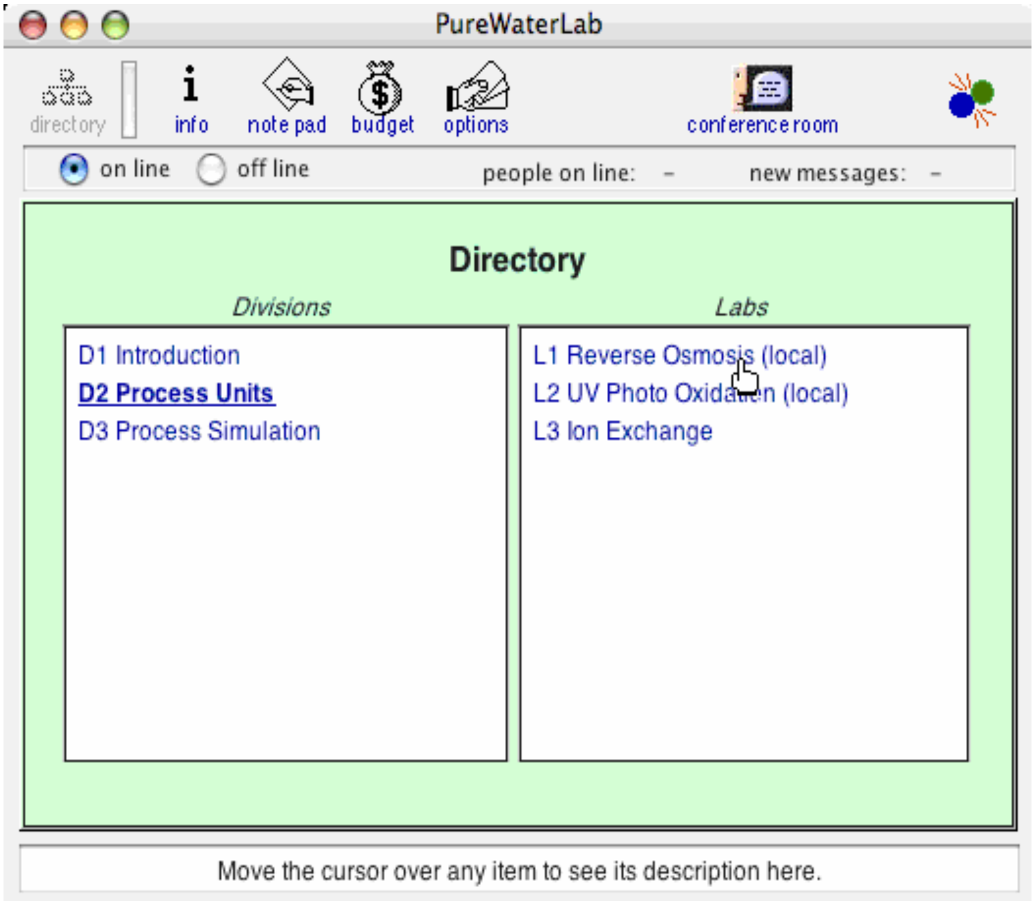
NSF Award DUE-0443044 Annual Report, April 2007

PureWaterLab - Conservation Education and Research Through Interactive Simulation

This attachment to the annual report presents screen shots from PureWaterLab. PureWaterLab is a desktop application that is integrated with the Internet and associated software on web servers. In the current web jargon, the Lab is a "rich Internet application." When on line, a student can access new modules and communicate in the Conference Room with other students. Updates to software are automatically downloaded and installed. When off line, the student can continue to work on the modules they previously accessed while on line.

Figure 1 is a screen shot of the Lab Directory, where modules are selected, when running under Mac OS X. The Lab modules are cross-platform and currently available on Windows and Mac. Operation under Linux will be available in the future.

