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**Chemical Engineering 4M03:  
Industrial Separations Processes  
Introduction to the WAVE Design Software**

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**Custom Courseware – Chapter 1**



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*Revision: R6*

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# 1. Introduction to Design Software for Membrane Processes

**Chapter #1 will introduce the following information:**

- The need for software tools
- Available software
- What WAVE is and what it is used for
- How WAVE is used in the water and wastewater industry

## 1.1 The Need for Software Tools



*As of 2017, the desalination plant in Carlsbad, California was the largest such plant in the Western Hemisphere, helping to provide the drought-stricken region with fresh water. In this photograph, the worker stands in front of 2,000 pressure vessels—a small subset of the entire plant. Designing and accurately simulating large membrane operations such as a desalination plant is infeasible to do by hand. Courtesy of: <https://www.dailynews.com/2015/11/01/questions-and-answers-about-huge-us-desalination-plant/>*

Designing a membrane-based water and wastewater treatment process can vary from case to case; the design of each system can be entirely different from the next. It is challenging as it requires the consideration of many application-specific factors such as the feedwater quality, environmental discharge/product water quality requirement, operating capacity, operating and capital cost constraints, safety constraints, etc. Software tools, like WAVE, make it possible for a user to assess the performance and feasibility of a water and wastewater treatment system before investing time and money building it. Engineers, process designers, consultants, and operators of

treatment systems use WAVE to design, simulate, and optimize water treatment processes, where doing so by hand would likely be infeasible, such as in systems like the one in the photograph above!

This courseware contains a set of chapters that are intended to introduce students to the WAVE design software. The chapters emphasize the use of WAVE to model commercial-scale water treatment operations, with a strong focus on membrane processes.

## 1.2 Software Options

This courseware will focus on using the WAVE software produced by DuPont (part of the Dow corporation). It is important to note that there are other design and optimization software options available. This section will outline the other programs for simulation of membrane processes such as ultrafiltration (UF), reverse osmosis (RO), and ion exchange (IX).

Alternative membrane-based design and simulation software:

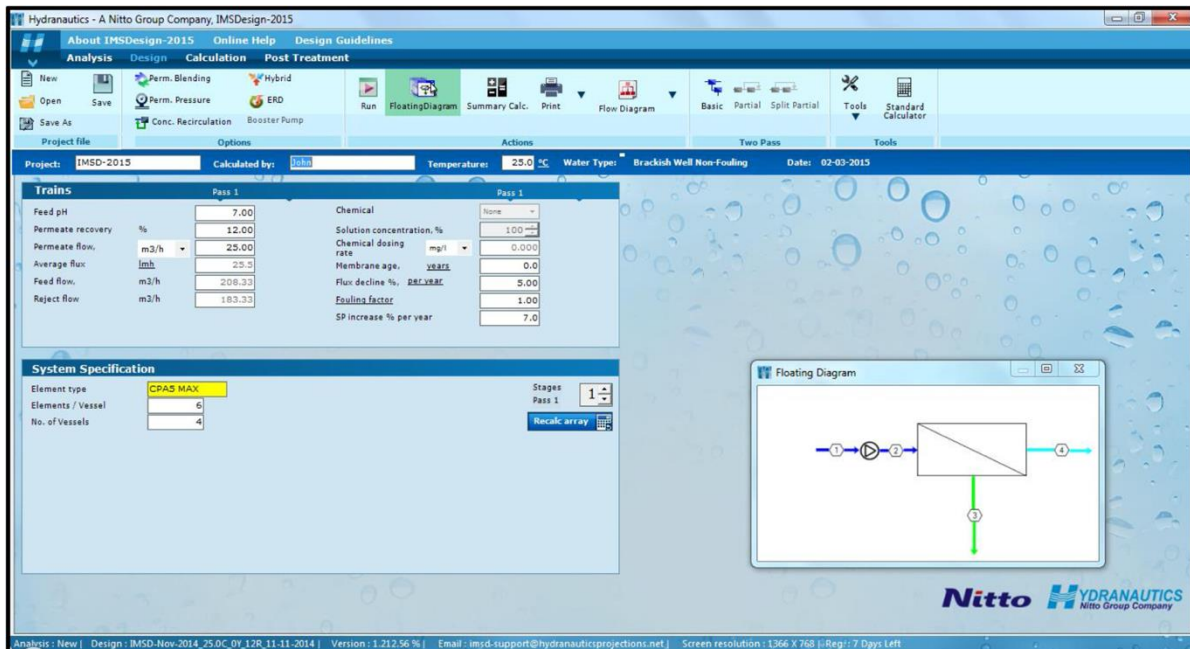
- **IMSDesign developed by Hydranautics Nitto Group Company.** The Integrated Membrane System Design (IMSDesign) application is a software that is used to design and analyze RO and nanofiltration (NF) membrane performance. This software has some interesting features such as allowing the user to add custom ions to the feedwater in addition to the default options. Users can add custom cations such as copper, chromium, manganese, iron, cobalt, nickel, molybdenum, silver, aluminum, lead, zinc, radium and uranium. Users can add custom anions such as bromide, iodide and sulfide. The software allows for post-treatment and chemical addition to the permeate stream. In addition, the software can provide a cost analysis which includes the cost of specific water, cost of materials, utilization of labor and total investment. An image of the IMSDesign project window can be seen in *Figure 1.1*.

☞ The IMSDesign-2015: User Guide by Hydranautics provides a detailed guide on how to use the software and can be found here:

<http://www.hydranauticsprojections.net/imsd/downloads/IMSD-UserGuide.pdf>

☞ The software can be downloaded for free here:

<http://www.hydranauticsprojections.net/imsd/downloads/>



**Figure 1.1:** The IMSDesign project window screen. Source: IMSDesign-2015: User Guide by Hydranautics <http://www.hydranauticsprojections.net/imsd/downloads/IMSD-UserGuide.pdf>

- **Toray Design System (TorayDS/DS2) by Toray Industries Inc.** The TorayDS allows the user to design and simulate a RO system. The TorayDS reports provide a detailed output for review and analysis of the designed system. This software has an interesting feature called the “Teach Mode” where the user can learn the software quickly.

☞ Visit the website to learn more about the software and to download it for free: <https://ap3.toray.co.jp/toraywater/>

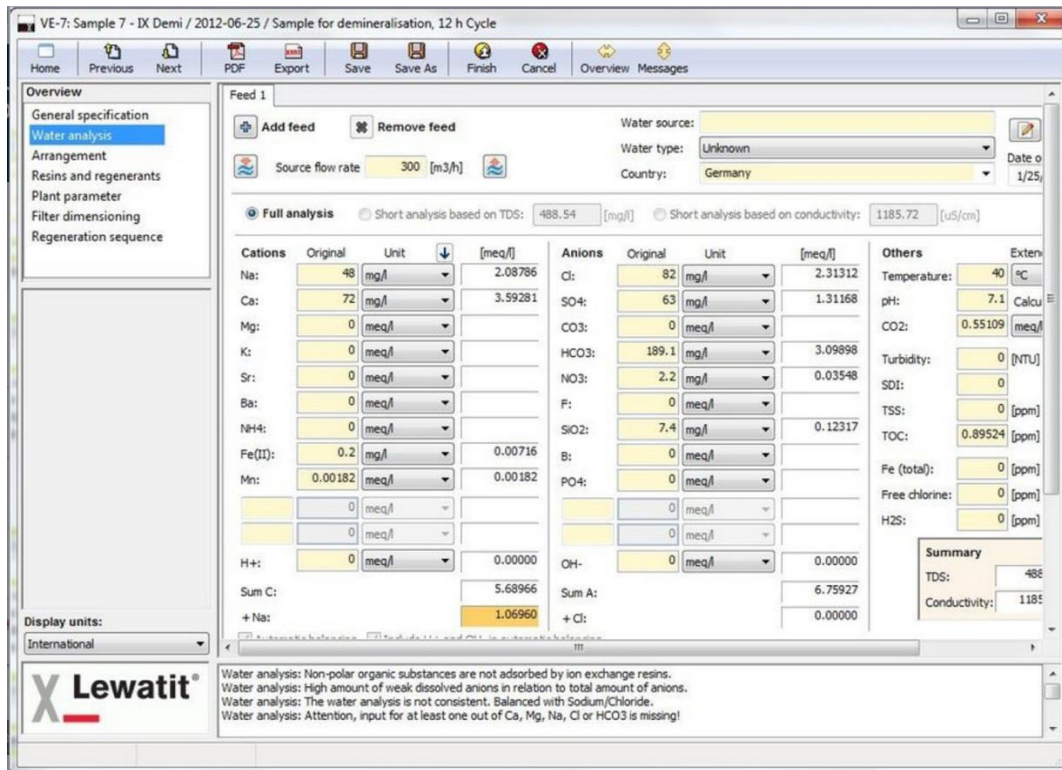
- **Winflows by Suez.** Winflows is a user-friendly software that allows the user to design and simulate simple or complicated RO system designs. Winflows’ features include 3-pass design systems, antiscalant dosing and more.

☞ Visit the website to learn more about the software and to download it for free: <https://www.suezwatertechnologies.com/resources/winflows>

- **LewaPlus® by LANXESS Engineering Chemistry.** LewaPlus® allows the user to design configurations consisting of UF, RO and IX. LewaPlus® offers a user-friendly interface that allows for simple drag and drop of technologies and understandable output for analysis. An image of the user interface can be seen in **Figure 1.2**.

LewaPlus® offers some key features for each membrane process:

For UF membranes used for RO pre-treatment and brackish water treatment, LewaPlus® offers information on membrane maintenance and cleaning.



**Figure 1.2:** The LewaPlus water analysis screen. Source: <https://lewaplus.software.informer.com/1.0/>

For RO, LewaPlus® offers calculation for system performance including feed pressure and permeate quality. LewaPlus® offers post treatment options and provides capital and operating costs based on prices sourced from historical data.

LewaPlus® has many more features, visit the website to learn more about this software and download it for free here: <https://lpt.lanxess.com/lewaplus-software/>

### 1.3 Background & Motivation

The “Water Application Value Engine” (WAVE) produced by DuPont (part of the Dow corporation) is a powerful software tool that enables the design and modelling of water treatment processes using three ubiquitous unit operations: UF, RO, and IX. WAVE supersedes previous DuPont software packages such as ROSA (for reverse osmosis) and CADIX (for ion exchange processes) to allow the integration of all three unit operations into a single model. According to the manufacturer, using WAVE offers engineers several important features:

- The ability to combine (in any order) UF, RO, and IX process combinations. *Think:* the sequencing of unit operations.
- The option to specify incoming feed rates or desired net product flow rates.
- A powerful solver able to accurately predict the performance of complex designs.

- Good predictive abilities with respect to varying water chemistries and species equilibria.
- Results that reflect “realistic” changes in chemical properties (*e.g.* volumetric flow rates) due to temperature, water composition, and compressibility.
- Embedded parameters reflective of the actual performance of real Dow membrane and IX technologies.
- “Default” parameters recommended by the manufacturer so that a design can be created quickly, or in the absence of applicable information.
- The ability to introduce and override parameters to improve the accuracy of calculations.

WAVE allows engineers and process designers to predict the performance of any combination of UF, RO, and IX processes where the feed water contains specified aqueous *salts* and/or *organic content*. The software combines theoretical models (*e.g.* Darcy’s Law) with operating data collected and analyzed by the manufacturer. As a result, WAVE can be used to predict the behavior of systems under a variety of conditions such as solution chemistries, temperatures, pressures, and unit operation choice/sequencing. WAVE computes process parameters such as:

- System performance, including stream compositions and flow rates for every major “stream” in the design. This includes the effectiveness of the separation;
- Operating requirements, including intervals between cleaning or regeneration; and
- Estimated operating costs required to meet separation objectives (*e.g.* feed flow rate, product composition).

Visit the DuPont website to learn more about this software and to download it for free:

<https://www.dupont.com/water/resources/design-software.html>



Much like design/simulation software that you have seen before (*e.g.* PIPE-FLO or Aspen), WAVE offers the user a multitude of features “under the hood” to manipulate or optimize. In this collection of chapters, we will merely introduce you to the software and a few of its features. Be aware that WAVE is a very powerful tool for the design and simulation of UF/RO membrane and IX systems. However, it is somewhat limited in that it was designed by the Dow corporation to market its membrane and IX products. As such, it only contains and supports Dow offerings and not membranes/IX resins manufactured by other companies.

## 1.4 Using WAVE in Research and Industry – Case Studies

WAVE has been successfully utilized to model and optimize new and existing membrane designs. DuPont outlines an example where WAVE was successfully used for a system design in Chino, California. The city has many dairy farms in the area which lead to the ground water being high in nitrates. DuPont's team used WAVE to simulate a series of membrane systems and then selected the one that gave the best combination of nitrate rejection and energy consumption profile.

☞ You can watch a video of the full story here: [https://www.youtube.com/watch?v=aQ-E8-F60M8&feature=emb\\_logo](https://www.youtube.com/watch?v=aQ-E8-F60M8&feature=emb_logo)

WAVE has also been successfully utilized in research-based applications. For example, Hirsimakia *et al.* used WAVE to simulate RO systems to desalinate and reuse high pH water associated with the extraction of coal seam gas (CSG) or otherwise called coal bed methane.

☞ The article titled “Process simulation of high pH reverse osmosis systems to facilitate reuse of coal seam gas associated water” by Caleb Hirsimaki, John G. Outram, Graeme J. Millar, and Ali Altaee can be found here: <https://doi.org/10.1016/j.jece.2020.104122>

Hirsimakia *et al.* explain that due to the worldwide increase in demand for energy, the extraction of CSG becoming more common and one of the by-products of this process is water containing high concentrations of dissolved salts, mainly sodium chloride and sodium bicarbonate. This water can be harmful to the environment and needs further treatment to be discharged or reused. The main idea presented in this article is to use an RO system to reuse the CSG water for livestock watering and crop irrigation. Hirsimakia *et al.* used WAVE to predict the performance of the designed system. For one scenario WAVE was used to simulate a two stage RO unit. The RO water recovery was predicted to be approximately 60% based on the fact that the WAVE software did not issue any design warnings. The results from WAVE were comparable with results from a different simulation software called Aqueous Material Balance (AqMB). It was concluded that the WAVE software predicted the RO performance well and the two software's results were in agreement with each other. One disadvantage the authors outlined is that WAVE was not able to complete the full desired pretreatment prior to desalination.

-End of Chapter-



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## 2. The Basics of WAVE

### Chapter #2 will introduce the following information:

- Downloading and installing the software
- Key features of the WAVE interface
- Assigning project units, water quality parameters and flow rates
- Saving and exporting WAVE files and reports
- Creating and managing cases in WAVE
- A practical design application for the software

### 2.1 Downloading & Installing the Software

WAVE is *free to use* and can be downloaded from the DuPont website using this URL: <https://www.dupont.com/water/resources/design-software.html>. Navigate towards the bottom of the page and click on the “Download WAVE Software” button.

 It is important to note that version 1.72 of WAVE is utilized throughout this courseware. WAVE is regularly updated so the version numbers are always changing to reflect these updates. Although the versions are updated frequently, they are not drastically different. No need to worry, simply download the latest version and adapt these downloading instructions as necessary.

On the next webpage entitled *Installation file for WAVE desktop for the first time*, DuPont will ask you to create an account to download the software. After you have created an account, return to the previous webpage. You are now able to select the “Download WAVE” hyperlink in the third list item. This will commence downloading the software. Note the process in **Figure 2.1**. After the .zip file downloads, extract the contents and run the installation file “`setup.exe`”. Follow the instructions provided by the software. As mentioned in the outlined instruction on the website, if you encounter problems when trying to run “`setup.exe`” and receive an error message about missing files, you must proceed to step 5.1. Download the “Microsoft SQL Server Compact 3.5 Service Pack 2” by clicking the link in step 5.1 and proceed to step 5.2. If WAVE is not yet downloaded proceed to step 5 again and then follow the remaining steps.

## WAVE 1.72 - Installation file for WAVE desktop for the first time

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PRINT NOTIFY ME ASK AN EXPERT

- Note: If you already have a copy of WAVE on your computer, go to: [WAVE - Updating WAVE Version](#)
  - 1. Log in to the Customer Portal
  - 2. System Requirements
  - 3. Download the program: Download WAVE, and select "Save".
  - 4. Unzip the folder.
  - 5. Right-click on **Setup.exe** and click on "run as administrator".
    - o Follow the on-screen instructions.
    - o If you receive an error message about missing files, the programs will need to be installed manually.
      1. Download [Microsoft SQL Server Compact 3.5 Service Pack 2](#)
      2. Run the executable file "SSCERuntime-ENU.exe" (preferably with administrative privileges). This will extract 2 installer programs.
        - If you have a 64 bit Operating System, you need both, "Microsoft SQL Server Compact 3.5 SP2 ENU" as well as "Microsoft SQL Server Compact 3.5 SP2 ENU x64"
        - If you have a 32-bit Operating System you will only need one instance of "Microsoft SQL Server Compact 3.5 SP2 ENU"
  - 6. Installation now complete!
  - 7. To open WAVE, go to the Start menu - All programs - DuPont and Right click on WAVE.
    - o Select Properties
    - o Click on Compatibility tab and select "Run this Program as an Administrator"
    - o Press Apply, then OK.
- In case of issues, please check the following: [WAVE Installation - WAVE Icon not Working](#)
- If you run into any problems, please contact us via "Ask an Expert" tab.
- Version of Windows (and if it is 32- or 64-bit)
  - Error message(s) you receive
  - Screen shots and other information that will help us troubleshoot your issues
- Reference: [WAVE User Manual](#)



**Figure 2.1:** The WAVE software can be downloaded from the DuPont website. An account must be created (see the top right of the screen) prior to downloading the installation files.

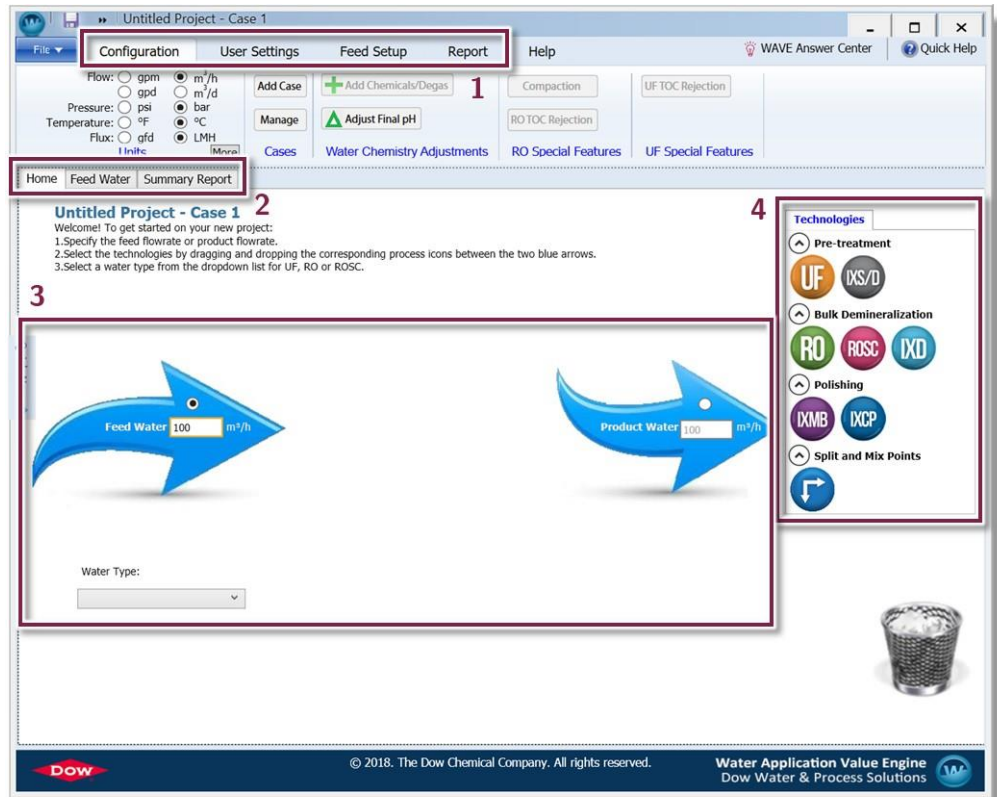
**!** WAVE is only supported on 32- or 64-bit **Windows** computers. If you use a Mac, the software will not be compatible with your computer unless you run a dedicated Windows partition.

🔗 Before you leave the *WAVE—Installation file for WAVE desktop for the first time* webpage, scroll down towards the bottom. The user manual for the software can be downloaded—for your reference—from the [WAVE User Manual](#) hyperlink. The WAVE user manual can be accessed here: <https://www.dupont.com/Wave/Default.htm>

## 2.2 The Software Interface

Begin by launching the WAVE software. You should see something similar to what is shown in *Figure 2.2*. In order to build and run a WAVE simulation, there are four main sections of features of which you should be aware:

1. **The menu bar tabs.** At the top of the screen, you can adjust a variety of simulation settings and preferences.
2. **The project settings tabs.** Under the menu bar, these tabs allow you to adjust settings with regards to your current project and view the results of the simulation.



**Figure 2.2:** The WAVE home screen. The interface is perhaps less complicated looking than other software you may have encountered. But do not be fooled: WAVE contains a multitude of features and parameters which can be manipulated—far more than what will be covered.

