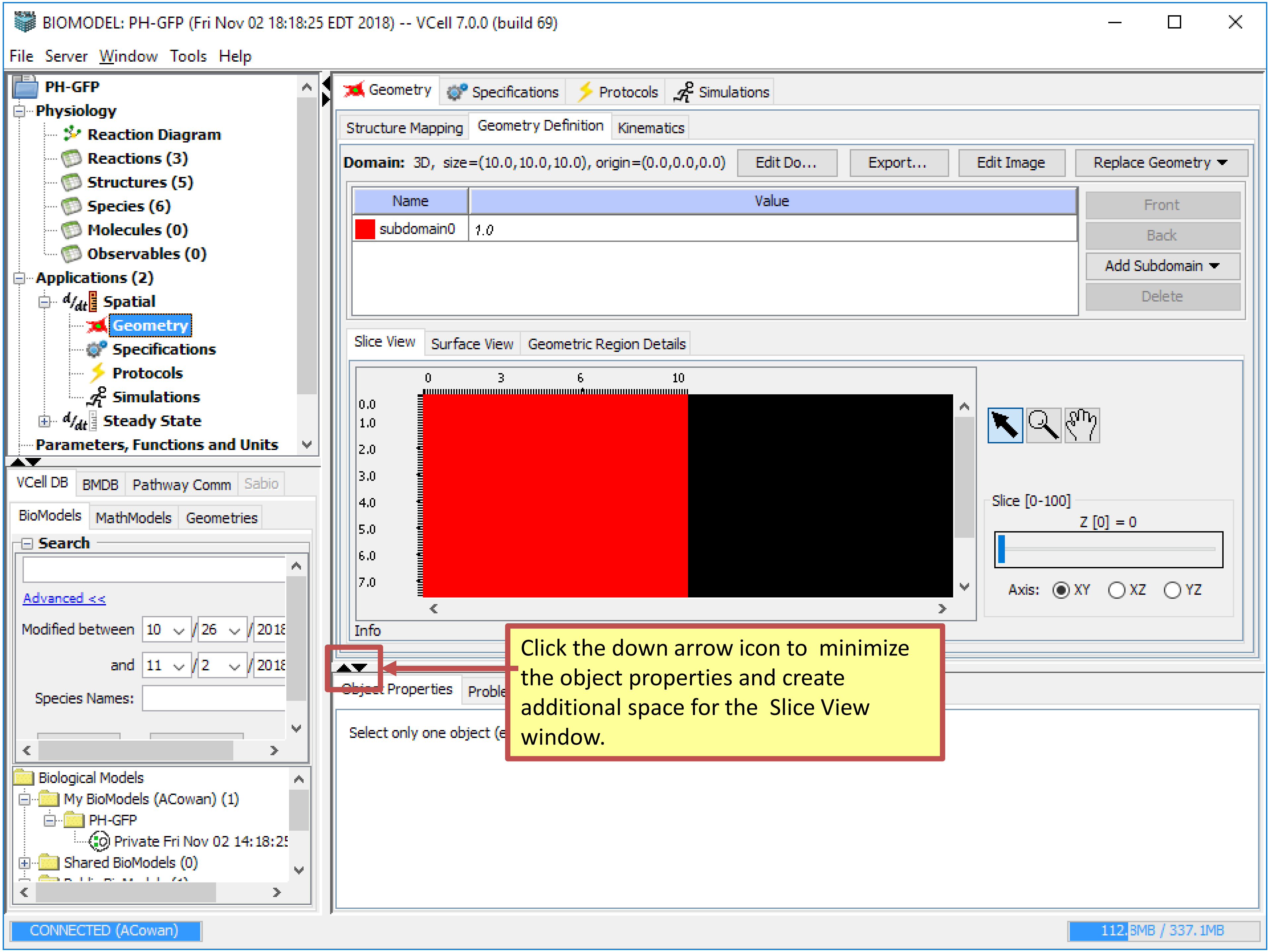
Choose new geometry type to create
Analytic Equations (1D)
Analytic Equations (2D)
Analytic Equations (3D)
Image based (import from file, zip or directory)
Mesh based (import from STL file)
New Blank Image Canvas
Constructed Solid Geometry (3D)
OK
Cancel
CONNECTED (ACowan)
60MB / 337.1MB


BIOMODEL: PH-GFP (Fri Nov 02 18:18:25 EDT 2018) -- VCell 7.0.0 (build 69)
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112.3MB / 337.1MB

Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)

Name	Value
🟥 subdomain0	1.0

Z [0] = 0

Axis: ● XY ○ XZ ○ YZ

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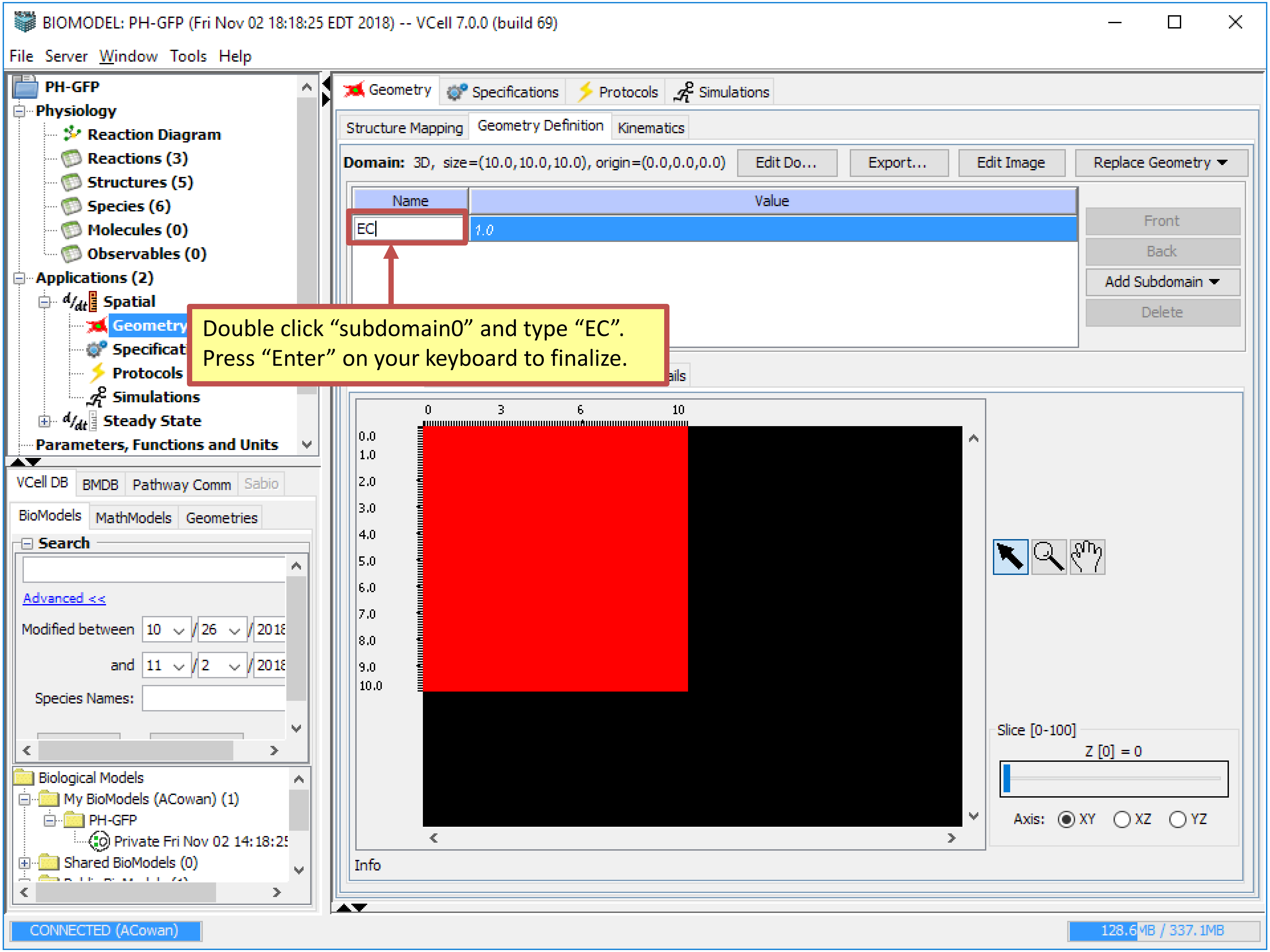
Species Names:

Select only one object (e

Click the down arrow icon to minimize the object properties and create additional space for the Slice View window.



Double click “subdomain0” and type “EC”. Press “Enter” on your keyboard to finalize.

BIOMODEL: PH-GFP (Fri Nov 02 18:18:25 EDT 2018) -- VCell 7.0.0 (build 69)

Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)

Name	Value
EC	1.0

Modified between 10 / 26 / 2018 and 11 / 2 / 2018

Slice [0-100] Z [0] = 0

Axis: ● XY ○ XZ ○ YZ

CONNECTED (ACowan)

128.6MB / 337.1MB

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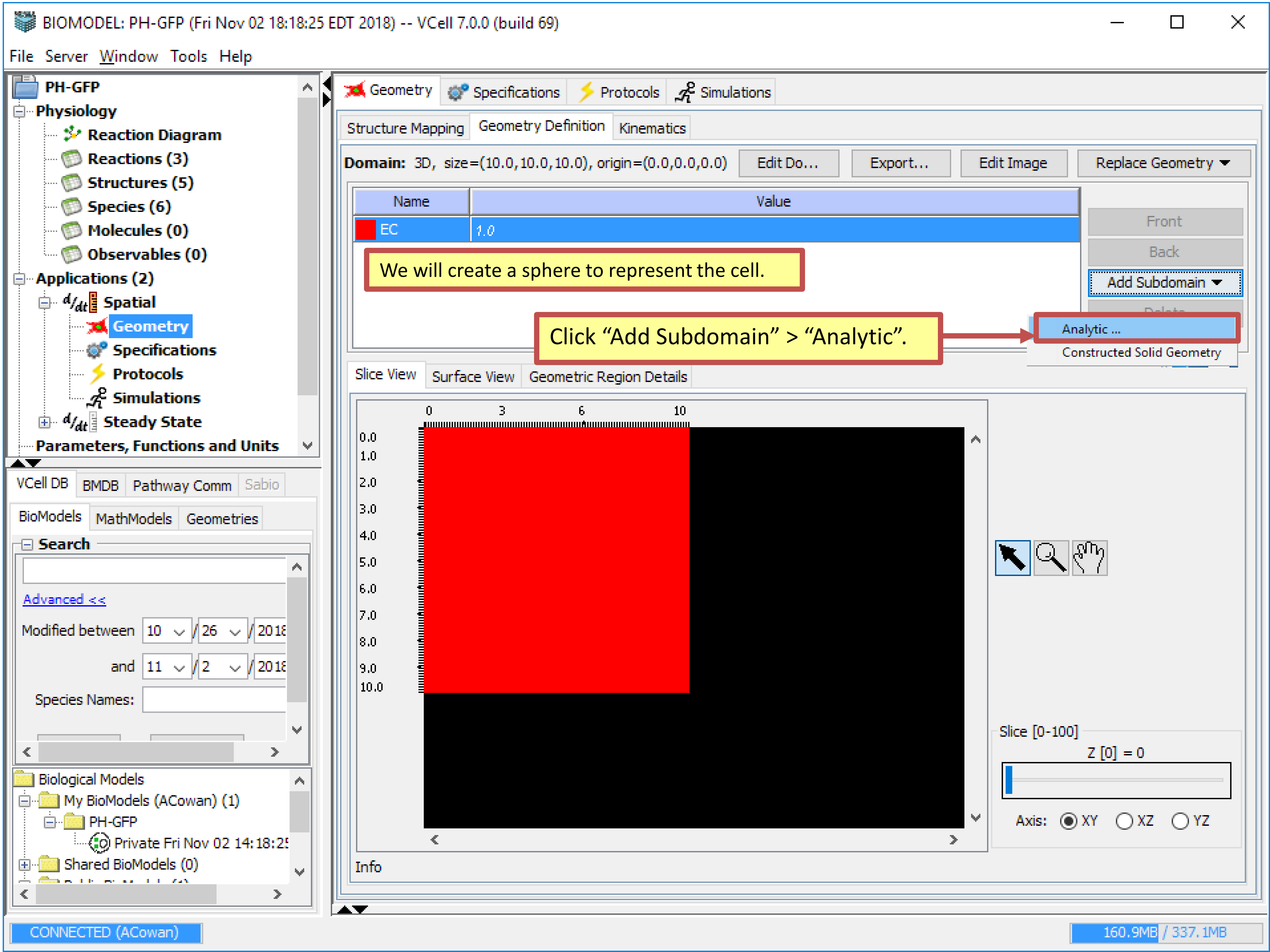
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Slice [0-100]
CONNECTED (ACowan)
160.9MB / 337.1MB

Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)

Name	Value
🟥 EC	1.0

Modified between 10 / 26 / 2018

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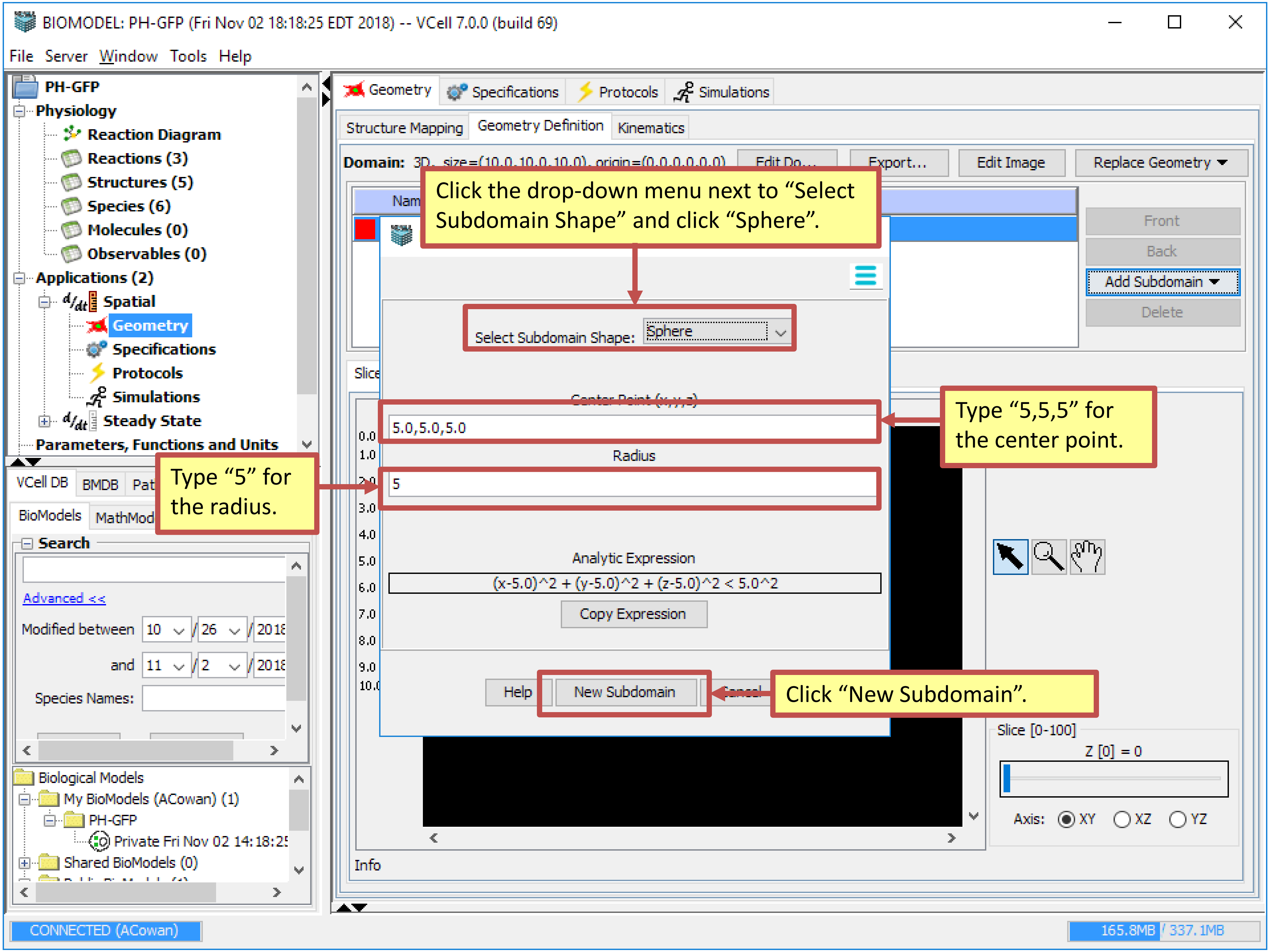
Species Names:

Z [0] = 0

Axis: ● XY ○ XZ ○ YZ

We will create a sphere to represent the cell.

Click “Add Subdomain” > “Analytic”.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Help
New Subdomain
Cancel
Slice [0-100]
Z [0] = 0
Axis:
● XY
○ XZ
○ YZ
Info
CONNECTED (ACowan)
165.8MB / 337.1MB

Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)

Click the drop-down menu next to "Select Subdomain Shape" and click "Sphere".

Select Subdomain Shape: Sphere

Center Point (x,y,z)

5.0,5.0,5.0

Type "5,5,5" for the center point.