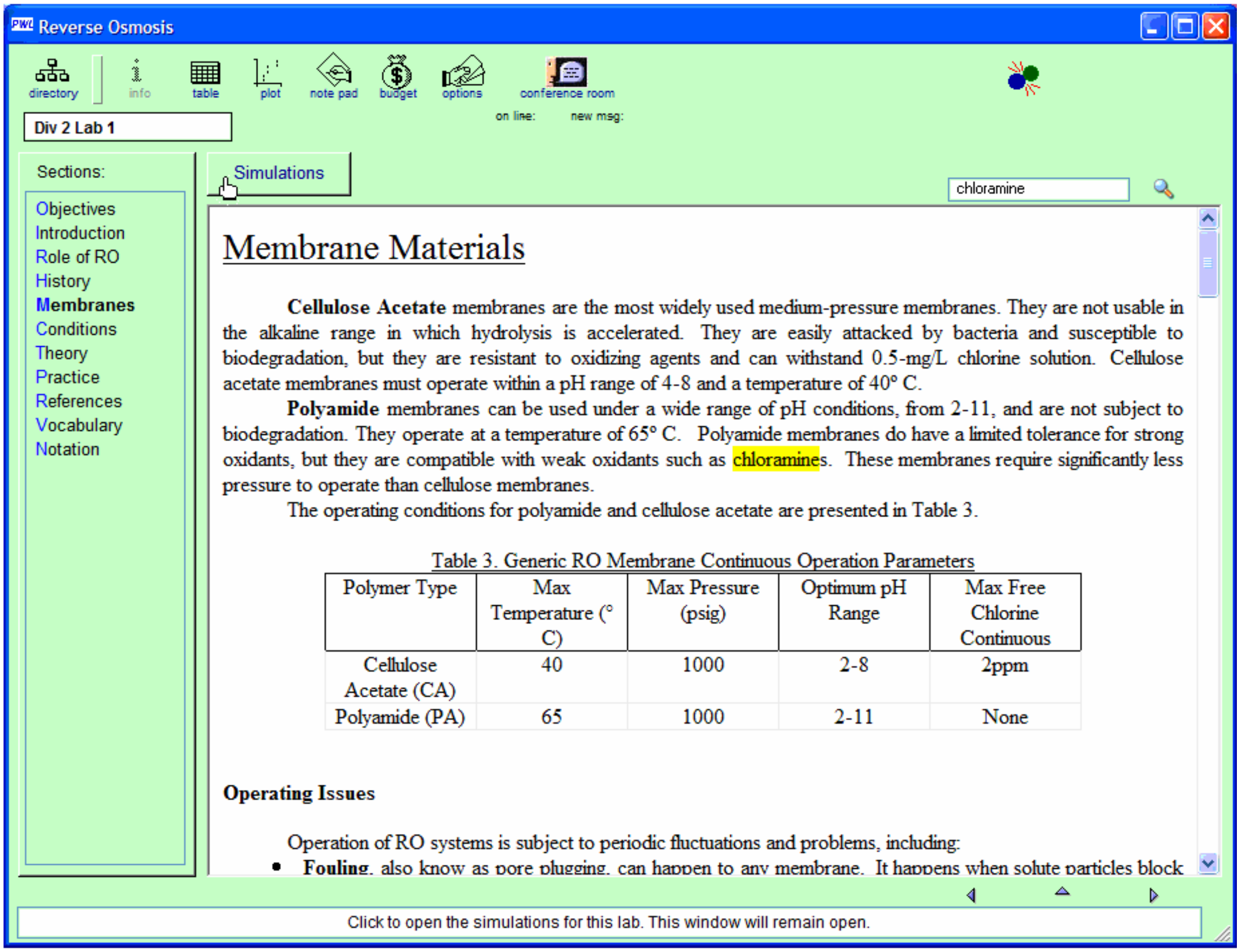


Move the cursor over any item to see its description here.

Figure 1

Figue 2 is a screen shot, when running under Windows XP, of the explanatory text of one of the modules. The software is written in a very high-level scripting language, Runtime Revolution, in order to allow us to develop the interactive simulations. To allow the collaborators at the University of Arizona flexibility in preparing the explanatory text, we use embedded web browser technology to display the text.

That is, the text that is shown below in Figure 2 is being displayed in the OS-default web browser, Internet Explorer in this case, as a web page that is embedded in the PureWaterLab software window. The embedded browser page is part of the parent window and moves and resizes with the parent window. Any web-page element that can be displayed by Internet Explorer, such as a Flash animation, can be displayed by PureWaterLab.



Membrane Materials

Cellulose Acetate membranes are the most widely used medium-pressure membranes. They are not usable in the alkaline range in which hydrolysis is accelerated. They are easily attacked by bacteria and susceptible to biodegradation, but they are resistant to oxidizing agents and can withstand 0.5-mg/L chlorine solution. Cellulose acetate membranes must operate within a pH range of 4-8 and a temperature of 40° C.