3. **The project flowsheet.** The project flowsheet is displayed when the *Home* tab is selected. Unlike programs such as Aspen or PIPE-FLO, the flowsheet in WAVE is a *block-flow diagram*. It merely exists to indicate what treatment technologies will be used, and in what order they will be used. The exact operating specifications of these “blocks” can be adjusted in due time.
4. **The treatment technologies.** The processes WAVE can model are located at the right side of the *project flowsheet*. These technologies can be added by dragging-and-dropping them between the *Feed Water* and *Product Water* arrows. They can be reordered or deleted in a similar manner. Seven technologies grouped into three categories are available:
  - **Pre-treatment:** ultrafiltration (UF), and ion exchange for softening/dealkalization (IXS/D).
  - **Bulk Demineralization:** reverse osmosis (RO), reverse osmosis for small commercial systems (ROSC), and ion exchange for demineralization (IXD).
  - **Polishing:** ion exchange mixed bed (IXMB), and ion exchange condensate polishing (IXCP).

In this courseware, we will focus on UF and RO membrane products but be aware that WAVE also supports these other technologies!

We will address some of the features of WAVE in greater detail in subsequent sections of this courseware, where we will learn to use WAVE to model UF and RO systems. But first, let us consider a real-life application where WAVE could be applied.

### 2.3 Treating Brackish Mine Wastewater – An Application of WAVE

The following is a short case study involving an iron ore mine. The process that extracts iron metal from ore produces a brackish (salty) wastewater stream. While current regulations do not directly dictate the effluent water quality, it is still inadvisable for the wastewater to be directly discharged from an environmental standpoint. Furthermore, it is expected that regulations will soon be enacted governing the maximum ion concentrations for the discharged water. Currently, the mining operation must deal with an average of 350 m<sup>3</sup>/h of brackish wastewater drawn from a tailings pond which has an average composition summarized in **Table 2.1** below. In this chapter we will focus on setting up the simulation and the design of the system will be revisited in Chapter 5.

As the mining company suspects that new, more stringent wastewater discharge regulations are forthcoming, they wish to study the available technologies to remove the salt from the wastewater prior to discharge. In particular, the company is interested in membrane processes (*e.g.* UF, RO) and seeks to answer the following questions:

- What effluent quality (*i.e.* composition) can be achieved using UF/RO processes?
- What UF/RO technologies are needed for this preliminary design?
- What operating considerations are there?

To address the company's questions and concerns, WAVE can be used to determine the effectiveness and feasibility of using UF/RO membrane processes in treating the wastewater.



Be sure that you have installed the WAVE software before proceeding. We will use it—along with the information presented in this section—to design a UF/RO system to treat the brackish water.

**Table 2.1:** Water quality analysis (WQA) of the effluent water stream from the actual iron mine. The valuable iron has been removed in previous steps.

Property	Value
Average Temperature (°C)	15±7
Turbidity (NTU)	85.2
pH (@ 15 °C)	7.52
Total Suspended Solids (mg/L)	80.9
Total Organic Carbon (mg/L)	11.2
Cationic Species	Concentration (mg/L)
Ammonium	1.56
Barium	0.065
Calcium	101
Magnesium	133
Potassium	25.7
Sodium	95.3
Strontium	0.875
Anionic Species	Concentration (mg/L)
Bicarbonate	83
Chloride	209
Nitrate	1.7
Sulfate	700
Neutral Species	Concentration (mg/L)
Boron	0.08
Silica	3.06

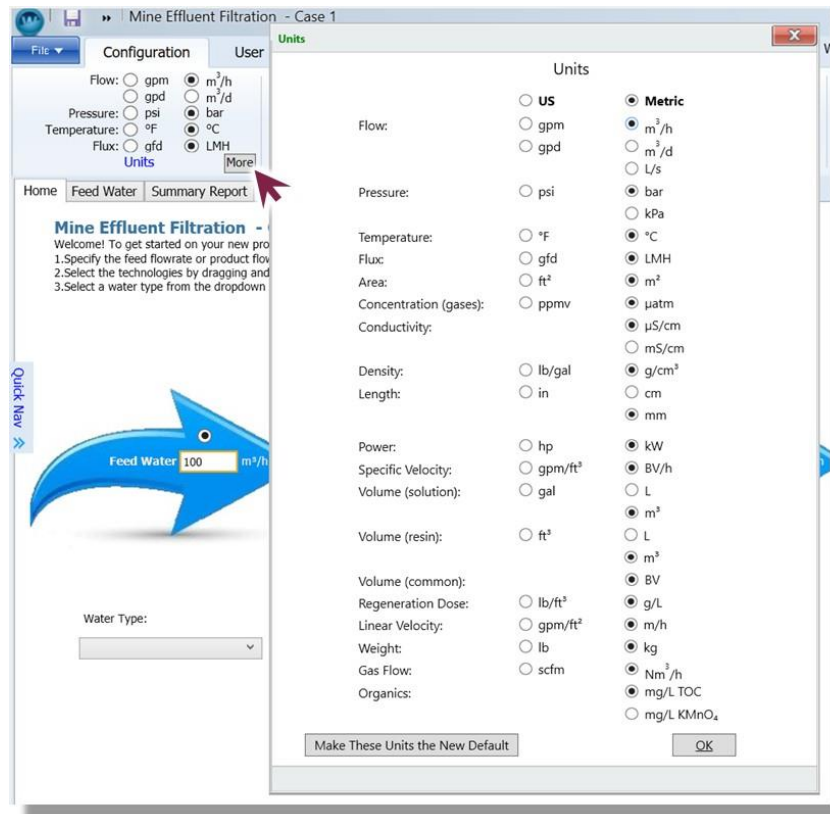
### 2.3.1 Setting Up the Simulation

Before we begin simulating the system at hand, we must set up a new project in WAVE.

**Setting the Display Units.** To ensure that your results match the ones presented in these chapters, you must ensure that your units of measurements match the units in **Figure 2.3**. To configure the units, navigate to the *Configuration* tab in the top menu and click “More”. We will use metric units by default, and it is recommended that you choose “m<sup>3</sup>/h” to match the influent flow rate given in **Section 2.3**. Verify your simulation’s units match the units in **Figure 2.3**. Click “OK” when you are finished.

**Specifying the Feed Water Quality.** In **Section 2.3**, we were given a WQA for the brackish effluent stream from the mine (*i.e.* **Table 2.1**). Now, we will input the data that we have into WAVE. Begin by navigating to the *Feed Setup* tab in the top menu bar and then navigate to the *Feed Water* in the project settings tab, as seen in **Figure 2.4**.

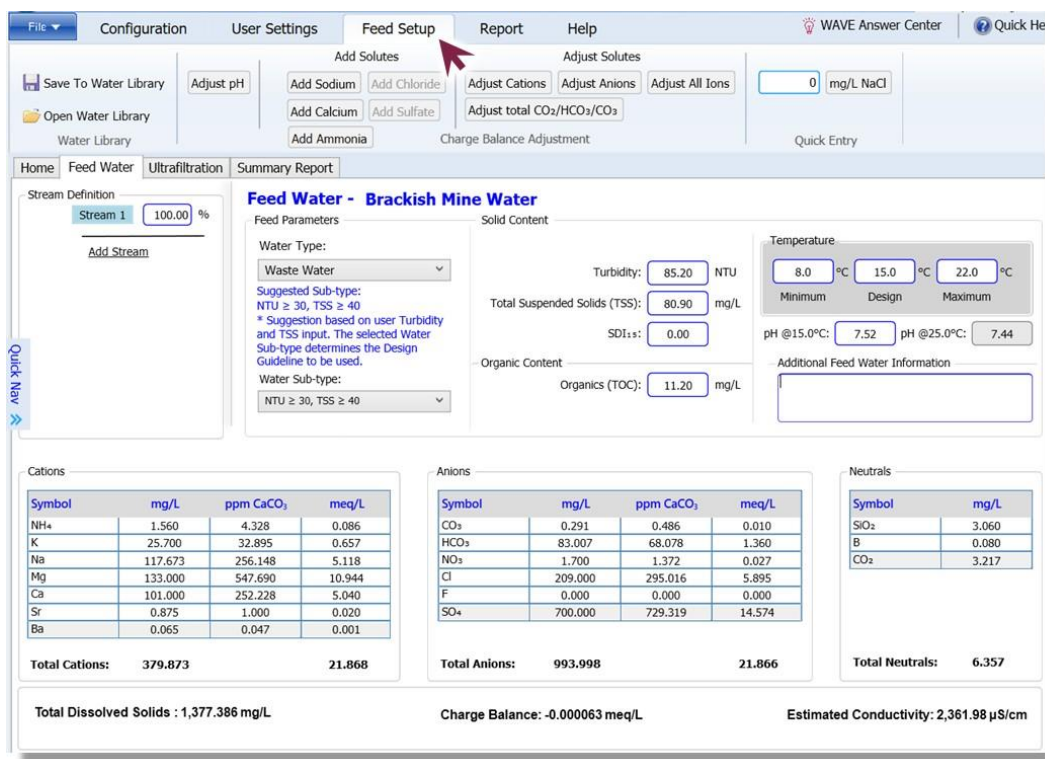




**Figure 2.3:** Setting the display unit preferences for the WAVE simulation.

- In the *Feed Parameters* panel, under the *Water Type* and *Water Subtype* drop-down menus, select the categories which *best describe your* water source with regards to total suspended solids (TSS) and *turbidity*<sup>1</sup>. Here, we will choose “Waste Water” and “NTU ≥ 30, TSS ≥ 40” to match our WQA. This guides WAVE in performing its calculations.
- In the *Solid Content* panel, we can specify the turbidity, TSS, Silt Density Index (SDI), and organics content (total organic carbon; TOC). Use the values from **Table 2.1** to fill in the *Solid Content* fields with exception to the SDI (*i.e.* the SDI value is 0 mg/L). All parameters in the *Solid Content* panel are *optional*.
- Beside the *Solid Content* parameters are fields to input the system temperature and pH. Fill in these values from **Table 2.1**. The “minimum” and “maximum” design temperatures are the bounds between which the system should operate. We can use the variation on the temperature (7°C) to populate these (albeit optional) fields.
- At the bottom of the screen, we can populate the tables of *Cations*, *Anions*, and *Neutrals* with values from **Table 2.1**. Be sure to use the columns with units of “mg/L”. If a species is not specified in our WQA, leave that row blank (*i.e.* 0 mg/L).

<sup>1</sup> The turbidity or “cloudiness” of water is reported in the standard *Nephelometric Turbidity Units* (NTU).



**Figure 2.4:** Assigning water quality parameters to the brackish feed stream.

Notice that several values update as you fill in the fields. For example, WAVE sums the total dissolved solutes to estimate the solution conductivity. WAVE also sums the total cations, anions and neutral species to calculate the overall “concentration of charge” (units: meq/L).<sup>2</sup>

Even though we have not specified any carbon dioxide concentration, WAVE has calculated this field to be a non-zero value due to chemical equilibria that exist in the water (*e.g.* bicarbonate  $\rightleftharpoons$  carbon dioxide equilibrium) at the given pH and temperature.



The calculations behind the water quality parameters (*e.g.* chemical equilibria) are quite complex; we will not delve into them in detail. Just be aware that WAVE performs calculations in the background based on thermodynamic models to ascertain which chemical species are present, and in what concentration/activity.

At the bottom of the *Feed Setup* screen, note the “*Charge Balance*” value of approximately -0.97 meq/L. What do you think that this means if you have ~ 0.97 milli-equivalents of negative charge per liter? Think of the net “milli-equivalent” of charge as being a milli-molar excess of positive or negative ions. The interpretation of this value is that given the composition of salts/solids that we have specified (based on the WQA), the solution has an *overall (net) negative charge* equal to this value. Our WQA analysis may not have detected additional cations in solution (*e.g.* residual Fe, Ni, etc.) that would balance out the negative charge. We know that a solution

<sup>2</sup> One mole of Na<sup>+</sup> ions produces one equivalent (+1 eq) of charge. One mole of Ca<sup>2+</sup> ions produces +2 eq of charge. One mole of Cl<sup>-</sup> ions produces -1 eq of charge.

cannot have a net charge: ions are always balanced by their counterions. As our solution has a net negative charge, we must “balance” it with *more positive ions*. In the software, we can do this by either (a) adding sodium ions, (b) adding calcium ions, (c) adding ammonia (ammonium) ions, or (d) adjusting the pH (adding  $H^+$  ions).


In our example here, we will balance the net charge by adding sodium ions. Using more sodium is unlikely to change critical results (*e.g.* fouling) as sodium salts are generally soluble over a wide range of process conditions. However, additional  $Na^+$  ions may decrease the quality of the permeate water due to the small size and ability for these ions to cross RO membranes (as opposed to  $Ca^{2+}$ ). Under the *Feed Setup* menu bar tab, click “Add Sodium” to automatically balance the charge with sodium ions. The charge balance should now be a very small value (approximately  $-0.000063$  meq/L), which is essentially zero. The completed result is shown in **Figure 2.4**. We are ready to continue; return to the flowsheet by clicking on the *Home* project setting tab.

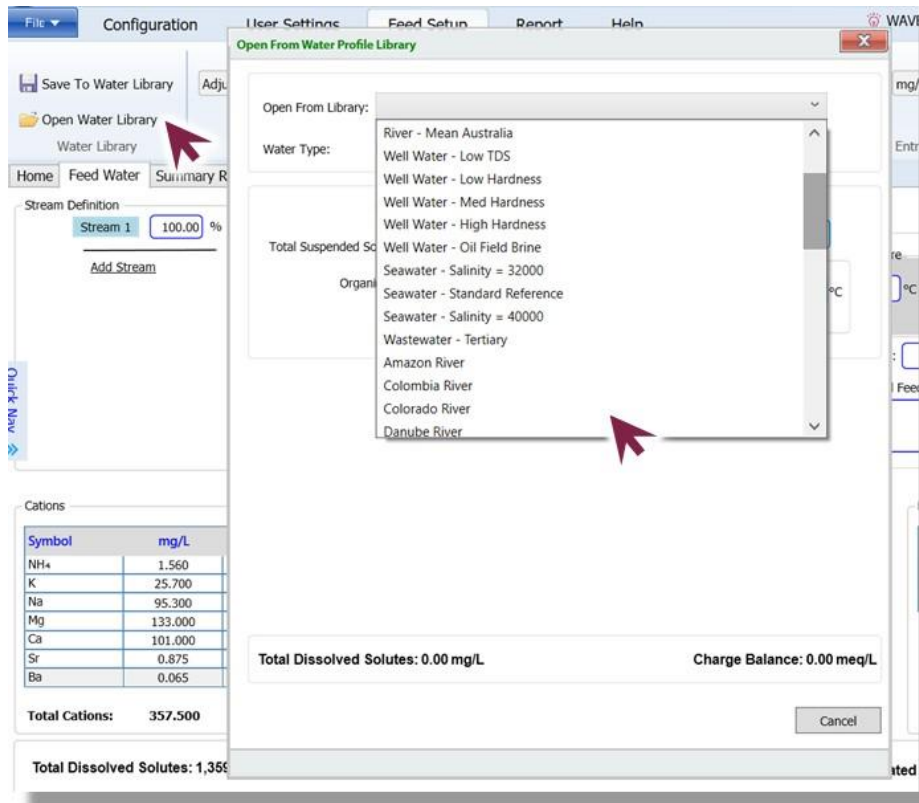


If you enter a water composition that is not charge-balanced, WAVE will not let you leave the *Feed Setup* screen until you make changes which set the net charge of the solution to zero.

As an aside, if you *do not* know much information about your feed water composition, WAVE offers a library of different water chemistries from all over the world. You can access them by clicking “Open Water Library” and selecting a suitable chemistry from the rather-extensive drop-down menu, as seen in **Figure 2.5**. We will use this feature in the chapters to come!

**Specifying Desired Flow Rates.** WAVE requires the user to specify either the total flow rate of the influent or effluent so that it can perform its calculations. In our scenario in **Section 2.3**, we were told that the mine produces  $350\text{ m}^3/\text{h}$  of brackish wastewater. This is the influent flow rate to the treatment system. Return to the *Home* tab and ensure that the “*Feed Water*” radio box () is ticked and set the flow rate in the field below. Check that your units are correct! Your flowsheet should look like that shown in **Figure 2.6**. If we knew how much treated water that we needed to produce, we could set the flow rate of *Product Water* instead. We are now ready to add membrane processes to our system. Save your project before moving on to the next chapter!

 Ensure that you have properly defined the feed water composition before continuing onto the next section. This example will be revisited in Chapter 5 where we will design the membrane system.



**Figure 2.5:** You can select from pre-loaded water chemistries as a starting point.



**Figure 2.6:** Specifying the flow rate.

## 2.4 How to Save a WAVE File

This section will outline how to save a WAVE project. Locate and click the “File” drop down menu and then select the “Save Project As” option, as seen in **Figure 2.7**. You will be prompted with a window titled “Project Information”, as seen in **Figure 2.8**. Rename your file in the “Project Name” field. Populate any of the additional fields with appropriate information as needed and then, press “Save”.

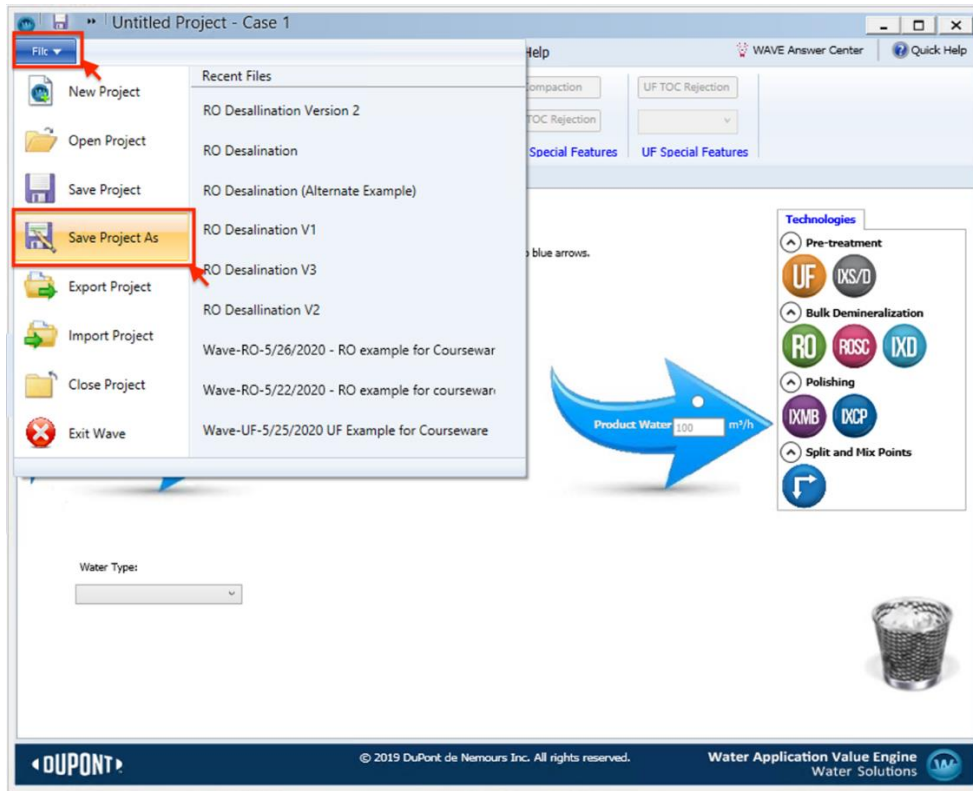


Figure 2.7: Saving a WAVE project.

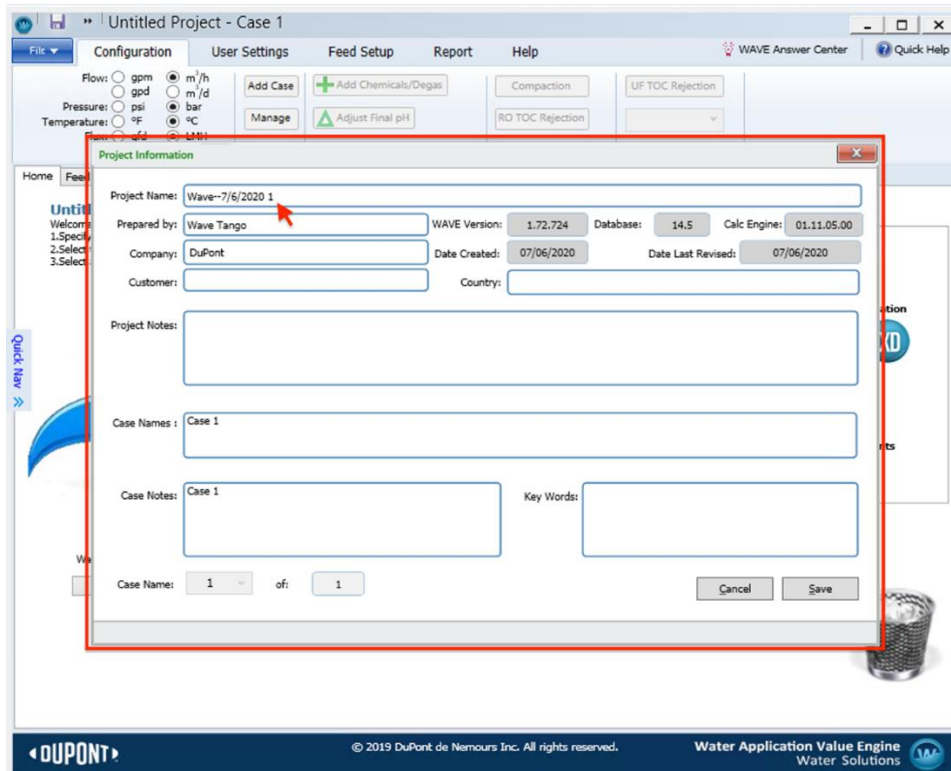


Figure 2.8: Saving and renaming a WAVE project.