Radius

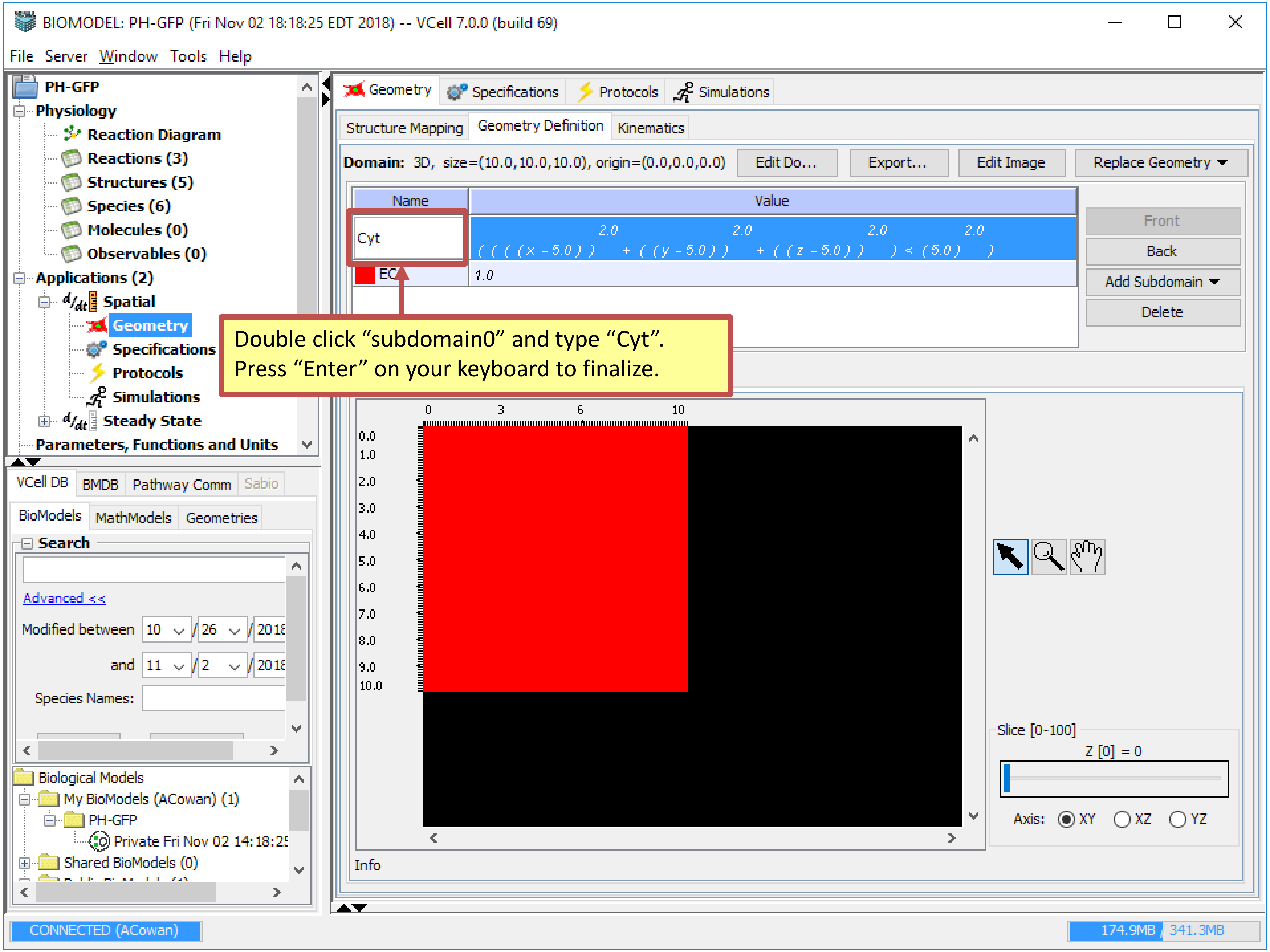
5

Type "5" for the radius.

Analytic Expression

(x-5.0)^2 + (y-5.0)^2 + (z-5.0)^2 < 5.0^2

Click "New Subdomain".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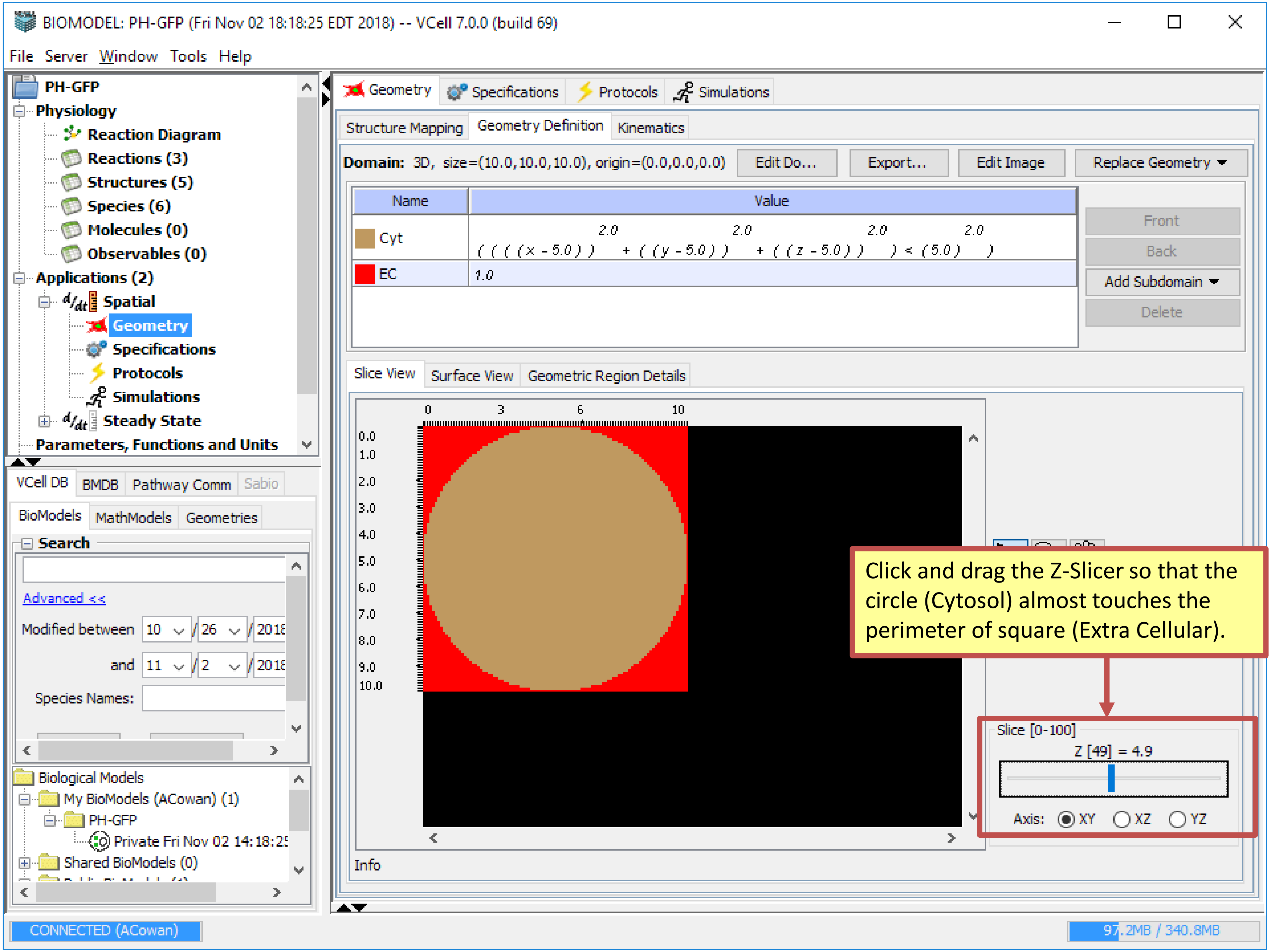
Slice [0-100]
Z [0] = 0
Axis: ● XY ○ XZ ○ YZ
Info
CONNECTED (ACowan)
174.9MB / 341.3MB

Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)

Name	Value
Cyt	$((((x - 5.0))^{2.0} + ((y - 5.0))^{2.0} + ((z - 5.0))^{2.0}) < (5.0)^{2.0})$
🟥 EC	1.0

Double click “subdomain0” and type “Cyt”.
Press “Enter” on your keyboard to finalize.



BIOMODEL: PH-GFP (Fri Nov 02 18:18:25 EDT 2018) -- VCell 7.0.0 (build 69)

Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)

Name	Value
🟫 Cyt	$((((x-5.0))^{2.0} + ((y-5.0))^{2.0} + ((z-5.0))^{2.0}) < (5.0)^{2.0})$
🟥 EC	1.0

Slice [0-100]

Z [49] = 4.9

Axis: ● XY ○ XZ ○ YZ

Click and drag the Z-Slicer so that the circle (Cytosol) almost touches the perimeter of square (Extra Cellular).

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CONNECTED (ACowan)

97.2MB / 340.8MB

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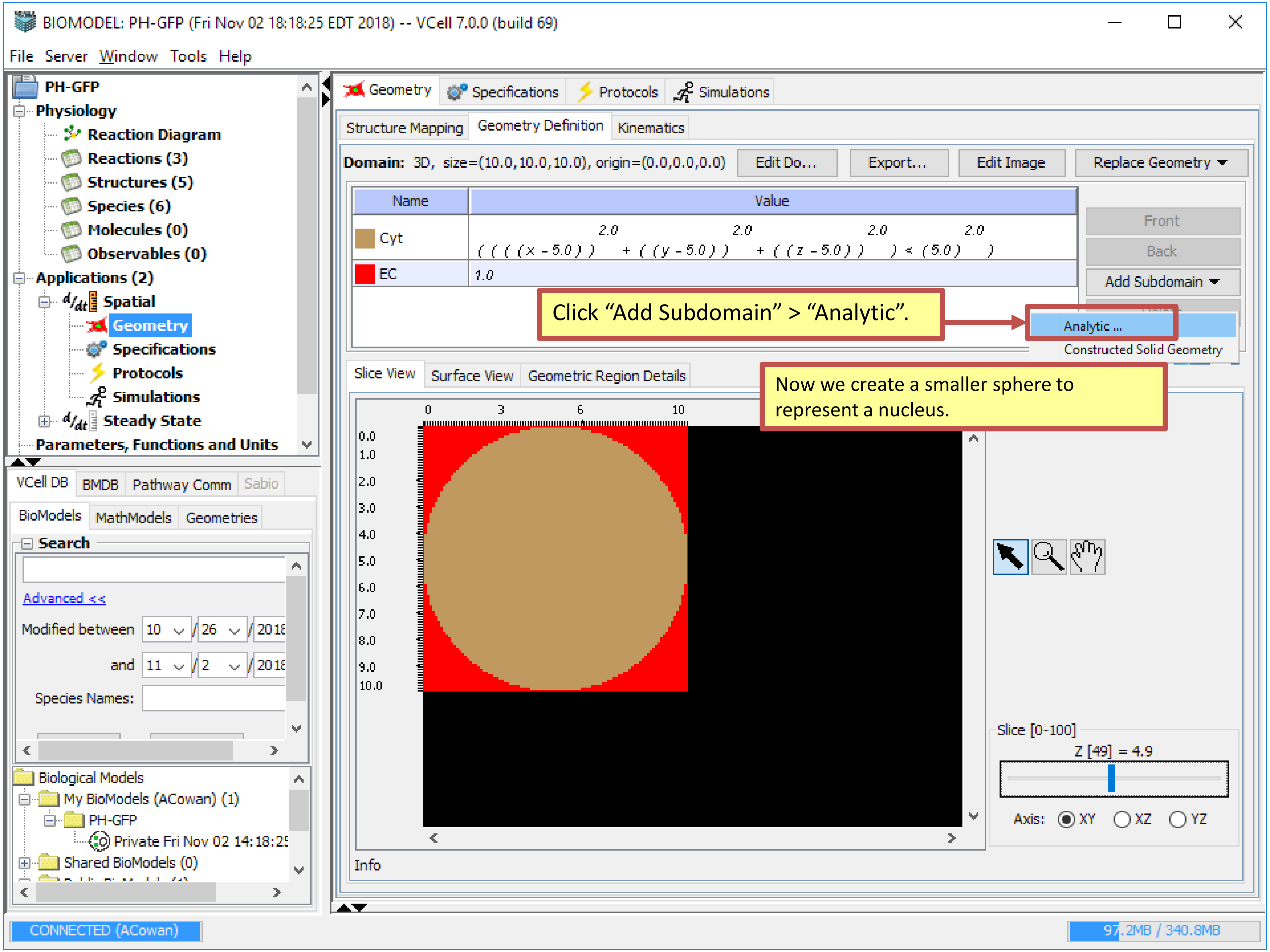

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Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)

Name	Value
🟫 Cyt	$((((x-5.0))^{2.0} + ((y-5.0))^{2.0} + ((z-5.0))^{2.0}) < (5.0)^{2.0})$
🟥 EC	1.0

Click “Add Subdomain” > “Analytic”.

Now we create a smaller sphere to represent a nucleus.

Slice [0-100]: Z [49] = 4.9

Axis: ● XY ○ XZ ○ YZ

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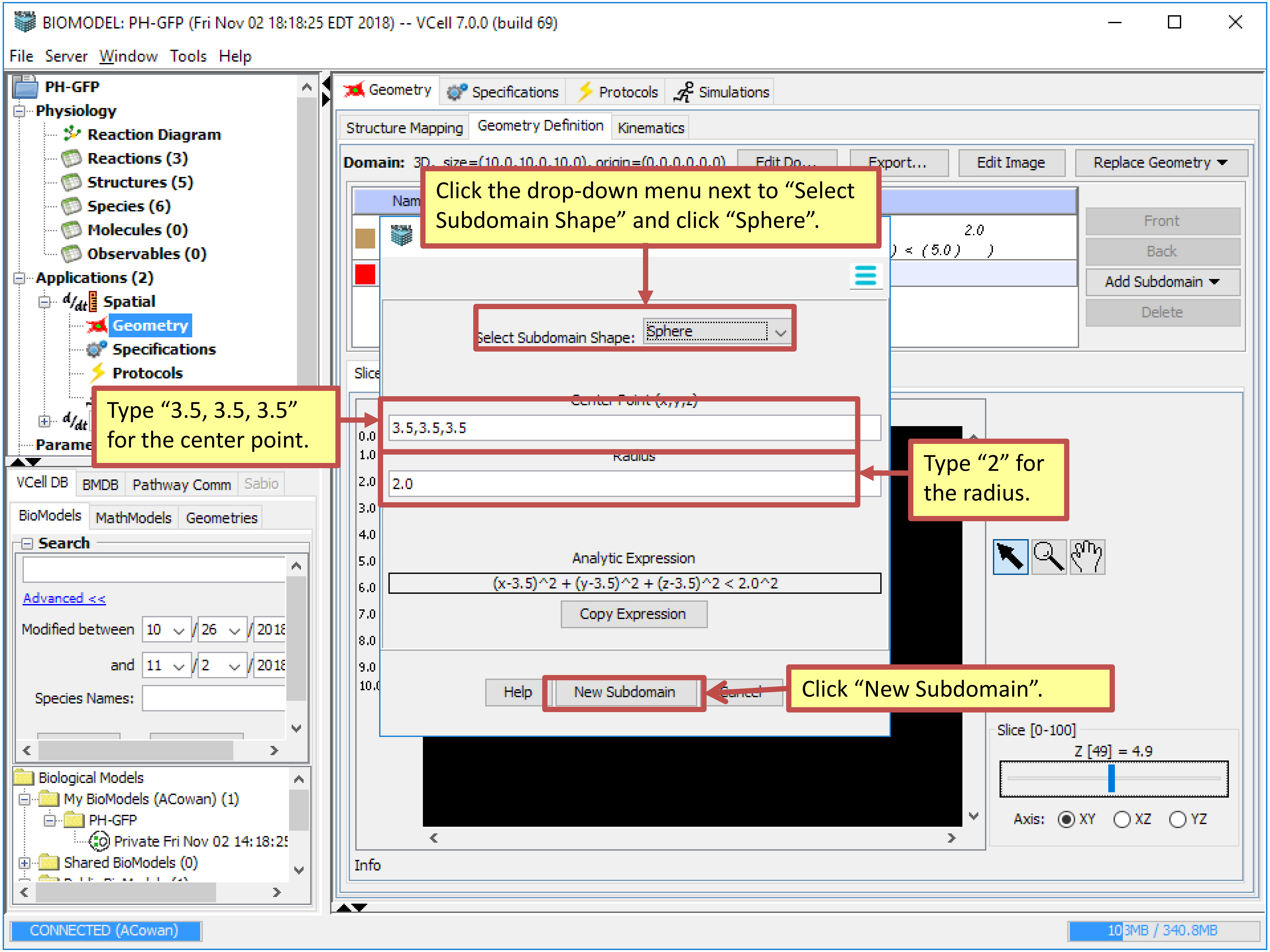
97.2MB / 340.8MB



BIOMODEL: PH-GFP (Fri Nov 02 18:18:25 EDT 2018) -- VCell 7.0.0 (build 69)

Click the drop-down menu next to “Select Subdomain Shape” and click “Sphere”.

Type “3.5, 3.5, 3.5” for the center point.

Type “2” for the radius.

Click “New Subdomain”.

Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)

Select Subdomain Shape: Sphere

Center Point (x,y,z): 3.5,3.5,3.5

Radius: 2.0

Analytic Expression: (x-3.5)^2 + (y-3.5)^2 + (z-3.5)^2 < 2.0^2

Slice [0-100]

Z [49] = 4.9

Axis: ● XY ○ XZ ○ YZ

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103MB / 340.8MB

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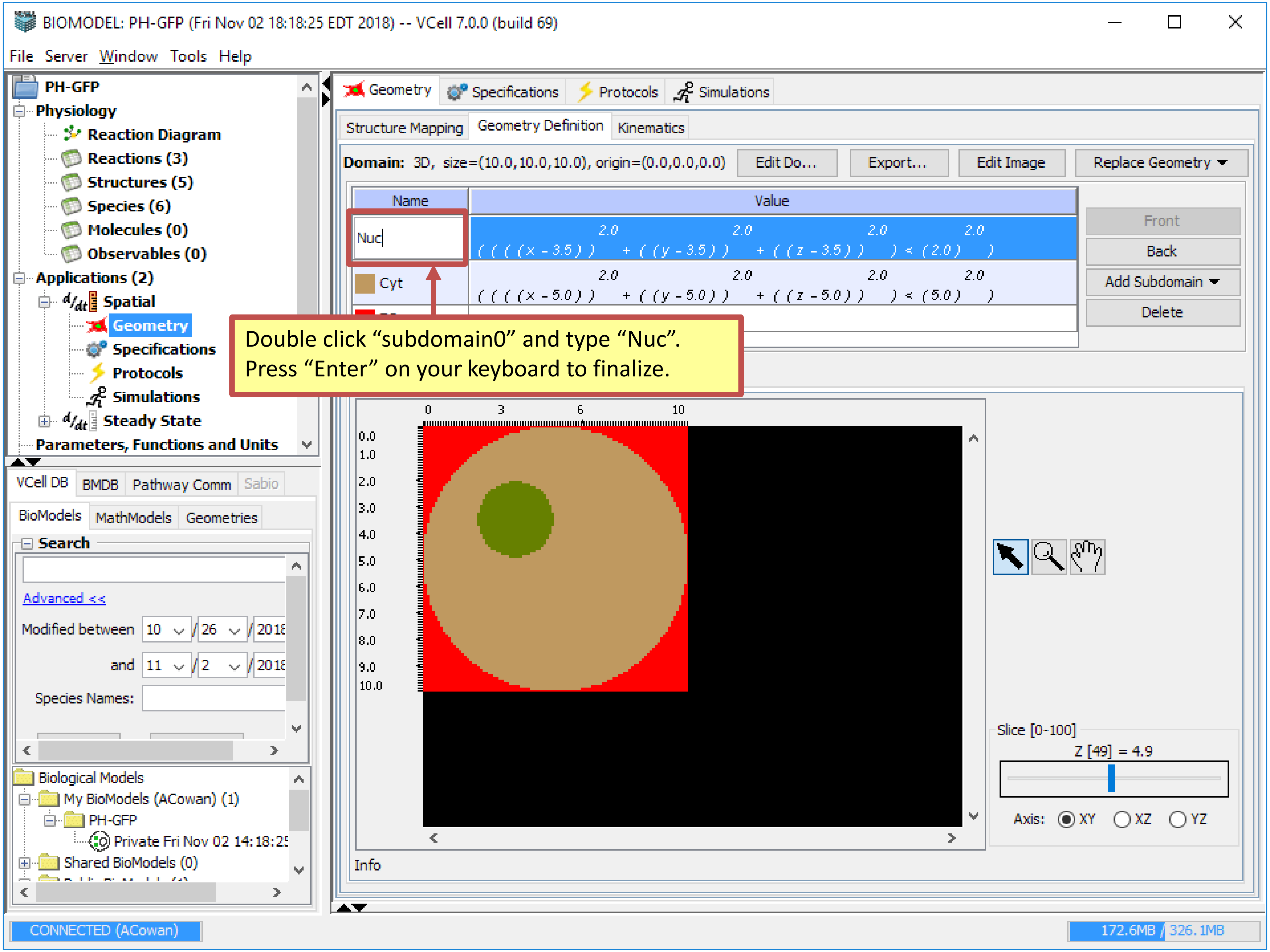
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CONNECTED (ACowan)
172.6MB / 326.1MB

Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)

Name	Value
Nuc	$((((x-3.5)^{2.0} + ((y-3.5)^{2.0} + ((z-3.5)^{2.0}) < (2.0)^{2.0})$
🟫 Cyt	$((((x-5.0)^{2.0} + ((y-5.0)^{2.0} + ((z-5.0)^{2.0}) < (5.0)^{2.0})$

Modified between 10 / 26 / 2018

and 11 / 2 / 2018

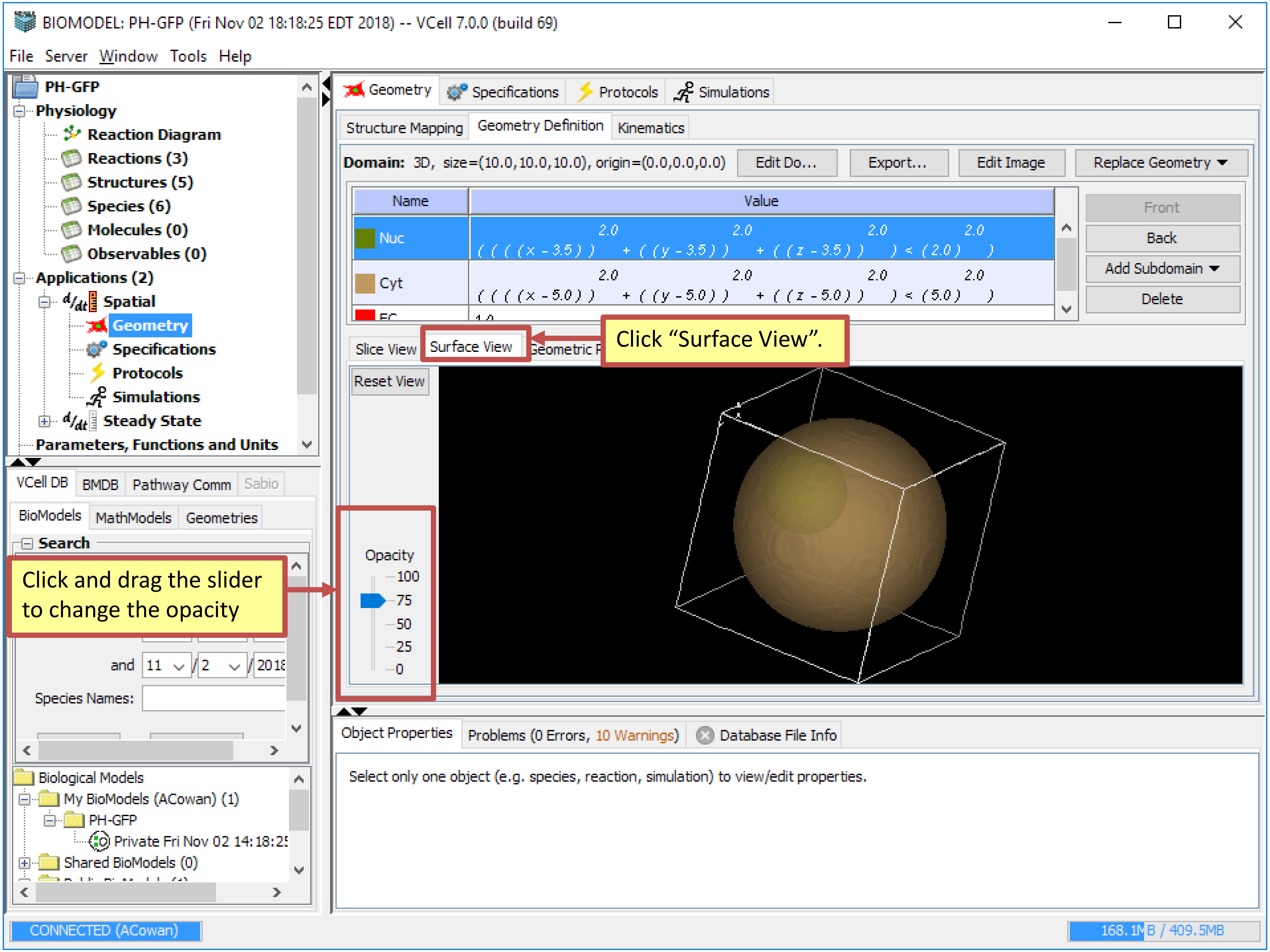
Species Names:

Slice [0-100]

Z [49] = 4.9

Axis: ● XY ○ XZ ○ YZ

Double click “subdomain0” and type “Nuc”. Press “Enter” on your keyboard to finalize.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Object Properties
Problems (0 Errors, 10 Warnings)
Database File Info
CONNECTED (ACowan)
168.1MB / 409.5MB

Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)

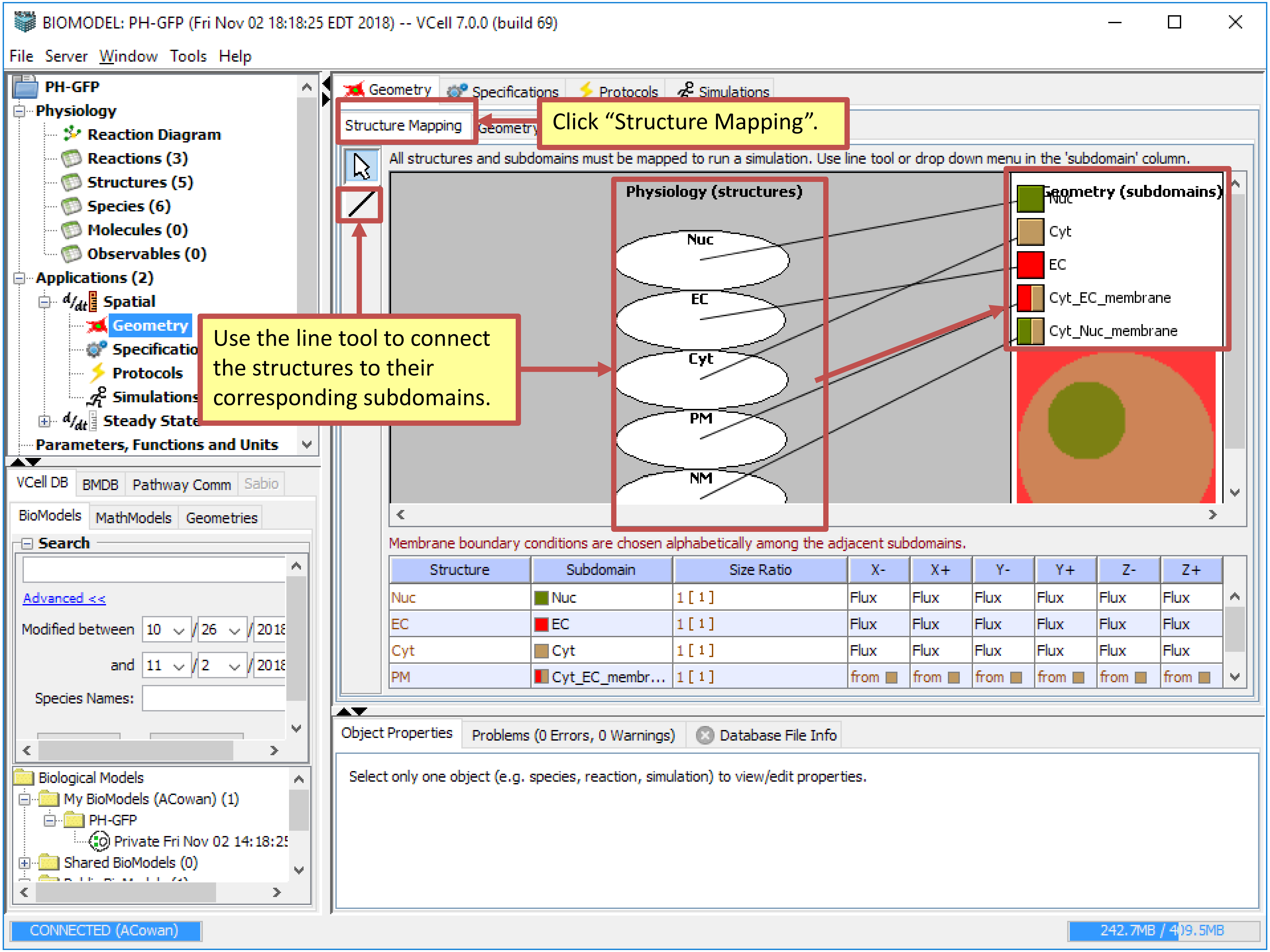
Name	Value
Nuc	$((((x-3.5))^{2.0} + ((y-3.5))^{2.0} + ((z-3.5))^{2.0}) < (2.0)^{2.0})$
Cyt	$((((x-5.0))^{2.0} + ((y-5.0))^{2.0} + ((z-5.0))^{2.0}) < (5.0)^{2.0})$
EC	1.0

and 11 / 2 / 2018

Select only one object (e.g. species, reaction, simulation) to view/edit properties.

Click "Surface View".

Click and drag the slider to change the opacity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CONNECTED (ACowan)
242.7MB / 409.5MB

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Click "Structure Mapping".

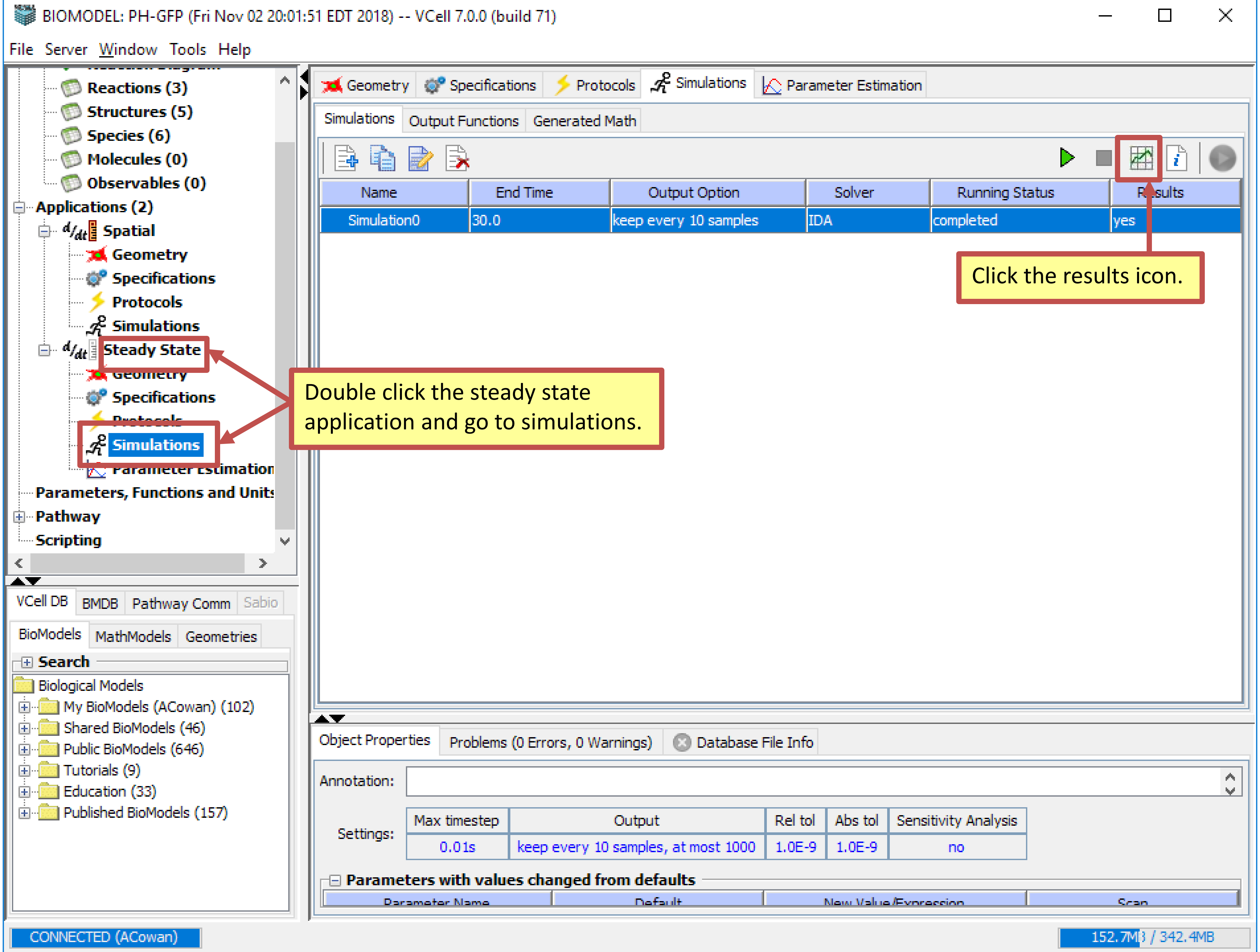
Use the line tool to connect the structures to their corresponding subdomains.

All structures and subdomains must be mapped to run a simulation. Use line tool or drop down menu in the 'subdomain' column.

Membrane boundary conditions are chosen alphabetically among the adjacent subdomains.

Structure	Subdomain	Size Ratio	X-	X+	Y-	Y+	Z-	Z+
Nuc	🟩 Nuc	1 [1]	Flux	Flux	Flux	Flux	Flux	Flux
EC	🟥 EC	1 [1]	Flux	Flux	Flux	Flux	Flux	Flux
Cyt	🟫 Cyt	1 [1]	Flux	Flux	Flux	Flux	Flux	Flux
PM	Cyt_EC_membr…	1 [1]	from 🟫	from 🟫	from 🟫	from 🟫	from 🟫	from 🟫

Select only one object (e.g. species, reaction, simulation) to view/edit properties.



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Problems (0 Errors, 0 Warnings)
Database File Info
CONNECTED (ACowan)
152.7MB / 342.4MB

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	30.0	keep every 10 samples	IDA	completed	yes

Click the results icon.

Double click the steady state application and go to simulations.

