**Year-1 Annual Report, 31 January, 2006**
**NSF DUE Award # 00443044**
**PureWaterLab - Conservation Education and Research Through Interactive Simulation**
**submitted by**

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## INTRODUCTION

This is the first annual report for this continuing grant. The report describes accomplishments during the first nine months of the project.

The mission of PureWaterLab is to teach students the importance of water conservation in manufacturing and to teach them how to use water efficiently through conservation, purification, and recycle. Water supply is a critical issue nationally, especially in the Western U.S. which is in the eighth year of an exceptional drought period. The project web site can be found at www.PureWaterLab.org.

PureWaterLab is a full-development project which continues the work of a prototype project. The prototype project, ReactorLab (NSF DUE-0125076), is continuing to be used and developed. It is available on the web at www.ReactorLab.net and on the CD included with the major textbook in the field of chemical reaction engineering (Fogler, 2006). ReactorLab is available in English, Spanish and Portuguese, and has been used in dozens of universities by thousands of students around the world.

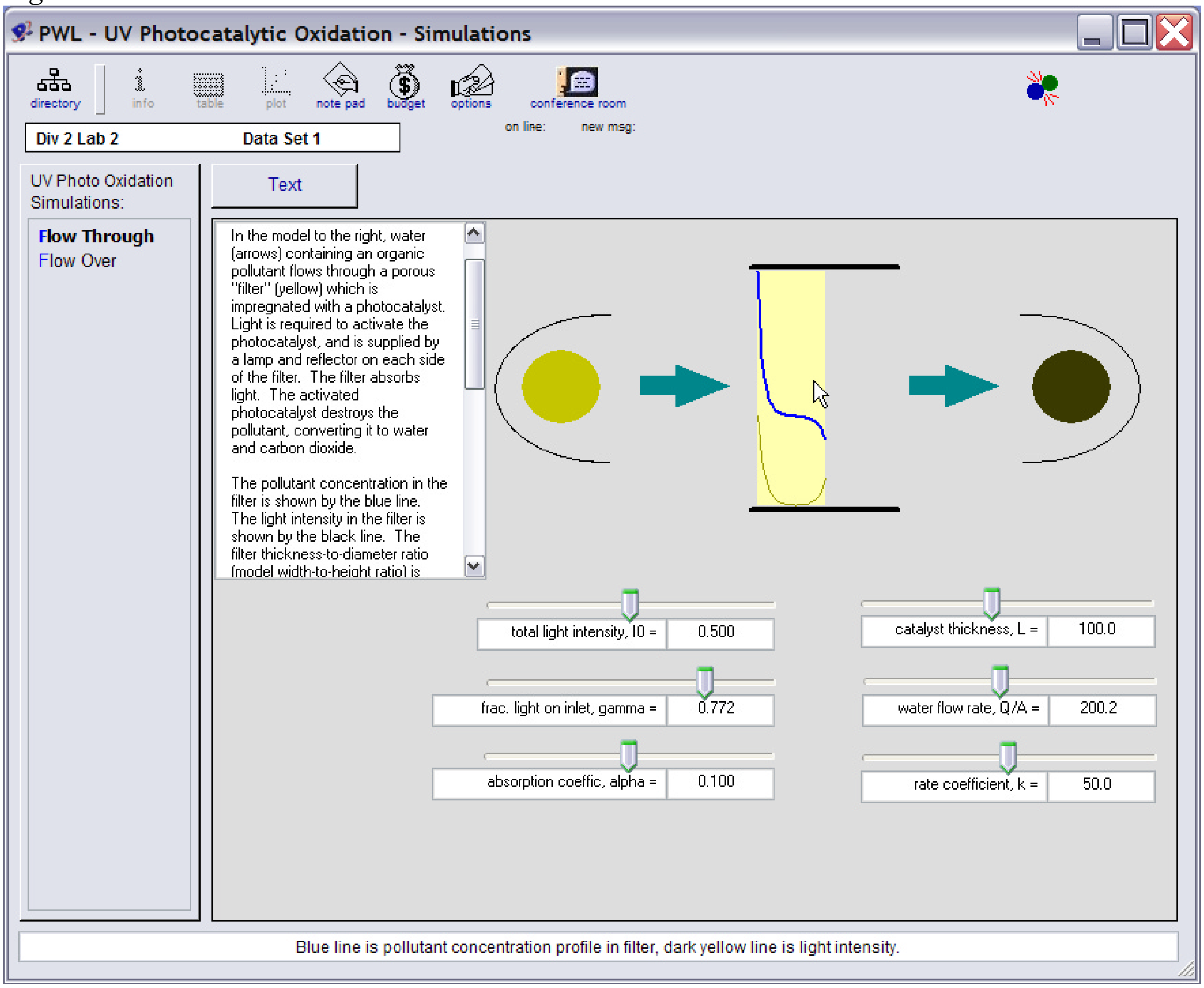
The prototype project developed an approach to teaching and learning about complex engineering systems that forms the basis for the current project. Through these continuing efforts the models and educational paradigms first implemented for ReactorLab continue to be developed and expanded.

They key feature of this approach is the use of interactive simulations of engineering systems. The simulations are based on detailed mathematical models and exhibit a wide range of output in response to inputs which are manipulated by the student. This richness of response is in contrast to movies or animations which, although valuable in context, play the same way each time.

Figure 1 shows one of the interactive simulations in PureWaterLab. Shown is one possible configuration of a photocatalytic unit which is used to destroy organic pollutants in water. The system is a permeable layer through which water flows (represented by the arrows). The layer is not to scale and is much thinner than shown. UV lamps on the inlet and outlet sides of the layer illuminate and activate photocatalyst which is distributed throughout the layer. The activated photocatalyst oxidizes organic pollutants in the water. The concentration of pollutant within the layer is represented by the blue curve and the light intensity is represented by the dark yellow curve.

A student can vary the input parameters with the slider controls and see the concentration and light intensity curves update as the sliders are dragged, as well as see the arrows change thickness as the water flow changes and see the lamp intensities change. By doing so, the student is taking an active part in the learning process and can get a real "feel" for the system as well as gain fundamental understanding of how the different processes interact in the system to produce its behavior.

*Figure 1. Interactive simulation.*




An important feature of the interactive simulations in PureWaterLab is that the graphical plots and animations shown are not approximate graphical representations but are driven by detailed mathematical models of the systems which are computed as the student changes input values. The same is true of numerical results presented, and the mathematical models are explained to students in the explanatory text and graphics associated with the simulation.