## 2.5 How to Export a WAVE file

First, ensure the project file is saved per *Section 2.4*. Locate and click the “File” drop down menu, then select the “Export Project” option, as seen in *Figure 2.9*. You will be prompted with a window titled “WAVE Export”, as seen in *Figure 2.10*. Choose a location on your computer where you want the exported file to be saved. Input an appropriate file name and ensure the file save type is “Dupont Export (\*.DWPX)”. Then, press “Save”, as seen in *Figure 2.10* (where the file is exported to the desktop).

! According to the WAVE User Manual WAVE projects are saved in a database that cannot be shared. Therefore, the file must be exported as a “DuPont Export (\*.DWPX)” so then the file can be saved and sent as an attachment to share with others via email.

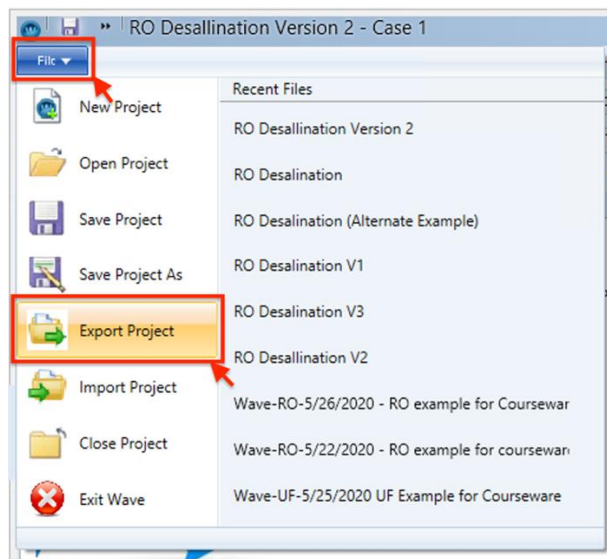


Figure 2.9: Exporting a WAVE project.

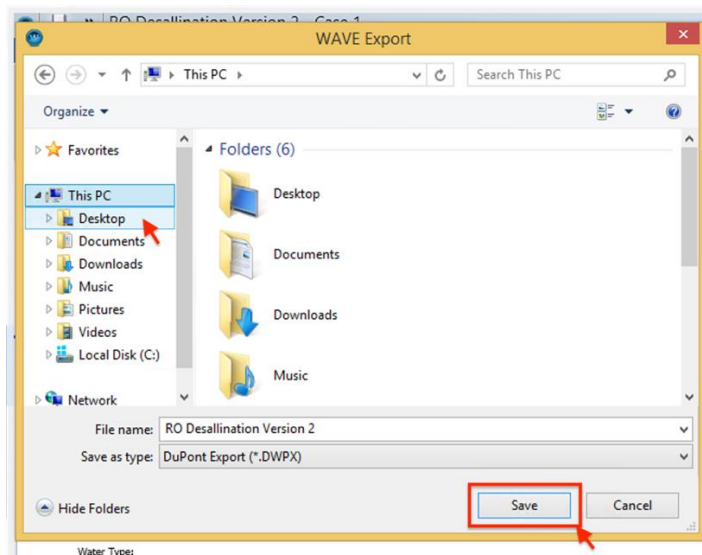


Figure 2.10: Exporting a WAVE file as a DuPont Export (.DWPX) file to desktop.

## 2.6 Simulating Related Designs in WAVE

WAVE has a useful feature, called *cases*, that allows users to efficiently simulate different design scenarios by modifying the initial project's parameters. The user can analyze the results without making a new WAVE project. WAVE automatically generates an initial case when you start a new project, but more cases can be added subsequently.

For example, generating a new case may be useful if you have a system and want to investigate the effect of changing the design water temperature, influent composition or membrane type etc. on the performance of your system.

To add another case to a project, press “Add Case” in the “Cases” section under the *Configuration* menu bar tab, as seen in **Figure 2.11**. Once you add a new case, the *Home* tab and screen will update the file name to reflect that you are now working on that particular case (*i.e.* “Case 2”).

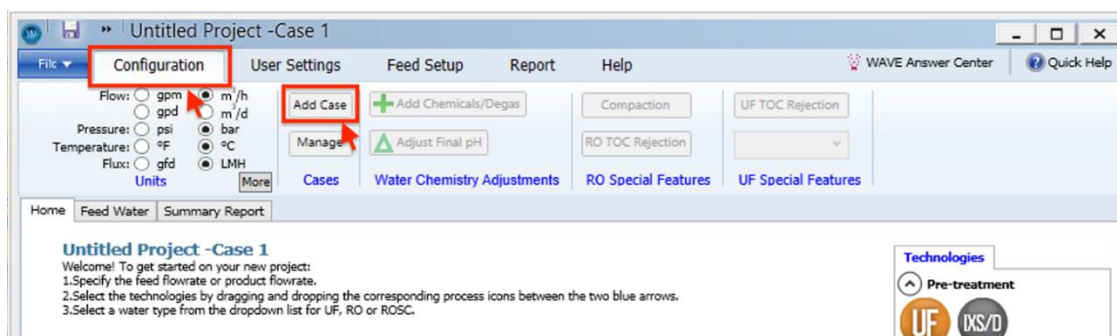
To manage cases, press “Manage” in the “Cases” section under the *Configuration* menu bar tab, as seen in **Figure 2.12**. A window will appear titled “Case Management”, as seen in **Figure 2.13**. Users can rename the existing cases by double clicking the previous case name and typing the desired name. In the same manner, a user can add notes to each case which is highly recommended to identify what each case is for.

Additionally, the user can add, open, and delete cases:

- A new case can be added by clicking the “Add Case” button.
- An existing case can be opened by clicking once on the desired case, which will highlight the field in blue, and then clicking the “Open Case” button.
- An existing case can be deleted by selecting the desired case and clicking the “Delete Case” button.



Consult the Case Management chapter of the WAVE User Manual for a more in-depth explanation of how to manage cases in WAVE. The User Manual can be found here: <https://www.dupont.com/Wave/Default.htm>.



**Figure 2.11:** Adding a case in WAVE.

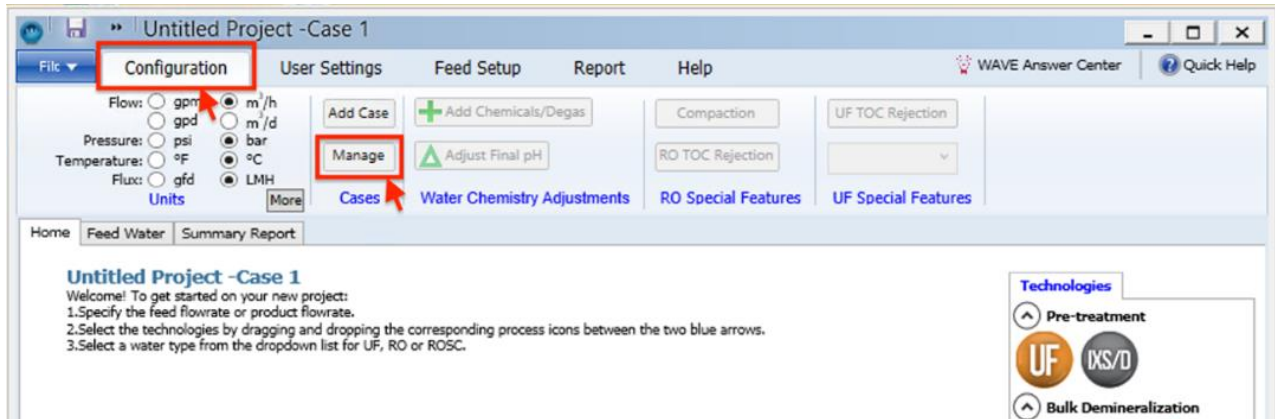


Figure 2.12: Opening the WAVE “Case Management” window.

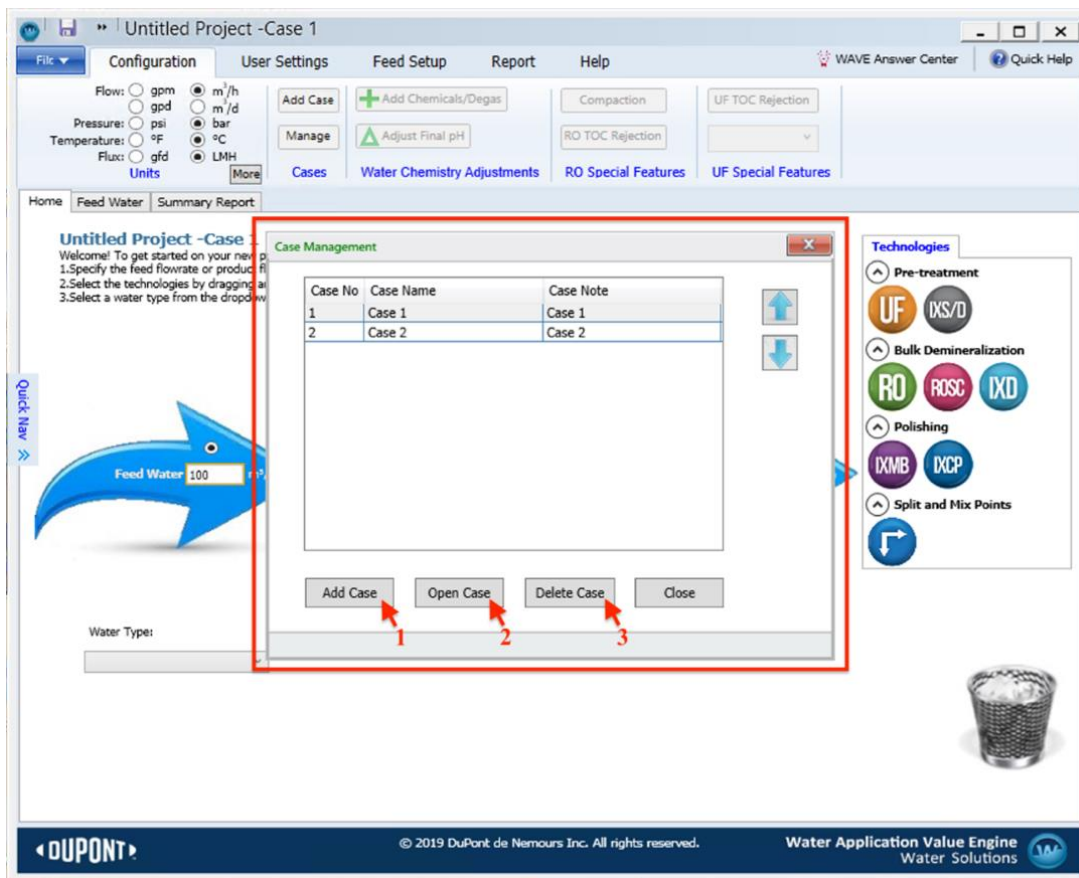


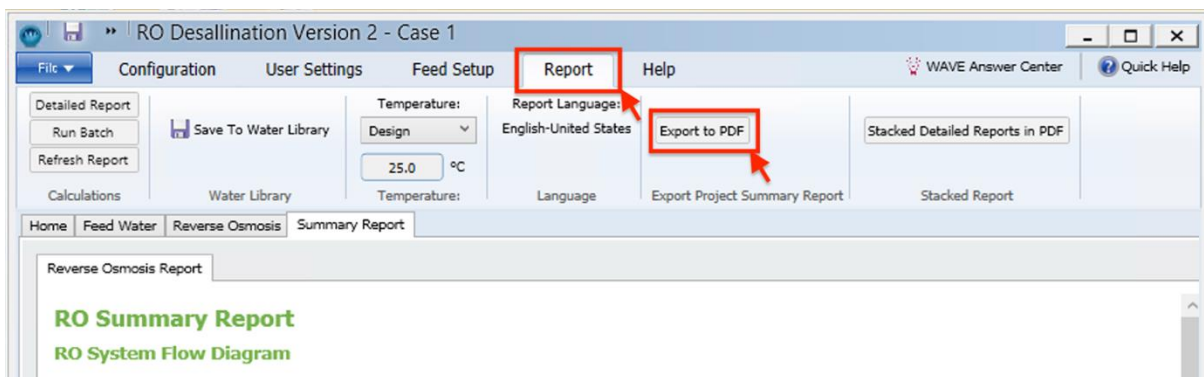
Figure 2.13: The WAVE “Case Management” window with options to add (1), open (2), delete cases (3).



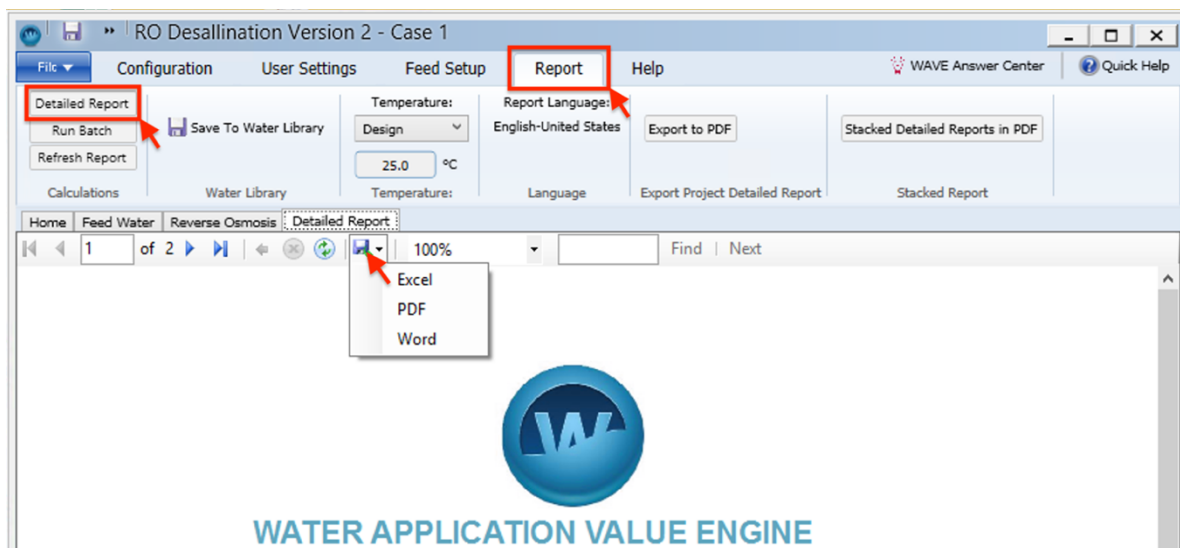
## 2.7 Summary and Detailed Reports

**Summary Report.** The summary report is a short report of key results from the simulation. It can be accessed by clicking the *Summary Report* project setting tab or the *Report* menu bar tab. To export a project summary report as a PDF file, click the “Export to PDF” button in the “Export Project Summary Report” section of the *Report* menu bar tab, as seen in **Figure 2.14**. A window will appear which will allow you to rename the file and choose the location to save it on your computer.

**Detailed Report.** The detailed report contains more information on the results of the simulation such as energy usage and operating costs in addition to the content from the summary report. To generate a detailed report, click the “Detailed Report” button in the “Calculations” section of the *Report* menu bar tab. WAVE will present the detailed report via a new project tab named *Detailed Report*. Note that the detailed report will be of the current case you have open. To save a detailed report, ensure you are on the *Detailed Report* project tab, click the small save button icon (📄), and then choose an appropriate file type, as seen in **Figure 2.15**. A window will appear which will allow you to rename the file and choose the location to save it on your computer.

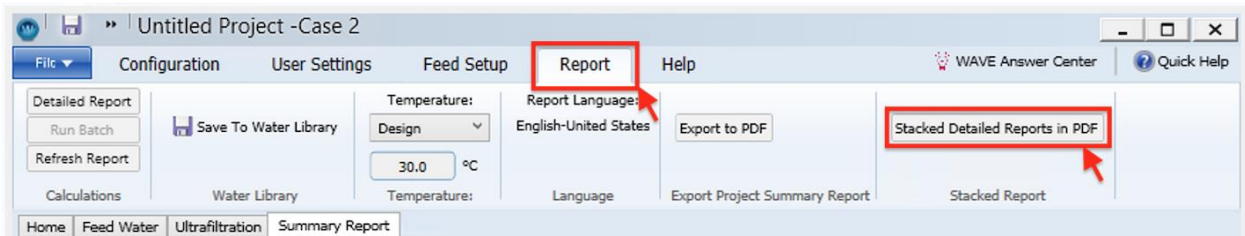


**Figure 2.14:** Exporting a WAVE project summary report.

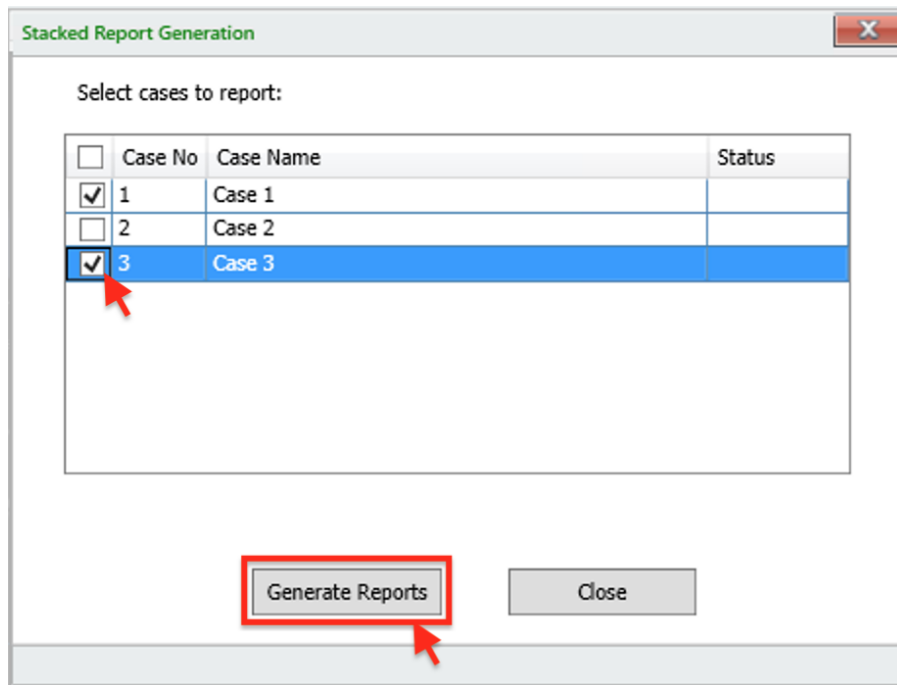


**Figure 2.15:** Exporting a WAVE detailed report.

**Stacked Detailed Report.** A stacked detailed report appends each selected case’s individual detailed report to create one large report. Note that the stacked detailed report can only be saved as a PDF file. To generate a stacked detailed report, click the “Stacked Detailed Reports in PDF” button in the “Stacked Report” section of the *Report* menu tab. A window will appear called “Stack Report Generation”, check the boxes (☑) of the cases you want to include in the report. Then click “Generate Reports” and a prompt will appear indicating this process may take a few moments, click “OK” to proceed. Once the report has been generated a window will appear which will allow you to rename the file and choose the location to save it on your computer.



**Figure 2.16:** Exporting a Stacked Detailed Report in WAVE.



**Figure 2.17:** Selecting desired cases to be included in the Stacked Detailed Report.

-End of Chapter-

## **Works Cited**

- [1] “WAVE Software for Water Treatment Plant Design,” *www.dupont.com*. [Online]. Available: <https://www.dupont.com/water/resources/design-software.html>.
- [2] “Water Application Value Engine DuPont Water Solutions,” *Dupont.com*, 2020. [Online]. Available: <https://www.dupont.com/Wave/Default.htm>.

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**Chemical Engineering 4M03:  
Industrial Separations Processes  
Introduction to the WAVE Design Software**

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**Custom Courseware – Chapter 3**



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*Revision: R4*

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### 3. Ultrafiltration Technologies in WAVE

#### Chapter #3 will introduce the following information:

- Configuring a membrane process
- Adding ultrafiltration process to the flowsheet
- Assigning ultrafiltration operating parameters
- Interpreting summary report results and design warnings
- Analyzing and optimizing the ultrafiltration process

Ultrafiltration (UF) technology is best suited to treat feedwater containing colloidal matter as UF membranes reject bacteria, viruses and suspended solids to produce permeate with low turbidity ( $\leq 0.1$  NTU). As a result, UF membranes solve many water and wastewater problems such as decontaminating industrial process water (*e.g.* oil-water separations), treating water for the food and beverage industry, pre-treating brackish water before reverse osmosis (RO) processes, recycling wastewater for local reuse. These are just a few examples.