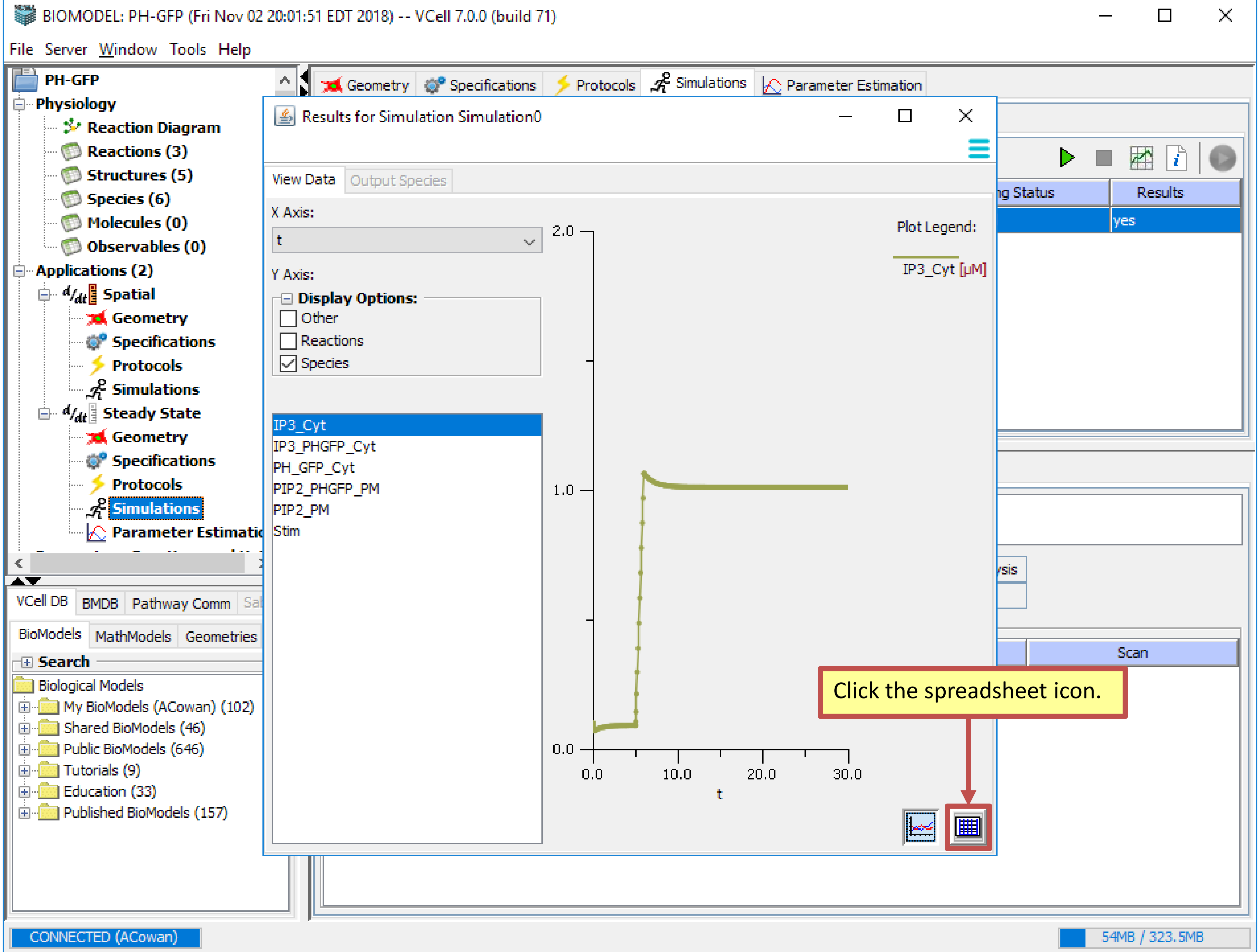
Annotation:

Settings:

Max timestep	Output	Rel tol	Abs tol	Sensitivity Analysis
0.01s	keep every 10 samples, at most 1000	1.0E-9	1.0E-9	no

Parameters with values changed from defaults

Parameter Name	Default	New Value/Expression	Scan


BIOMODEL: PH-GFP (Fri Nov 02 20:01:51 EDT 2018) -- VCell 7.0.0 (build 71)
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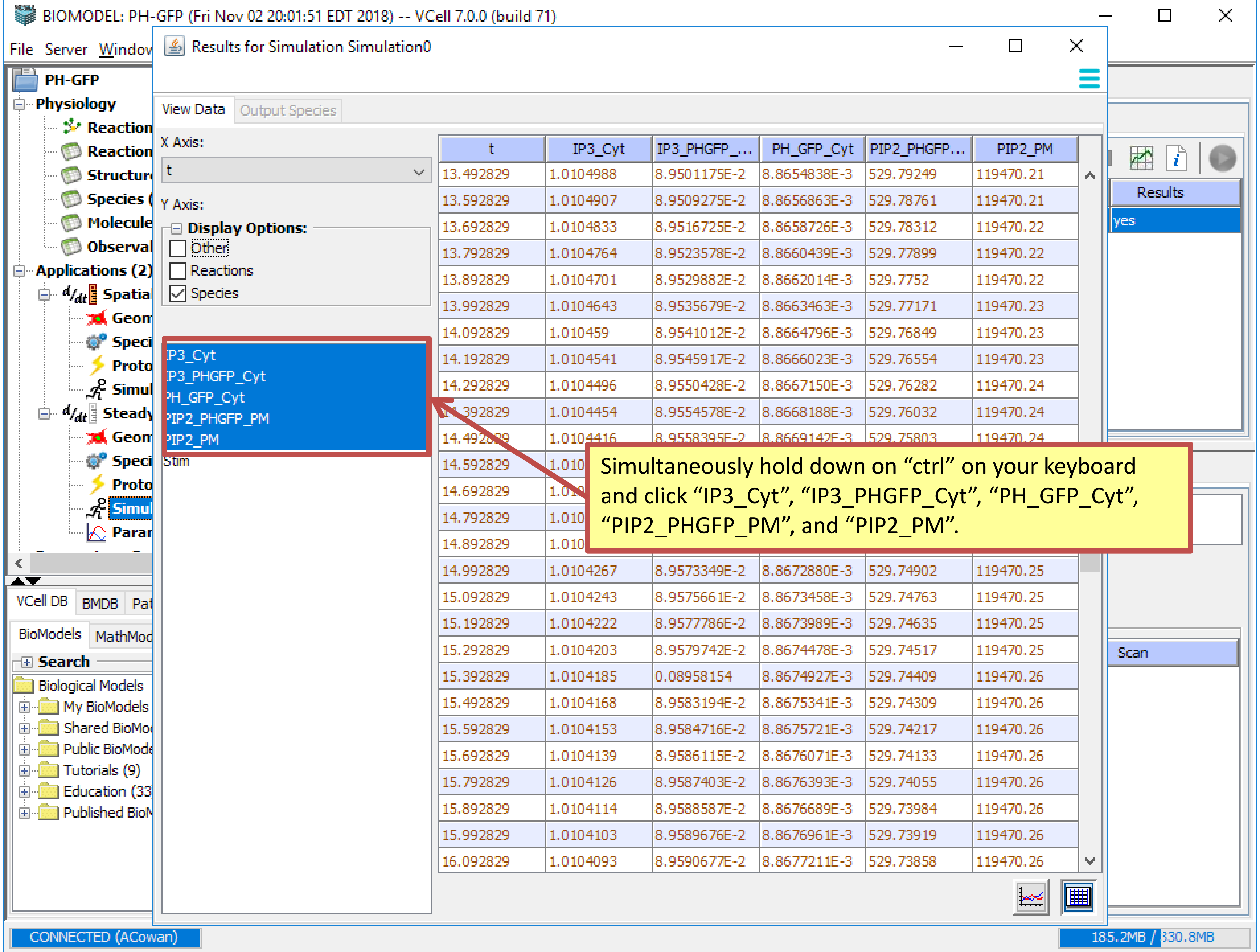
Click the spreadsheet icon.


BIOMODEL: PH-GFP (Fri Nov 02 20:01:51 EDT 2018) -- VCell 7.0.0 (build 71)
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☐ Other
☐ Reactions
☑ Species

IP3_Cyt
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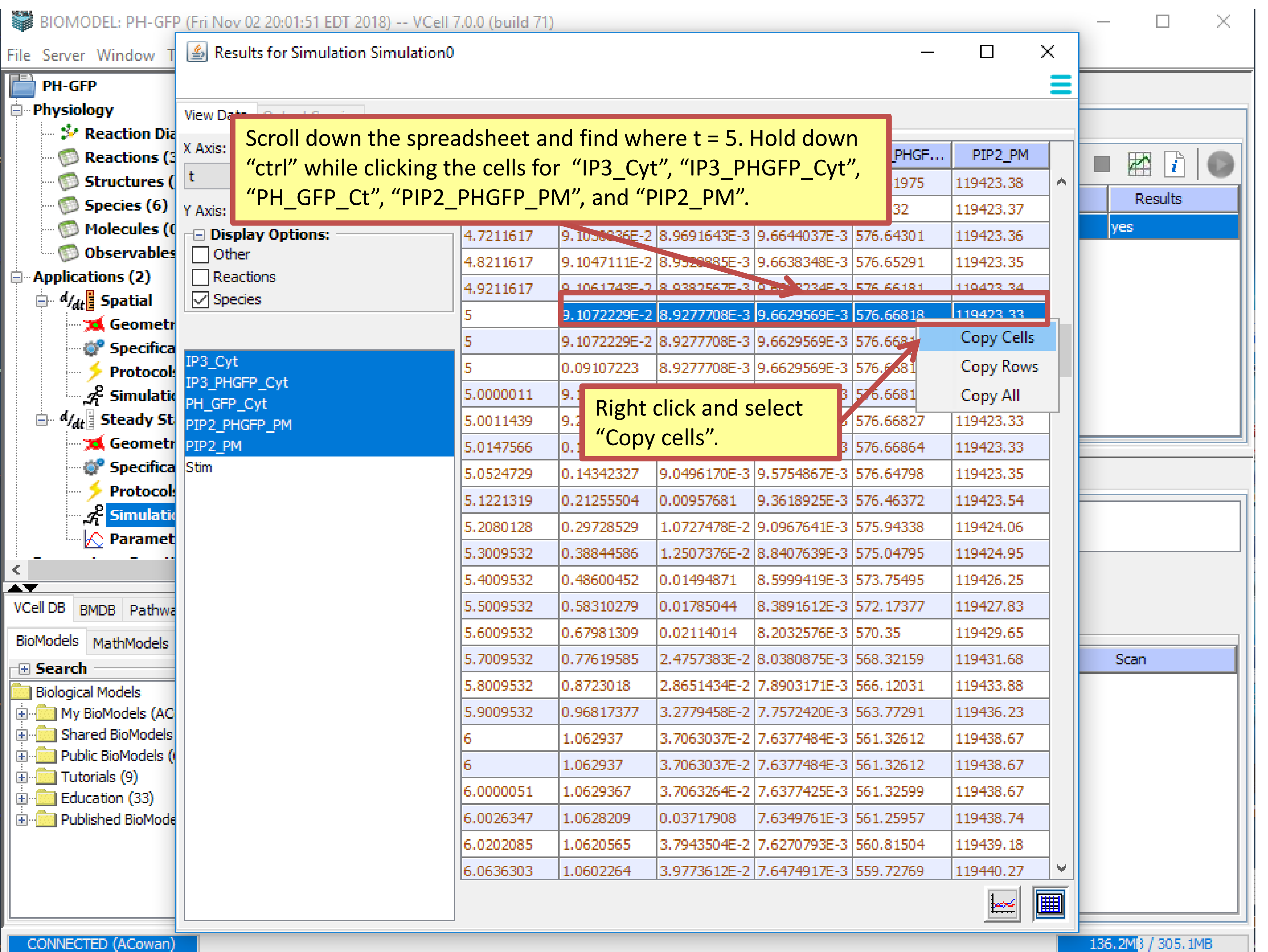
PH_GFP_Cyt
PIP2_PHGFP_PM
PIP2_PM
Stim

t	IP3_Cyt	IP3_PHGFP_...	PH_GFP_Cyt	PIP2_PHGFP...	PIP2_PM
13.492829	1.0104988	8.9501175E-2	8.8654838E-3	529.79249	119470.21
13.592829	1.0104907	8.9509275E-2	8.8656863E-3	529.78761	119470.21
13.692829	1.0104833	8.9516725E-2	8.8658726E-3	529.78312	119470.22
13.792829	1.0104764	8.9523578E-2	8.8660439E-3	529.77899	119470.22
13.892829	1.0104701	8.9529882E-2	8.8662014E-3	529.7752	119470.22
13.992829	1.0104643	8.9535679E-2	8.8663463E-3	529.77171	119470.23
14.092829	1.010459	8.9541012E-2	8.8664796E-3	529.76849	119470.23
14.192829	1.0104541	8.9545917E-2	8.8666023E-3	529.76554	119470.23
14.292829	1.0104496	8.9550428E-2	8.8667150E-3	529.76282	119470.24
14.392829	1.0104454	8.9554578E-2	8.8668188E-3	529.76032	119470.24
14.492829	1.0104416	8.9558395E-2	8.8669142E-3	529.75803	119470.24
14.592829	1.010				
14.692829	1.01				
14.792829	1.010				
14.892829	1.010				
14.992829	1.0104267	8.9573349E-2	8.8672880E-3	529.74902	119470.25
15.092829	1.0104243	8.9575661E-2	8.8673458E-3	529.74763	119470.25
15.192829	1.0104222	8.9577786E-2	8.8673989E-3	529.74635	119470.25
15.292829	1.0104203	8.9579742E-2	8.8674478E-3	529.74517	119470.25
15.392829	1.0104185	0.08958154	8.8674927E-3	529.74409	119470.26
15.492829	1.0104168	8.9583194E-2	8.8675341E-3	529.74309	119470.26
15.592829	1.0104153	8.9584716E-2	8.8675721E-3	529.74217	119470.26
15.692829	1.0104139	8.9586115E-2	8.8676071E-3	529.74133	119470.26
15.792829	1.0104126	8.9587403E-2	8.8676393E-3	529.74055	119470.26
15.892829	1.0104114	8.9588587E-2	8.8676689E-3	529.73984	119470.26
15.992829	1.0104103	8.9589676E-2	8.8676961E-3	529.73919	119470.26
16.092829	1.0104093	8.9590677E-2	8.8677211E-3	529.73858	119470.26

Simultaneously hold down on “ctrl” on your keyboard and click “IP3_Cyt”, “IP3_PHGFP_Cyt”, “PH_GFP_Cyt”, “PIP2_PHGFP_PM”, and “PIP2_PM”.



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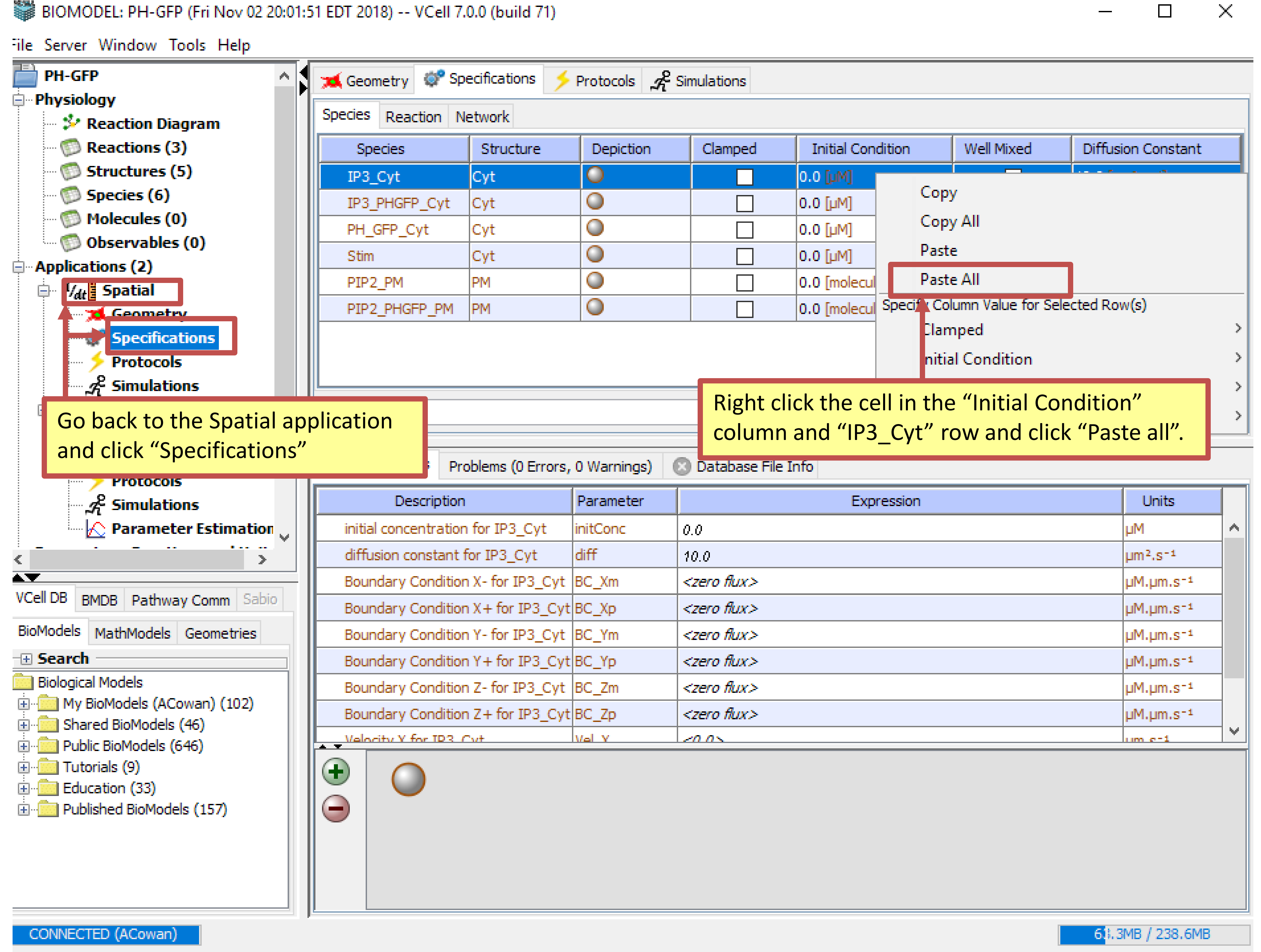
PIP2_PM
Stim
Copy Cells
Copy Rows
Copy All
Results
yes
Scan
CONNECTED (ACowan)
136.2MB / 305.1MB

Scroll down the spreadsheet and find where t = 5. Hold down "ctrl" while clicking the cells for "IP3_Cyt", "IP3_PHGFP_Cyt", "PH_GFP_Ct", "PIP2_PHGFP_PM", and "PIP2_PM".

Right click and select "Copy cells".