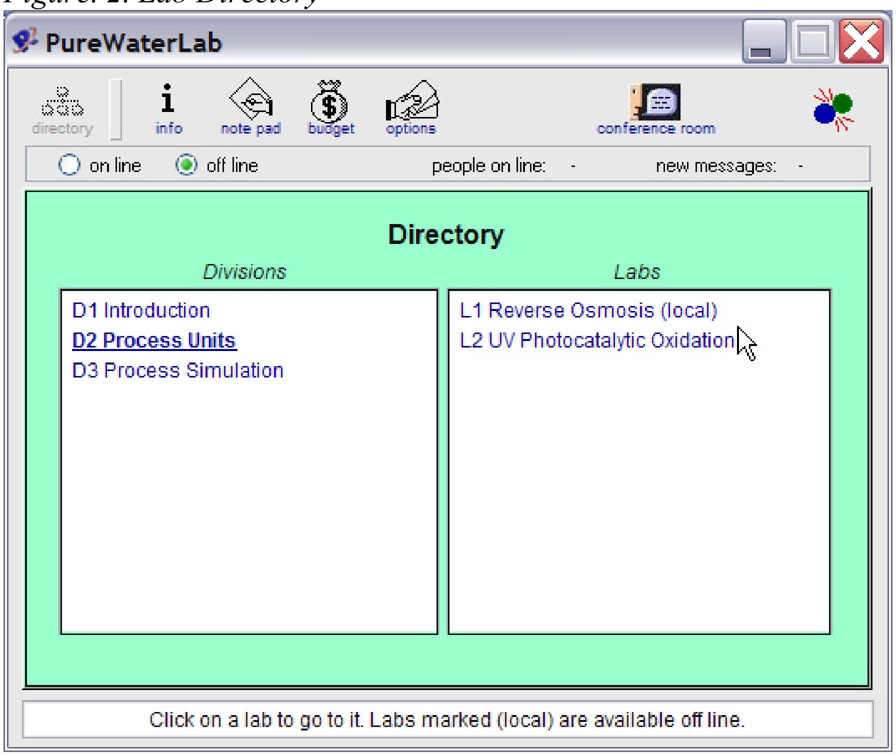
An educational unit that only displayed the mathematical model and a static image of one set of curves would not actively involve the student in the educational experience nor be as instructive as the interactive simulations that are being developed for PureWaterLab.

Note in the figure above that information about the object under the mouse cursor is displayed to the user in the information field at the bottom of each window. This allows a student to use the software with little or no prior training.

The software approach is based on a desktop application with full Internet connectivity. The use of a dedicated desktop application as opposed to a generic web browser allows a more consistent user interface and full access to disk functions and printing.

The PureWaterLab desktop application can be connected to the project web server when desired by the student. When connected or "on line," the student can access individual educational modules on the server. When accessed, a module copy is also written to the local disk and can also be used "off line" when no web connection is available. This off-line use is not available when a generic web browser is used. Figure 2 shows the Lab Directory with a model available off line denoted as "(local)."

*Figure. 2. Lab Directory*




When connected or "on line", the software automatically updates its files when new versions are available. With few exceptions, files are written in a cross-platform, very high-level "scripting" language. Both of these features provides for easy update of students using different types of computers to the current version of the software.

The exceptions to the cross-platform script files occur when platform-specific, compiled executable files (e.g., Windows .dll files) are required to obtain the desired speed of execution. The software can detect the platform on which it is running and download only the executable files for that platform.

In the sections below, we will list the personnel involved in the project, the Year 1 task objectives and the accomplishments achieved during the first nine months, and further explanation of some of the features of PureWaterLab.

## PERSONNEL

The project is jointly performed by researchers at the University of California, San Diego (UCSD) and The University of Arizona (UA). The work at UA is subcontracted.

UCSD is working on software development of the overall lab and for the interactive simulations. In addition, UCSD is developing the mathematical models that drive the simulations.

Arizona is working on the text and graphic parts of the modules as well as assessment.

The PI is Professor Richard Herz of UCSD. During the summer of 2005, an undergraduate student was hired and worked on development of models for the reverse osmosis and UV photocatalytic oxidation units. A graduate student was hired as a Research Assistant at the start of the 2005-2006 academic year to work on model development. The student is currently an MS student but is anticipated to continue working on the project as a PhD student with dissertation research associated with the Lab's process simulator. Another MS student worked on the project during Fall Quarter 2005 as an unpaid student doing independent research, and worked on development of models of ion exchange beds.

The principal at UA is Professor Greg Ogden. Professor Ogden was previously on the chemistry and environmental science faculty of Pima Community College in Tucson, AZ. The project will utilize his association with the community college to help assess use of the software in that environment. Two undergraduate students are employed by the project and are working on developing text and graphical explanations for the modules. The UA team also includes a professional educational assessment expert, Vivian Harte.

## YEAR 1 TASKS AND ACCOMPLISHMENTS IN FIRST 9 MONTHS

<u>Task 1. The PureWaterLab web site will be established, and prototype's software framework will become the core of PureWaterLab."</u>

The project's web site was established at www.PureWaterLab.org. Distributions of the Lab for Windows and Macintosh operating systems are provided for download. In the future, a distribution for Linux on Intel PC will be provided.

The software framework of the prototype, ReactorLab, is used as the starting point for development of PureWaterLab. As PureWaterLab is developed, improvements and new features are added to the software framework in a way that they are fully compatible with ReactorLab. Currently, we are maintaining separate copies of the software and distribution sites so as not to inadvertently corrupt ReactorLab. In the future, we plan to merge the software and distribution sites for the two Labs as we build a set of educational packages which are maintained and distributed under a common software and distribution framework.

Task 2. "Design decisions will be made about the structure of the new complete educational modules and about how to handle display text in order to facilitate translation."

The key features of the project are interactive simulations driven by detailed mathematical models. The prototype is being extended to provide textual (plus associated graphics) explanations of the simulated processes in order to provide complete educational modules.

Our main design challenge is to decide how best to display explanatory text and simulations to the student.

In the current version of the lab modules, we provide the text in one window and the simulations in a separate window. This approach allows each component to be displayed in a full window and also allows the student to easily switch between windows and also allows the student to resize and juxtapose the two windows on the same screen. Figure 3 shows a page in the reverse osmosis module with the mouse cursor ready to click on the "Simulations" button in order to open the simulation window.