UF systems are often used before RO membranes in order to remove colloidal matter that would otherwise foul the RO membranes.

! Before you proceed to design and simulate in WAVE on your own it is important to note that your results may vary slightly from other simulation results even for the same design with the exact same design parameters. This is due to the following three factors:

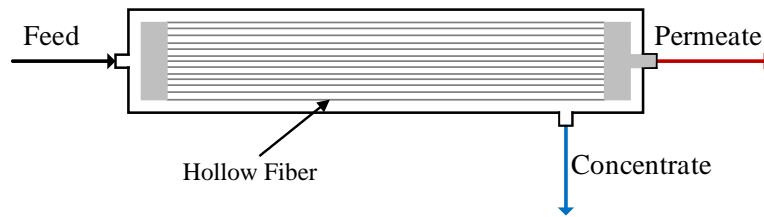
- The version of WAVE you are using
- Previous simulation results
- The order in which you input parameters on WAVE

#### 3.1 Background

Designing and simulating UF technology in WAVE requires understanding the basic UF terms:

- **Module:** The smallest “membrane unit” in a UF process. Depending on the manufacturer and application, modules may be constructed using hollow fibre, tubular, or flat sheet membranes, and designed to use outside-in or inside-out flow. A visual representation of a module can be seen in *Figure 3.1*.

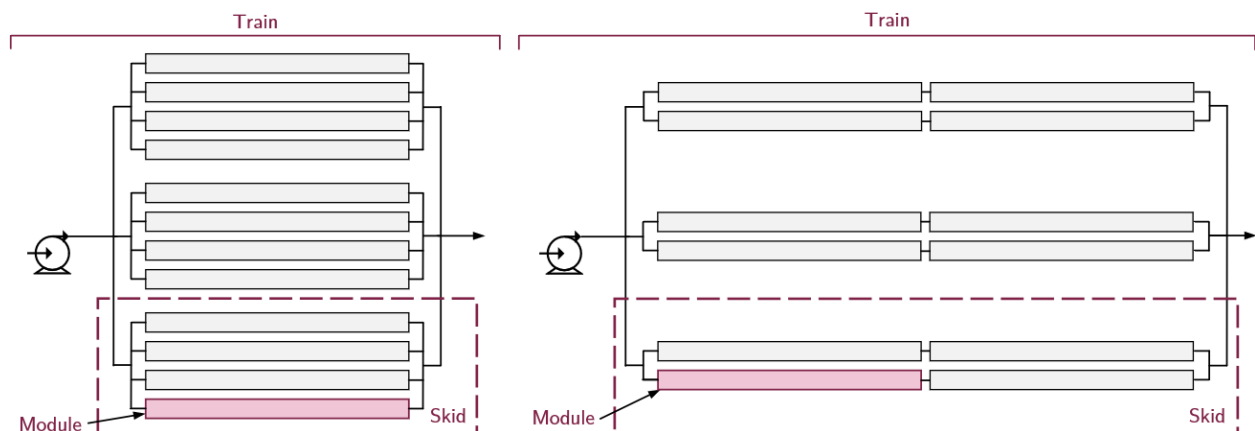
🔗 To get an idea of what this module looks like, check out the video at the link, below:  
<https://www.youtube.com/watch?v=tIAAoCBYfN0>



**Figure 3.1:** A representation of a cross-section of a hollow fiber UF module, showing the individual hollow fibers in grey. The feed stream is coloured in black, the permeate stream is coloured in red, and the concentrate stream is coloured in blue. This module is operated in an outside-in configuration.

- **Skid:** A prefabricated assembly of modules, piping, process instrumentation and control hardware that is often mounted on a modular pallet/frame. Depending on the manufacturer and end-user requirements, modules within a skid can be arranged horizontally or vertically, and in series or in parallel (or a combination of both).
- **Train:** A complete treatment system consisting of multiple skids. A train may consist of the same technology (e.g. many UF skids), or a train may consist of different technologies (e.g. pre-treatment, primary treatment, and then post-treatment). Skids can be arranged in series to meet separation quality objectives, while skids in parallel are used to meet capacity requirements. Furthermore, a plant may use multiple trains in parallel to meet capacity *and* operability (i.e. maintenance, flexibility) needs.

**Figure 3.2** illustrates the relationship between elements, modules, skids, and trains.



**Figure 3.2:** Illustration of the relationship between modules, skids and trains. In this diagram, each skid has 4 modules, and each train has 3 parallel skids:  $4 \times 3 = 12$  modules total. The left panel features modules arranged in parallel within a skid, while the right panel features modules arranged both in series and in parallel within a skid.

## 3.2 Problem Definition & Background

Let us consider how ultrafiltration membranes are used in municipal wastewater treatment processes. Typically, municipal wastewater is treated via preliminary, primary, secondary, and tertiary treatment processes before the effluent is discharged to a local water body. To be discharged, it is critical that certain parameters of the product water (such as total suspended solids (TSS), total phosphorus (TP), ammonia, pH, etc.) meet regulatory limits, which may vary depending on location. As these regulations are projected to become more stringent in the future, ultrafiltration membranes can be used to further treat secondary and tertiary municipal wastewater.

☞ Check out this article titled “Ultrafiltration as an advanced tertiary treatment process for municipal wastewater” by George Tchobanoglous, Jeannie Darby, Keith Bourgeois, John McArdle, Paul Genest, and Michael Tylla found here: [https://doi.org/10.1016/S0011-9164\(98\)00175-1](https://doi.org/10.1016/S0011-9164(98)00175-1)

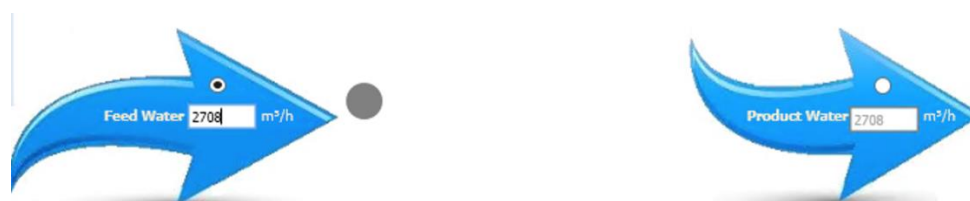
In this chapter’s problem, it is found that more stringent wastewater discharge regulations will be enforced. You are asked to design and simulate the addition of UF membranes to a wastewater treatment plant (WWTP). The WWTP has a maximum capacity of 65,000 m<sup>3</sup>/d (~2,708 m<sup>3</sup>/h). Though on average, the WWTP typically treats 50,000 m<sup>3</sup>/d (~2,083 m<sup>3</sup>/h). In North America, this plant is sized to serve a population of 130,000 to 140,000 people.

## 3.3 Setting Up the Simulation

Let us set up the simulation! First, open WAVE and then create a new file by clicking “File” and then “Save As”. Make sure to name this file something descriptive so that you can easily return to it in the future. Refer to **Section 2.4** for additional details on how to save a WAVE file.

**Specifying Desired Flow Rates.** We will design our system to intake the maximum amount effluent produced by the WWTP: ~2,708 m<sup>3</sup>/h. For now, we will assume that the flow rate of water which flows out of the WWTP will equal the flow rate of water that enters the membrane process. Ensure that the “Feed Water” radio box (●) is ticked and set the flow rate in the field below it. Check that your units are correct! Your flowsheet should look like that shown in **Figure 3.3**. If we knew how much treated water we needed to produce, we would set the flow rate of *Product Water* instead. We will look at an example of this in the following chapter.

? You may be tempted to select the “Product Water” radio box instead of the “Feed Water” radio box in this application. Why is it a good idea to select the latter option, here?

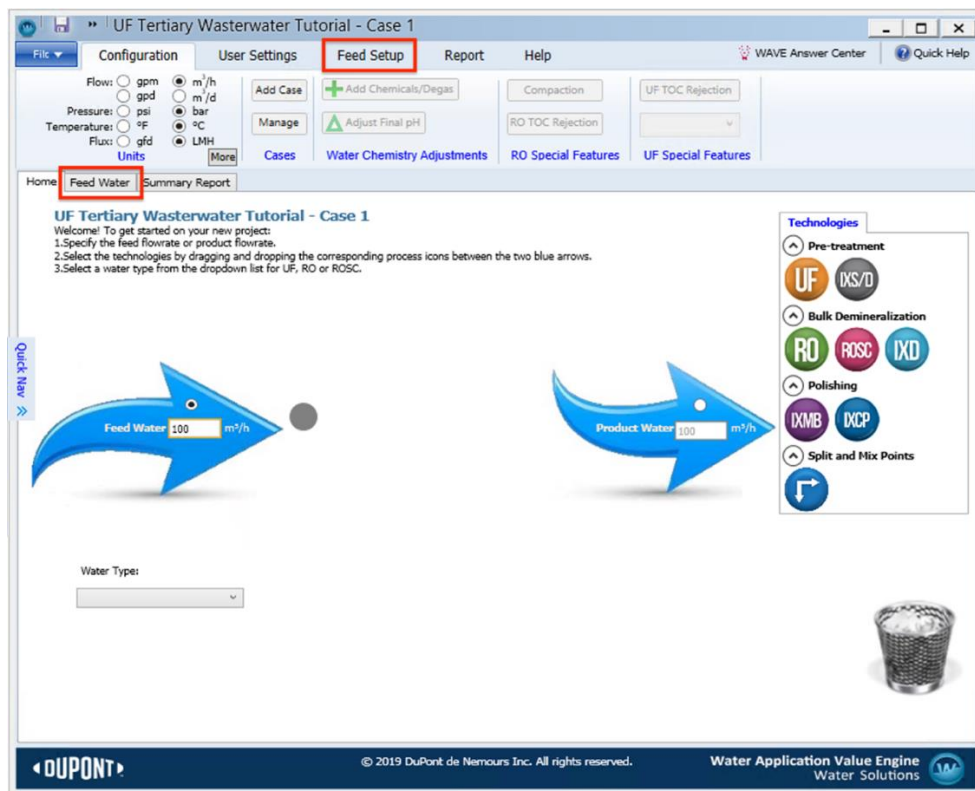


**Figure 3.3:** *Specifying the influent flow rate.*



**Specifying the Feed Water Quality.** We will utilize the *Water Library* feature built into WAVE to specify our feed water quality. Navigate to the *Feed Water* project setting tab or the *Feed Setup* menu tab, as seen in **Figure 3.4**. The contents in *Feed Water* project setting tab will be blank because no information has been input, as seen in **Figure 3.5**. To populate these fields using WAVE’s *Water Library*, click the “Open Water Library” button under the *Feed Setup* menu tab, as highlighted in **Figure 3.5**. A new window will appear titled “Open From Water Profile Library”. As shown in **Figure 3.6**, click the “Open From Library” drop-down menu, select “Wastewater - Tertiary”, and then click “Copy to Feed Water”. You will now see the tables and fields populated in the *Feed Water* project tab. Note that the suggested “Water Sub-type” is based on turbidity and total suspended solids.

WAVE does not have a correlation for the solid content, so we must input the turbidity, TSS and SDI<sup>1</sup>. For this scenario, we will refer to **Table 3.1** for the turbidity, TSS and SDI for our feedwater. After inputting the turbidity, TSS and SDI values, the *Feed Water* project tab should look like that in **Figure 3.7**.



**Figure 3.4:** The “*Feed Water*” and “*Feed Setup*” tab outlined on the main flow sheet.

<sup>1</sup> The SDI is the silt density index – a common water quality metric that is related to how likely the water is in fouling a membrane

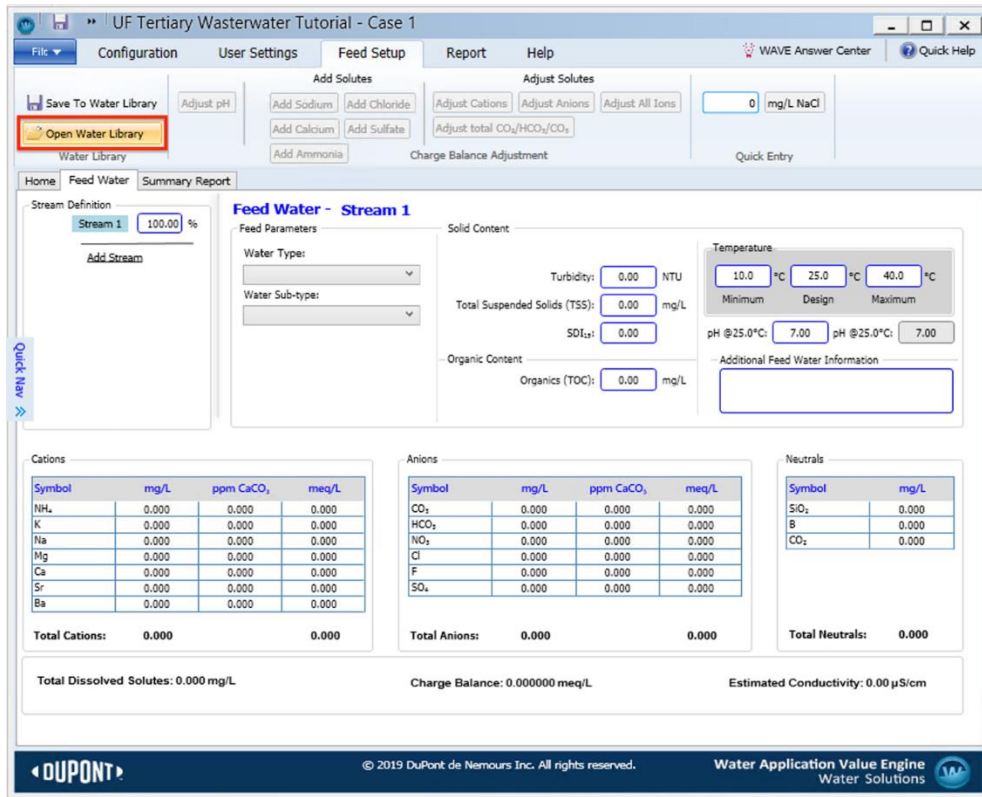


Figure 3.5: Accessing WAVE's Water Library.

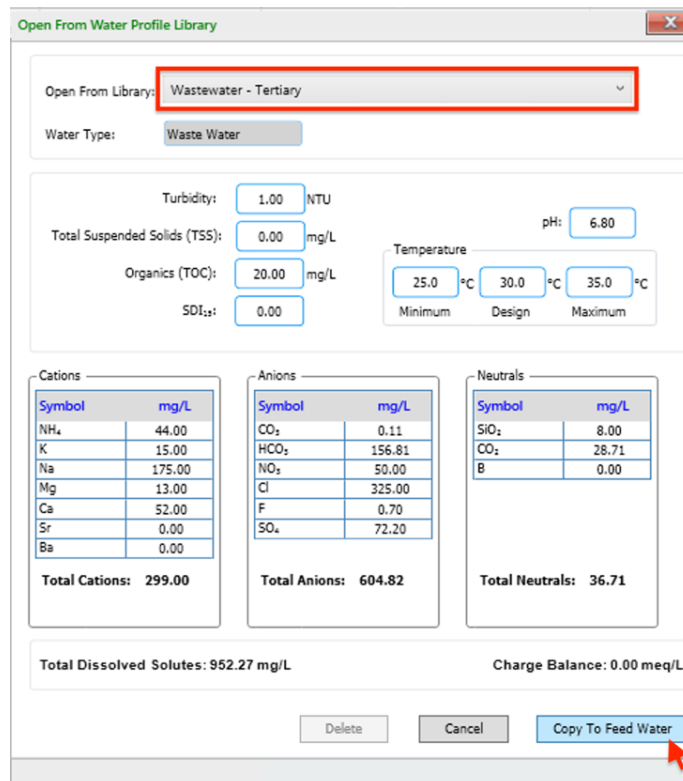
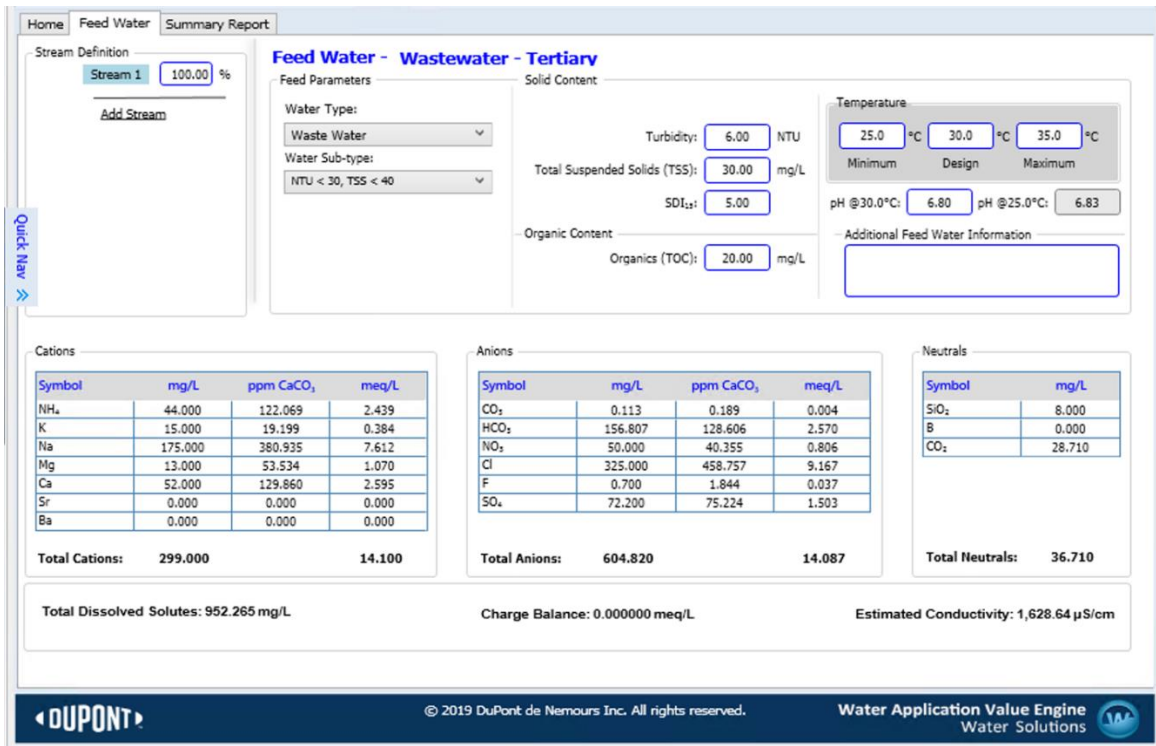


Figure 3.6: The Water Library window where multiple sources of water may be chosen from to be used as the feed water source and can be copied to the Feed Water tab.

**Table 3.1:** Water quality analysis parameters TSS, Turbidity and SDI for tertiary wastewater.

Parameter	Value
Turbidity (NTU)	6.00
TSS (mg/L)	30.00
SDI (-)	5.00



**Figure 3.7:** Assigning water quality parameters to the tertiary wastewater feed stream.

### 3.4 Adding UF Technologies to the Flowsheet

Navigate to the *Home* project tab; your empty flowsheet will be displayed. Locate the orange UF icon in the *Technologies* panel. Drag and drop the icon onto the flowsheet, beside the feed arrow. A gray circle may appear when the UF icon has been dragged to the right location. Notice how a new *Ultrafiltration* project tab appears.

The UF process is now applied onto the flowsheet, as seen in **Figure 3.8**. By adding the UF process to the flowsheet, WAVE applies reasonable parameters for the system and immediately calculates a solution. Unlike other software programs, WAVE automatically computes the results of the simulation after changes are made to the process settings and before the simulation report is viewed. We will now learn how to modify the settings associated with the design and operation of the UF system.



Figure 3.8: Adding a UF system to the flowsheet.

### 3.5 UF Process & Design Specifications in WAVE

Navigate to the new *Ultrafiltration* project tab—you can modify the UF process settings here, as seen in *Figure 3.9*. On the left side of the screen, note the navigation tabs (*Design, Configuration, Backwash, CEB, CIP, Additional Settings*). By default, the *Design* screen is shown with WAVE’s default parameters applied automatically.

**Components of a Membrane System.** Let us go into further detail with regards to the parameters shown in the *Design* screen. Firstly, locate the *UF System Diagram* at the bottom left of the screen, which illustrates the different parts of the UF system’s design, including required equipment, flow rates, pressures, and concentrations. Let us go through the components of each train one-by-one:

- **Strainer.** The strainer on the feed line is a coarse filter designed to remove large aggregates from the feed water before they can reach the membrane modules. This helps prevent fouling and damage to the system. The size of the strainer mesh and its recovery can be defined in the *Strainer Specification* panel above the diagram.