				PHGF…	PIP2_PM
[illegible]	[illegible]	[illegible]	[illegible]	1975	119423.38
[illegible]	[illegible]	[illegible]	[illegible]	32	119423.37
4.7211617	9.10[illegible]36E-2	8.9691643E-3	9.6644037E-3	576.64301	119423.36
4.8211617	9.1047111E-2	8.9[illegible]885E-3	9.6638348E-3	576.65291	119423.35
4.9211617	9.1061743E-2	8.9382567E-3	9.[illegible]234E-3	576.66181	119423.34
5	9.1072229E-2	8.9277708E-3	9.6629569E-3	576.66818	119423.33
5	9.1072229E-2	8.9277708E-3	9.6629569E-3	576.668[illegible]	[illegible]
5	0.09107223	8.9277708E-3	9.6629569E-3	576.681[illegible]	[illegible]
5.0000011	9.1[illegible]	[illegible]	[illegible]	576.6681	[illegible]
5.0011439	9.2[illegible]	[illegible]	[illegible]	576.66827	119423.33
5.0147566	0.1[illegible]	[illegible]	[illegible]	576.66864	119423.33
5.0524729	0.14342327	9.0496170E-3	9.5754867E-3	576.64798	119423.35
5.1221319	0.21255504	0.00957681	9.3618925E-3	576.46372	119423.54
5.2080128	0.29728529	1.0727478E-2	9.0967641E-3	575.94338	119424.06
5.3009532	0.38844586	1.2507376E-2	8.8407639E-3	575.04795	119424.95
5.4009532	0.48600452	0.01494871	8.5999419E-3	573.75495	119426.25
5.5009532	0.58310279	0.01785044	8.3891612E-3	572.17377	119427.83
5.6009532	0.67981309	0.02114014	8.2032576E-3	570.35	119429.65
5.7009532	0.77619585	2.4757383E-2	8.0380875E-3	568.32159	119431.68
5.8009532	0.8723018	2.8651434E-2	7.8903171E-3	566.12031	119433.88
5.9009532	0.96817377	3.2779458E-2	7.7572420E-3	563.77291	119436.23
6	1.062937	3.7063037E-2	7.6377484E-3	561.32612	119438.67
6	1.062937	3.7063037E-2	7.6377484E-3	561.32612	119438.67
6.0000051	1.0629367	3.7063264E-2	7.6377425E-3	561.32599	119438.67
6.0026347	1.0628209	0.03717908	7.6349761E-3	561.25957	119438.74
6.0202085	1.0620565	3.7943504E-2	7.6270793E-3	560.81504	119439.18
6.0636303	1.0602264	3.9773612E-2	7.6474917E-3	559.72769	119440.27


BIOMODEL: PH-GFP (Fri Nov 02 20:01:51 EDT 2018) -- VCell 7.0.0 (build 71)
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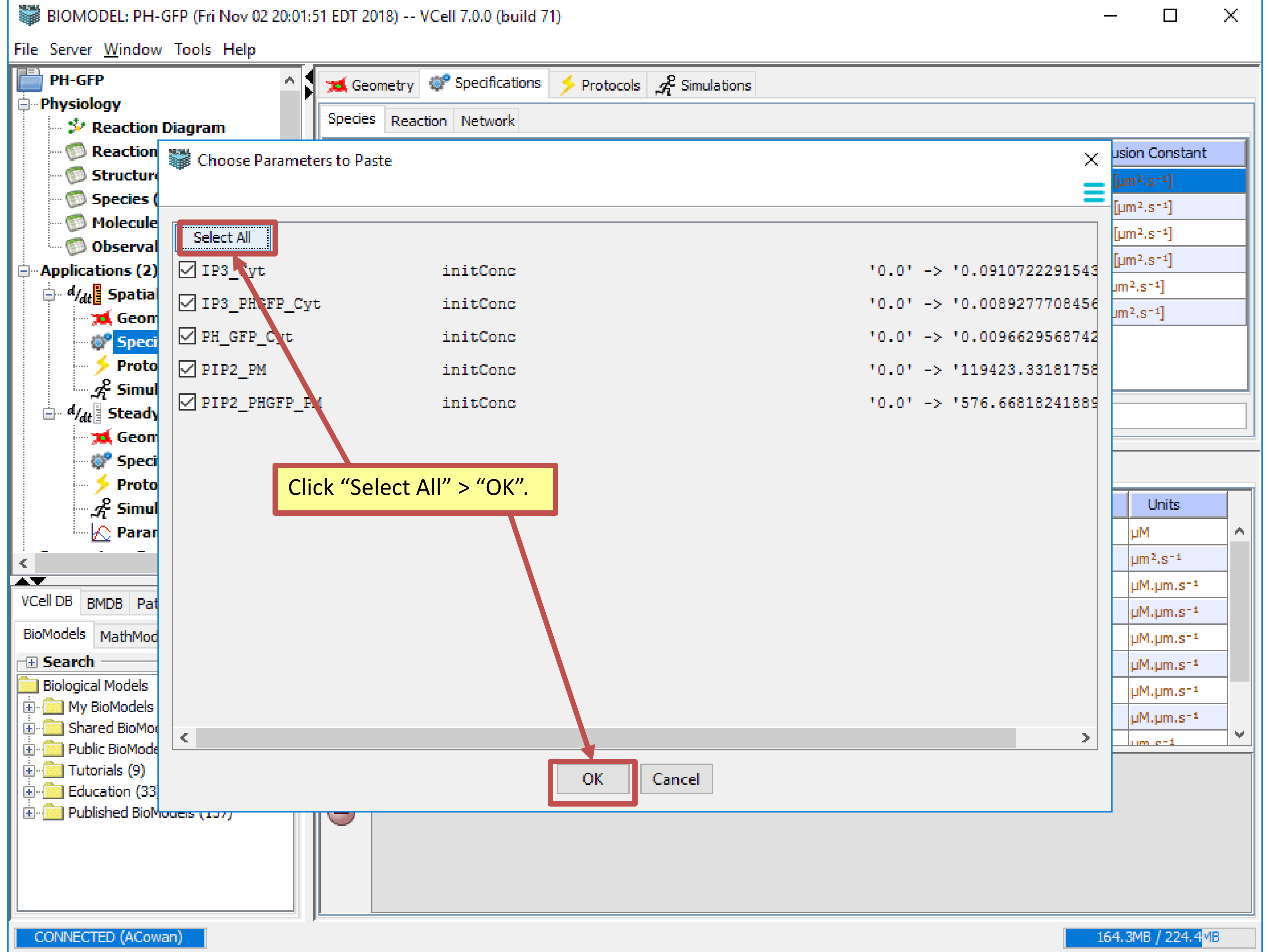
Paste
Paste All
Specify Column Value for Selected Row(s)
Clamped
Initial Condition
Problems (0 Errors, 0 Warnings)
Database File Info
CONNECTED (ACowan)
63.3MB / 238.6MB

Species	Structure	Depiction	Clamped	Initial Condition	Well Mixed	Diffusion Constant
IP3_Cyt	Cyt	●	☐	0.0 [µM]		
IP3_PHGFP_Cyt	Cyt	●	☐	0.0 [µM]		
PH_GFP_Cyt	Cyt	●	☐	0.0 [µM]		
Stim	Cyt	●	☐	0.0 [µM]		
PIP2_PM	PM	●	☐	0.0 [molecul		
PIP2_PHGFP_PM	PM	●	☐	0.0 [molecul		

Description	Parameter	Expression	Units
initial concentration for IP3_Cyt	initConc	0.0	µM
diffusion constant for IP3_Cyt	diff	10.0	$\mu m^2.s^{-1}$
Boundary Condition X- for IP3_Cyt	BC_Xm	<zero flux>	$\mu M.\mu m.s^{-1}$
Boundary Condition X+ for IP3_Cyt	BC_Xp	<zero flux>	$\mu M.\mu m.s^{-1}$
Boundary Condition Y- for IP3_Cyt	BC_Ym	<zero flux>	$\mu M.\mu m.s^{-1}$
Boundary Condition Y+ for IP3_Cyt	BC_Yp	<zero flux>	$\mu M.\mu m.s^{-1}$
Boundary Condition Z- for IP3_Cyt	BC_Zm	<zero flux>	$\mu M.\mu m.s^{-1}$
Boundary Condition Z+ for IP3_Cyt	BC_Zp	<zero flux>	$\mu M.\mu m.s^{-1}$
Velocity X for IP3_Cyt	Vel_X	<0.0>	$\mu m.s^{-1}$

Go back to the Spatial application and click “Specifications”

Right click the cell in the “Initial Condition” column and “IP3_Cyt” row and click “Paste all”.



BIOMODEL: PH-GFP (Fri Nov 02 20:01:51 EDT 2018) -- VCell 7.0.0 (build 71)

Choose Parameters to Paste

```
☑ IP3_Cyt          initConc    '0.0' -> '0.0910722291543
☑ IP3_PHGFP_Cyt    initConc    '0.0' -> '0.0089277708456
☑ PH_GFP_Cyt       initConc    '0.0' -> '0.0096629568742
☑ PIP2_PM          initConc    '0.0' -> '119423.33181758
☑ PIP2_PHGFP_PM    initConc    '0.0' -> '576.66818241889
```

Click “Select All” > “OK”.

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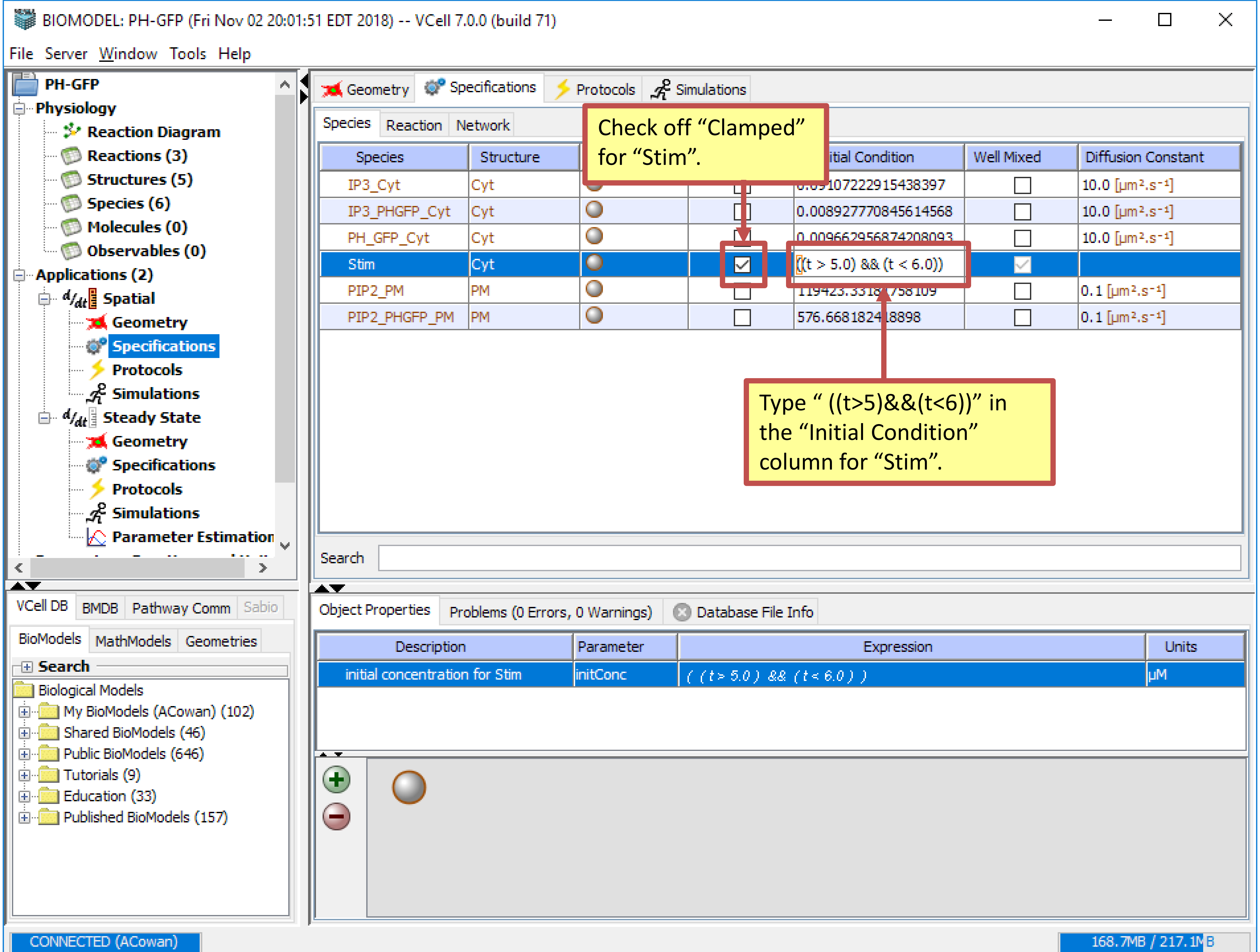
Cancel
CONNECTED (ACowan)
164.3MB / 224.4MB


BIOMODEL: PH-GFP (Fri Nov 02 20:01:51 EDT 2018) -- VCell 7.0.0 (build 71)
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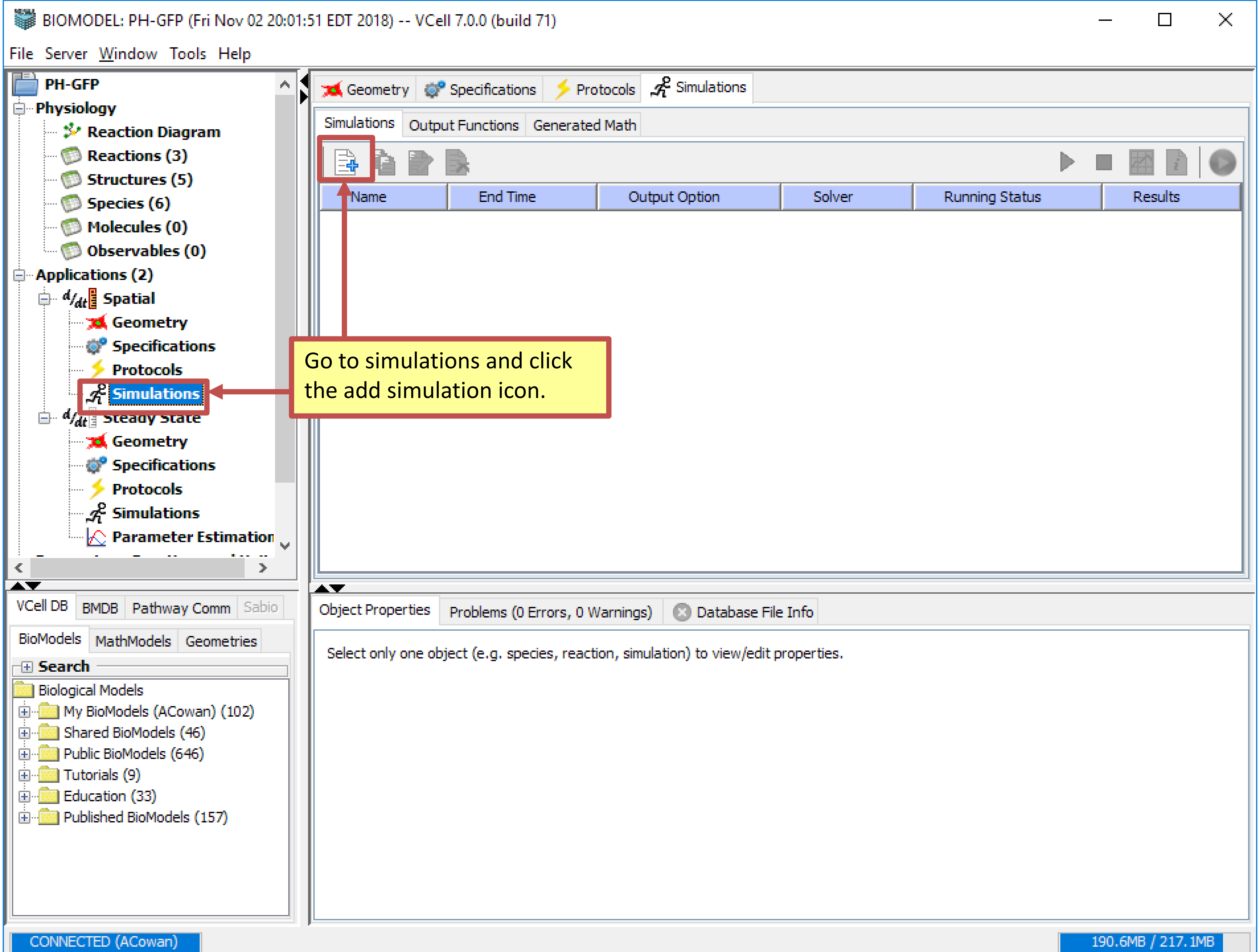
CONNECTED (ACowan)
168.7MB / 217.1MB

Species	Structure			Initial Condition	Well Mixed	Diffusion Constant
IP3_Cyt	Cyt	●	☐	0.09107222915438397	☐	10.0 [µm².s⁻¹]
IP3_PHGFP_Cyt	Cyt	●	☐	0.008927770845614568	☐	10.0 [µm².s⁻¹]
PH_GFP_Cyt	Cyt	●	☐	0.009662956874208093	☐	10.0 [µm².s⁻¹]
Stim	Cyt	●	☑	((t > 5.0) && (t < 6.0))	☑	
PIP2_PM	PM	●	☐	119423.3318[illegible]758109	☐	0.1 [µm².s⁻¹]
PIP2_PHGFP_PM	PM	●	☐	576.6681824[illegible]18898	☐	0.1 [µm².s⁻¹]

Description	Parameter	Expression	Units
initial concentration for Stim	initConc	((t > 5.0) && (t < 6.0))	µM

Check off “Clamped” for “Stim”.

Type “ ((t>5)&&(t<6))” in the “Initial Condition” column for “Stim”.


BIOMODEL: PH-GFP (Fri Nov 02 20:01:51 EDT 2018) -- VCell 7.0.0 (build 71)
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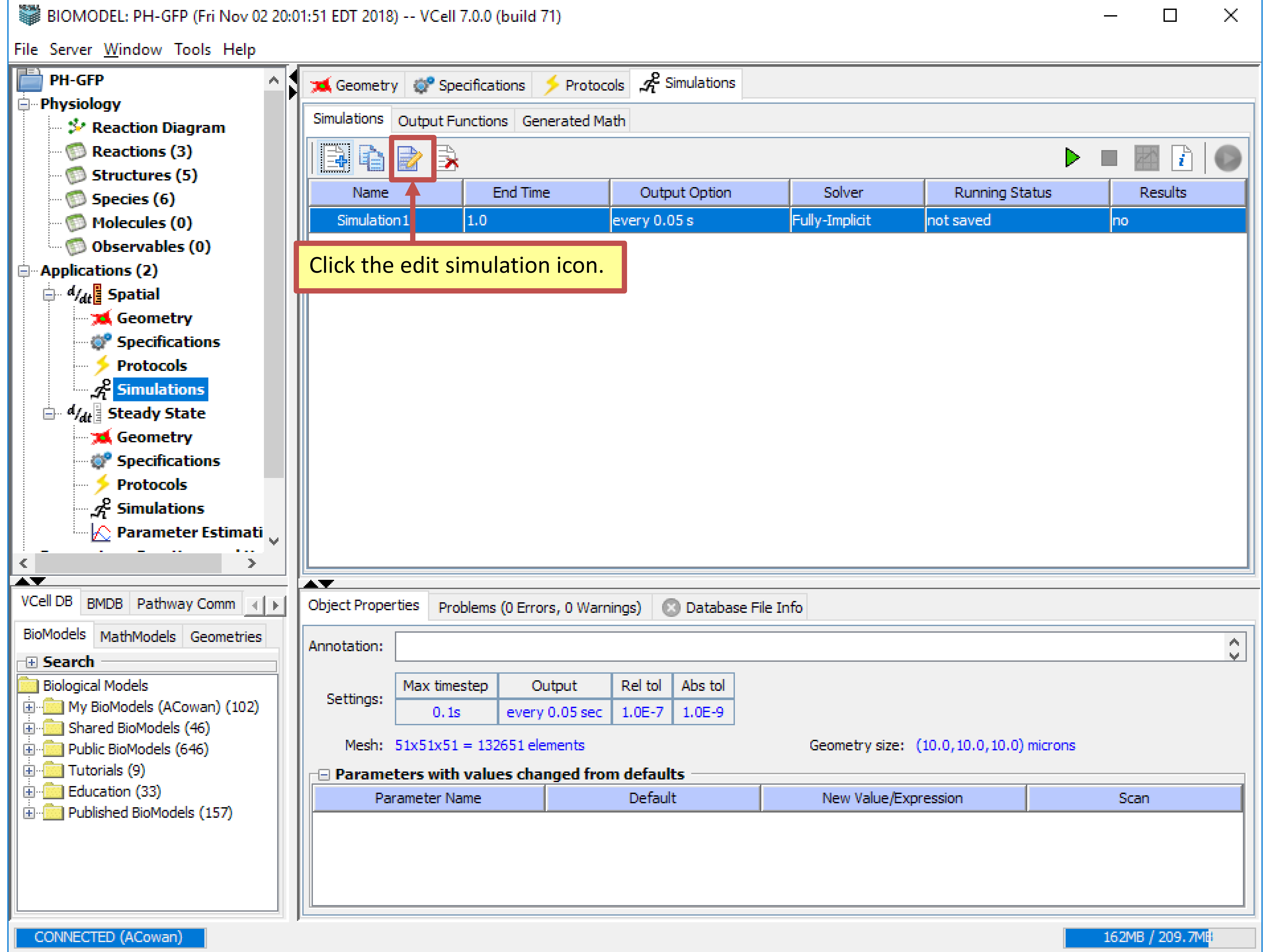
190.6MB / 217.1MB

Select only one object (e.g. species, reaction, simulation) to view/edit properties.