*Figure 3. Text explanation window in module with button linking to associated simulations.*

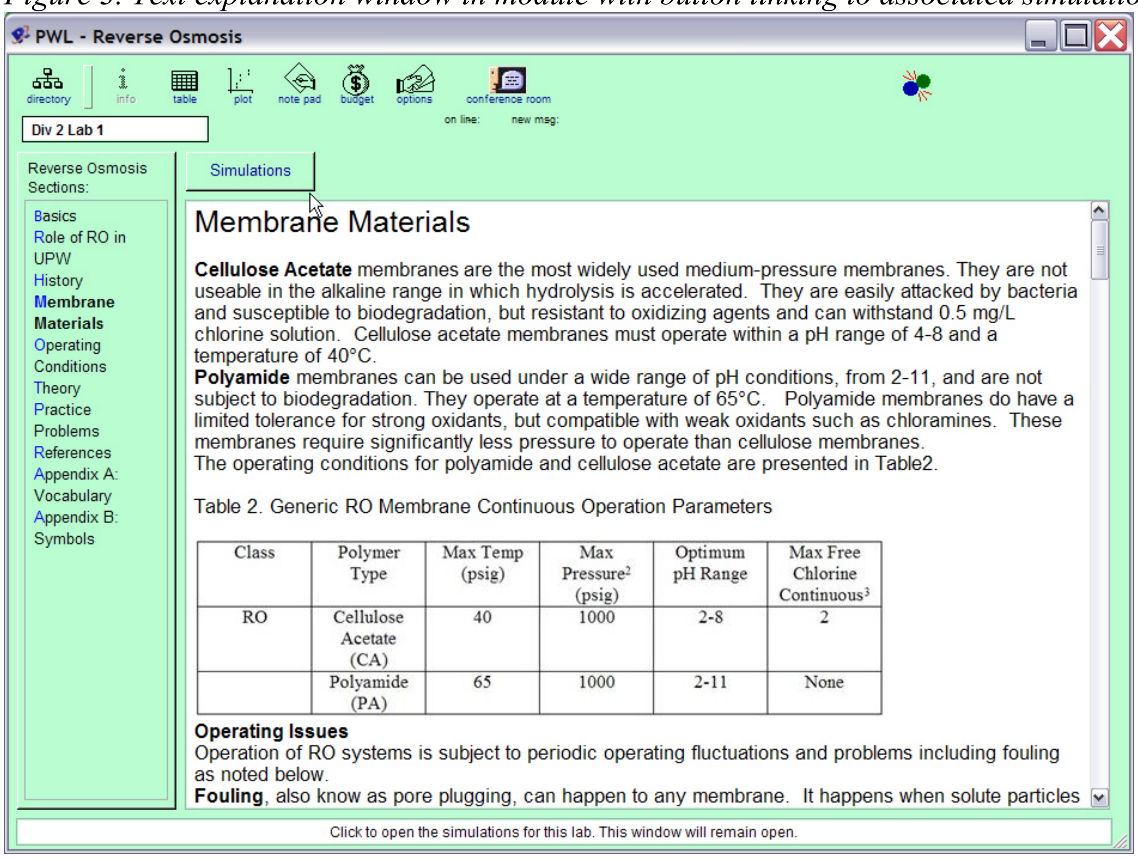
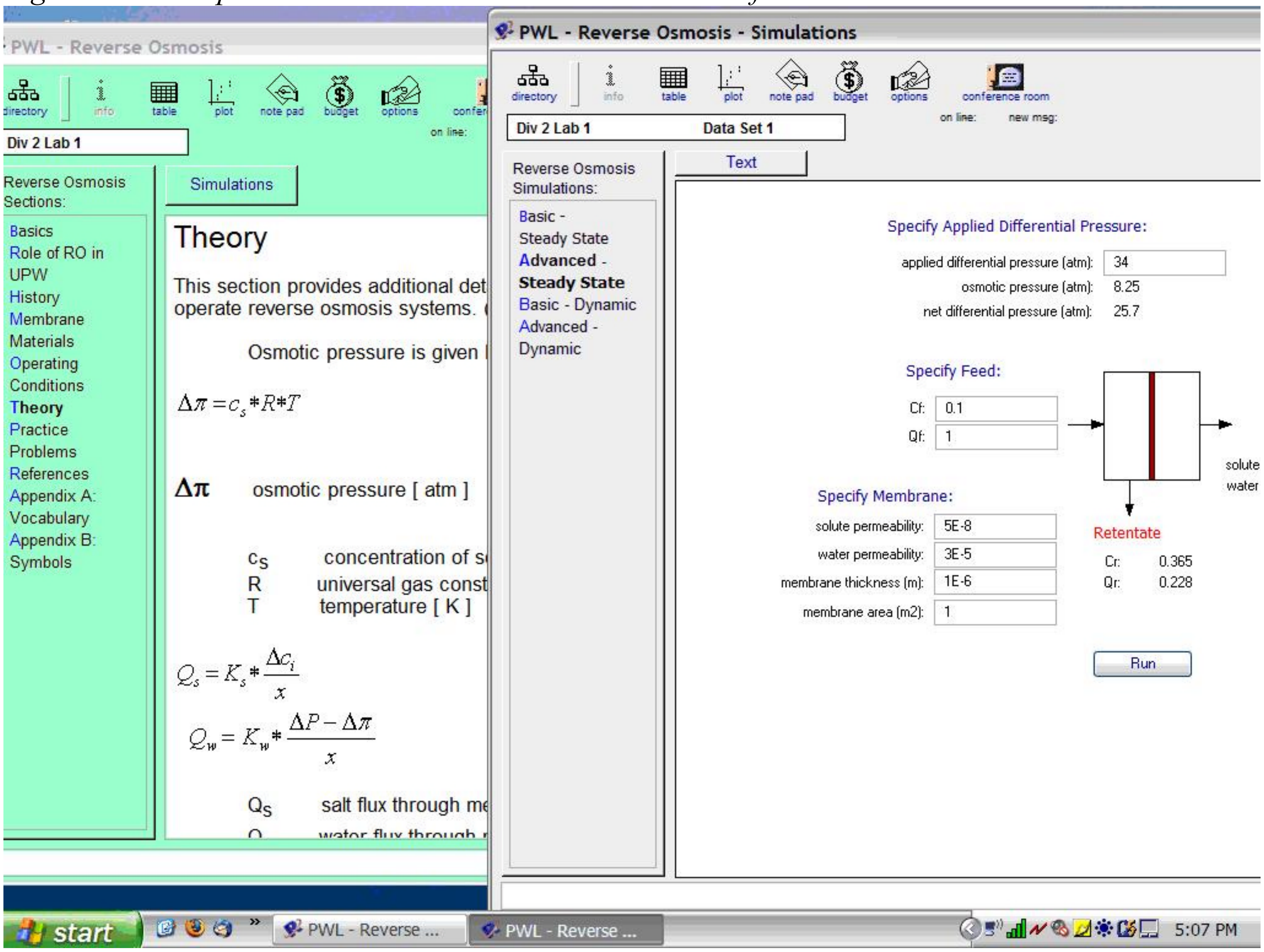


Figure 4 shows the text explanation window and the simulation window both open on the screen.