The screenshot displays the 'Design' configuration for an Ultrafiltration system. Key parameters include:

- UF Feed Flow Rate:** Automatic, 2708 m³/h
- Strainer Specification:** Strainer Recovery: 99.5%, Strainer Size: 150 µm
- Filtration TMP Increase:** Backwash: 0.0 mbar/h, Acid CEB: 0.0 mbar/h, Alkali CEB: 0.0 mbar/h, CIP: 0.0 mbar/h, mini-CIP: 0.0 mbar/h
- Design Instantaneous (Gross) Flux and Flow Rates:**
  - Filtrate Flux (for 25 °C): 40.0 (Recommended Range: 1.00 - 75.00 LMH)
  - Backwash Flux: 120.0 (Recommended Range: 100.00 - 150.00 LMH)
  - CEB Flux: 60.0 (Recommended Range: 60.00 - 120.00 LMH)
  - Forward Flush Flow: 1.32 (Recommended Range: 0.00 - 2.50 m³/h/module)
  - Air Flow: 7.0 (Recommended Range: 5.00 - 12.00 Nm³/h/module)
  - CIP Recycle Flow Rate: 1 (Recommended Range: 1 - 4 m³/h/module)
  - mini-CIP Recycle Flow Rate: 1 (Recommended Range: 1 - 4 m³/h/module)
- Design Cycle Intervals:**
  - Filtration Duration: 20 min
  - Acid CEB: 36 h
  - Alkali/Oxidant CEB: 12 h
  - CIP: 30 d
  - mini-CIP: 0 d
  - Membrane Integrity Testing: Offline Time per Train: 0 min/day

The schematic diagram at the bottom shows the flow from a Feed Pump through a Strainer (150 µm) to a CIP Tank (30 L) and then to the UF modules. It also shows the Backwash Pump (BW: 4.0 m³/h / CEB: 2.0 m³/h) and Filtrate Tank (711 m³) components.

Figure 3.9: Settings for the UF system can be heavily customized and adjusted.

- **Membrane Module.** A depiction of a single membrane module is found in the center of the diagram. The specific membrane modules (and its internal elements) that you want to use in your design can be chosen from the *Module Selection* drop-down menu. Note that all the modules are manufactured by Dow/DuPont!

For now, we will leave the membrane module as the Ultrafiltration SFP-2660. A product data sheet for this module can be found here: <https://www.lenntech.com/Data-sheets/Dow-UF-SFD-2660-L.pdf>

The module naming code gives insight to the product specifications. Let us look at the DuPont UF Module SFP-2660. We will break up the module name to further understand the naming convention:

<b>A</b>		<b>B</b>		<b>C</b>		<b>D</b>		<b>E</b>
DuPont UF Module		SFP		2		6		60

**A.** This section of the code outlines the supplier, DuPont, and its intended type of filtration: ultrafiltration.

**B.** This is the application code, which indicates what application the module is used for. There are two options:

- SFP: non-drinking water applications;
- SFD: drinking water applications.

**C.** This is a code to indicate the material of which the membrane is made. The “2” is for polyvinylidene fluoride or polyvinylidene difluoride (PVDF).

**D.** This is the module diameter reported in inches. For the specific module SFP-2660, the module diameter is 6 inches.

**E.** This is the module length reported in inches. For the specific module SFP-2660, the module length is 60 inches.

Additionally, “XP” may be added to the end of the module name to indicate that it is a higher permeability module.


- **Filtrate Tank.** A tank is positioned on the line filtrate (also known as permeate) leaving the membrane module. It acts as both a swing tank and as a reservoir for water with which to backwash the membrane. Backwashing is a frequent (*e.g.* every ~15 mins) process by which foulants and debris on or inside the membrane structure are loosened and removed. Backwashing occurs by pumping filtrate water backwards through the membrane at high pressure for a short period of time (duration ~1 minute). Backwashing parameters can be modified in the *Backwash* tab at the left of the screen. Also, a chemically enhanced backwash (CEB) can be performed where a cleaning chemical (*e.g.* bleach, acid, base) is added to the backwash water to help solubilize foulants and scale. Along with backwashing, CEB is a regularly occurring process (~ daily). These features are accessed

in the *CEB* tab to the left of the screen. There is more to come on these terms and on cleaning procedures!

- **Air Scour.** Like backwashing and other cleaning processes, air scouring is used to maintain long-term membrane performance. This process often occurs every few backwashes. Air scouring settings can be accessed under the *CEB* tab.
- **Cleaning-In-Place Tank.** This tank holds cleaning-in-place (CIP) chemicals dissolved in water. CIP is an occasional process (~ monthly) whereby a membrane module or set of modules are taken offline and CIP solution is pumped into the modules to perform a very thorough cleaning of the entire membrane, such as for the removal of adhered foulants. These settings can be accessed in the *CIP* tab.
- **Pumps.** Several pumps (*e.g.* feed, backwash, CIP) are required to operate each membrane skid/train. Note that the flow rate values associated with the pumps in the *UF System Diagram* are not for any single module or pump: they are the sum of the flow rates in the entire system (*i.e.* across multiple pumps). While the diagram illustrates only one membrane module, the flow values are representative of the entire process.
- **Valves, Split & Mix Points.** The valves and split/mix points required to operate a single module are also indicated in the *UF System Diagram*.

For now, we will leave the process settings at their default values. More on this to come!

The use of periodic backwashing, cleaning processes, and air scouring can help maintain the performance and health of the membranes. The frequency of these maintenance processes are generally dictated by the propensity of the feed water to foul the membranes. These design cycle parameters—as well as the flow rates of air/water—can be tuned in their respective tabs, or in the *Design Cycle Intervals* panel and the *Design Instantaneous (Gross) Flux and Flow Rates* panel of the *Design* tab. Physical experimentation, simulation, literature searches, prior experience, and manufacturer knowledge all play a role in the complex process of choosing operating parameters, as well as the exact membrane manufacturer/module/membrane type/etc.!

 To learn more about individual values on the screen, hover your mouse over the text. A tooltip will appear when available!

**The Configuration Screen.** Now under the *Configuration* tab to the left side of the screen, you can set up the membrane system with regards to numbers of modules and trains, and modules per train. The WAVE software offers recommendations of configurations based on the water quality of your feed as well as the required flow rate. The suggested options can be seen in **Figure 3.10**. Notice that the total number of modules is quite consistent (2,340–2,376) even though the number of trains and modules per train varies. This is because the design requires a certain *total membrane area* to effectively treat the specified influent flow rate of water. This area is almost independent of the arrangement of modules into trains. Now, WAVE requires you to select one of the recommended configurations (or enter your own)—the “default” option is to have only one train

and one module. Check out the operating flux in the *Selected Configuration* panel: 97,095 LMH (L/m<sup>2</sup>/h).

☞ How does this compare to the expected design flux for a single module? Check out the product data sheet here: <https://www.lenntech.com/Data-sheets/Dow-UF-SFD-2660-L.pdf>.

Based on the “default” configuration the calculated flux is massive and unreasonable as all the feedwater is passing through a single module! We need to add more modules to the system. At this point, we do not know what exact configuration of (multiple) modules/trains is best from a design or operational standpoint, so let us select a reasonable middle-ground option: Option 6, with 18 trains and 130 modules/train (2,340 total modules). Double-click on that row in the table to populate the *Selected Configuration* panel. Now the operating flux through a given membrane is 40 LMH—much more reasonable!

Each specific membrane module has a maximum operating flux. If the operating flux is greater than modules maximum operating flux, WAVE will warn us when we review the summary report, more on this later to come. Now, how does the operating flux compare to the expected design flux for a single module?

Note that there is a cost trade-off when choosing the number of trains and number of modules per train: each train tends to have its own pumping system and tanks for CIP/CEB. Increasing the number of trains increases the capital costs as you need more pump/tanks/piping/valves/etc. But, with more trains, you obtain greater operational flexibility (*e.g.* for maintenance) and perhaps a lower operating cost too.

The screenshot shows the WAVE software interface with the 'Configuration' panel selected. The 'Selected Configuration' panel shows: Online Trains: 1, Standby Trains: 0, Redundant Trains: 0, Total Trains: 1, Modules/Train: 1, Total Modules: 1, and Operating Flux: 97095 LMH. Below this is a table of 'Recommended Configurations' with 8 options. A red box highlights the table. The table columns are: Option, Online Trains, Standby Trains, Total Trains, Max Offline BW/CEB, Modules/Skid, Skids/Train, Modules/Train, Online Modules, and Total Modules.

Option	Online Trains	Standby Trains	Total Trains	Max Offline BW/CEB	Modules/Skid	Skids/Train	Modules/Train	Online Modules	Total Modules
1	13	0	13	5	-	-	180	2340	2340
2	14	0	14	5	-	-	168	2352	2352
3	15	0	15	5	-	-	156	2340	2340
4	16	0	16	6	-	-	148	2368	2368
5	17	0	17	6	-	-	138	2346	2346
6	18	0	18	6	-	-	130	2340	2340
7	19	0	19	7	-	-	124	2356	2356
8	20	0	20	7	-	-	118	2360	2360

**Figure 3.10:** WAVE suggests various configurations in terms of number of modules and number of modules per train. WAVE arranges the options in order of increasing number of trains and decreasing modules per train. The options are not arranged in order of preference.

Back on the *Design* navigation tab, check out the gray box at the top left of the *UF System Diagram*. The operating parameters have now been adjusted for our choice of configuration. In particular, note the UF System Recovery value: 81.4%. What does this mean? Consider the *Feed Water*, *Net Filtrate* and *Waste* stream flow rates on the diagram: approximately 81% of the feed water is filtered through the membrane and enters the filtrate stream. The other ~19% is rejected to the waste concentrate stream. What does this mean in terms of the operation of the process? What happens to the 500.2 m<sup>3</sup>/h of water that is “wasted”? Some other process must be used to deal with the rejected concentrate stream—perhaps a settling pond or a second UF process. Or perhaps, the water is recycled back to the start of the process. At the end of this chapter, we will attempt to improve the recovery of water by optimizing the system.

### 3.5.1 Backwashing, CEB, CIP & Additional Settings

Let us go through the additional navigation tabs that are offered for the UF membrane. First, we will define some additional terms to improve our understanding of fouling and the typical cleaning procedures used to help mitigate fouling.

Fouling can deteriorate many aspects of membrane performance: some of the signs of fouling include loss of capacity, decrease in permeability, and increase in transmembrane pressure (TMP). There are four main types of fouling that can occur:

**Inorganic/Precipitation Fouling or Scaling.** This type of fouling is caused by metal salts. These species are dissolved in the feedwater and their concentration increases (*i.e.* past solubility limits) as the membranes filter feedwater. Once the saturation concentration is exceeded, the salts precipitate on surfaces and can scale the membrane surface. This does not happen often in UF because the salt ions easily permeate through the larger membrane pores.

**Particle Fouling.** This type of fouling refers to non-biological particles such as silt or clay that deposits on the membrane surface and can block or clog the membrane pores.

**Biological and Microbial Fouling.** This type of fouling occurs as a result of microorganisms such as bacteria or algae attaching and growing on the membrane surface. The microorganisms excrete a gel-like polymeric based substance, called extracellular polymeric substance (EPS) or biofilm, that can significantly block the membrane pores.

**Organic Fouling.** This type of fouling occurs when carbon-based macromolecules and compounds deposit onto the membrane surface. Typical carbon-based materials are found in plant and animal material. Naturally-occurring humic and alginic substances are common organic membrane foulants.

It is important to tailor your type of cleaning to the type of fouling that is present. For example, acids are often used to clean inorganic scale, and bases are often used to strip away organics. Note that it is possible for multiple types of fouling to occur simultaneously. Therefore, more than one of the methods below can be used in tandem for cleaning (*i.e.* backwashing then air scouring and repeat). Let us describe the cleaning methods in more detail and introduce some additional terms.



**Air Scouring.** Air is introduced at the bottom of the module to allow the air bubbles to rise to the top of the module and in the process dislodging and loosening any foulants on the outside of the membrane surface (~20 – 30 seconds). The dislodged material is removed by draining the modules after the air scouring is complete. Air scouring is usually followed by backwashing the membrane.

**Backwashing.** Is the process where water, usually the UF permeate, is pumped in the opposite direction through the membrane to remove and dislodge foulants that may be present on the membrane surface. This is a physical cleaning and occurs automatically approximately every 5 – 15 minutes depending on the foulants present in the feedwater.

☞ Check out this video on backwashing, notice the change in direction of flow. Find the link to the video here: <https://www.youtube.com/watch?v=Upm2KBHgbo>

**Chemically Enhanced Backwash (CEB).** This is the same process of a backwash, except that chemicals are injected into the water used to backwash and is therefore considered to be a chemical cleaning. The frequency of CEB is determined by the feedwater quality, where high quality feedwater will require less frequent CEBs. DuPont suggests a frequency of 1–7 days for a CEB. Typical chemicals used for CEB include acids—such as hydrochloric acid (HCl) and sulphuric acid (H<sub>2</sub>SO<sub>4</sub>)—that remove colloids and inorganic salts. Alkali chemicals are also used—such as sodium hydroxide (NaOH) and sodium hypochlorite (NaOCl)—that remove organics and bio-foulants. The choice of chemicals and dose are dependent on the foulants present in the feed water.

☞ Check out this video on CEB; notice the chemical injection site. Find the link to the video here: <https://www.youtube.com/watch?v=RnjiABNg5aI>

**Clean-in-Place (CIP).** A CIP is a more vigorous cleaning process than the CEB and is completed when the train is offline. This process involves an initial backwashing step, then a chemical clean where the cleaning solution is recycled/circulated within the system for some time (~ 1 hour), then the modules are soaked in the solution without any circulation (~ 2 hours) prior to performing a final backwash. The chemicals can be heated to increase the effectiveness of the CIP. Typical chemicals used in a CIP are acids and alkalis. Typical acids include hydrochloric acid (HCl), sulphuric acid (H<sub>2</sub>SO<sub>4</sub>), oxalic acid and citric acid. Typical alkalis again include sodium hydroxide (NaOH) and sodium hypochlorite (NaOCl). Unlike CEB, the CIP does not occur automatically. Instead, CIP is performed as needed and is determined by monitoring performance parameters like the transmembrane pressure (TMP). A typical “rule of thumb” outlined by DuPont is to trigger a CIP when the TMP becomes 1 bar (or 14.5 psi) greater than the initial TMP of new, unfouled membranes. DuPont provides a general range of how often a CIP should be performed, which can range from every 1–12 months.

☞ Check out this video of a CIP being performed on a module here: <https://www.youtube.com/watch?v=IRDR4-1VQLE>

Notice in the video linked above that the CIP tank contains the cleaning chemicals, and the chemical circulation is followed by a chemical soak, and then a filtrate backwash.

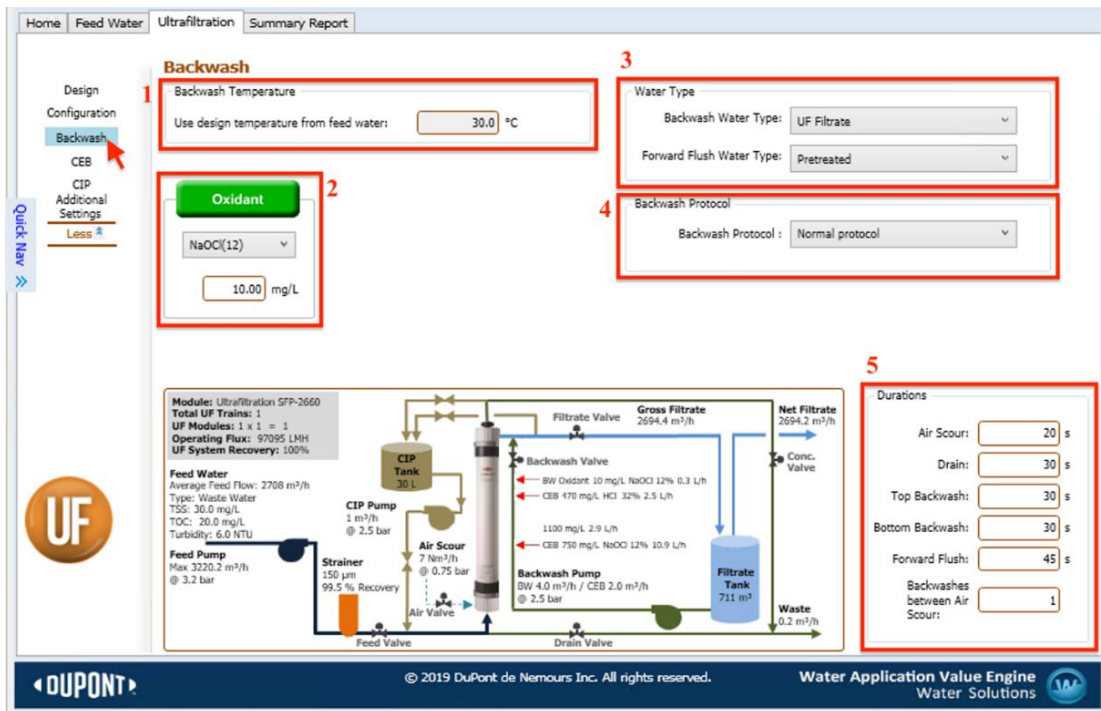
As mentioned earlier, WAVE has additional tabs where users can edit the parameters for *Backwash*, *CEB*, *CIP* and *Additional Settings*. Let us look at these tabs in more detail.

① For additional details about these tabs consult the WAVE user manual which can be accessed here: <https://www.dupont.com/Wave/Default.htm>

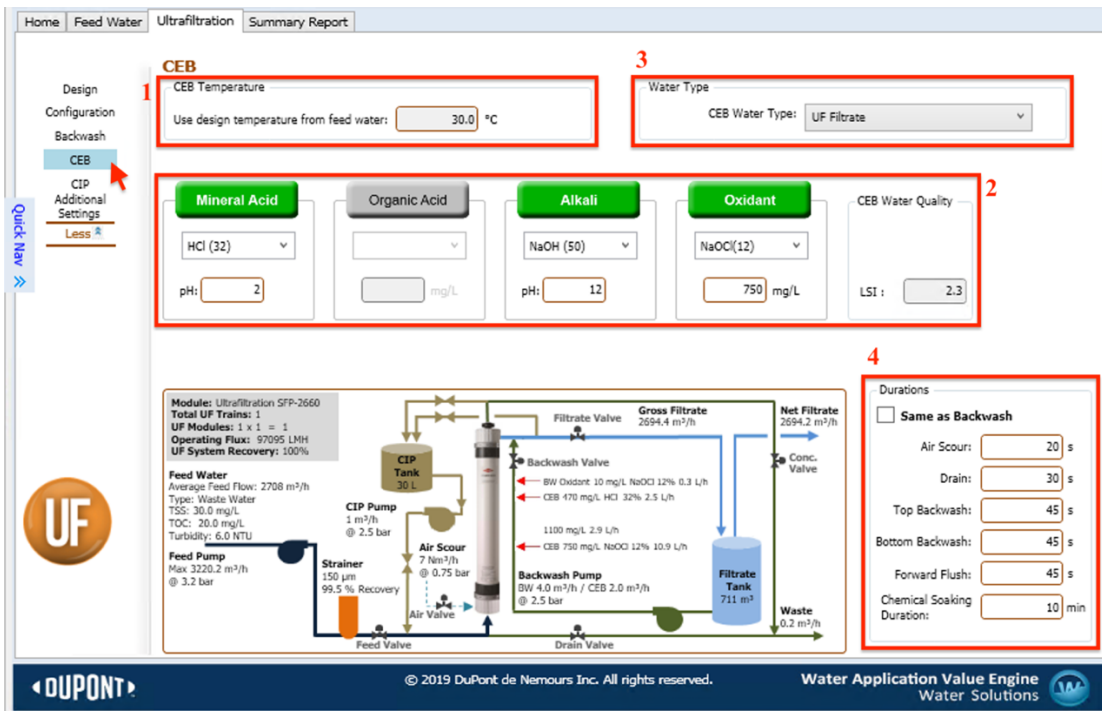
**The Backwash Tab.** This tab allows you to change specifications associated with backwashing. There are five main categories in which the backwashing specifications can be altered. *Figure 3.11* outlines the five sections that can be modified.

**CEB tab.** This tab allows the user to modify the CEB specifications. There are four main sections that the user can modify, as seen in *Figure 3.12*.