Go to simulations and click the add simulation icon.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162MB / 209.7MB

BIOMODEL: PH-GFP (Fri Nov 02 20:01:51 EDT 2018) -- VCell 7.0.0 (build 71)

Click the edit simulation icon.

Name	End Time	Output Option	Solver	Running Status	Results
Simulation1	1.0	every 0.05 s	Fully-Implicit	not saved	no

Annotation:

Settings:

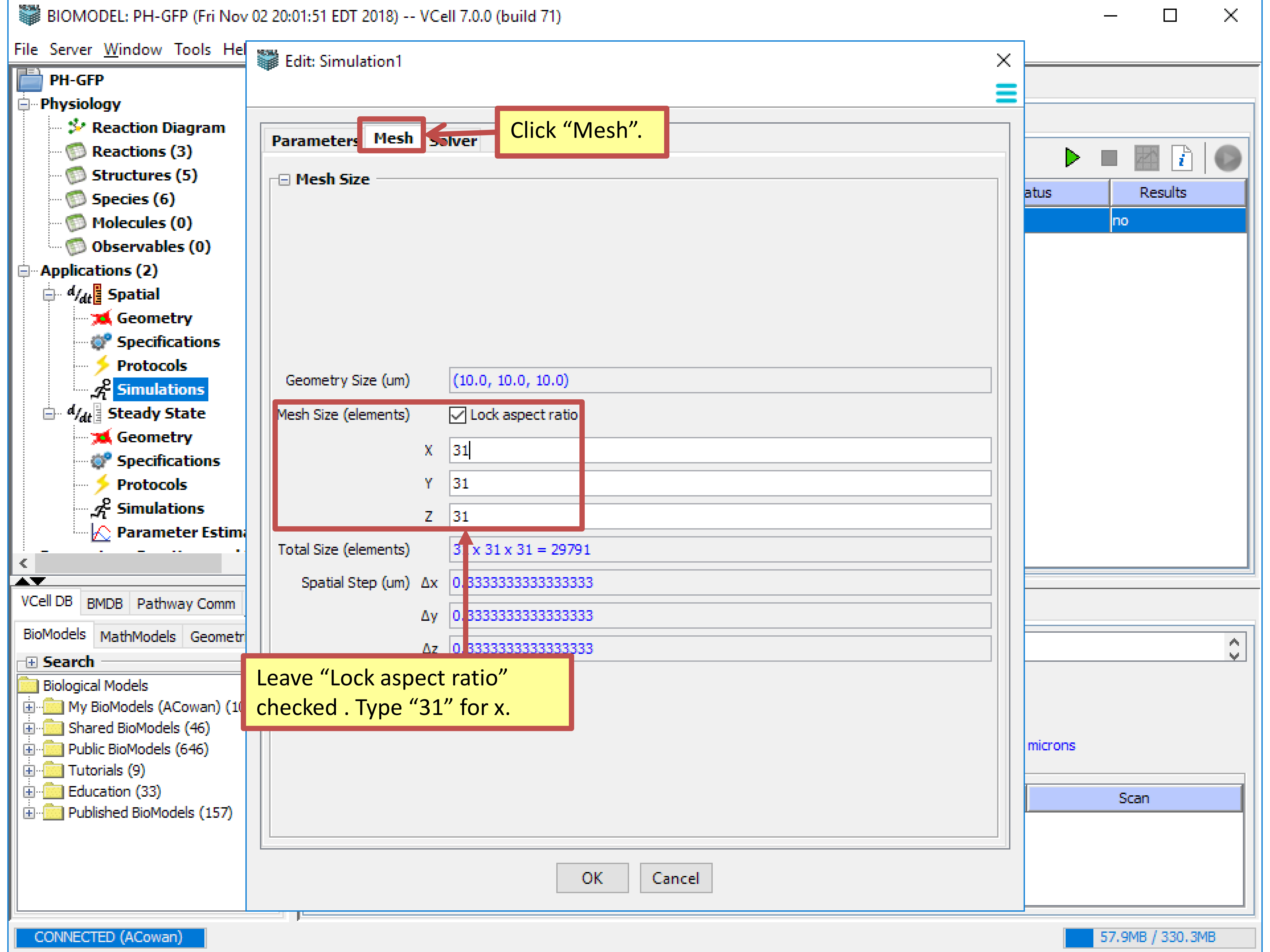
Max timestep	Output	Rel tol	Abs tol
0.1s	every 0.05 sec	1.0E-7	1.0E-9

Mesh: 51x51x51 = 132651 elements

Geometry size: (10.0,10.0,10.0) microns

Parameters with values changed from defaults

Parameter Name	Default	New Value/Expression	Scan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OK
Cancel
CONNECTED (ACowan)
57.9MB / 330.3MB

Click “Mesh”.

Geometry Size (um) (10.0, 10.0, 10.0)

Mesh Size (elements) ☑ Lock aspect ratio

X 31

Y 31

Z 31

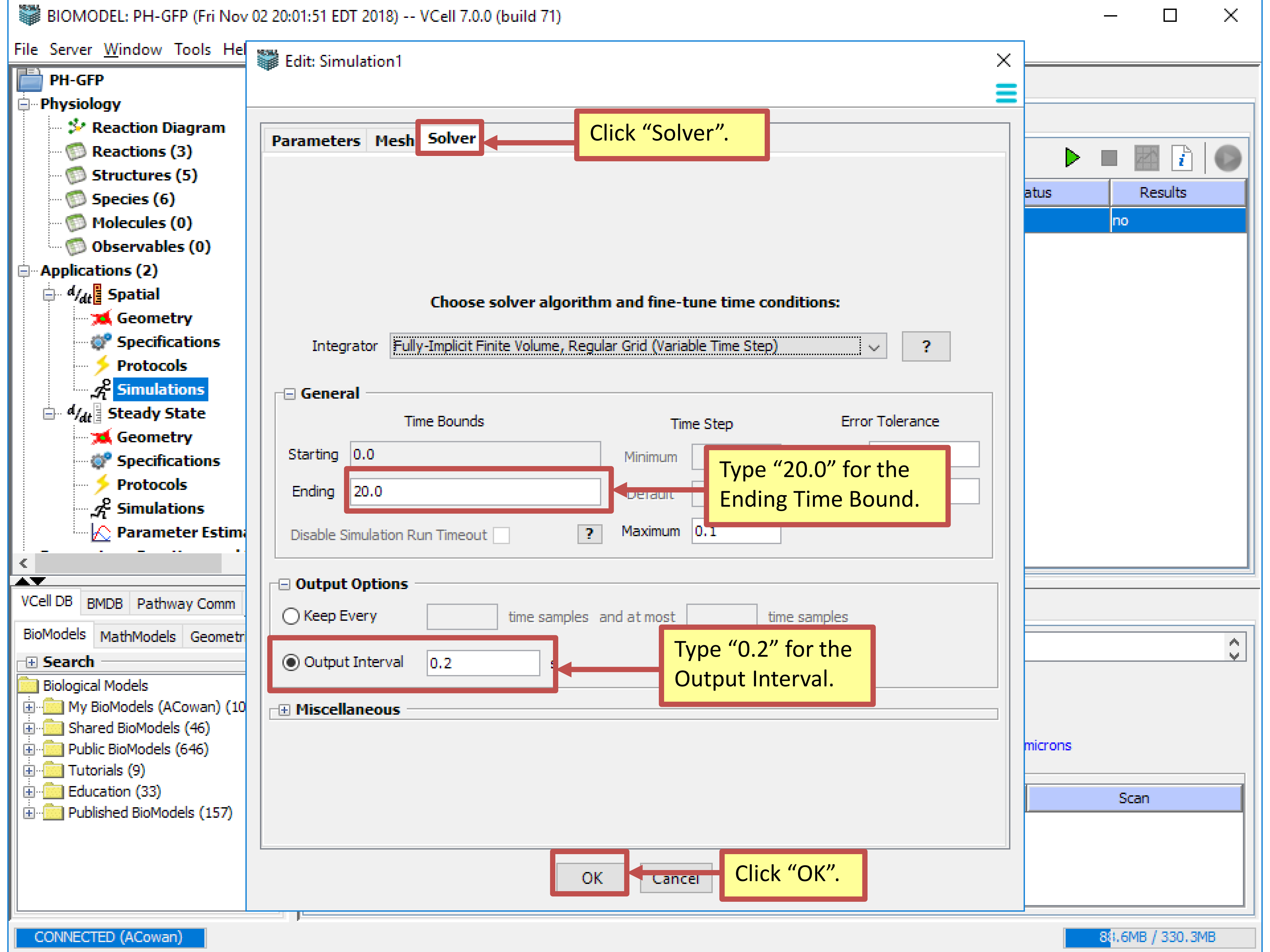
Total Size (elements) 31 x 31 x 31 = 29791

Spatial Step (um) Δx 0.33333333333333333

Δy 0.33333333333333333

Δz 0.33333333333333333

Leave “Lock aspect ratio” checked . Type “31” for x.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8.6MB / 330.3MB
Edit: Simulation1
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OK
Cancel

Click “Solver”.

Choose solver algorithm and fine-tune time conditions:

Integrator: Fully-Implicit Finite Volume, Regular Grid (Variable Time Step)

General

Time Bounds		Time Step		Error Tolerance
Starting	0.0	Minimum		
Ending	20.0	Default		
Disable Simulation Run Timeout ☐		Maximum	0.1	

Type “20.0” for the Ending Time Bound.

Output Options

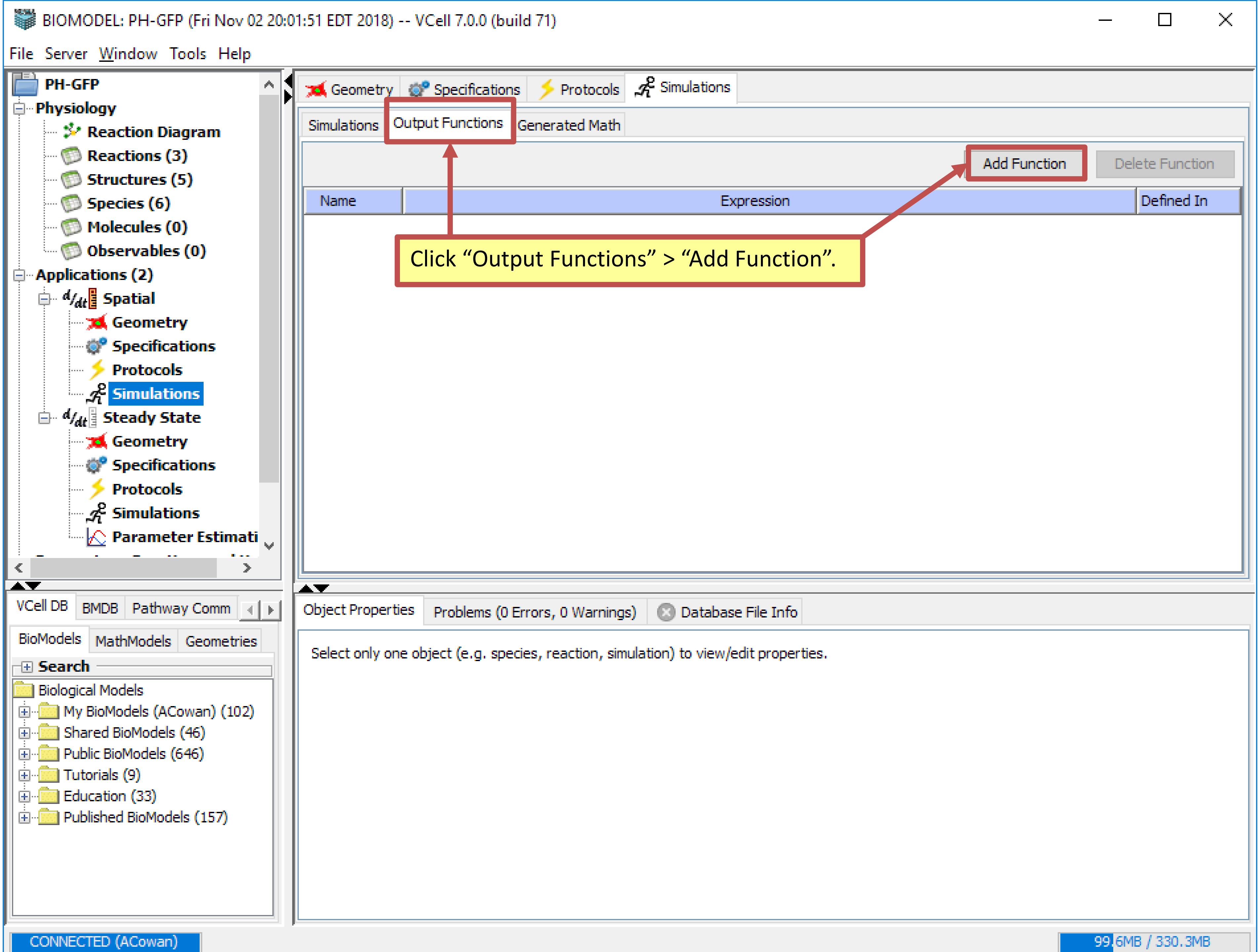
○ Keep Every ___ time samples and at most ___ time samples

● Output Interval 0.2

Type “0.2” for the Output Interval.

Miscellaneous

Click “OK”.


BIOMODEL: PH-GFP (Fri Nov 02 20:01:51 EDT 2018) -- VCell 7.0.0 (build 71)
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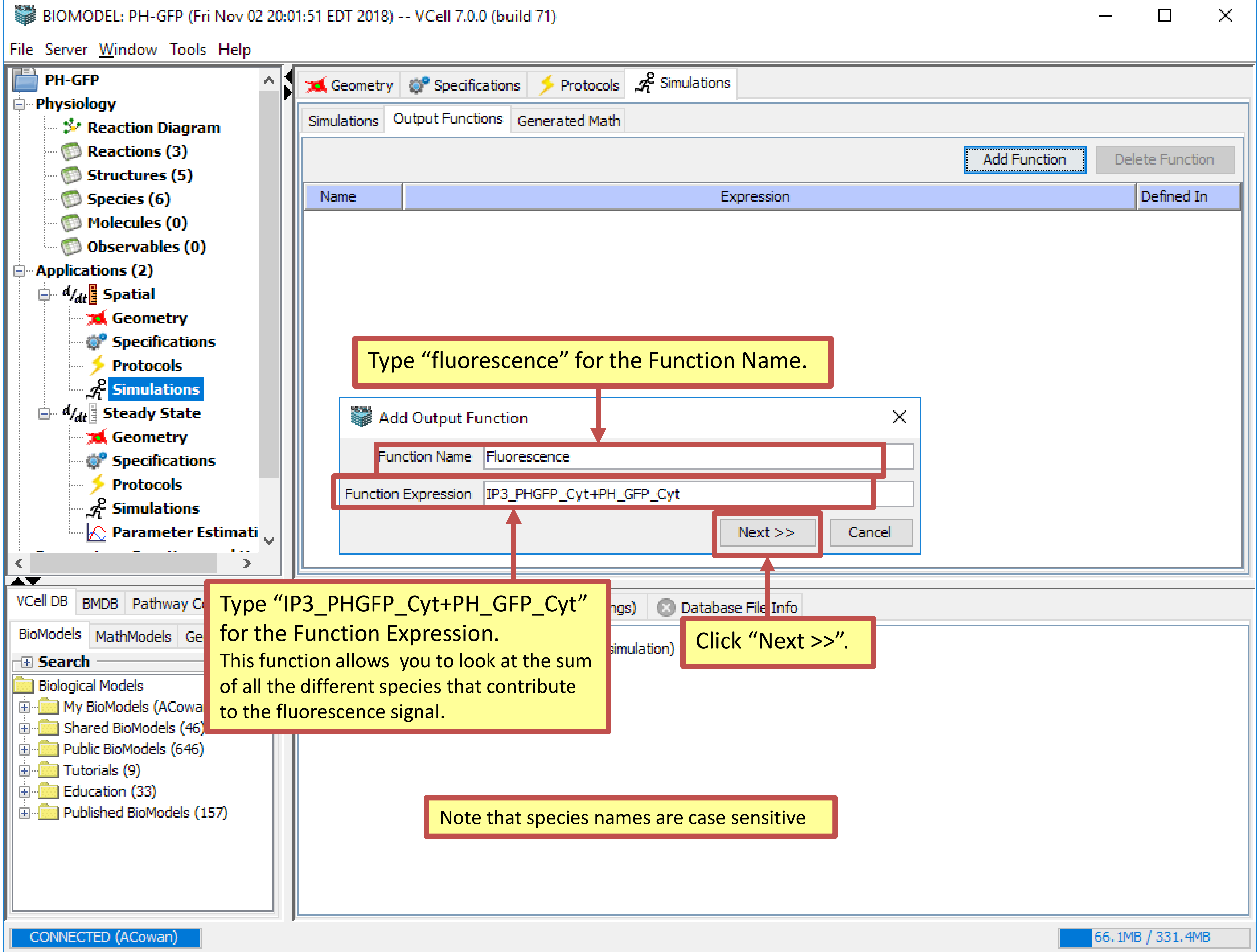
Database File Info
CONNECTED (ACowan)
99.6MB / 330.3MB

Click “Output Functions” > “Add Function”.