Polyamide membranes can be used under a wide range of pH conditions, from 2-11, and are not subject to biodegradation. They operate at a temperature of 65° C. Polyamide membranes do have a limited tolerance for strong oxidants, but they are compatible with weak oxidants such as chloramines. These membranes require significantly less pressure to operate than cellulose membranes.

The operating conditions for polyamide and cellulose acetate are presented in Table 3.

Table 3. Generic RO Membrane Continuous Operation Parameters

Polymer Type	Max Temperature (° C)	Max Pressure (psig)	Optimum pH Range	Max Free Chlorine Continuous
Cellulose Acetate (CA)	40	1000	2-8	2ppm
Polyamide (PA)	65	1000	2-11	None

Operating Issues

Operation of RO systems is subject to periodic fluctuations and problems, including:

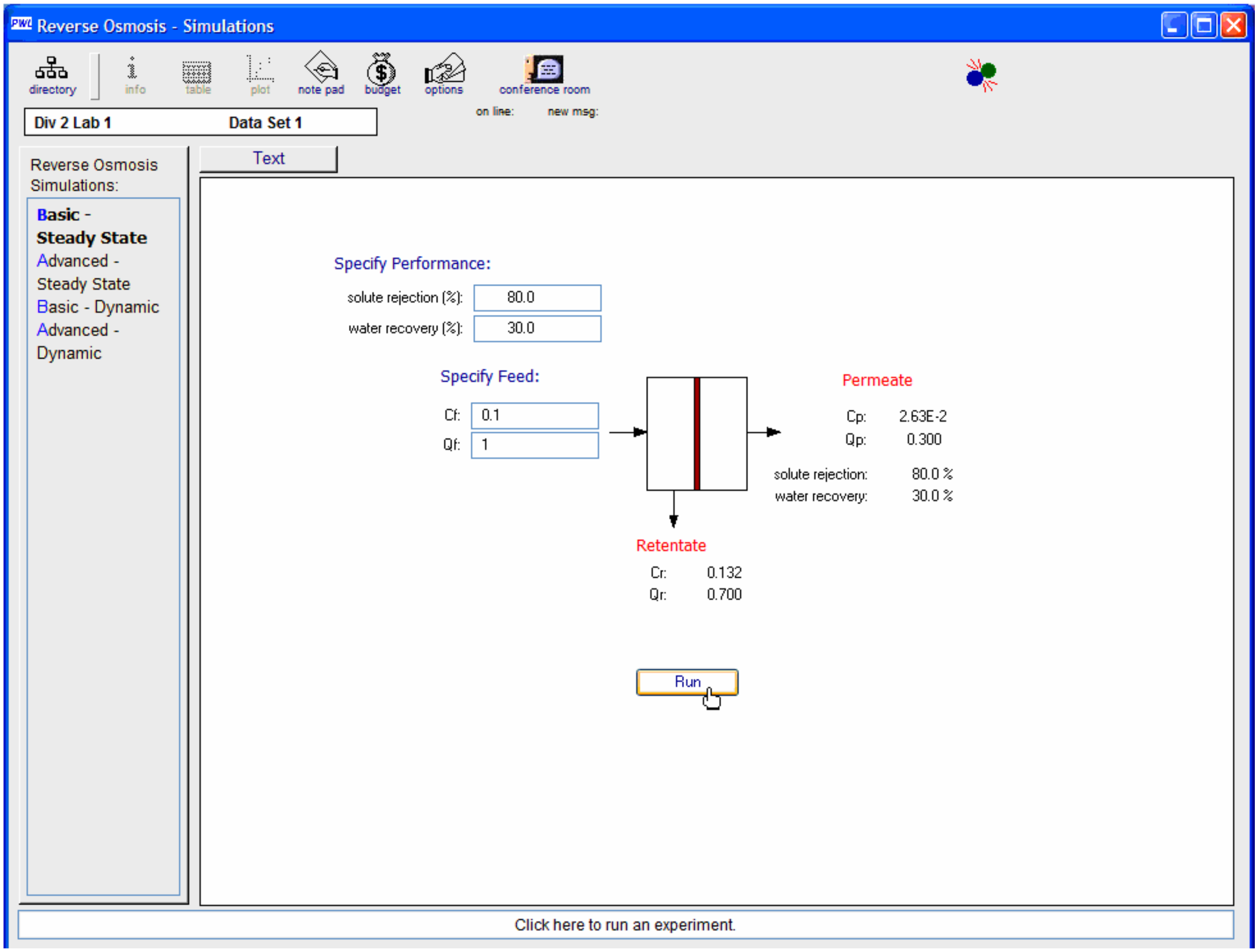
- **Fouling**, also know as pore plugging, can happen to any membrane. It happens when solute particles block

Click to open the simulations for this lab. This window will remain open.