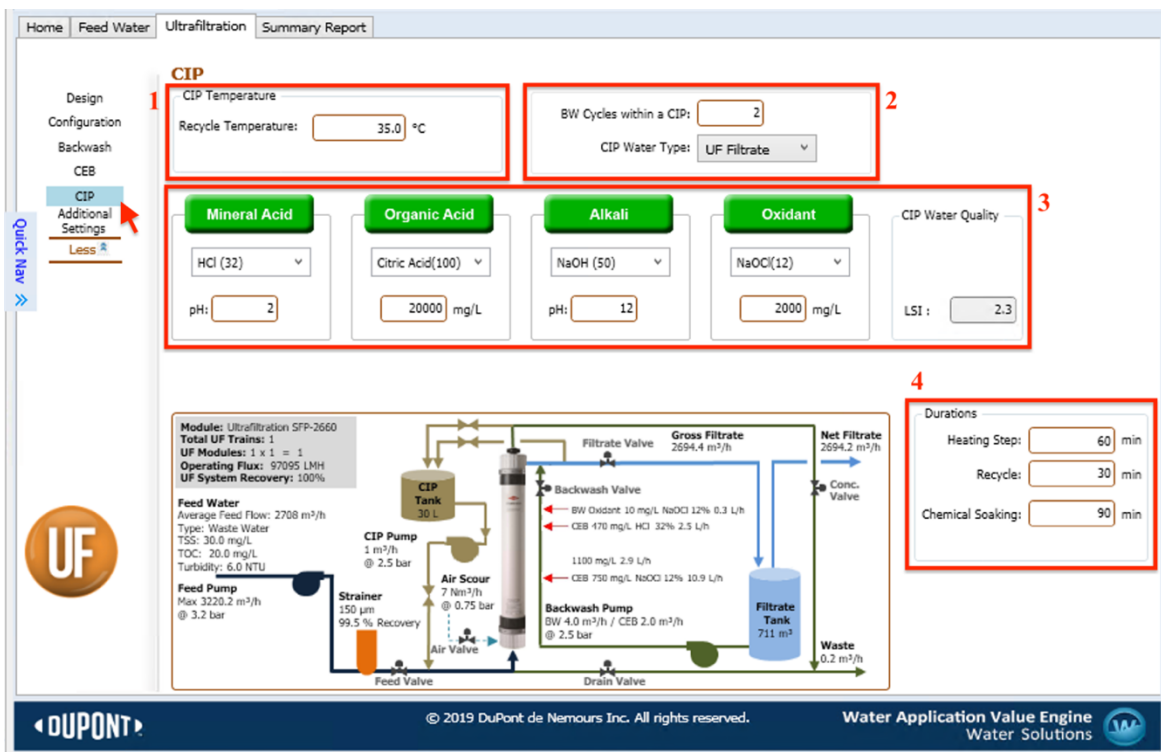
**CIP Tab.** Similar to the backwash and CEB tab, the user can modify the CIP specifications. There are four main sections that the user can modify. *Figure 3.13* outlines the four main sections that can be modified.



**Figure 3.11:** The backwash tab on WAVE allows the user to adjust settings in five categories including: (1) backwash temperature, (2) oxidant addition, (3) water type, (4) backwash protocol, and (5) durations.



**Figure 3.12:** The CEB tab on WAVE allows the user to adjust settings in four categories including: (1) CEB temperature, (2) chemical addition, (3) water type, and (4) durations.



**Figure 3.13:** The CIP tab on WAVE allows the user to adjust settings in four categories including: (1) CIP temperature, (2) CIP water type and BW cycles, (3) chemical addition, and (4) durations.

We will briefly go through each section that can be modified throughout these three tabs.

**Backwash & CEB temperature.** By default, WAVE uses the design temperature of the feedwater, which was specified by the user in the *Feed Water* tab in the *Temperature* panel. This temperature cannot be changed on the backwash tab but can be updated via the design temperature.

**CIP Temperature.** WAVE allows the user to specify the temperature of the chemical solution being recycled during the CIP. To change the temperature, simply enter the desired temperature in the “Recycle Temperature” field in the CIP temperature panel. The CIP recycle temperature can range from 1–40°C. The upper limit exists because high temperature can damage the membranes.

**Backwash Oxidant.** An oxidant can be added during backwashing to aid in the cleaning process. In our case the default is 10 mg/L of sodium hypochlorite (NaOCl). The type of oxidant and its dose can be updated by the user. To deactivate the oxidant, simply click the green oxidant box and it will turn grey when deactivated.

**CEB and CIP Mineral Acid, Organic Acid, Alkali, Oxidant Selection and Dose.** WAVE allows the user to specify the chemical type and dosage for CEBs and CIPs. To change the defaulted chemicals and dose, click the name of the desired addition. The chemical does can be activated/deactivated by clicking the chemical box, it will be green when it is activated and grey when it is not activated. For each addition, the user can click the drop-down menu to select the desired chemical from the list. Depending on the desired addition, the user can specify the dose in mg/L for organic acid and oxidants, or target pH for mineral acids and alkali. The CEB and CIP water quality box will indicate the Langelier Saturation Index (LSI) or Stiff & Davis Stability Index (S&DI) depending on the TDS in the feedwater. The LSI is applicable for feedwater with less than 10,000 mg/L TDS, whereas the SDI is applicable for feedwater with greater than 10,000 mg/L TDS.

**Backwash, CEB and CIP Water Type.** WAVE gives users the ability to choose the source water type for each cleaning procedure by clicking the drop-down menu.

**Backwash Protocol.** The backwash protocol can be chosen from the drop-down menu and in our case, defaults to “Normal protocol” as the only option available.

**BW Cycles within a CIP.** WAVE allows the user to choose the number of backwashes within a CIP. The default is two backwashes in a CIP.

**Durations.** WAVE provides default durations for steps during a backwash, CEB and CIP. The backwash durations include air scour, drain, top backwash, bottom backwash, forward flush, and the number of backwashes between air scours. The CEB durations include air scour, drain, top backwash, bottom backwash, forward flush, and chemical soak duration. The user has the ability to choose “same as backwash”, which will copy the durations from the backwash tab. Lastly, the CEB durations include the heating step, the chemical recycle step, and the chemical soaking step. The default values are based on the feed water and sub

water type. The user can change these durations in their corresponding fields. These exact values for these parameters are based on experimentation and a lot of experience.

Note that DuPont defines the following CIP duration terms as follows:

- **Heating Step:** the time in a CIP cycle that is required to heat up the chemicals from the initial temperature (design temperature) to the final temperature (CIP recycle temperature).
- **Recycle:** the time that the chemical solution is recycled through the UF modules.
- **Chemical Soaking:** the time that the UF modules are soaked in each chemical.

Furthermore, WAVE allows the user to change additional settings such as pressure settings, tank storage and size factors, power settings and valves.

### 3.6 Interpreting the UF Report

Let us view the results from the simulation of the UF system as it stands currently. Navigate to the *Summary Report* tab in the project tabs. Now, WAVE will automatically calculate the remaining design and operating parameters from the information that has been provided to the software.

WAVE divides the results into four categories: UF System Overview, UF Operating Conditions, UF Water Quality, and UF Design Warnings. Let us go through each category and interpret the results.

! Like in other software packages, WAVE may at times display an error that the simulation cannot converge. This restricts you from viewing the summary report. If this is the case, ensure that your design parameters are as specified in this courseware. Otherwise, restarting the software can help to clear previous solutions from the software's memory and may enable convergence.

**UF System Overview.** This table provides general information for the designed system such as the number of trains, number of modules, the system and train flow rate, the system recovery, the TMP and utility water. In our case we have 18 trains at an average TMP of 0.22 bar (at 25°C) and a system recovery of 81.44% as seen in *Figure 3.14*.

**UF System Overview**

Module Type	Ultrafiltration SFP-2660	
# Trains	Online = 18	Standby = 0
		Redundant = 0
# Modules	Per Train = 130	Total = 2340
System Flow Rate (m <sup>3</sup> /h)	Gross Feed = 2708.0	Net Product = 2194.3
Train Flow Rate (m <sup>3</sup> /h)	Gross Feed = 150.4	Net Product = 121.9
UF System Recovery (%)	81.44	
TMP (bar)	0.22 @ 25.0 °C	0.20 @ 30.0 °C
Utility Water	Forward Flush: Pretreated water	Backwash: UF filtrate water

**Figure 3.14:** A portion of the Summary Report, the UF System Overview, providing general details of the designed system such as the system recovery, in this case the system recovery is 81.44%.

**UF Operating Conditions.** This table gives insight into each cycle. It provides users with a summary of each cycle’s duration, interval, and flux. In our case we can see that the filtration cycle has an average flux of 34 LMH (L/m<sup>2</sup>/h) as seen in **Figure 3.15**.

**UF Water Quality.** This table compares the feedwater versus the expected UF product water quality for a few parameters to determine if the proposed design is sufficient. For our case, the UF water quality can be observed in **Figure 3.16**.

- Turbidity has decreased from 6 NTU to less than 0.1 NTU.
- All the TSS has been removed.
- The TOC content has decreased from 20 to 18 mg/L of TOC. The remaining TOC is most likely a dissolved fraction that has passed through the UF membranes. We will deal with TOC rejection in more detail, soon.
- The SDI has decreased from 5 to less than 2.5.
- The dissolved solids content, TDS, remains unchanged at 952 mg/L!

**UF Operating Conditions**

	Duration	Interval	Flux/Flow
Filtration:	20.0 min	23.1 min	-
Instantaneous			
18 Online Trains			40 LMH
18 Total Trains			40 LMH
Average			34 LMH
Net			28 LMH
Backwash	3.1 min	23.1 min	120 LMH
Acid CEB	15.8 min	36 h	60 LMH
Alkali CEB	15.8 min	12 h	60 LMH
CIP	311.3 min	30 d	1.00 m <sup>3</sup> /h

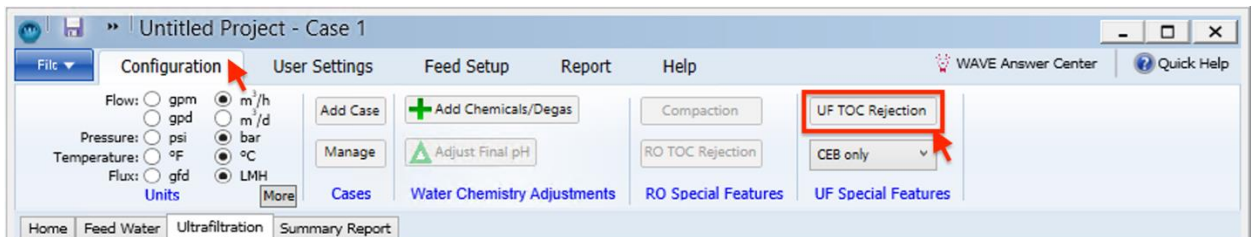
**Figure 3.15:** A portion of the Summary Report, the UF System Overview, providing general details on the operating conditions of the designed system, this specific system has an average flux of 34 LMH.

**Critical Point:** When we look at the TOC rejection value output by the software, it is critical to note that WAVE cannot actually theoretically calculate rejection. WAVE uses a default value of 10% rejection for all cases! The user can input their own system specific TOC rejection based on experiments conducted. Therefore the TOC rejection does not change when other system parameters are updated. Navigate to the “UF Special Features” section on the *Configuration* menu bar at the top of the screen, and click the “UF TOC Rejection” button as seen in **Figure 3.17**. The TOC rejection can be changed accordingly, by updating the field as seen in **Figure 3.18**. Therefore the user must specify their own TOC rejection, but for this example we will use the default value.

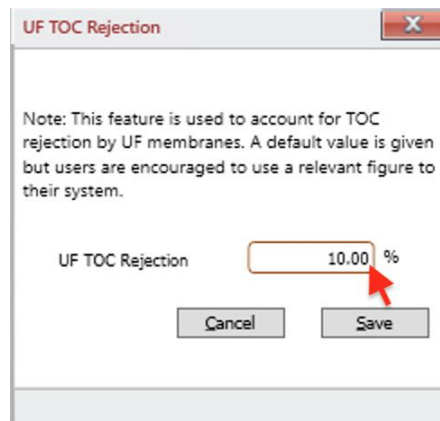
### UF Water Quality

Stream Name	Wastewater - Tertiary	
Water Type	Waste Water (25.0 - 35.0 °C)	
	Feed	Expected UF Product Water Quality
Temperature (°C)	30.0	30.0
Turbidity (NTU)	6.0	≤ 0.1
TSS (mg/L)	30.0	-
Organics (TOC) (mg/L TOC)	20.0	18.0
SDI <sub>15</sub>	5.0	≤ 2.5
TDS (mg/L)	952	952
pH	6.8	6.8

**Figure 3.16:** Water quality report for the UF system (Dow SFP-2660) treating tertiary municipal wastewater.



**Figure 3.17:** Accessing the UF TOC rejection feature in WAVE.



**Figure 3.18:** Users have the ability to update the UF TOC rejection in WAVE.

? Take a moment to think and ask yourself why the TDS did not change. How would you remove the remaining TDS?

**UF Design Warnings.** This table presents any design warnings by providing the type of design warning with the parameter's estimated value versus the limit. In our case, we currently have no design warnings. This may not always be the case. It is also important to understand that even though there are no design warnings, it does not mean we cannot improve our design.

Now let us look at the detailed report. Refer to **Section 2.6** on how to generate a detailed report. In addition to the content from the summary report, the detailed report contains the following tables: UF Configuration Options, UF System Size and Module Details, UF Flow Details, UF Pump Hydraulics and Electricity Cost, UF Pressure Ratings, UF Storage Tanks, Filtration Mode and Backwash Parameters, and UF Utility and Chemical Costs. As you can see the detailed report contains an extensive amount of information. Let us investigate some of this information to further analyze our design.

Make your way to the bottom of the detailed report and look at the specific water cost: it is 0.213 \$/m<sup>3</sup>. The specific water cost is the cost to produce one cubic meter of treated water. The costs encompassed in the specific water cost are electricity costs, chemical costs, and service water costs, which are all outlined in the detailed report. Notice that in this case, the majority of the cost comes from the service water cost, which is associated with handling the concentrate stream. We will attempt to optimize our system to recover more water and reduce the total amount of concentrate.

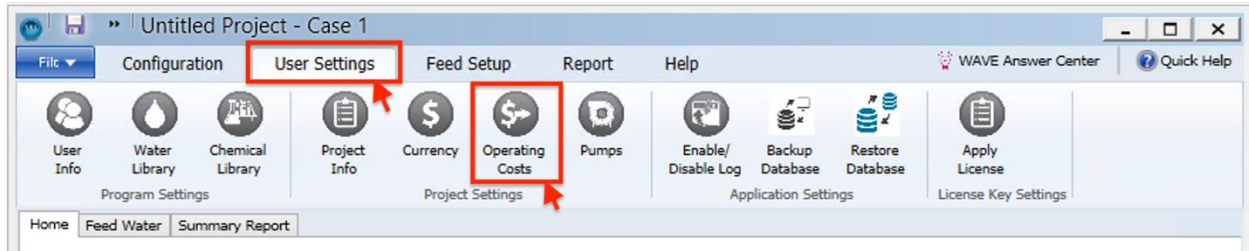
Note that these costs are calculated using WAVES default operating costs. The user has the ability to change the default operating costs by clicking the *Operating Costs* icon in the "Project Settings" section of the *User Settings* menu tab as seen in **Figure 3.19**. A new window will appear titled "Project Operating Costs" (**Figure 3.20**) where the user has the ability to update any operating cost by changing the value in the corresponding field. For now, we will leave the default values, but this is a great way to predict operating costs more accurately if specific costs are known.

☞ At this point save your current file as the original file. We will be modifying our scenario and will be analyzing and comparing our results to other scenarios

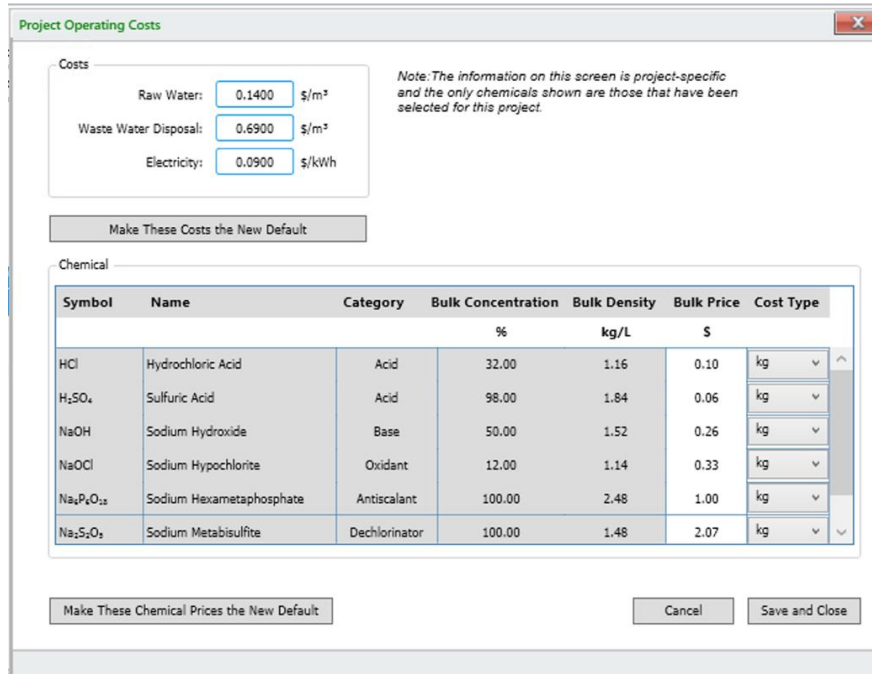
**Addressing Design Warnings.** We are going to introduce warnings into the system to learn how to deal with them. Recall when we were selecting the configuration and WAVE gave a default of one train and one module with a flux of 97,095 LMH.

☞ To avoid overwriting the working the system that we have built already, create and save a new file to test run the default configuration of one train and one module.





**Figure 3.19:** Accessing operating costs in WAVE.



**Figure 3.20:** WAVE allows users to update default costs for electricity, water disposal and chemicals.

Now, navigate to the summary report and look at all the design warnings at the bottom! Let us look at one as an example, it reads:

1. “Filtration Cycle: Filtration Flux > Max (LMH)”: this is indicating that the operating flux is greater than the max limit of 75 LMH: it is actually calculated to be 97,095 LMH.

The flux is calculated using the following equation:

$$J = \frac{Q_P}{A} \quad (3.1)$$

where  $J$  is the flux of the system in LMH (L/m<sup>2</sup>/h),  $Q_P$  is the permeate flow in L/h, and  $A$  is the membrane surface area in m<sup>2</sup>.

Based on Equation 3.1, the flux and area are inversely proportional. Therefore, the default configuration of one module and one train has a small membrane surface area of 33 m<sup>2</sup> (355 ft<sup>2</sup>) and a large operating flux of 97,095 LMH. By increasing the number of modules and thus the total

membrane surface area,  $A$ , the flux decreased to a reasonable value below the maximum filtration flux which is 75 LMH.

The remaining design warnings are a result of exceeding the guideline design limits, which are based on the “Water Sub-type” that is selected on the *Feed Water* tab.


### 3.7 Chapter Questions

#### Question 1.

Sketch a UF configuration with a single train consisting of three skids and three modules per skid. Sketch the configuration in both series and parallel. Label your diagram indicating the train, skids, and modules. How many modules are there in total?

#### Question 2.

What can you determine about the DuPont UF Module SFD-2880 just by looking at its name? Verify this by using the product data sheet and confirming the module specifications.

 The product data sheet can be found here:  
<https://www.dupont.com/content/dam/dupont/amer/us/en/water-solutions/public/documents/en/45-D01048-en.pdf>

#### Question 3.

Consider the original chapter example to complete this question. We used the default module, the DuPont UF Module SFP-2660. Is there a different module that would yield greater recovery? If so, replace it to optimize the system and save this as a new file. Take this opportunity to explore the membrane module options that DuPont has to offer. Is the removal of the solids content affected? What about the associated electricity costs, chemical costs, service water costs and the specific cost of water?

#### Question 4.

Using the original chapter example, investigate the relationship between filtration duration and system recovery. Navigate to the *Design* screen on the *Ultrafiltration* tab and locate the *Design Cycle Intervals* panel on the bottom right hand corner. Alter the filtration duration by 5-minute increments ranging from 15 to 35 minutes. Monitor the system recovery as you change the filtration duration. What do you observe? Are there any consequences or benefits when having an extreme scenario such as a short or long filtration duration? Explain your results.

Filtration Duration (min)	System Recovery (%)
15	
20	
25	
30	
35	

-End of Chapter-

### Works Cited

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- [2] G. Tchobanoglous, J. Darby, K. Bourgeois, J. McArdle, P. Genest, and M. Tylla, “Ultrafiltration as an advanced tertiary treatment process for municipal wastewater,” *Desalination*, vol. 119, no. 1–3, pp. 315–321, Sep. 1998 [Online]. Available: [https://doi.org/10.1016/S0011-9164\(98\)00175-1](https://doi.org/10.1016/S0011-9164(98)00175-1).
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**Chemical Engineering 4M03:  
Industrial Separations Processes  
Introduction to the WAVE Design Software**

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**Custom Courseware – Chapter 4**



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*Revision: R8*

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## 4. Design & Simulation of Reverse Osmosis and Nanofiltration

### Chapter #4 will introduce the following information:

- Designing reverse osmosis system using DuPont's steps
- Simulating reverse osmosis systems
- Choosing reverse osmosis parameters
- Interpreting the results of the reverse osmosis simulation
- Addressing simulation design warning messages

Reverse Osmosis (RO) is used in a variety of applications such as seawater desalination, industrial process water, wastewater treatment, and the concentration of dairy products. In this chapter, we will use RO membranes to reject small “dissolved” species and produce highly purified product water.

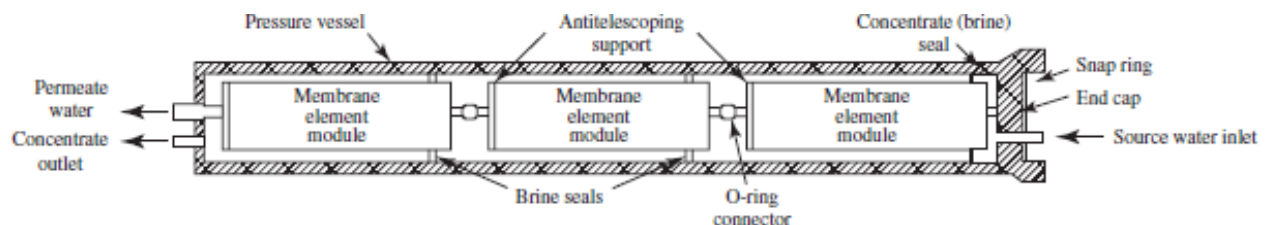


For clarification, the term “dissolved” in this context (*i.e.* versus *suspended* solids) does not literally mean that the particles themselves are actually dissolved, like salt ions. While a large fraction of “dissolved” solids are indeed ions, this category includes organic species which may be very small colloids and are not by necessity solubilized!