Select only one object (e.g. species, reaction, simulation) to view/edit properties.


BIOMODEL: PH-GFP (Fri Nov 02 20:01:51 EDT 2018) -- VCell 7.0.0 (build 71)
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CONNECTED (ACowan)
66.1MB / 331.4MB

Add Output Function

Function Name: Fluorescence

Function Expression: IP3_PHGFP_Cyt+PH_GFP_Cyt

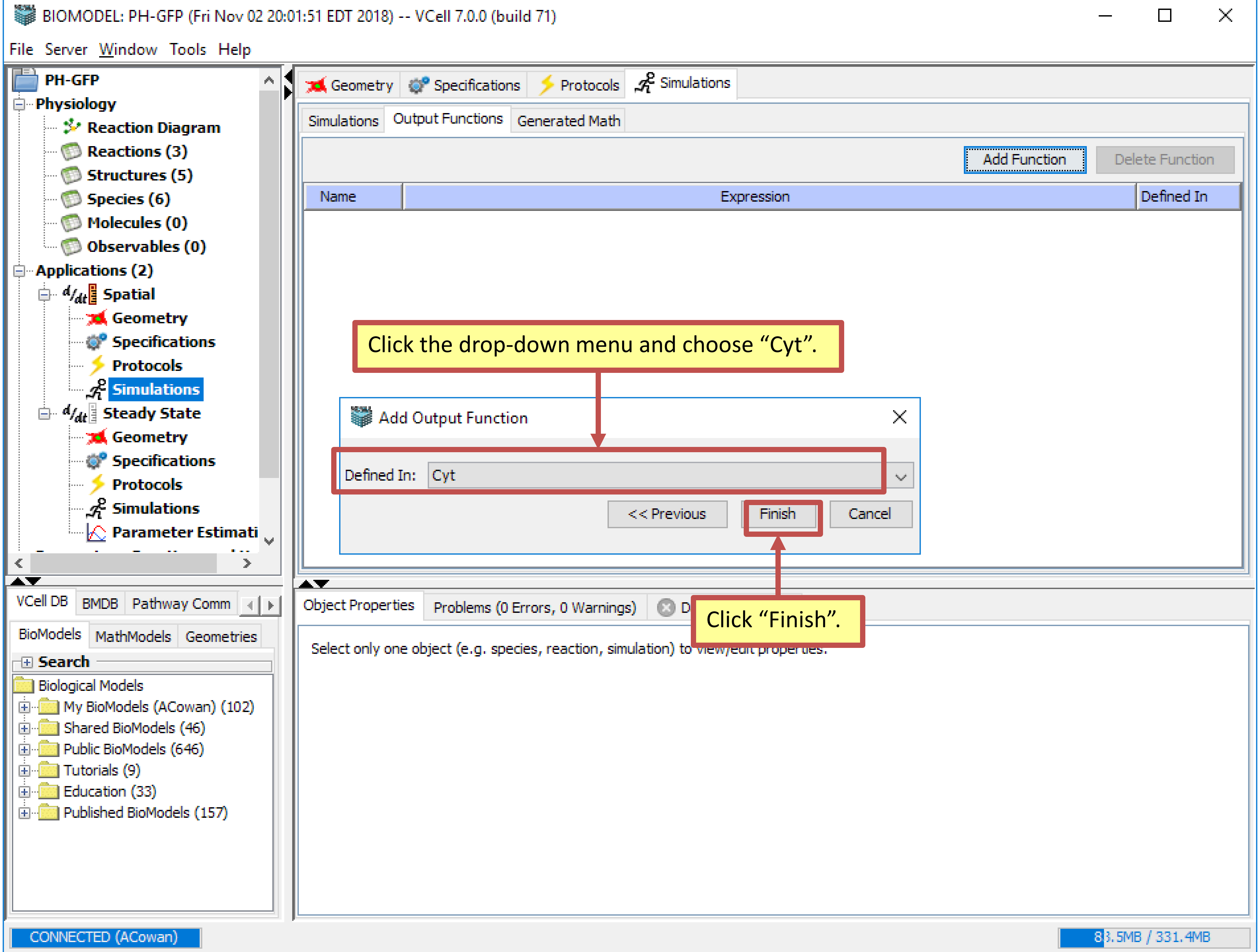
Next >>
Cancel

Type “fluorescence” for the Function Name.

Type “IP3_PHGFP_Cyt+PH_GFP_Cyt” for the Function Expression.
This function allows you to look at the sum of all the different species that contribute to the fluorescence signal.

Click “Next >>”.

Note that species names are case sensitive


BIOMODEL: PH-GFP (Fri Nov 02 20:01:51 EDT 2018) -- VCell 7.0.0 (build 71)
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<< Previous
Finish
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Select only one object (e.g. species, reaction, simulation) to view/edit properties.
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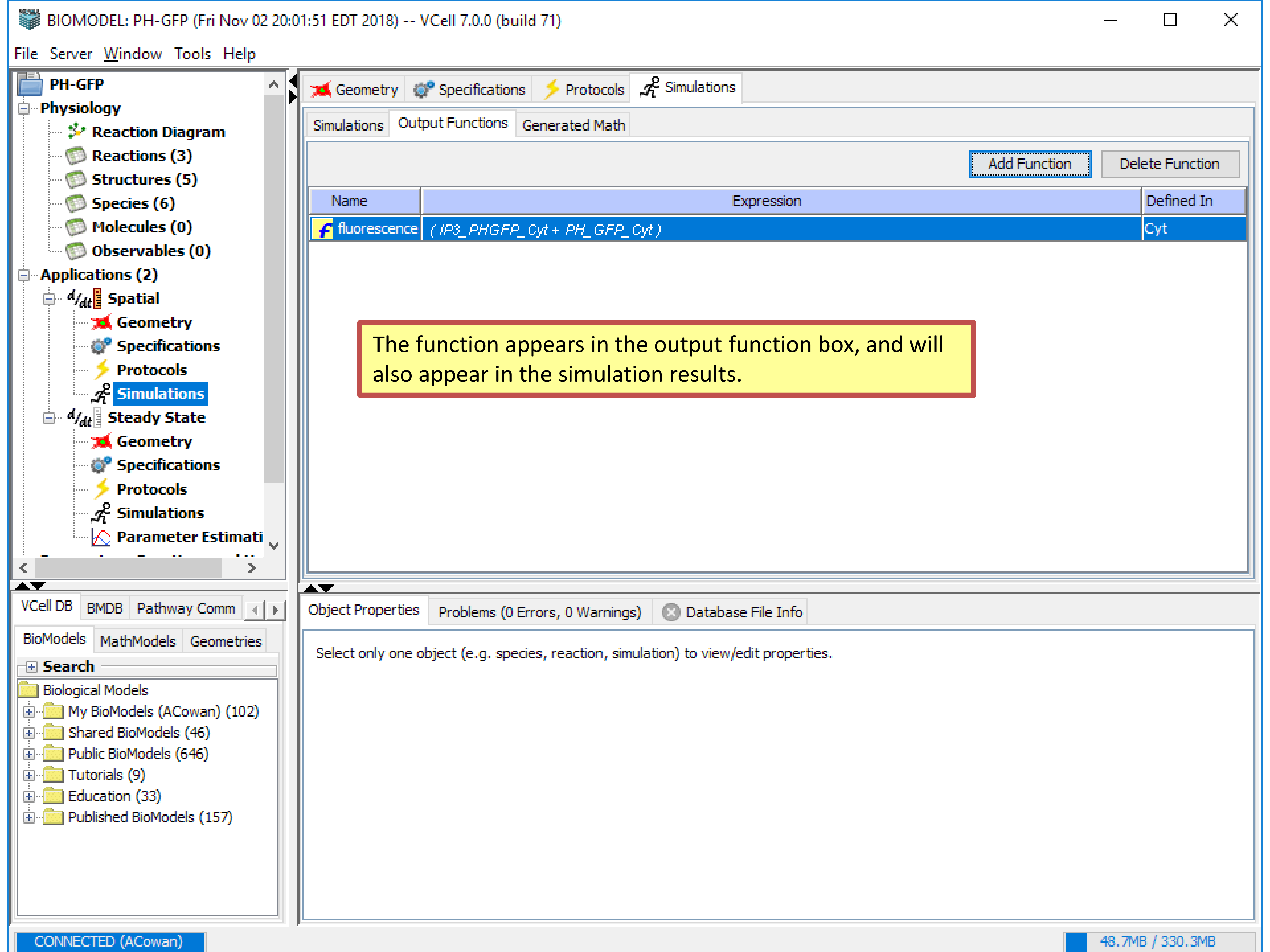
83.5MB / 331.4MB

Click the drop-down menu and choose “Cyt”.

Click “Finish”.


BIOMODEL: PH-GFP (Fri Nov 02 20:01:51 EDT 2018) -- VCell 7.0.0 (build 71)
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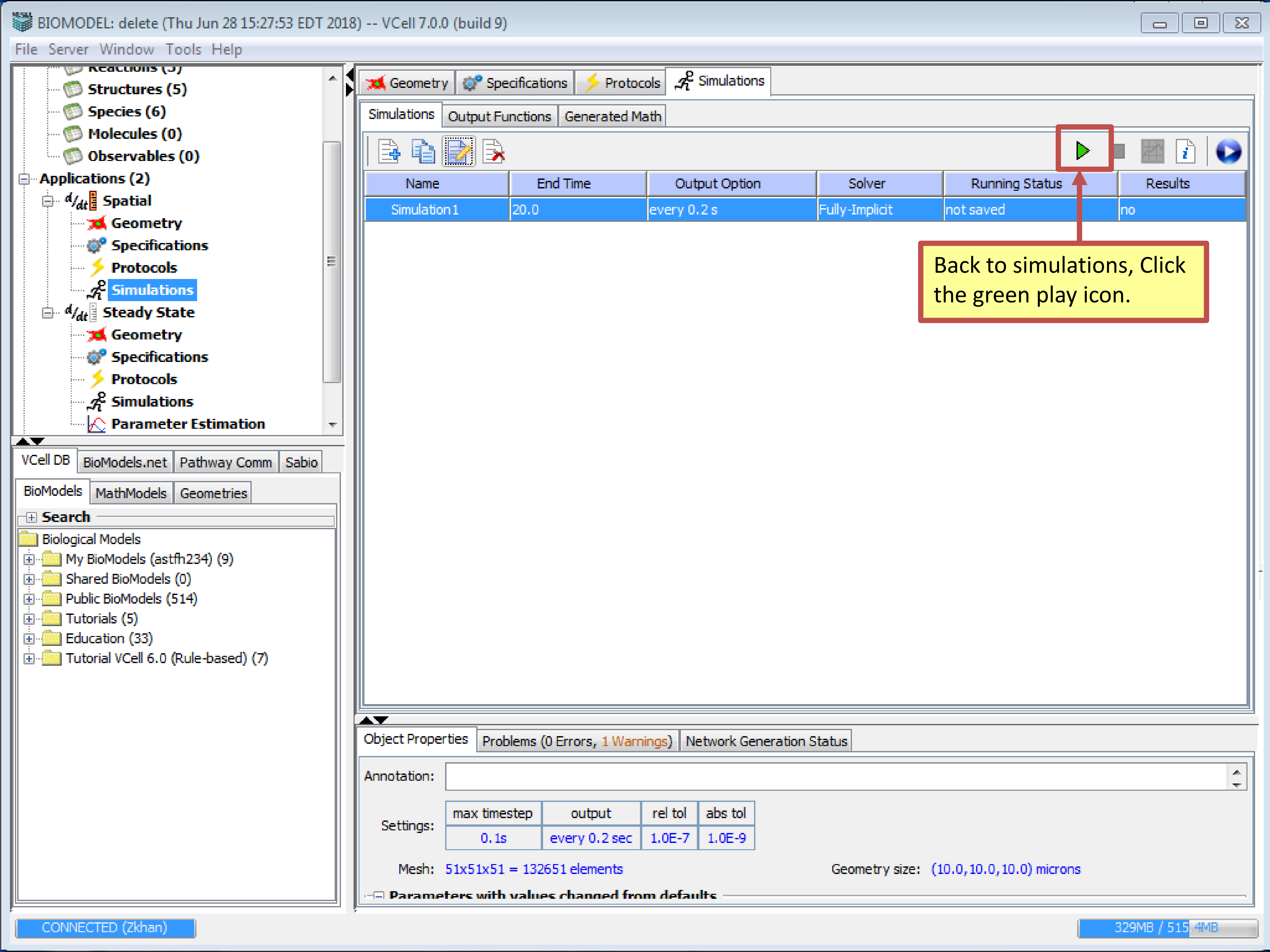
48.7MB / 330.3MB

Name	Expression	Defined In
fluorescence	(IP3_PHGFP_Cyt + PH_GFP_Cyt)	Cyt

The function appears in the output function box, and will also appear in the simulation results.

Select only one object (e.g. species, reaction, simulation) to view/edit properties.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CONNECTED (Zkhan)
329MB / 515.4MB

Back to simulations, Click the green play icon.

Name	End Time	Output Option	Solver	Running Status	Results
Simulation1	20.0	every 0.2 s	Fully-Implicit	not saved	no

Annotation:

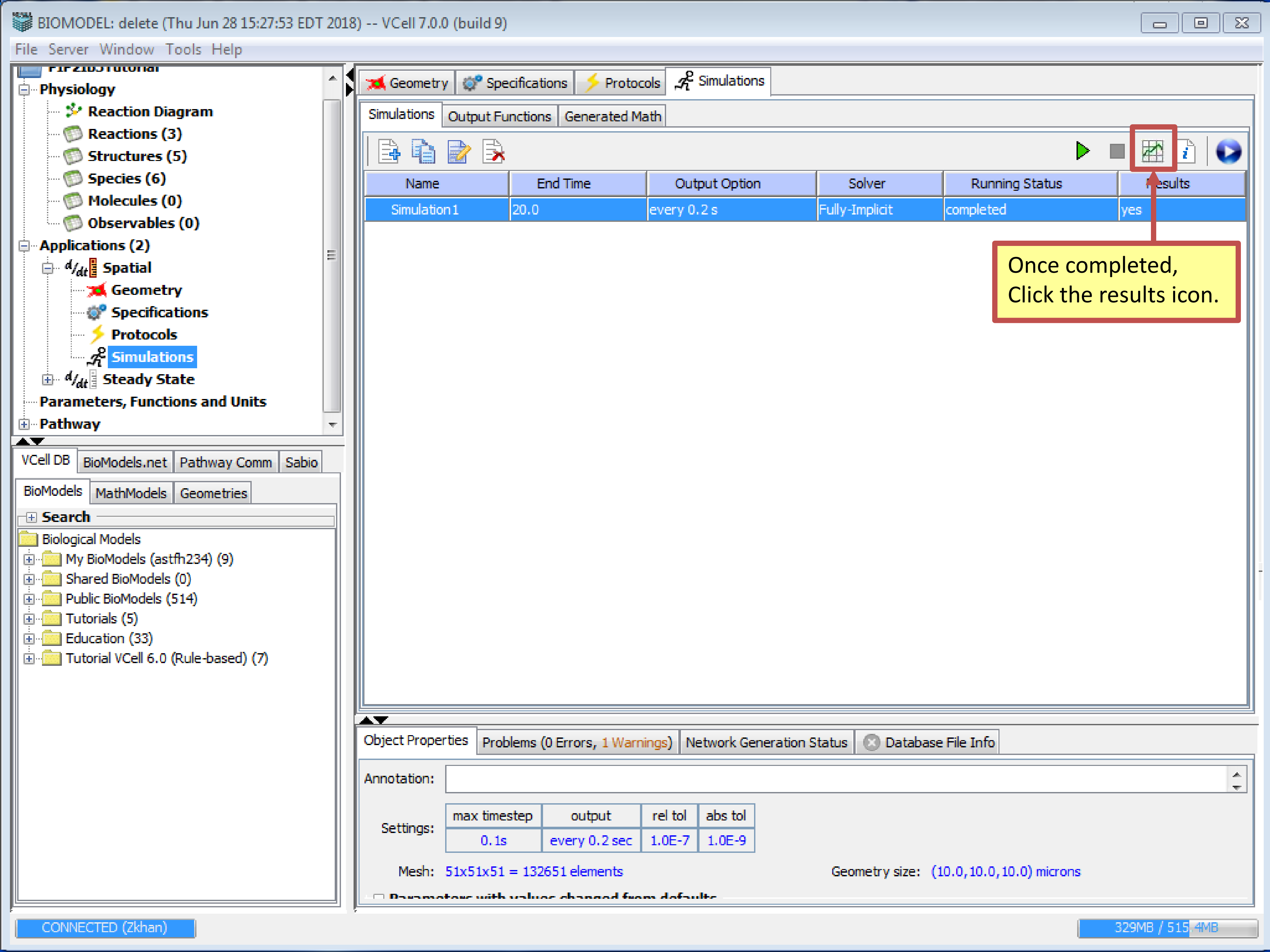
Settings:

max timestep	output	rel tol	abs tol
0.1s	every 0.2 sec	1.0E-7	1.0E-9

Mesh: 51x51x51 = 132651 elements

Geometry size: (10.0,10.0,10.0) microns

Parameters with values changed from defaults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CONNECTED (Zkhan)
329MB / 5154MB

Name	End Time	Output Option	Solver	Running Status	Results
Simulation1	20.0	every 0.2 s	Fully-Implicit	completed	yes

Once completed,
Click the results icon.