*Figure 4. Text explanation window and simulation window for reverse osmosis module.*




An alternative is to display only one window which is divided into a section for the text and a section for the simulation. This alternative will be tried and considered. It was not chosen first because it is more difficult to divide one window in a way that allows the text, graphics and simulation sections to all be used easily.

The display text in ReactorLab has been translated from English into Spanish and Portuguese by volunteers. One objective of the current project is to provide a way to facilitate translation and switching between different languages. In the first nine months of the project we have experimented with one way to do this. We haven't yet made a final decision, and are developing the lab modules solely in English for the time being.

<u>Task 3. "Educational modules for water use in the semiconductor manufacturing industry will be designed, constructed, tested and evaluated."</u>

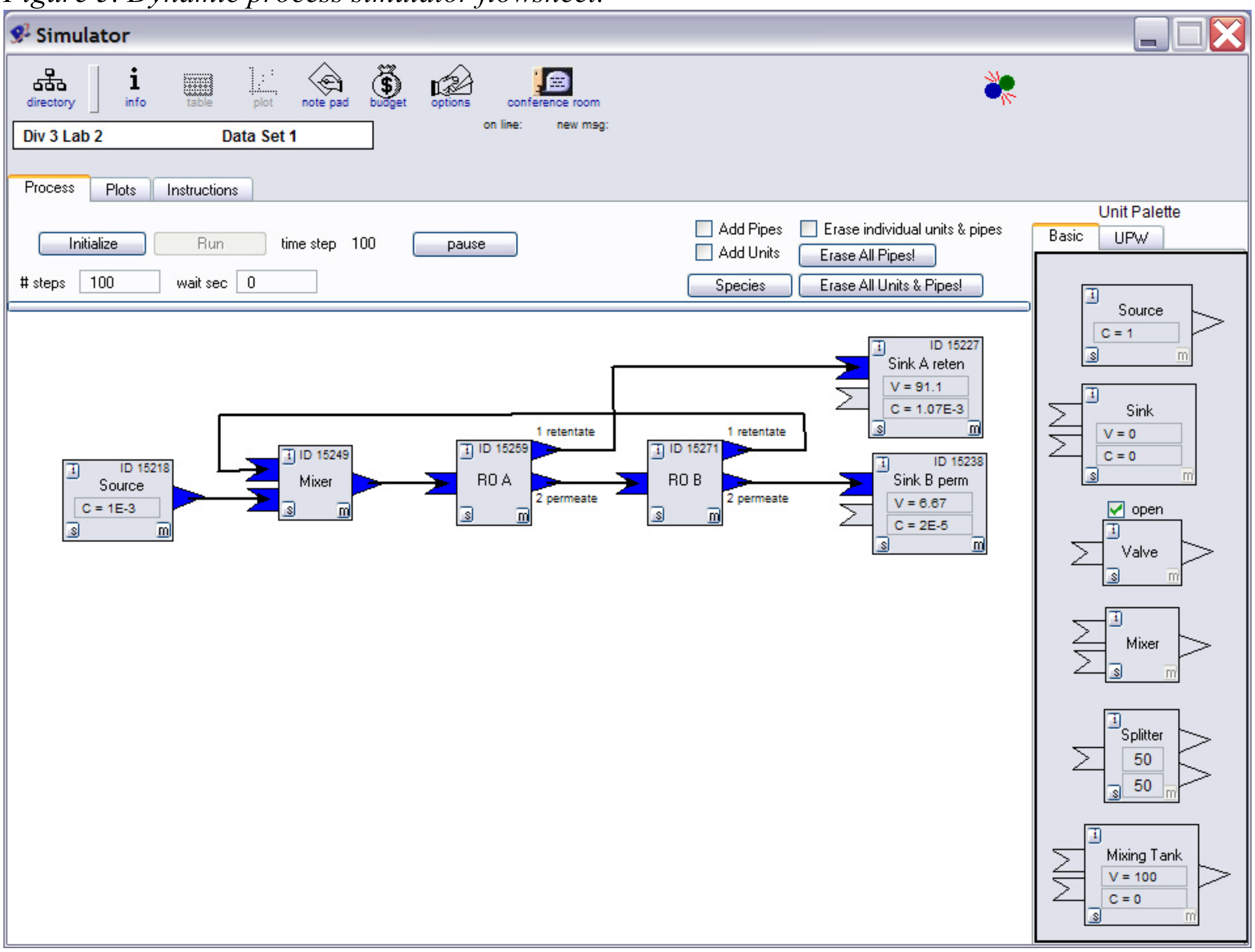
We have developed, and are continuing to develop, several modules relating to water use in the semiconductor industry. The Lab Directory currently has three divisions: Introduction, Process

Units and Process Simulation. The modules in the Process Units division currently include reverse osmosis and UV oxidation. During the first nine months of the project we have also developed the math models governing the ion exchange simulation.

In addition to providing modules on individual water purification units, a water system simulator is included in the Process Simulation division. Water systems are complex networks of many types of interconnected processes, and it is important to teach the dynamics of integrated systems (Brown, 1992). A significant portion of the UCSD effort during the first nine months of the project has been devoted to the process simulation module.