### 4.1 Background

Before we learn to simulate RO processes, let us consider a few additional terms related to the arrangement of membranes in RO systems:

- **Element:** like the *module* in a UF system, an element is the smallest “membrane unit” in a RO process.
- **Pressure Vessel (PV):** a container for one or more *elements* that are arranged in series. A cross section of three elements in series within a single pressure vessel can be seen in *Figure 4.1*.

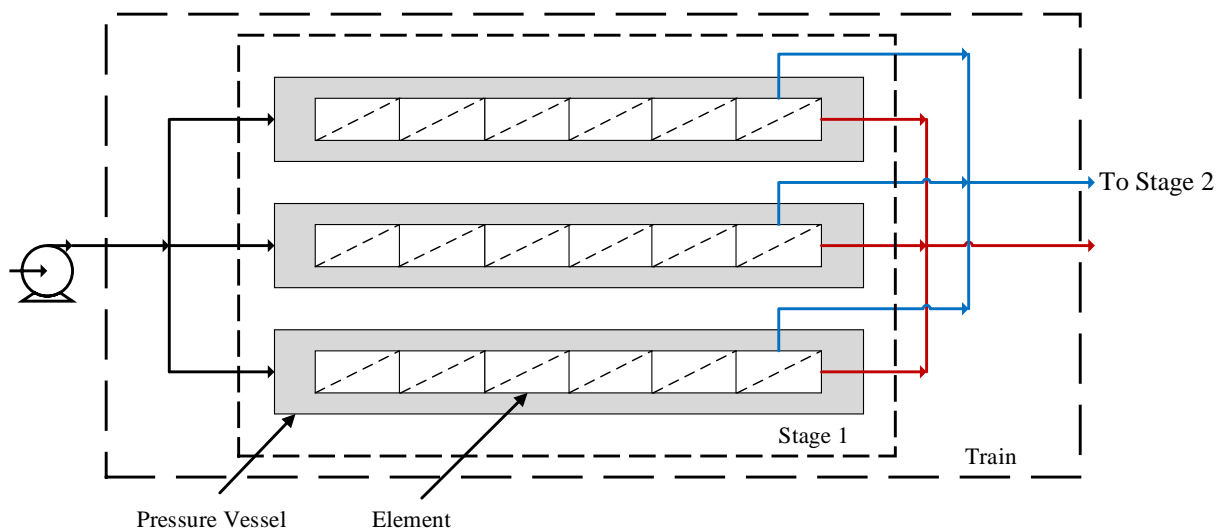


**Figure 4.1:** The cross section of a pressure vessel with spiral wound elements. Original Source: U.S. AID, 1980. Sourced from: Mackenzie L. Davis, Ph.D., P.E., BCEE. *Water and Wastewater Engineering: Design Principles and Practice, Second Edition*.

- **Train:** like UF processes, trains in RO systems are self-contained arrangements of PVs with the necessary process equipment (e.g. pumps, tanks, etc.). The relationship between an element, pressure vessel and train can be seen in **Figure 4.2**.
- **Passes:** in a multiple-pass system within a *train*, permeate water from the first pass becomes the feed water in the second pass, and so on. Passes are used to improve the permeate water quality. The first image in **Figure 4.3** displays a three-pass system.
- **Stages:** in a multiple-stage system within a *train*, the first stage *retentate* becomes the second stage feed water, and so on. Stages are used to concentrate retentate water further and/or obtain a greater water recovery. The second image in **Figure 4.3** displays a three-stage system in comparison to a three-pass system.
- **Array:** an array is defined as multiple *stages*. Therefore, the three-stage system in **Figure 4.3** is an array because it has more than one stage.

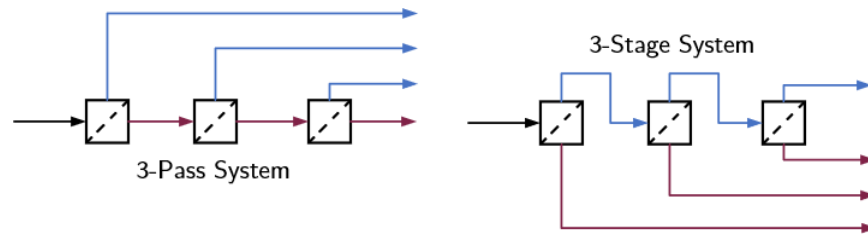
① For additional information, refer to Chapter 9 of the textbook “The Water and Wastewater Engineering: Design Principles and Practice” written by Mackenzie Davis. It is accessible via the following link: <https://www.accessengineeringlibrary.com/content/book/9781260132274>

① If you do not have access to this site, you may request a free trial for Access Engineering here: [https://learn.mheducation.com/ACE\\_FreeTrialRequest.html](https://learn.mheducation.com/ACE_FreeTrialRequest.html).



**Figure 4.2:** Illustration of the relationship between element, pressure vessel, stage and train for an RO system. In this diagram the stage has three pressure vessels in parallel containing six elements in series for a total of  $3 \times 6 = 18$  elements in the first stage. Feed streams are coloured in black, permeate streams are coloured in red, and concentrate streams are coloured in blue.





**Figure 4.3:** Examples of 3-pass (left) and 3-stage (right) RO systems. The separator symbol in this case represents the elements inside the pressure vessels. Feed streams are coloured in black, permeate streams are coloured in red, and concentrate streams are coloured in blue.

It is important to understand the governing equations for passive membrane transport: the relationship between the concentration gradient, hydrostatic pressure, and fluxes are represented by the Kedem–Katchalsky (K–K) equations. These equations are beyond the scope of this courseware.

🔗 For more information on the K–K equations check out the following article:  
[https://doi.org/10.1016/S0376-7388\(00\)00367-7](https://doi.org/10.1016/S0376-7388(00)00367-7).

Now that you have a basic understanding of the components in a RO system and we know the terminology, the challenge is now designing the system. The Dow Chemical Company (DuPont) outlines steps to follow when designing a RO membrane system. The detailed steps can be found in their WAVE academy Webinar “Reverse Osmosis Basics” and in Section 3.11 of the “FilmTec™ Reverse Osmosis Membranes Technical Manual”. Additionally, Chapter 8 of the textbook titled “Membrane Technology for Water and Wastewater Treatment in Rural Regions” written by Rosalam Sarbatly outlines the steps to design a membrane system (from the DOW chemical company in 2019).

📌 As mentioned earlier, Dow (DuPont) produces excellent webinars. They provide a great webinar titled “Reverse Osmosis Design Basics” led by Scott Beardsley. It is highly recommended to supplement this chapter. The webinar can be accessed here:  
<https://gateway.on24.com/wcc/gateway/dowwaterandprocessso/906323?showId=906323&showCode=dowwaterandprocessso&partnerref=LP>

The steps to design a membrane system are outlined in section 3.11 of the FilmTec™ Reverse Osmosis Membranes Technical Manual and can be found here:  
<https://www.dupont.com/content/dam/dupont/amer/us/en/water-solutions/public/documents/en/45-D01504-en.pdf>

The steps to design a membrane system are outlined in Chapter 8 (pages 204 – 208) of “Membrane Technology for Water and Wastewater Treatment in Rural Regions” written by Rosalam Sarbatly and can be accessed here: <https://www-igi-global-com.libaccess.lib.mcmaster.ca/gateway/book/237021>

A slightly modified version of the steps to designing a membrane system are briefly outlined below.

**Step 1.** Define the scope for the membrane system of interest. This includes the feedwater source and composition, required permeate flow and quality, and the system recovery. The system recovery is defined as the fraction or percent of permeate flow produced from the feed flow, as shown in the following equation:

$$\text{System Recovery (\%)} = \frac{\text{Permeate Flow}}{\text{Feed Flow}} \times 100\% \quad (4.1)$$

**Step 2.** Determine the configuration of the system. The system may be plug flow or be a concentrate recirculation system. Plug flow indicates that the water passes once through the system, whereas a concentrate recirculation system indicates that the concentrate is being recycled to the beginning of the pass/stage. Membrane processes are commonly continuous but a batch process may be used in certain applications. Batch processes are commonly used in the pharmaceutical industry and the food and beverage industry.

**Step 3.** Choose the appropriate membrane element. DuPont offers many FilmTec™ element types depending on the application. A general rule of thumb they suggest is based on the TDS of the feed water as seen in **Table 4.1**. Additional parameters to consider are the energy requirements, element length, diameter, and the spacer thickness (for spiral-wound geometry).

**Step 4.** Determine the average membrane flux. This can be found from the manufacturer; DuPont provides design guidelines and suggests average flux ranges for their FilmTec™ elements based on feed water source and pretreatment.

① “Membrane System Design Guidelines for 8-inch FilmTec™ Elements” can be found in Table 22 of “FilmTec™ Reverse Osmosis Membranes Technical Manual” here: <https://www.dupont.com/content/dam/dupont/amer/us/en/water-solutions/public/documents/en/45-D01504-en.pdf>

**Step 5.** Calculate the number of elements needed using the following formula:

$$N_E = \frac{Q_P}{J \times A} \quad (4.2)$$

where  $N_E$  is the number of elements,  $Q_P$  is the permeate flow rate (defined in Step 1),  $J$  is the flux (from Step 4), and  $A$  is the active membrane area of the element (from Step 3).

**Table 4.1:** The “Rule of Thumb” for selecting membrane element types based on TDS recommended from DuPont. Reproduced from DuPont’s “Reverse Osmosis Design Basics” Webinar.

TDS (mg/L)	Membrane Elements
< 1,000	NF270, NF90, XLE, ECO, TW30, XFR, BW30
< 10,000	BW30, XFR
10,000 – 30,000	SEAMAXX, SW30ULE, SW30XLE
30,000 – 50,000	SW30HR, SW30XHR, SW30HRLE, SW30XLE

**Step 6.** Calculate the number of pressure vessels required using the following formula:

$$N_V = \frac{N_E}{N_{E/V}} \quad (4.3)$$

where  $N_V$  is the number of pressure vessels,  $N_E$  is the number of elements (from Step 5), and  $N_{E/V}$  is the number of elements per vessel.

The number of vessels per element can be chosen and will depend on the desired system recovery. We will revisit how to determine this later in the chapter.

**Step 7.** Choose the number of stages. This can be determined by referencing the tables provided by Dow (DuPont) which are dependent on the feed source and desired system recovery as seen in **Table 4.2** for brackish water RO systems and **Table 4.3** for seawater RO systems.

A common term used is the number of “elements in series”, as seen in **Table 4.2** and **Table 4.3**. This does not refer to the total number of elements. Let us look at an example: imagine a two-stage configuration, each with six elements per pressure vessel in each stage. Imagine a single water molecule that travel from the feed side through to the end of the system as retentate – the water molecule would travel through 12 elements. Therefore, there are 12 elements in series.

**Table 4.2:** Recommended number of stages for brackish water systems, with corresponding number of elements in series and number of stages. Reproduced from the DuPont FilmTec™ Reverse Osmosis Membranes Technical Manual.

System recovery (%)	Number of elements in series	Number of stages (6-element vessels)
40 – 60	6	1
70 – 80	12	2
85 – 90	18	3

**Table 4.3:** Number of stages for seawater systems, with corresponding number of elements in series and number of stages. Reproduced from the DuPont FilmTec™ Reverse Osmosis Membranes Technical Manual.

System recovery (%)	Number of elements in series	Number of stages (6-element vessels)	Number of stages (7-element vessels)	Number of stages (8-element vessels)
35 – 40	6 – 7	1	1	-
45	7 – 12	2	1	1
50	8 – 12	2	2	1
55 – 60	12 – 14	2	2	-

For example, if you desire 45% recovery in a seawater application (refer to **Table 4.3**) you will see that the number of elements in series should range from 7–12. The range is dependent on the number of elements per pressure vessel, and number of stages. There may be two stages with six elements per pressure vessel thus 12 elements in series. There may be one stage with seven elements per pressure vessel and thus seven elements in series. The same applies for eight-element vessels.

**Step 8.** Calculate the staging ratio,  $R$ . The staging ratio is the number pressure vessels in one stage to the following stage and can be calculated using the following formula:

$$R = \left[ \frac{1}{1 - Y} \right]^{\frac{1}{n}} \quad (4.4)$$

where  $Y$  is the system recovery, and  $n$  is the number of stages (from Step 7).

**Step 9.** Calculate the number of vessels in the first stage using the following formula:

$$N_V(1) = \frac{N_V}{(1 + R^{-1})} \quad (4.5)$$

where  $N_V(1)$  is the number of pressure vessels in stage 1,  $N_V$  is the total number of pressure vessels (from Step 6).

**Step 10.** Input the system design parameter into WAVE and analyze its performance. The system can be analyzed and optimized based on the simulation output. This gives the user the opportunity to assess the preliminary design and verify its feasibility. In the following section we will use these steps to design and simulate a RO system.

## 4.2 Problem Definition

Seawater desalination is a common application for RO technology. The complexity of these membrane systems varies. This example will walk through the design of a RO membrane system using the steps outlined by DuPont as a starting point. We will then implement our design into WAVE and interpret the report. At the end of this chapter, there will be questions for additional practice on designing and simulating RO processes.

**?** Take a moment to think. What are some of the advantages to using a simulation after the design stage and before implementation? Write down some of your thoughts and discuss them with a colleague or classmate.

Consider that certain areas around the world have limited access to fresh water sources. As populations increase and climates change, currently used fresh water sources may be insufficient or negatively affected. Therefore, alternative sources and methods, such as seawater desalination, may be required to produce potable drinking water for coastal areas.

🔗 Check out this article that discusses the challenges the coastal city of Miami may face in the future and how RO may be a solution. Find the article here:

[https://getpocket.com/explore/item/miami-will-be-underwater-soon-its-drinking-water-could-go-first?utm\\_source=pocket-newtab](https://getpocket.com/explore/item/miami-will-be-underwater-soon-its-drinking-water-could-go-first?utm_source=pocket-newtab)

The goal and purpose of this example is that we want to treat 5,500 m<sup>3</sup>/h of seawater, so that it can be used as potable water. We can visualize how much treated water this plant would produce per day. The approximate volume of an Olympic size swimming pool is 2,500 m<sup>3</sup>. That means we could fill approximately 53 Olympic sized swimming pools with desalinated seawater each day! This quantity of treated water would be for a largely populated coastal area that requires potable water and may have limited access to ground water or other surface water sources such as lakes. It is important to note that further treatment may be required after the RO process to ensure the water meets the water quality requirements of that area, but for now let us focus on the desalination aspect of the treatment process.

Let us understand the capacity of the plant we are interested in designing by doing a quick calculation. In California, the average resident uses 85 US gallons of water per person per day, which is approximately 0.32 m<sup>3</sup> per person per day. If we are producing 132,000 m<sup>3</sup>/day, then we can supply approximately 412,500 people. A typical coastal city of this size may be Bakersfield, California, which has a population of approximately 384,000 (as of 2018) according to the US Census Bureau. This is rough estimate, provides a way to understand the magnitude of the plant we are designing.

### 4.3 Setting up the Simulation

Let us get started on setting up the simulation and completing step one of our membrane system design. Create a new file and name it appropriately so you can easily reference the file in the future. On the home page, enter the product water amount (5,500 m<sup>3</sup>/h) into the “Product Water” box in the blue arrow. We require a WQA of the feed water; in this case we will use a great resource built into the WAVE software, the Water Library.



What if you do not know the composition of your feedwater? The quality of the water can be assessed by collecting a sample from the water of interest and performing various lab tests, such as chemical testing, to determine the water quality of the feed water.

Navigate to the grey *Feed Water* project settings tab and click on it. Or, you can choose to click the blue *Feed Setup* menu bar tab at the top of the window, as seen in **Figure 4.4**. The contents in the *Feed Water* tab will be blank at this point because no information has been input. Navigate to the “Open Water Library” button as outlined in **Figure 4.5**. Click this button and a new window should appear.

The new window, seen in **Figure 4.6**, is called “Open from Water Profile Library” and has a drop-down menu where the water source can be selected from a list. We will choose “Seawater – Standard Reference”. Once this is chosen, a summary of the WQA should appear. Click the

“Copy to Feed Water” button on the bottom right hand corner of the window. The WQA will populate the parameters and tables on the *Feed Water* tab.

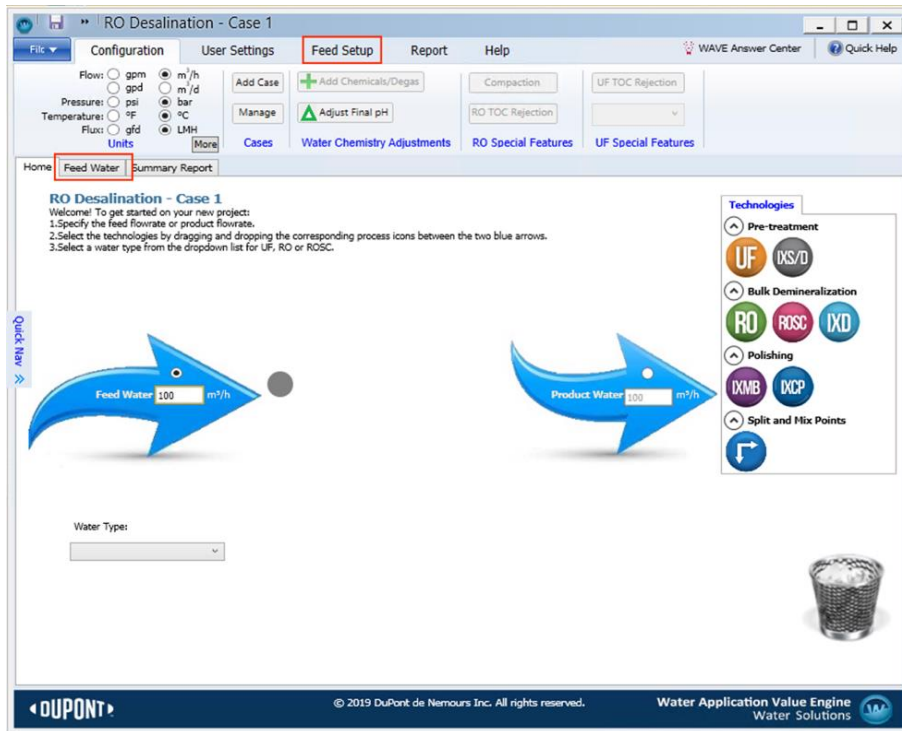


Figure 4.4: The main flowsheet showing the “Feed Water” and “Feed Setup” tabs.

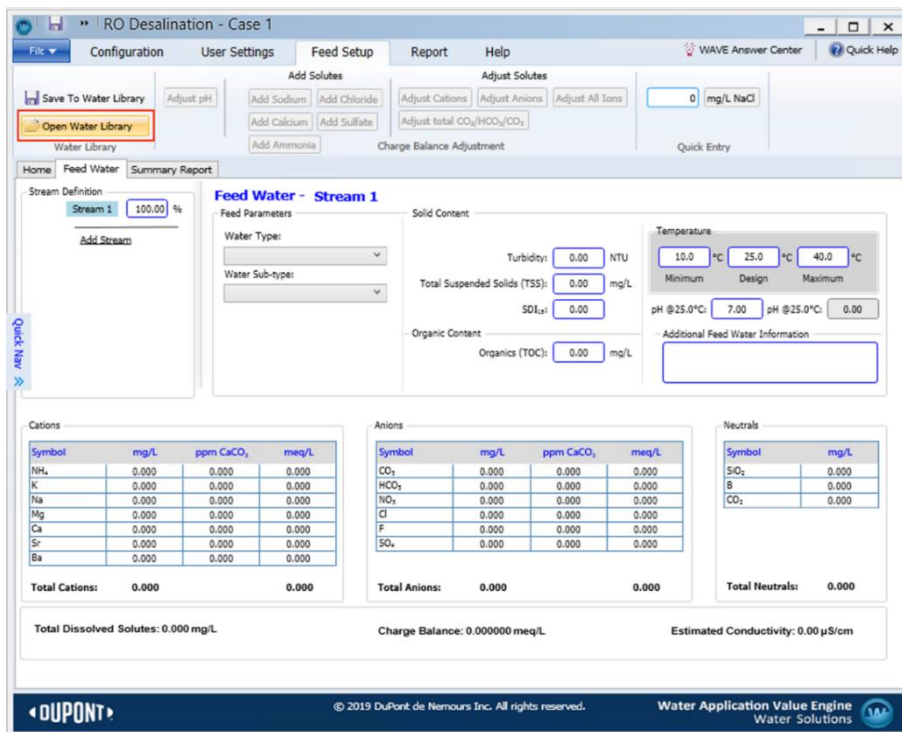
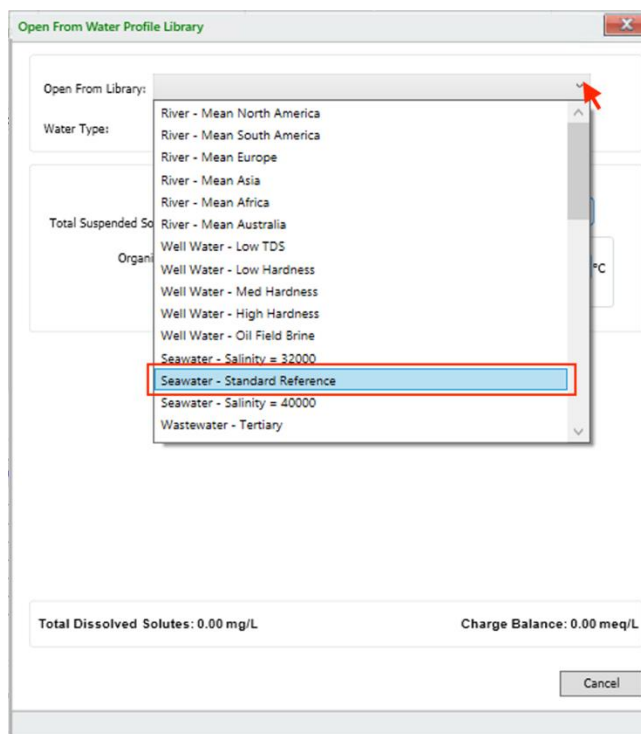


Figure 4.5: The “Feed Water” screen showing the location of the “Open Water Library” button.