Figure 2

Developers working on the project at the University of Arizona develop their web pages with standard web content creation software and publish files to the project server. Students using the Lab have files automatically updated when the desktop software detects new files on the server.

A button in the module text window links to the interactive simulations for the module. Figure 3 shows a basic steady-state simulation for this module on the reverse osmosis water purification process. In this module, both basic and advanced, and steady-state and dynamic-response simulations are provided. Students can select the level of detail they need.



Div 2 Lab 1 Data Set 1

Specify Performance:

solute rejection (%): 80.0

water recovery (%): 30.0

Specify Feed:

Cf: 0.1

Qf: 1

Permeate

Cp: 2.63E-2

Qp: 0.300

solute rejection: 80.0 %

water recovery: 30.0 %

Retentate

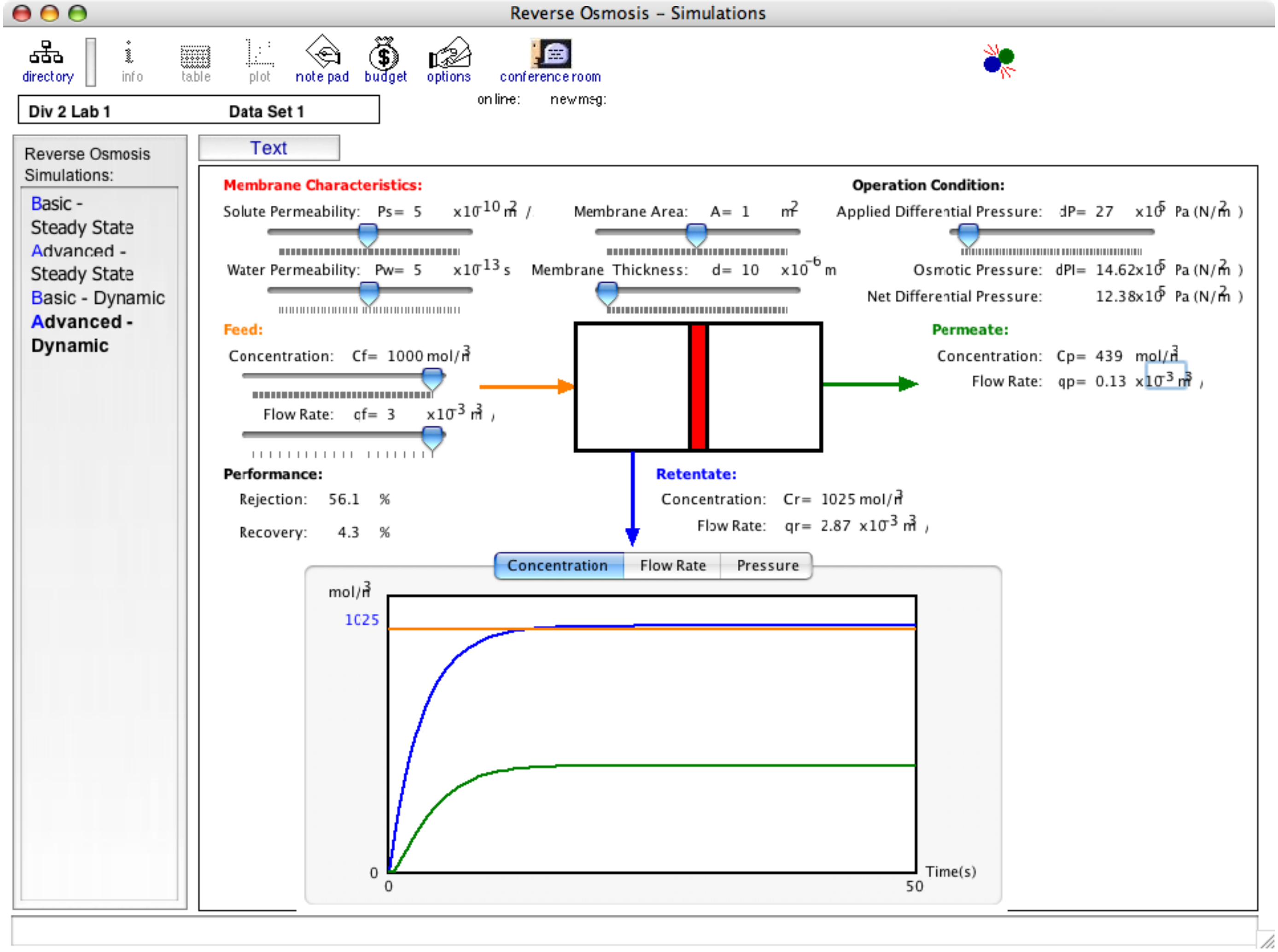
Cr: 0.132

Qr: 0.700

Click here to run an experiment.

Figure 3

Figure 4 shows a more advanced simulation of a reverse osmosis cell.



Div 2 Lab 1 Data Set 1

Reverse Osmosis Simulations:

- Basic - Steady State
- Advanced - Steady State
- Basic - Dynamic
- **Advanced - Dynamic**

Membrane Characteristics:

Solute Permeability: Ps= 5 x10^{10} m^2 /

Membrane Area: A= 1 m^2

Water Permeability: Pw= 5 x10^{13} s

Membrane Thickness: d= 10 x10^{-6} m

Operation Condition:

Applied Differential Pressure: dP= 27 x10^5 Pa (N/m^2)

Osmotic Pressure: dPI= 14.62x10^5 Pa (N/m^2)

Net Differential Pressure: 12.38x10^5 Pa (N/m^2)

Feed:

Concentration: Cf= 1000 mol/m^3

Flow Rate: qf= 3 x10^3 m^3 /

Permeate:

Concentration: Cp= 439 mol/m^3

Flow Rate: qp= 0.13 x10^3 m^3 /

Performance:

Rejection: 56.1 %

Recovery: 4.3 %

Retentate:

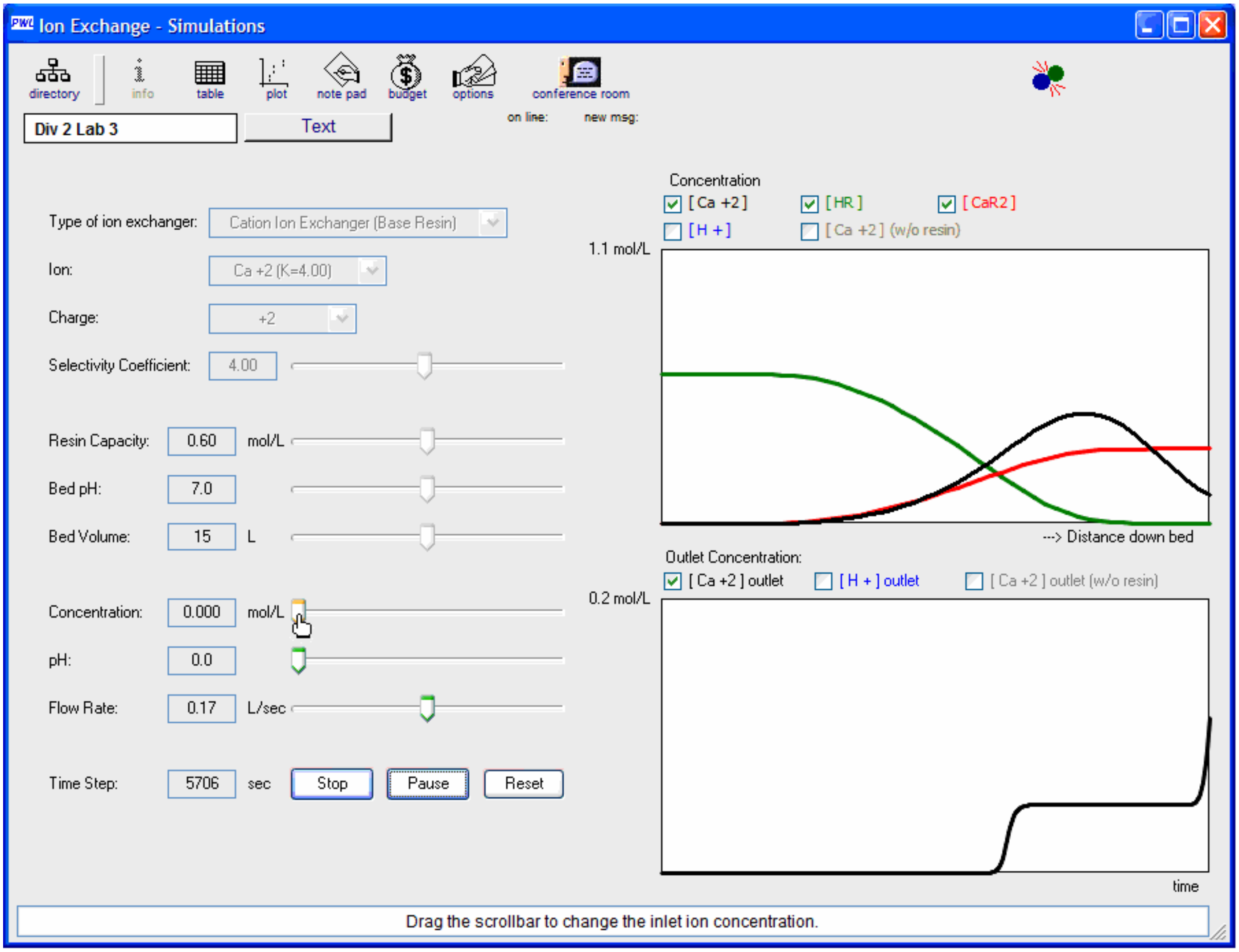
Concentration: Cr= 1025 mol/m^3

Flow Rate: qr= 2.87 x10^3 m^3 /

Figure 4

Figure 5 shows a simulation of an ion exchange bed which is used to remove contaminant ions from water. The top plot on the right shows concentrations of species vs. position within the bed (inlet on left, outlet on right). The bottom plot on the right shows concentrations of species vs. time in the stream flowing out of the bed. The simulation runs continuously and the plots update continuously to show the changing conditions. Check boxes above the plots allow species to be added or removed from the plots as the simulation is running. The student can vary operational parameters such as feed concentration and feed pH while the simulation is running. The simulation can be paused to study the results and then resumed.

This simulation provides a student with an unprecedented ability to see - and get a "feel" for - what is happening in this complex process that is far beyond what a list of equations and static plots can provide.



Div 2 Lab 3

Type of ion exchanger: Cation Ion Exchanger (Base Resin)

Ion: Ca +2 (K=4.00)