Annotation:

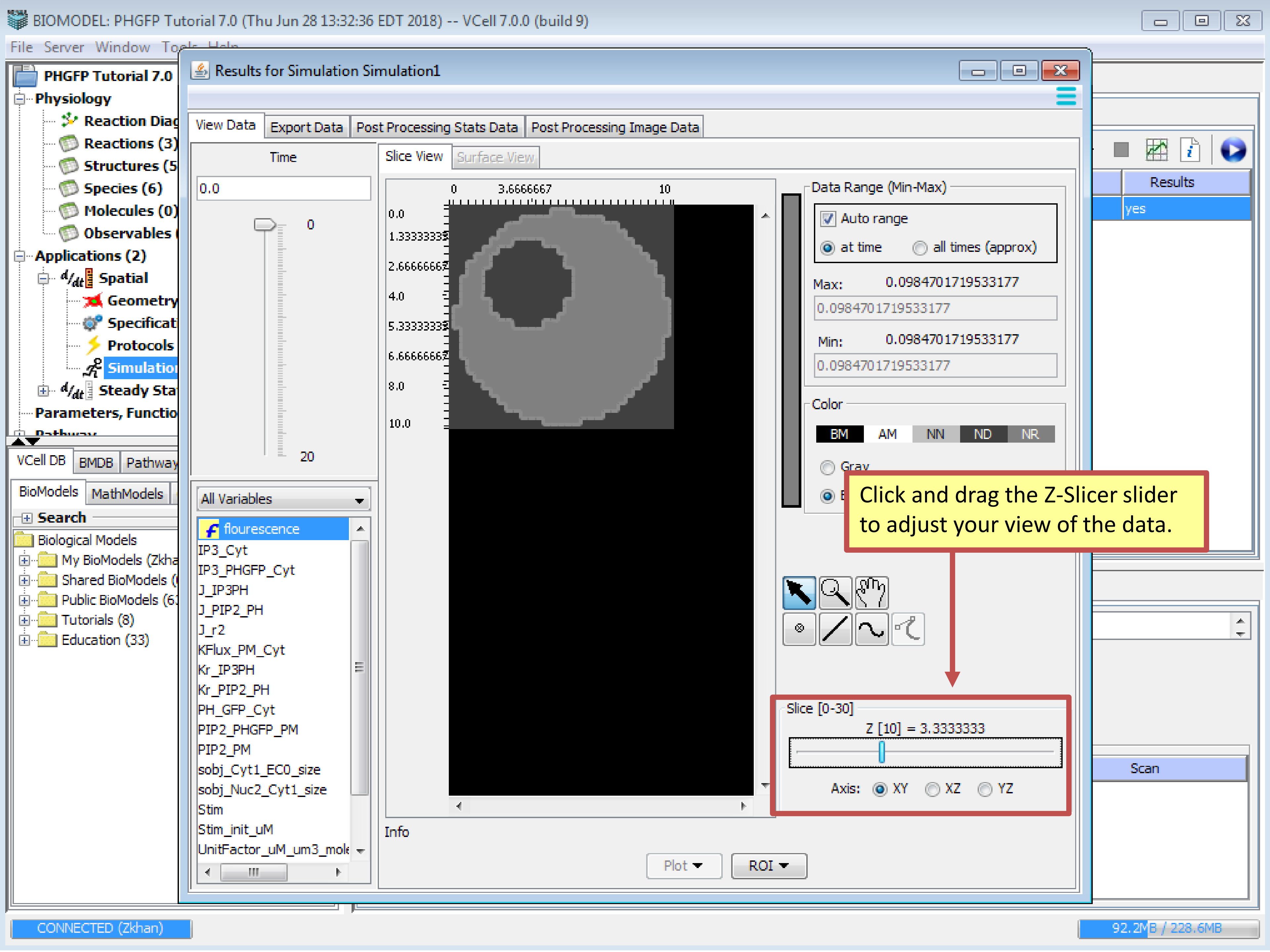
Settings:

max timestep	output	rel tol	abs tol
0.1s	every 0.2 sec	1.0E-7	1.0E-9

Mesh: 51x51x51 = 132651 elements

Geometry size: (10.0,10.0,10.0) microns

☐ Parameters with values changed from defaults


BIOMODEL: PHGFP Tutorial 7.0 (Thu Jun 28 13:32:36 EDT 2018) -- VCell 7.0.0 (build 9)
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KFlux_PM_Cyt
Kr_IP3PH
Kr_PIP2_PH
PH_GFP_Cyt
PIP2_PHGFP_PM
PIP2_PM
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Surface View
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Slice [0-30]
Results
yes
Scan
CONNECTED (Zkhan)
92.2MB / 228.6MB

☑ Auto range

● at time ○ all times (approx)

Max: 0.0984701719533177

0.0984701719533177

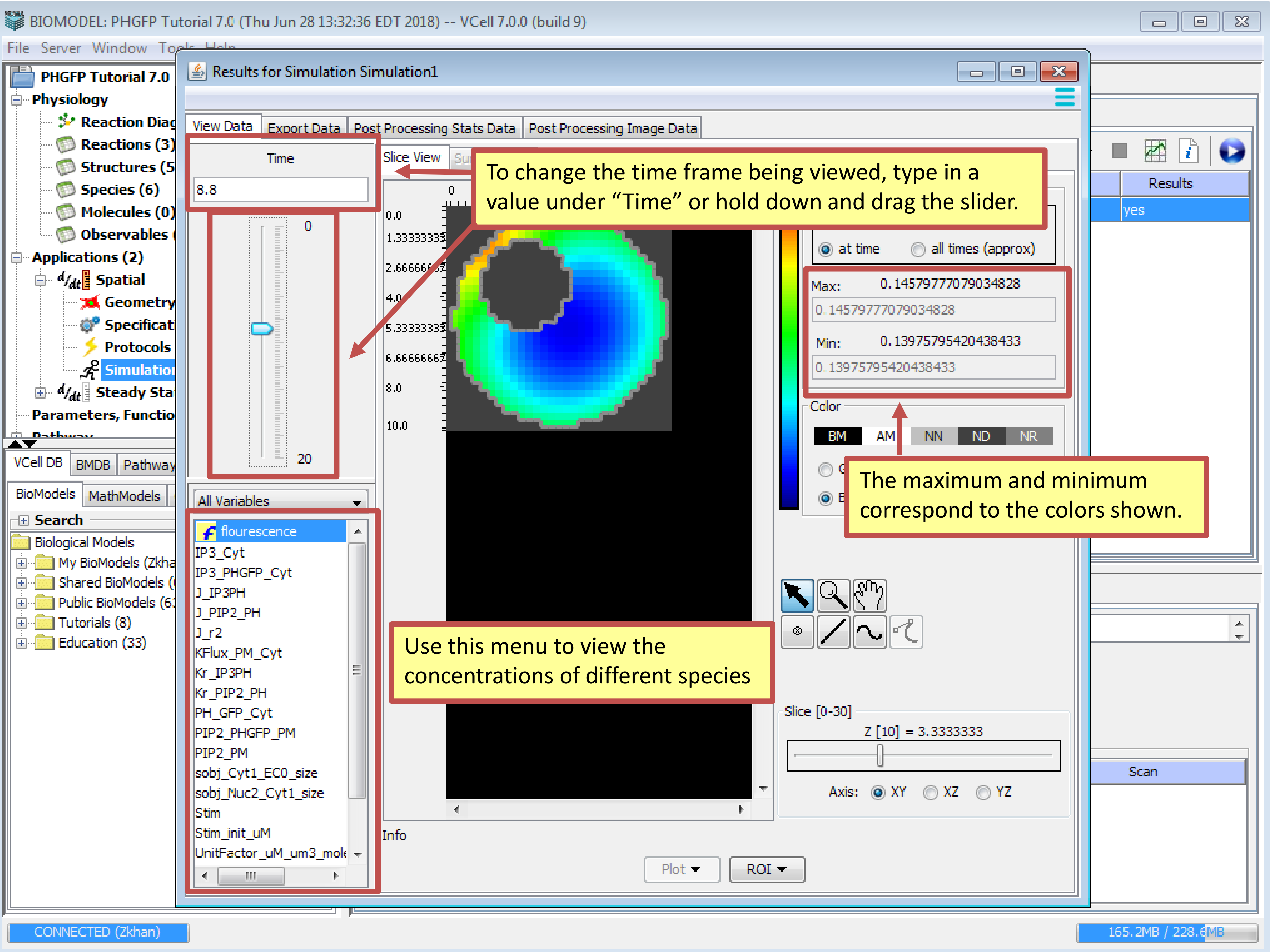
Min: 0.0984701719533177

0.0984701719533177

Z [10] = 3.3333333

Axis: ● XY ○ XZ ○ YZ

Click and drag the Z-Slicer slider to adjust your view of the data.



BIOMODEL: PHGFP Tutorial 7.0 (Thu Jun 28 13:32:36 EDT 2018) -- VCell 7.0.0 (build 9)

Results for Simulation Simulation1

Time: 8.8

● at time ○ all times (approx)

Max: 0.14579777079034828

Min: 0.13975795420438433

Slice [0-30]

Z [10] = 3.3333333

Axis: ● XY ○ XZ ○ YZ

To change the time frame being viewed, type in a value under “Time” or hold down and drag the slider.

The maximum and minimum correspond to the colors shown.

Use this menu to view the concentrations of different species

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Kr_PIP2_PH
PH_GFP_Cyt
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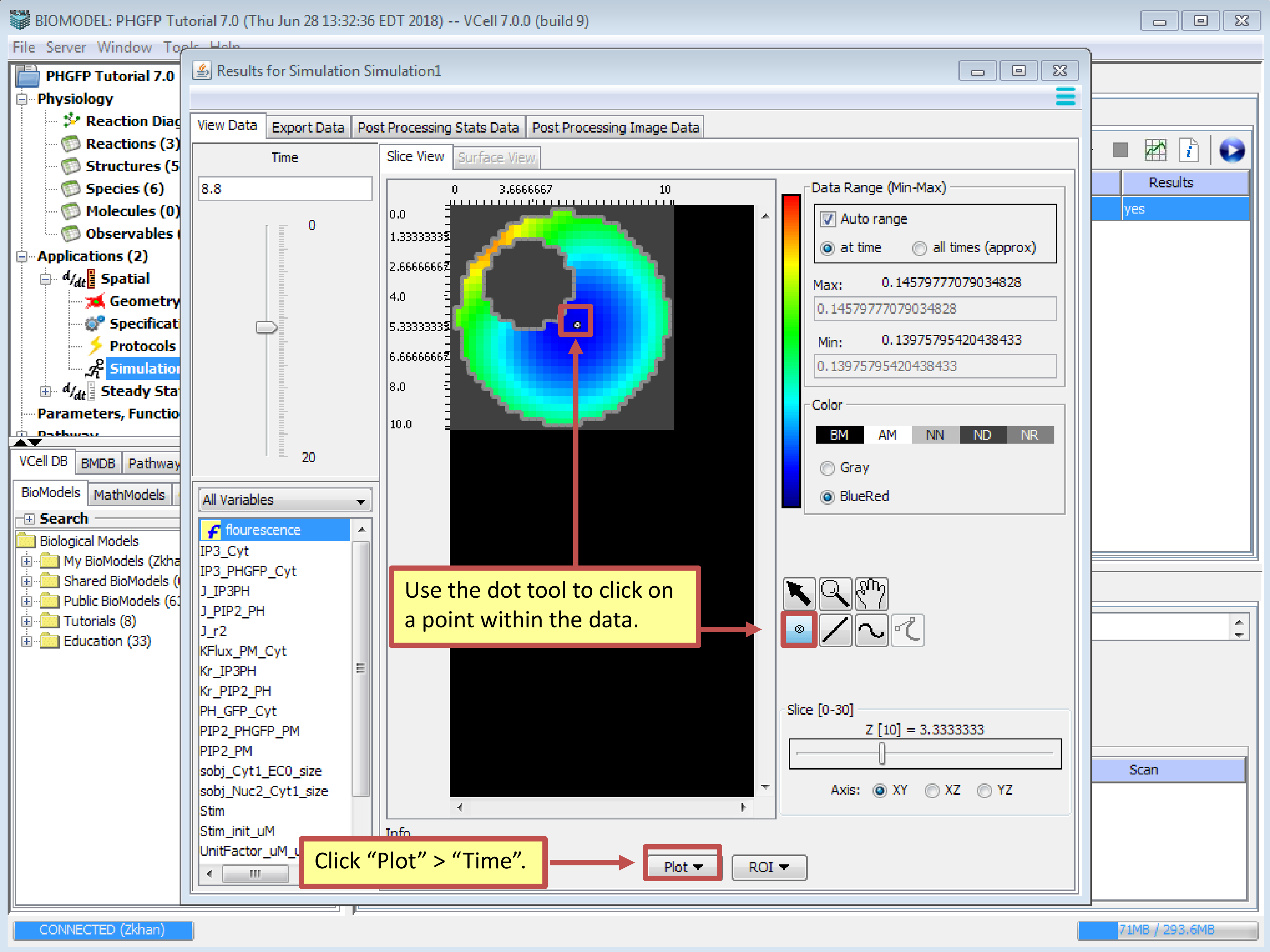
165.2MB / 228.6MB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J_PIP2_PH
J_r2
KFlux_PM_Cyt
Kr_IP3PH
Kr_PIP2_PH
PH_GFP_Cyt
PIP2_PHGFP_PM
PIP2_PM
sobj_Cyt1_EC0_size
sobj_Nuc2_Cyt1_size
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2.6666666
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Data Range (Min-Max)
Color
BM
AM
NN
ND
NR
Gray
Slice [0-30]
Info
Plot
ROI
Results
yes
Scan
CONNECTED (Zkhan)
71MB / 293.6MB

Time: 8.8

☑ Auto range

● at time ○ all times (approx)

Max: 0.14579777079034828

Min: 0.13975795420438433

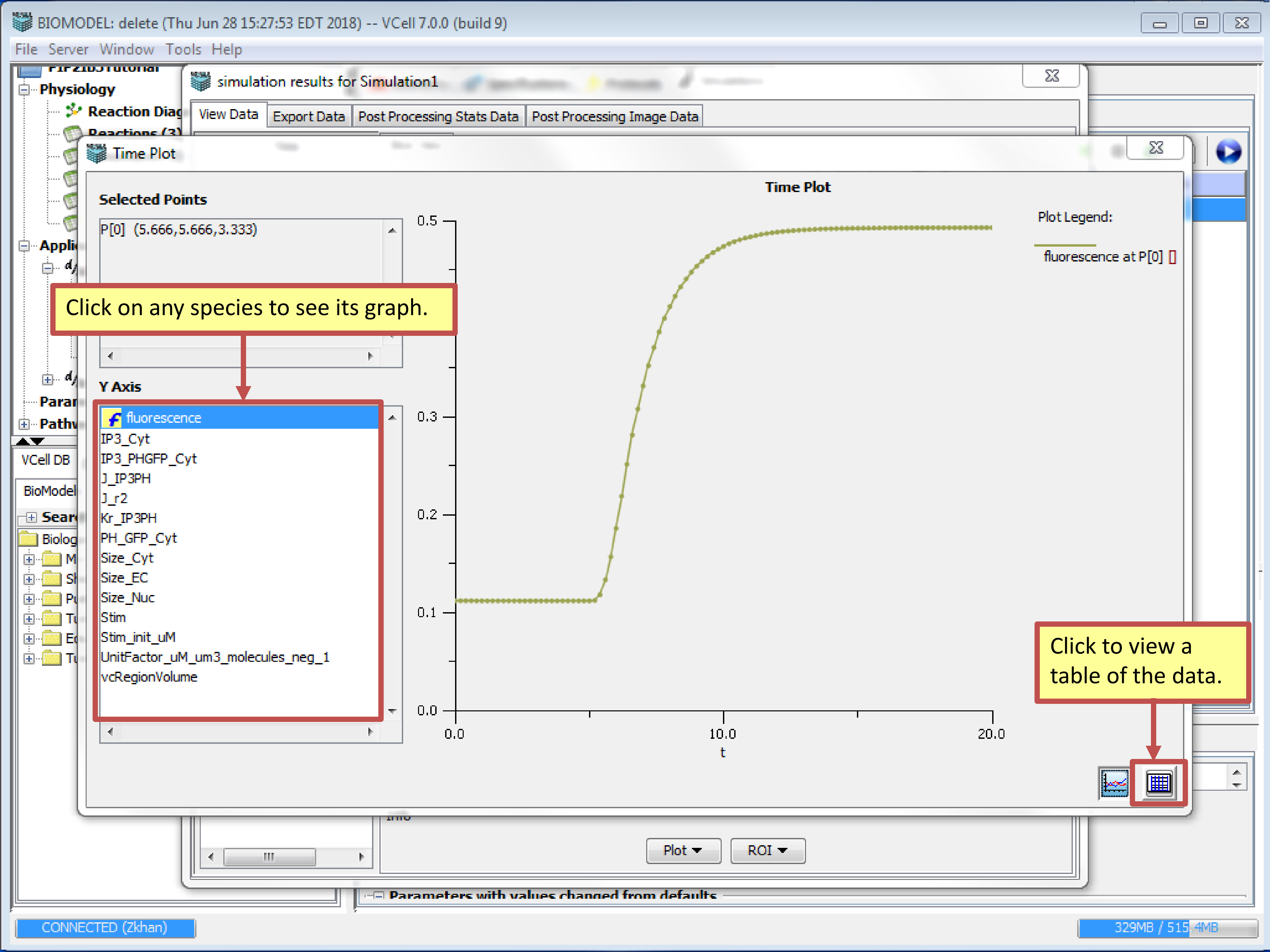
● BlueRed

Z [10] = 3.3333333

Axis: ● XY ○ XZ ○ YZ

Use the dot tool to click on a point within the data.

Click “Plot” > “Time”.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J_IP3PH
J_r2
Kr_IP3PH
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fluorescence at P[0]
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CONNECTED (Zkhan)
329MB / 515.4MB

Click on any species to see its graph.

Click to view a table of the data.

Acknowledgements

The following students worked on this tutorial:

Arundeep Singh (2018) – Sport and Medical Sciences Academy
Zaiba Khan (2018) – East Windsor High School

Their work was supported by the Department of Health Career Opportunity Programs; the Aetna Foundation, Connecticut Collegiate Awareness and Preparation Program, Office of Higher Education; Connecticut State Legislative Fund; The Hartford; William and Alice Mortensen Foundation; John and Valerie Rowe Health Professions Scholars Program; the University of Connecticut Foundation; the Friends of the Department of Health Career Opportunity Programs and UConn Health.