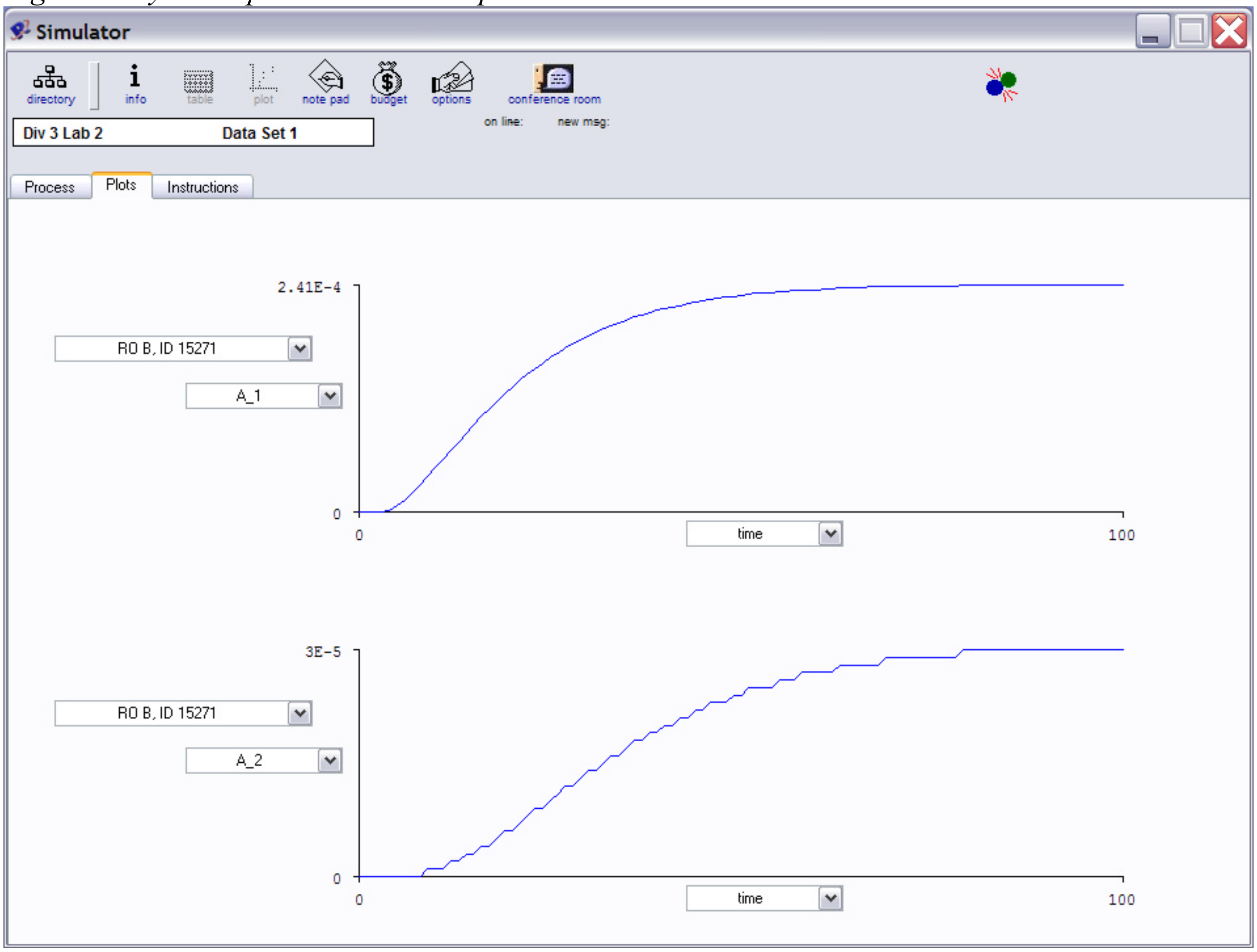
A student can select units from a palette and place them on a flowsheet, connect the units with pipes, and then run the simulation. Figure 5 shows a simulation of two reverse osmosis units in series.

*Figure 5. Dynamic process simulator flowsheet.*




After the simulation runs, plots of selected values can be viewed on the plot page, as shown below.

*Figure 6. Dynamic process simulator plots.*




<u>Task 4. "The PureWaterLab desktop application and the first educational modules will be posted at the web site for distribution and the presence of the site will be advertised to educators"</u>

As explained under Task 1 above, distributions of the Lab for Windows and Macintosh operating systems are provided for download. In the future, a distribution for Linux on Intel PC will be provided.

At the nine-month stage, we do not feel that the modules are developed to the point where they are ready for distribution on the web site. We plan to further develop the current modules, add two more, and then advertise the site to educators near the end of year-one of the project as planned.

<u>Task 5. "PureWaterLab will be introduced into courses at UCSD, the University of Arizona, and Pima Community College and will be evaluated."</u>

By the end of the first year of the project, as planned, modules will be used and evaluated in courses at UCSD and the University of Arizona.

Task 6. "Start assessment in Year 1 by conducting a questionnaire of industry experts."

We have been working with our assessment consultant to develop several types of assessment components. The following assessment tools have been developed to date and are included as appendices of this document:

- questionnaire of industry experts,
- quiz to assess prior knowledge upon starting a new educational module,
- quizzes and sample questions to reinforce and assess student learning during and at the end of a module.

## INTERACTIVE SIMULATIONS

To conclude this report, explanation of some of the features of PureWaterLab will be provided.

By supplying simplified simulations for a system, and then providing more complex simulations, students can gradually increase their depth of understanding. Figure 7 shows a basic simulation of a reverse osmosis membrane in which the user specifies the feed to the unit and the operational performance of the unit and can see as output the resulting product stream flows and compositions.

*Figure 7. Basic-level simulation.*

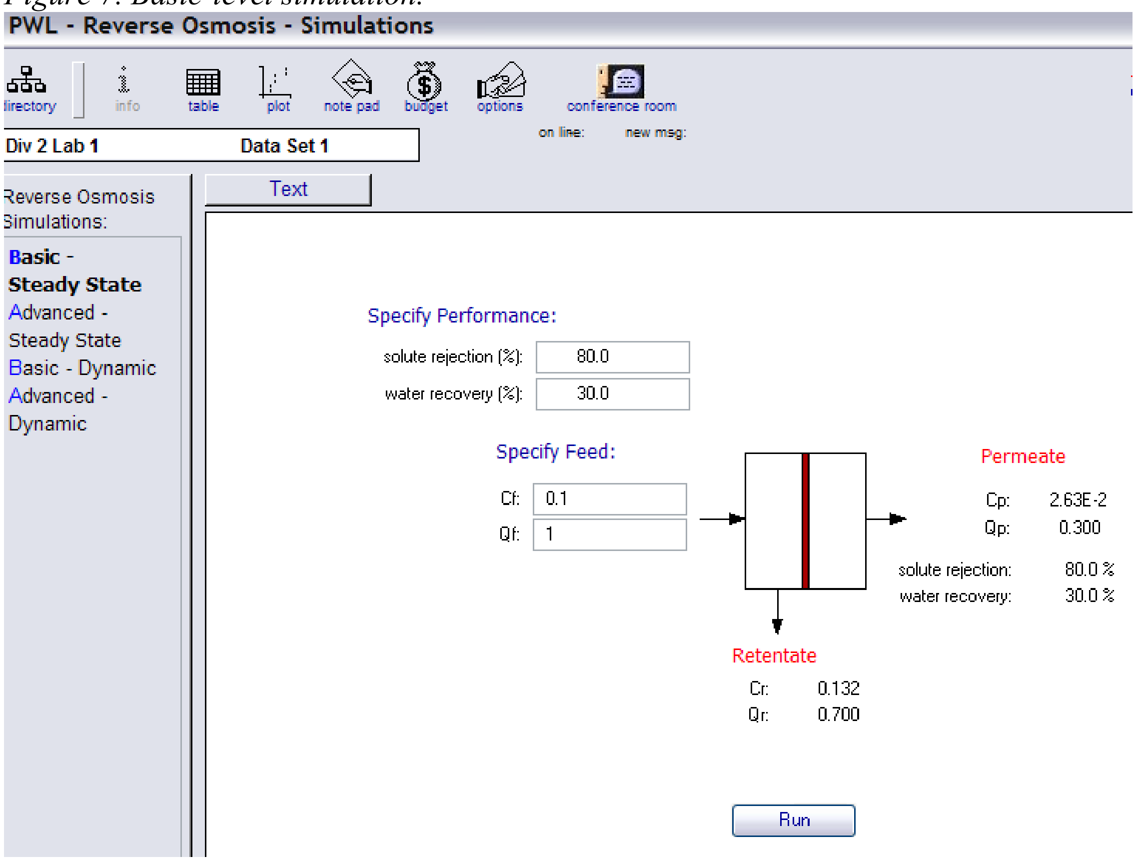
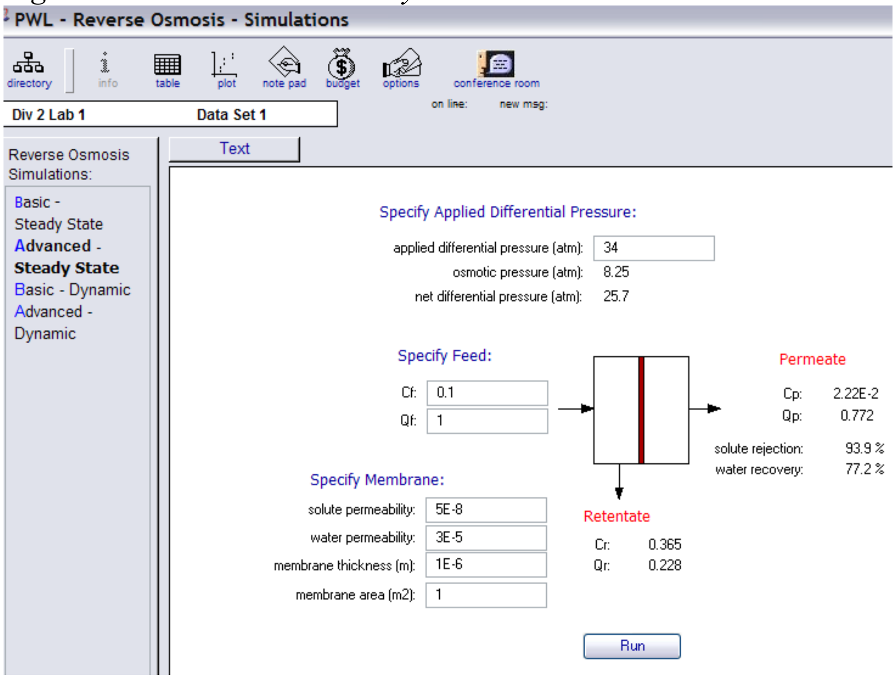