Charge: +2

Selectivity Coefficient: 4.00

Resin Capacity: 0.60 mol/L

Bed pH: 7.0

Bed Volume: 15 L

Concentration: 0.000 mol/L

pH: 0.0

Flow Rate: 0.17 L/sec

Time Step: 5706 sec

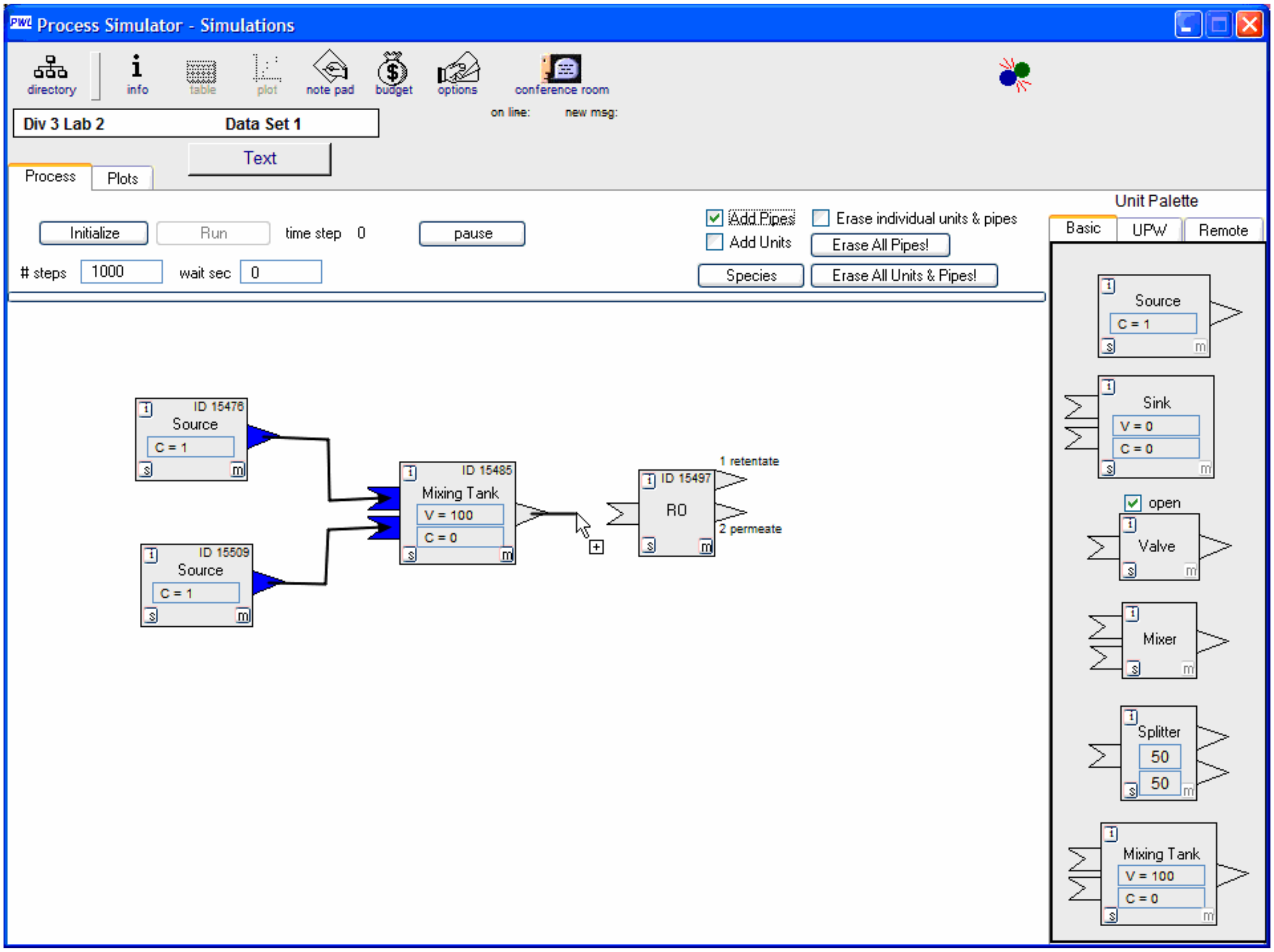
Concentration
☑ [Ca +2] ☑ [HR] ☑ [CaR2]
☐ [H +] ☐ [Ca +2] (w/o resin)

Outlet Concentration:
☑ [Ca +2] outlet ☐ [H +] outlet ☐ [Ca +2] outlet (w/o resin)

Drag the scrollbar to change the inlet ion concentration.

Figure 5

The module shown in Figures 2-5 concern an individual water purification process. The project also includes a water purification plant simulator, as shown in Figure 6. The plant simulator allows a student to design and experiment with their own water purification plant. Figure 6 shows a pipe being added to connect two units.