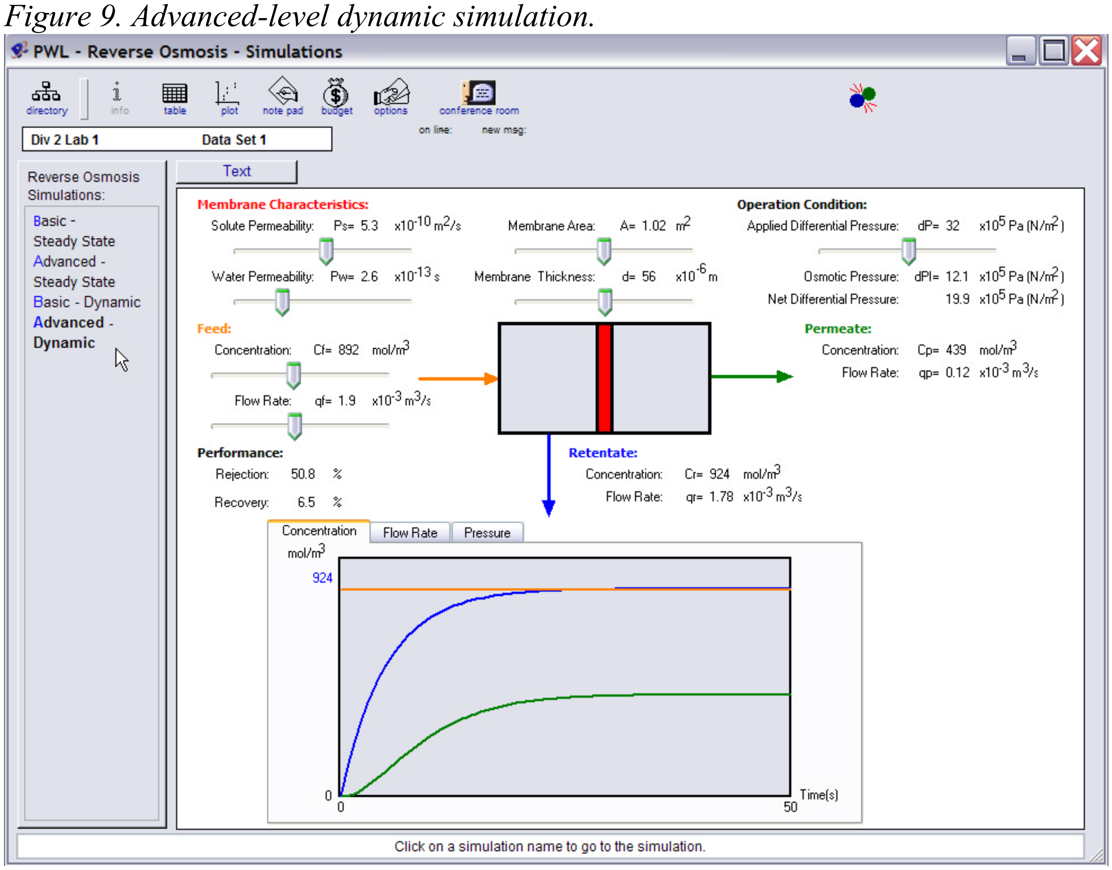

Figure 8 shows a more advanced simulation in which the user specifies all of the operational parameters of the system and then can see the output stream values and the performance measures.

*Figure 8. Advanced-level steady-state simulation.*



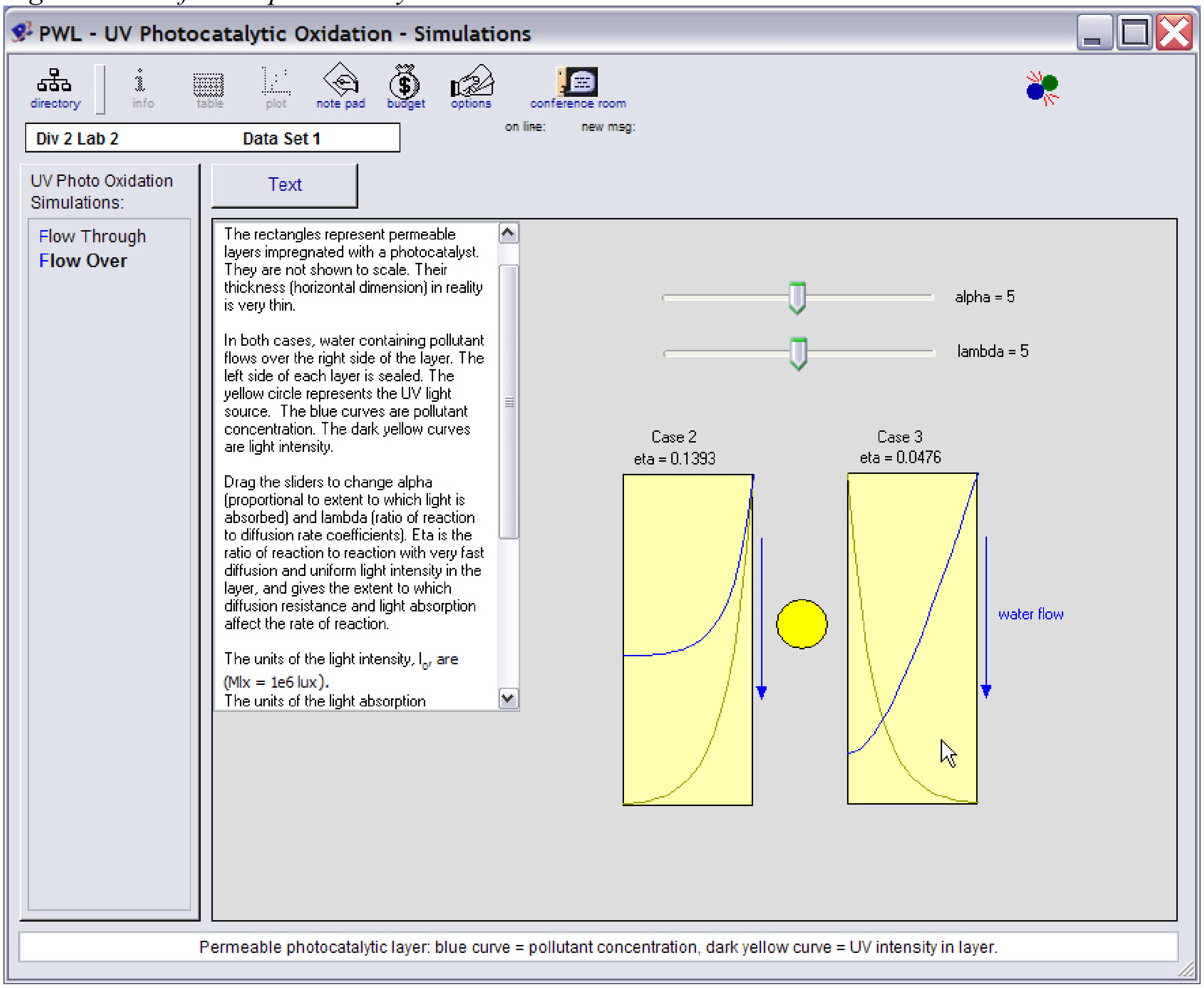

As yet another level of detail for the reverse osmosis process, the student can see the dynamic response of the unit to a step change in feed concentration in the simulation shown in Figure 9.

*Figure 9. Advanced-level dynamic simulation.*



The speed of execution of the simulations allows complex models to be updated in real time in response to input changes made by the student. Figure 10 shows two alternate configurations for photocatalytic units in which water flows over a thin catalyzed layer.

*Figure 10. Profiles in photocatalyst.*




In Case 2 shown, the layer is illuminated from its right-hand side over which water flows, with its left-hand side sealed. The blue curve is pollutant concentration and the dark yellow curve is UV intensity within the layer. In Case 3, the UV illumination is on the left-hand, sealed side of the layer. The output value "eta" given under the "Case 2" and "Case 3" labels show the relative overall activity of the two layers.

As the student slides the input controls, the four curves continuously and smoothly update.

The model equations in these two cases are rather complex and were developed by the PI in an associated research paper (Herz, 2004). For example, the concentration curve for Case 2 as a function of the horizontal direction $x$ within the layer is given by the following equation:

$$C(x) = C_o \frac{\mathrm{K}_1(\mathrm{f}_1)\ \mathrm{I}_0(\mathrm{f}_2(x)) + \mathrm{K}_0(\mathrm{f}_2(x))\ \mathrm{I}_1(\mathrm{f}_1)}{\mathrm{K}_1(\mathrm{f}_1)\ \mathrm{I}_0(\mathrm{f}_3) + \mathrm{K}_0(\mathrm{f}_3)\ \mathrm{I}_1(f_1)}$$

where $K_{0/1}$ and $I_{0/1}$ are modified (hyperbolic) Bessel functions, and where

$$\mathrm{f}_1 = 2\left(\frac{\lambda}{\alpha}\right)e^{-\alpha/2} \quad ; \quad \mathrm{f}_2(x) = 2\left(\frac{\lambda}{\alpha}\right)e^{-\alpha x/2} \quad ; \quad \mathrm{f}_3 = 2\left(\frac{\lambda}{\alpha}\right)$$

$\alpha$ = dimensionless light absorption coefficient.

$x$ = dimensionless distance into photocatalytic layer from surface exposed to water.

$$\lambda = L\sqrt{\frac{kI_0}{D_{eff}}}$$

$D_{eff}$ = effective diffusion coefficient of pollutant in photocatalytic layer.

$I_o$ = incident intensity of UV illumination (*italic*, Bessel functions $\mathrm{I}_0$ are not italic)

$k$ = photocatalytic reaction rate coefficient.

$L$ = thickness of photocatalytic layer.

For each of the two cases, six hyperbolic Bessel function values are approximated by numerical series expansions and two hyperbolic trigonometric functions are computed as the input sliders are dragged by the student. This computation is done with sufficient speed by the cross-platform scripting language such that the curves update smoothly.

**REFERENCES**

Brown, G. S., "Improving education in public schools: Innovative teachers to the rescue," *System Dynamics Review*, vol. 8, no. 1, p. 83 (1992).

Fogler, H. S., Elements of Chemical Reaction Engineering, 4th ed., Prentice-Hall, New York (2006).

Herz, R. K., "Intrinsic kinetics of first-order reactions in photocatalytic membranes and layers," *Chemical Engineering Journal*, vol. 99, p. 237 (2004).

**APPENDIX 1 - MODULE PRE-SURVEY**

**REVERSE OSMOSIS MODULE**
**PRE-SURVEY – DRAFT 1**

1. What is membrane filtration?

2. The difference between conventional filtration and cross-flow filtration is:

a. With conventional filtration, there is a cake buildup onto the membrane that blocks the flow. In cross-flow filtration, the cake buildup is prevented.
b.
c.