Div 3 Lab 2 Data Set 1

time step 0

steps 1000

wait sec 0

☑ Add Pipes

☐ Add Units

☐ Erase individual units & pipes

Source C = 1

Source C = 1

Mixing Tank V = 100 C = 0

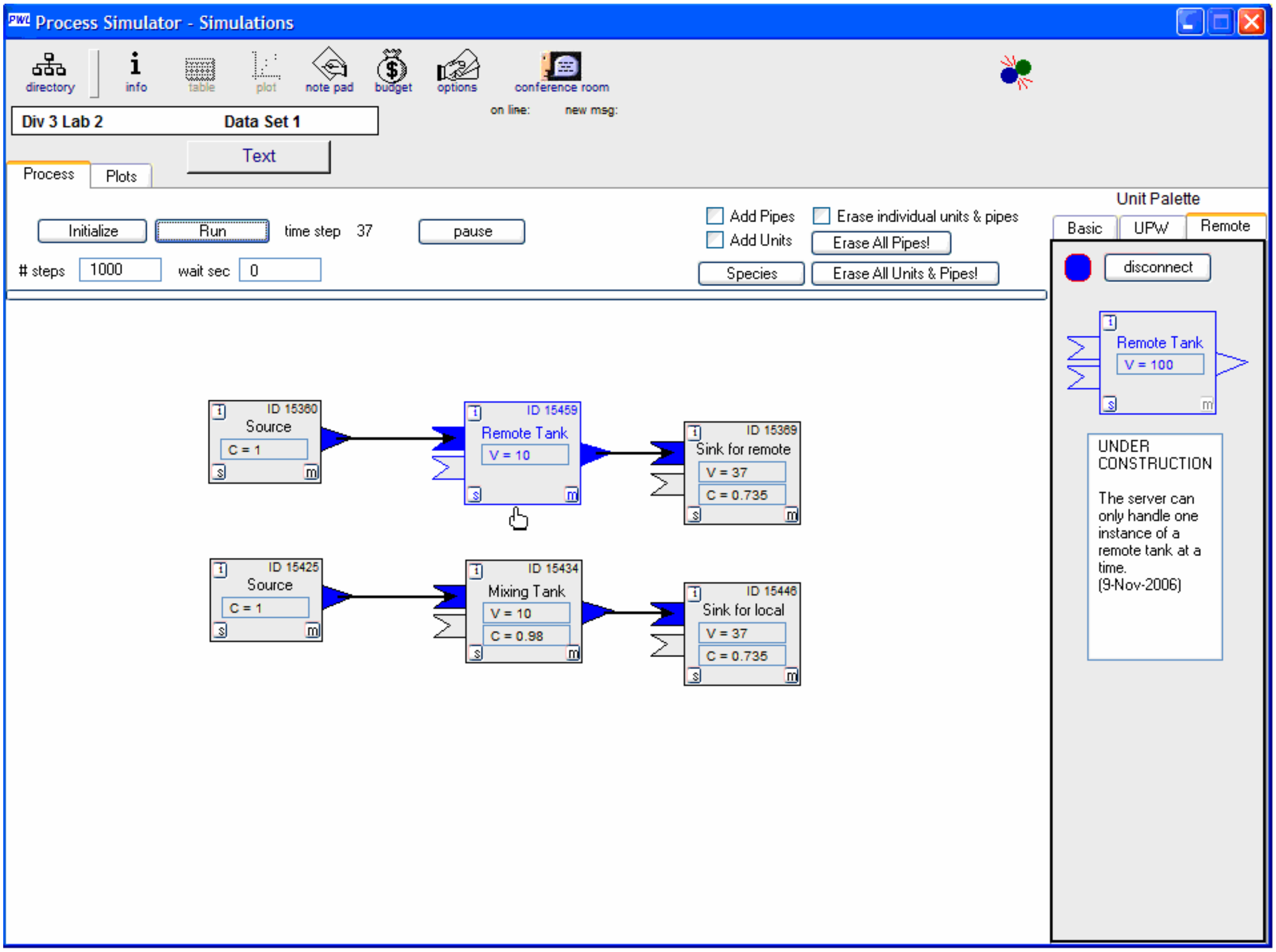
Palette: Source C = 1; Sink V = 0 C = 0; ☑ open Valve; Mixer; Splitter 50 50; Mixing Tank V = 100 C = 0

Figure 6

One of the most innovative aspects of the project is the development of the ability for student groups at different colleges to collaborate together in a plant simulation. This development of the distributed dynamic plant simulator is still at a relatively early stage.

Figure 7 shows two simple, parallel plants, each consisting of a water source, a mixing tank, and a sink. The mixing tank in the top process is a remote unit. That is, the computations which simulate the mixing tank are located on another computer. Messages, which represent water flow, are sent from the water source on the local computer over the Internet to the remote computer which hosts the remote mixing tank. Messages representing the output of the remote mixing tank then return to the local computer and "flow" to the next unit in the plant, the sink. The local-to-remote messages are written in extensible markup language (XML) text in order to provide hardware and software independence. The bottom plant in Figure 7 contains only local units and runs in parallel in order to check the remote simulation during development.

During the next year of the project, this concept will be extended to allow multiple student teams at different schools to collaborate in real-time on one plant simulation. Planning, communication, teamwork and complex system dynamics and behavior are skills and concepts that will be taught.



time step 37

steps 1000

wait sec 0

UNDER CONSTRUCTION

The server can only handle one instance of a remote tank at a time.
(9-Nov-2006)

Figure 7