3. What is osmosis?

4. What equation is used to estimate the osmotic pressure of saline solutions with respect to pure solvent?

5. The semi-permeable membrane used in the reverse osmosis process is impermeable to what two substances and permeable to what substance?

6. The pro and con of heating the water prior to using the reverse osmosis process are:

   a.
   b. It improves the hydraulic performance allowing increased permeate flow, but it also increases the contaminant flux.
   c.

## APPENDIX 2 - SURVEY WITHIN MODULE

### REVERSE OSMOSIS MODULE
### SURVEY WITHIN MODULE – DRAFT 1

1. How useful were the following sections of the Reverse Osmosis (RO) module? Please mark one box for each line (1-7) below:

| | **Very useful** | **Somewhat useful** | **Not very useful** | **Not useful at all** |
|---|---|---|---|---|
| Basics | | | | |
| Role of RO in UPW | | | | |
| History | | | | |
| Materials | | | | |
| Operating Conditions | | | | |
| Theory (Equations) | | | | |
| Practice Problems | | | | |

[OR]

Please rank each section below to indicate how useful it is to you in understanding RO. Rank the most useful section "1," the second most useful "2," etc.

______ Basics
______ Role of RO in UPW
______ History
______ Materials
______ Operating Conditions
______ Theory (Equations)
______ Practice Problems

2. Of all the sections of the RO module, the section you will probably use the most will be (mark only one):

______ Basics
______ Role of RO in UPW
______ History
______ Materials
______ Operating Conditions
______ Theory (Equations)
______ Practice Problems
______ I won't use any of the sections

3. The RO module was:

| | **Strongly agree** | **Agree** | **Disagree** | **Strongly disagree** |
|---|---|---|---|---|
| Easy to use | | | | |
| Easy to navigate between sections | | | | |
| Easy to work the controls to make the simulation occur | | | | |

4. The RO module was arranged in the following order: Basics, Role of RO in UPW, History, Materials, Operating Conditions, Theory (Equations), Practice Problems. Was this the best order?

- ❑ Yes
- ❑ No

If you answered no, what do you think would be a better order?
______________________________________________________________________________
______________________________________________________________________________
______________________________________________________________________________
______________________________________________________________________________
________________________________________

5. The contents of the RO module were easy to understand.

- ❑ Yes
- ❑ No

If you answered no, please indicate any section that was difficult to understand.

______________________________________________________________________
______________________________________________________________________
______________________________________________________________________
______________________________________________________________________
______________________________

6. There were several instructions regarding the simulator content. Did you find these:

- ❑ Very beneficial
- ❑ Somewhat beneficial
- ❑ Not very beneficial
- ❑ Not beneficial at all

7. There were numerous examples in the simulator content. Did you find these:

- ❑ Very beneficial
- ❑ Somewhat beneficial
- ❑ Not very beneficial
- ❑ Not beneficial at all

8. Do you feel there is a need for demonstrations throughout the module?

- ❑ Yes
- ❑ No

If you marked yes, in what section(s) do you think demonstrations would be most helpful to you?

______________________________________________________________________
______________________________________________________________________
______________________________________________________________________
______________________________________________________________________
______________________________

9. When you missed a question in the Practice Problems section, how effective did you find it to link to the appropriate section to review?

- ❑ Very effective
- ❑ Somewhat effective
- ❑ Not very effective
- ❑ Not effective at all

10. Should the answers to the Practice Problems include:

| | Yes | No | Undecided |
|---|---|---|---|
| Unit conversions | | | |
| Step-by-step solutions | | | |
| The complete answer | | | |

11. In comparison to learning this material by lecture and reading the textbook, how effective is using this RO module?

- ❑ The RO module is more effective than lecture/reading
- ❑ They are about the same
- ❑ Lecture/reading is more effective than the RO module
- ❑ I'm not able to make a judgment at this time.

If you marked any of the three answers above, please explain your answer.

____________________________________________________________________________

12. Did learning from the RO module increase your interest in science?

- ❑ Yes, very much
- ❑ Yes, somewhat
- ❑ Undecided
- ❑ No, probably not
- ❑ No, not at all

13. Did learning from the RO module increase your interest in purifying water?

- ❑ Yes, very much
- ❑ Yes, somewhat
- ❑ Undecided
- ❑ No, probably not
- ❑ No, not at all

14. Please list any ideas you may have to improve the contents of the RO module.

____________________________________________________________________________

## APPENDIX 3 - SURVEY OF INDUSTRY REPRESENTATIVES

**SURVEY FOR**
**INDUSTRY REPRESENTATIVES – DRAFT 1**

Name ____________________________________________________________

Company Name ____________________________________________________

Company Address__________________________________________________
____________________________________________________________

Phone Number ____________________________________________________

E-mail Address ____________________________________________________

1. As part of a National Science Foundation project, PureWaterLab is developing interactive computer simulation modules to educate people on ways to conserve water and meet discharge regulations in manufacturing plants. The first people to learn from these modules will be college students. Please indicate how useful the knowledge gained from each of these modules would be to your industry.

| | **Very useful** | **Somewhat useful** | **Not very useful** | **Not useful at all** |
|---|---|---|---|---|
| Reverse Osmosis | | | | |
| UPW in Semiconductor Fabs | | | | |
| UV Photocatalytic Oxydation | | | | |
| Process Simulator | | | | |
| Ion Exchange | | | | |
| Importance of Fresh Water | | | | |

2. What other simulation modules do you believe would be useful to a prospective employee?
____________________________________________________________
____________________________________________________________
____________________________________________________________
____________________________________________________________
______________________________________

3. Each module has two levels: basic and advanced. Using a chemical reactor as an example, the basic level would include a stoichiometric equation and the conversion of the key reactant, whereas the advanced level would involve reaction orders, pre-exponentials, and activation energies. The modules will be designed so that users can click on any unit and call up the level that is desired. Users will be able to switch back and forth between basic and advanced levels

whenever they want. What do you think should be included in the basic and advanced levels of the modules listed in Question 1 and those you have added in Question 2?

4. 

________________________________________________________________________________
________________________________________________________________________________
________________________________________________________________________________
________________________________________________________________________________
____________________________________________

5. As part of our project, we are required to have each of the modules evaluated by industry representatives. Would you be willing to evaluate at least one of the modules?

   - ❑ Yes
   - ❑ No
   - ❑ Undecided

6. Once the modules have been completed, do you believe they would be useful in educating the employees in your company?

   - ❑ Yes
   - ❑ No
   - ❑ Undecided

If you answered yes, may we contact you when the modules are ready?

- ❑ Yes
- ❑ No