**Figure 4.6:** The list of multiple water sources that can be chosen from to be used as the feed water source, with Seawater – Standard Reference chosen.

It is important to note that there is a limited selection of ions that can be included in the feed water quality. In certain cases, the feed water may be composed of ions that cannot be modelled even though they are of interest. For example, one application may be recovering lithium ions from batteries. The article “Cost Effective Recovery of Lithium from Lithium Ion Battery by Reverse Osmosis and Precipitation: A Perspective” by Basudev Swain discusses how it is possible for lithium ions to be recovered by RO, a link to the article is provided below. As you can see in the feedwater tab, there is no option for lithium ions. Some applications may be outside of the limits of WAVE.

🔗 “Cost Effective Recovery of Lithium from Lithium Ion Battery by Reverse Osmosis and Precipitation: A Perspective” by Basudev Swain can be found here:  
<https://doi.org/10.1002/jctb.5332>

#### 4.4 Reverse Osmosis Process & Design Specifications in WAVE

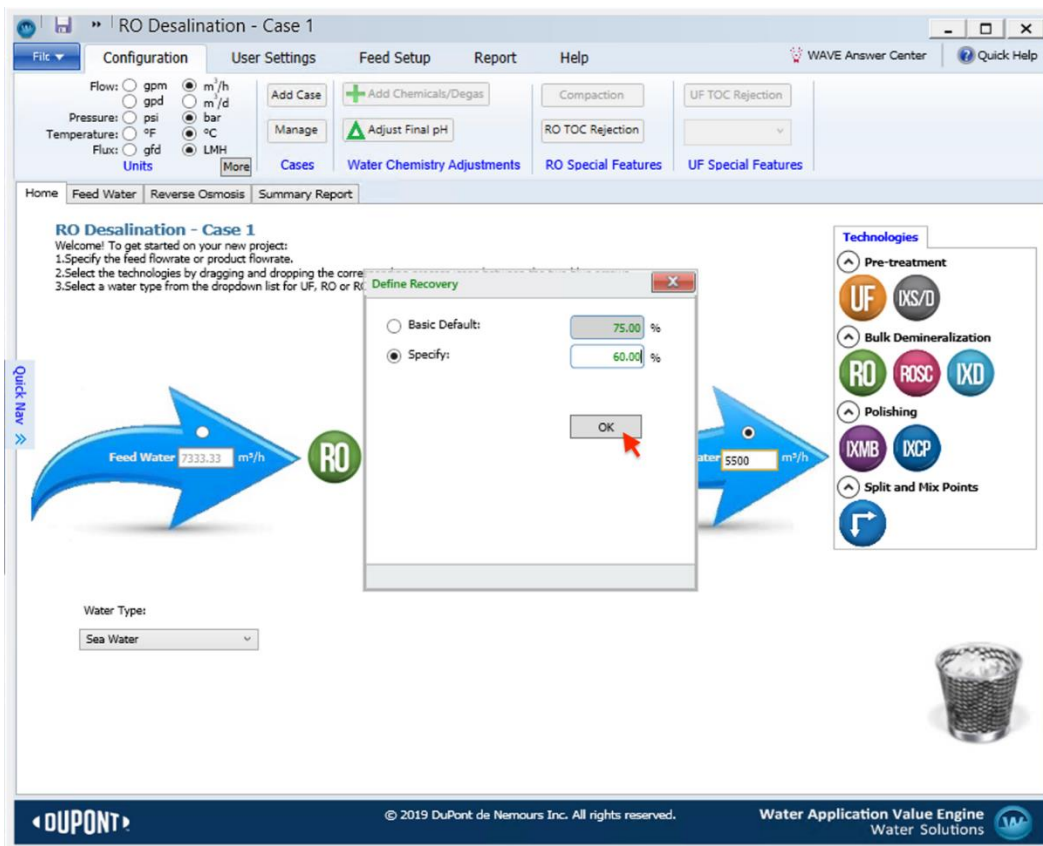
Now that we have set up our feed water source, we can add the RO process to our blank flowsheet. Navigate to the *Home* tab and drag and drop the “RO” icon from the “Technologies” section into the grey circle that appears after the feed arrow. If you hover your mouse over the icon you will notice that there is a pre-defined recovery of 75%. This is the default system recovery that WAVE uses.

In real RO systems, seawater system recovery generally ranges from 35% to 60%. System recovery for seawater desalination is normally lower than that of other applications such as brackish water systems due to the following:

- The seawater is abundant and free, therefore recovery does not have to be high.
- Recovery is not high because the concentrated brine is difficult to treat with RO membranes due to scaling and the process requires high pressures to overcome the osmotic pressure.

**Step 1.** We will try to recover as much water as possible and therefore choose 60%. Recall equation 4.1, the system recovery is defined as the fraction or percent of permeate flow produced from the feed flow. As seen in **Figure 4.7**, we will specify our recovery to be 60% in this example. To do this, right click on the RO icon and choose “Define Recovery”. Then click the radio box corresponding to “Specify”, type 60% and press “OK”.

Now, navigate to the *Reverse Osmosis* project setting tab. **Figure 4.8** shows the initial screen where the user can adjust RO parameters. Note the passes are numbered on the left-hand side of the tab, and the default layout is for a single-stage, single-pass system. Features that can be modified include:



**Figure 4.7:** The RO system recovery is redefined to be 60% instead of the default 75%.



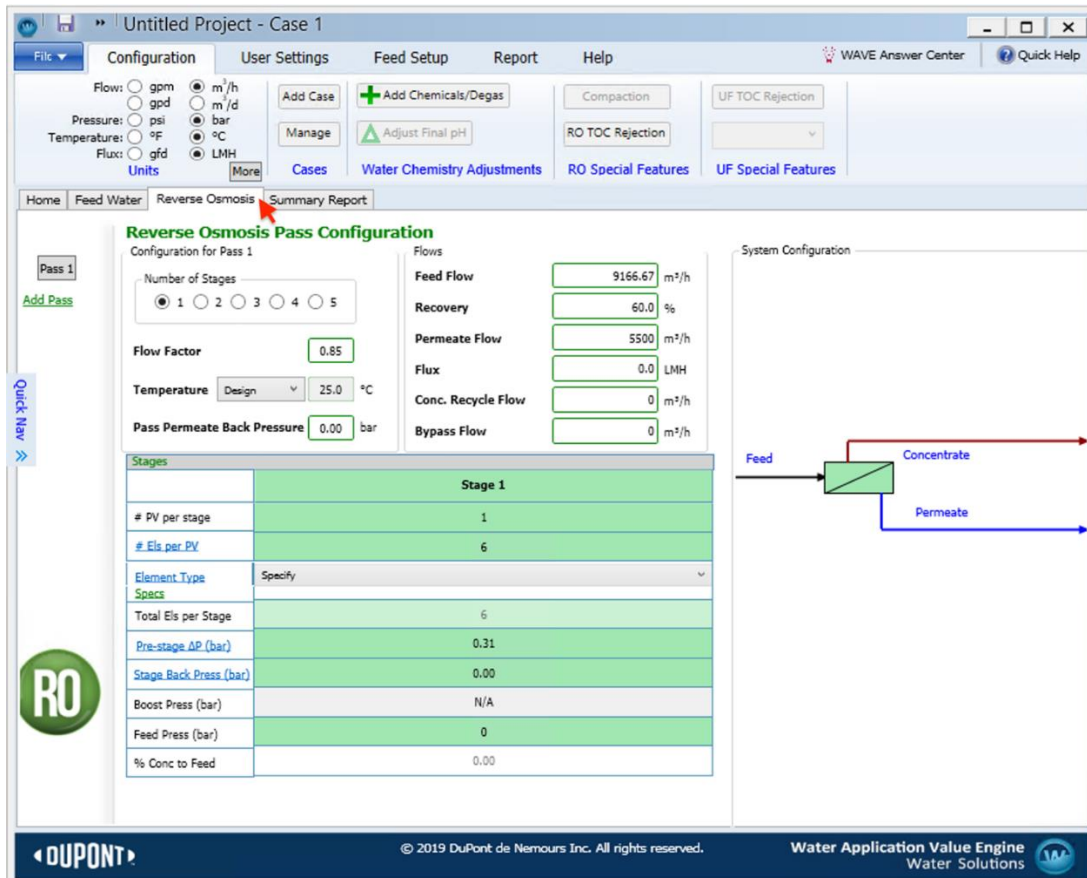


Figure 4.8: Default Reverse Osmosis tab on WAVE.

- **Pass Configurations.** At the top-left of the tab, you can specify parameters such as the number of stages in each pass.



It is important to note the flow factor here, which accounts for the loss flow through a pass due to fouling. The default is 0.85 but it can be adjusted for passes with no loss of flow (i.e. flow factor of 1.0) or to account for passes with loss of flow due to fouling (i.e. flow factor: 0.6). This is an import factor because greater pressures are required for fouled membranes and is an important aspect that will affect the pump sizing process for the system.

- **Flows.** To the right of the pass configurations, WAVE displays the flow rates and flux present in that particular pass. Note that these values cannot be edited independently; they are the result of system constraints and calculations. In some cases, you can manipulate the flows by clicking on certain fields to open the *Reverse Osmosis Flow Calculator* dialog box. In the dialog box, you can specify any bypasses (i.e. fraction of the feed that bypasses a stage/pass) and concentrate recycles (i.e. fraction of final concentrate stream which is recycled back to the beginning of the pass/module) to adjust your flow parameters.

- **Stage Parameters.** In the table at the bottom-left of the screen, the user can adjust parameters with regards to the system layout: the number of PVs per stage, the number of elements per PV, the exact membrane element that is used, pressure parameters, and more.

Now let us use the steps outlined by DuPont to work through the rest of the process to design our RO membrane system.

**Step 2.** The next step requires us to define the configuration of the system. Here, the system we are designing will be plug flow and will operate as a continuous process. Plug flow indicates that the water passes once through the system. In our case recirculation is not needed because we have an endless supply of seawater to draw from. This avoids the need for a complicated and expensive recirculation. We may choose to implement concentrate recirculation after we analyze the summary report.

**Step 3.** We will choose the element type based on the feedwater TDS. Navigate back to **Table 4.1** where the TDS “Rule of Thumb” is summarized.

You can observe in the *Feed Water* tab that there is a total of ~35,946 mg/L of TDS. Therefore, we will choose an element in the 30,000 – 50,000 mg/L range.

Let us investigate the SW30XHR-400 element. Click on the link below to access the product data sheet for this element which describes the membrane, outlining its typical properties, and more.

☞ The product data sheet for the FilmTec™ SW30XHR-400 element can be found here: <https://www.dupont.com/content/dam/dupont/amer/us/en/water-solutions/public/documents/en/45-D00973-en.pdf>

☞ All of DuPont’s products can be found by searching for a product or refining the search. Find the link to their product search here: <https://www.dupont.com/solution-finder/results.html?BU=water-solutions>

Let us note some important information from the product datasheet.

- The product description tells us that this element is useful for drinking water applications
- The active area of the membrane is 400 ft<sup>2</sup>, or 37.2 m<sup>2</sup>

You may have noticed after reading the product datasheet that the element name gives insight to the application for the specific element. For example, the “SW” in the membrane name indicates “seawater” and the “400” at the end of the membrane element name indicates the active area of the membrane in ft<sup>2</sup>. Thus, the SW30XHR-400 element is a reasonable starting point for this application. We will add it to our design in the software later.

We can also easily verify the active area of the element in WAVE. Ensure you are on the *Reverse Osmosis* project tab and navigate to the “Stages” table, which can be seen in **Figure 4.8**. Click on the “Specs” link under “Element Type” to open a window that displays the product specifications for each available element, including the membrane area. Ensure you watch the units here – look at the value in brackets for meters squared.

**Step 4.** For our next step we must determine the flux through the membrane for our calculations in later steps. The flux values can be found from the manufacturer itself in Table 22 in Section 3.9.1 of “FilmTec™ Reverse Osmosis Membranes Technical Manual”. There is an average flux for seawater with open intake. The average flux ranges from 11-17 LMH (L/m<sup>2</sup>/h), so we can use a flux value in this range.

It is important to note that conservative estimates should be made if possible. Just for the purpose of this chapter we will use the higher value of an average flux range of 17 LMH in our calculation.

① “Membrane System Design Guidelines for 8-inch FilmTec™ Elements” can be found in Table 22 of “FilmTec™ Reverse Osmosis Membranes Technical Manual” here: <https://www.dupont.com/content/dam/dupont/amer/us/en/water-solutions/public/documents/en/45-D01504-en.pdf>

**Step 5.** Now that we have determined the flux based on the suggested range from the guidelines, we can easily calculate the number of elements using the equation 4.2.

$$N_E = \frac{5,500 \text{ m}^3/\text{h}}{17 \text{ LMH} \times 37.2 \text{ m}^2} \times \frac{1000 \text{ L}}{1 \text{ m}^3} = 8,697 \text{ elements}$$

Therefore, we require approximately 8,697 elements in our entire configuration. We will not input this value directly into WAVE yet as we still have to determine the number of stages and the staging ratio to determine the elements in each stage.

**Step 6.** The next step requires we calculate the total number of pressure vessels needed. Note that this is not the number of pressure vessels per stage. Once we determine the staging ratio, we can determine the number of pressure vessels per stage.

Use equation 4.3 to determine the total number of pressure vessels needed. The number of elements per vessel ranges from 1 through 8 on WAVE. We will leave the default (6) for now.

$$N_V = \frac{8,697 \text{ elements}}{6 \text{ elements/vessel}} = 1,450 \text{ vessels}$$

Therefore, we require 1,450 pressure vessels.

**Step 7.** This step requires we select the number of stages. With reference to **Table 4.3**, we will use two stages because we desire 60% recovery and are using six elements per pressure vessel. Navigate to the “Configuration of Pass 1” box on the *Reverse Osmosis* project tab and choose “2” stages by clicking the radio box. You will notice that the image on the right will update to show two stages. Additionally, the “Stages” table will now have two columns; this is so you can enter in the required information for the second stage. We will return to this table after we have finished our design and input all the necessary information.

**Step 8.** Now we will determine the staging ratio. Recall this is the ratio of the number of pressure vessels in one stage to the following stage. For example, a staging ratio of 2:1 or 2 is outlined in

the black dashed boxes in **Figure 4.9 Error! Reference source not found.**– the first stage contains four pressure vessels and the second stage contains two pressure vessels.

① A common name for a staging ratio of 2:1 is called the Christmas tree design.

The staging ratio,  $R$ , can be calculated using equation 4.4 In our case, we want 60% recovery and two stages:

$$R = \left[ \frac{1}{1 - 0.60} \right]^{\frac{1}{2}}$$

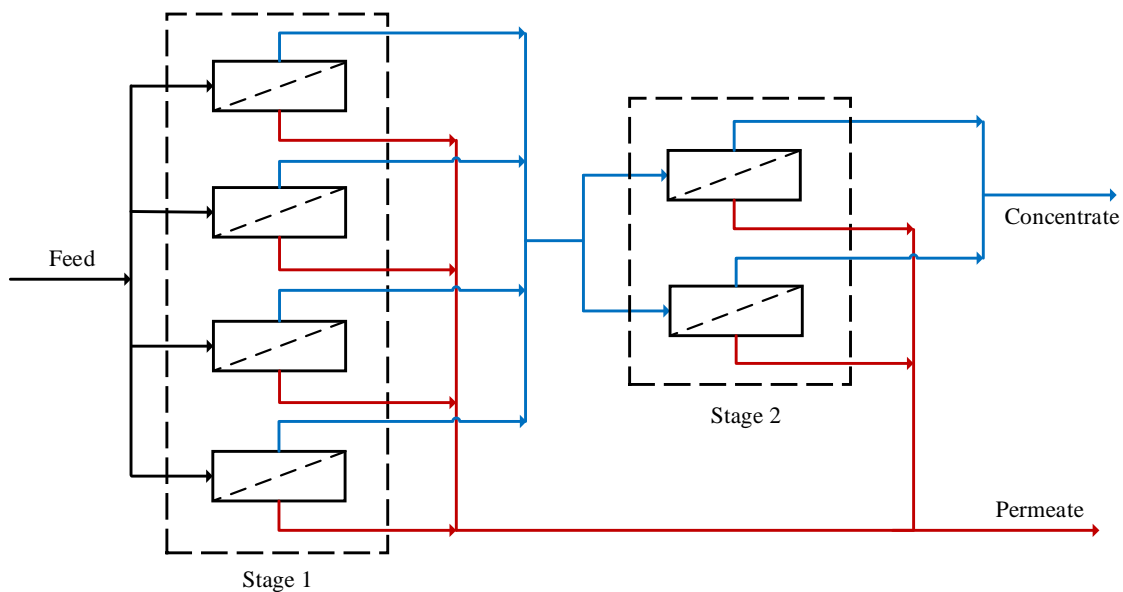
$$R = 1.58$$

Therefore,  $R$  is calculated to be approximately 1.58.

**Step 9.** Now, with the staging ratio, we can calculate the number of PVs per stage. For two stages use equation 4.5 to calculate the PV in stage one.

$$N_V(1) = \frac{1,450 \text{ vessels}}{(1 + 1.58^{-1})} = 888 \text{ vessels}$$

Therefore, in the first stage 888 pressure vessels are required.



**Figure 4.9:** Example of a RO configuration with a staging ratio of 2:1. Outlined in black dashed lines are four pressure vessels in the first stage and two pressure vessels in the second stage. The feed stream is coloured in black, permeate streams are coloured in red, and concentrate stream are coloured in blue.

By the staging ratio's definition, we can calculate that the second stage requires 562 PVs (888 divided by 1.58). Or, since there are only two stages and we know there must be a total of 1,450 PVs, we can calculate the number of PVs in the second stage based on the difference (1,450 minus 888).

The previous equation can be adapted for any number of total stages. For any number of stages, the number of PVs in the first stage is calculated as follows:

$$N_V(1) = \frac{N_V}{1 + \sum_{i=1}^{n-1} R^{-i}} \quad (4.6)$$

For configurations with more than two stages, you must use the staging ratio to determine the number of PVs per stage in the second stage, third stage, etc. For example, to determine the number of PVs in the second stage for a three-stage configuration, divide the number of PVs in the first stage by the staging ratio. Likewise, to determine the number of PVs in the third stage of a three-stage configuration, divide the number of PVs in the second stage by the staging ratio. Be sure to verify your calculations by summing your calculated number of stages and checking the sum against the total number of vessels calculated in step 6 using Equation 4.3. This is assuming that the staging is consistent throughout the configuration.

**Step 10.** Now that we have our design complete, let us input it into WAVE and analyze the results.

Ensure you are on the *Reverse Osmosis* project tab and that you have chosen two stages as mentioned earlier. We will now input the number of pressure vessels, the elements per pressure vessel and the element type (indicated by the columns in WAVE as “# PV per stage”, “# Els per PV”, and “Element Type”, respectively). Enter the number of pressure vessels for stage one by typing the number in the corresponding table section. Notice that the stage you are editing is highlighted in green on the table and the image to the right. Leave the default of six elements per PV in the row indicated by “# Els per PV”. Finally choose the element type by clicking the drop-down menu in the row “Element Type” and select the desired element: SW30XHR-400. You can now repeat this for the second stage by inputting the corresponding design information.

Ensure you are editing stage two by verifying that the column on the table is highlighted in green and so is the corresponding stage on the image on the right of the screen. Once you have input all the information from our design, your *Reverse Osmosis* tab should look like the one in **Figure 4.10**.

Be sure to check your parameters. Press the “Summary Report” tab when ready and WAVE will generate the results from the simulation. It is important to note that sometimes WAVE's calculations fail to converge, especially with RO systems. A window will appear to inform you if this happens. If this is the case, ensure that your design parameters are as specified in this courseware. Otherwise, restarting the software can help to clear previous solutions from the software's memory and may enable convergence.

We will analyze the system using WAVE in the following section and any warnings will be addressed.

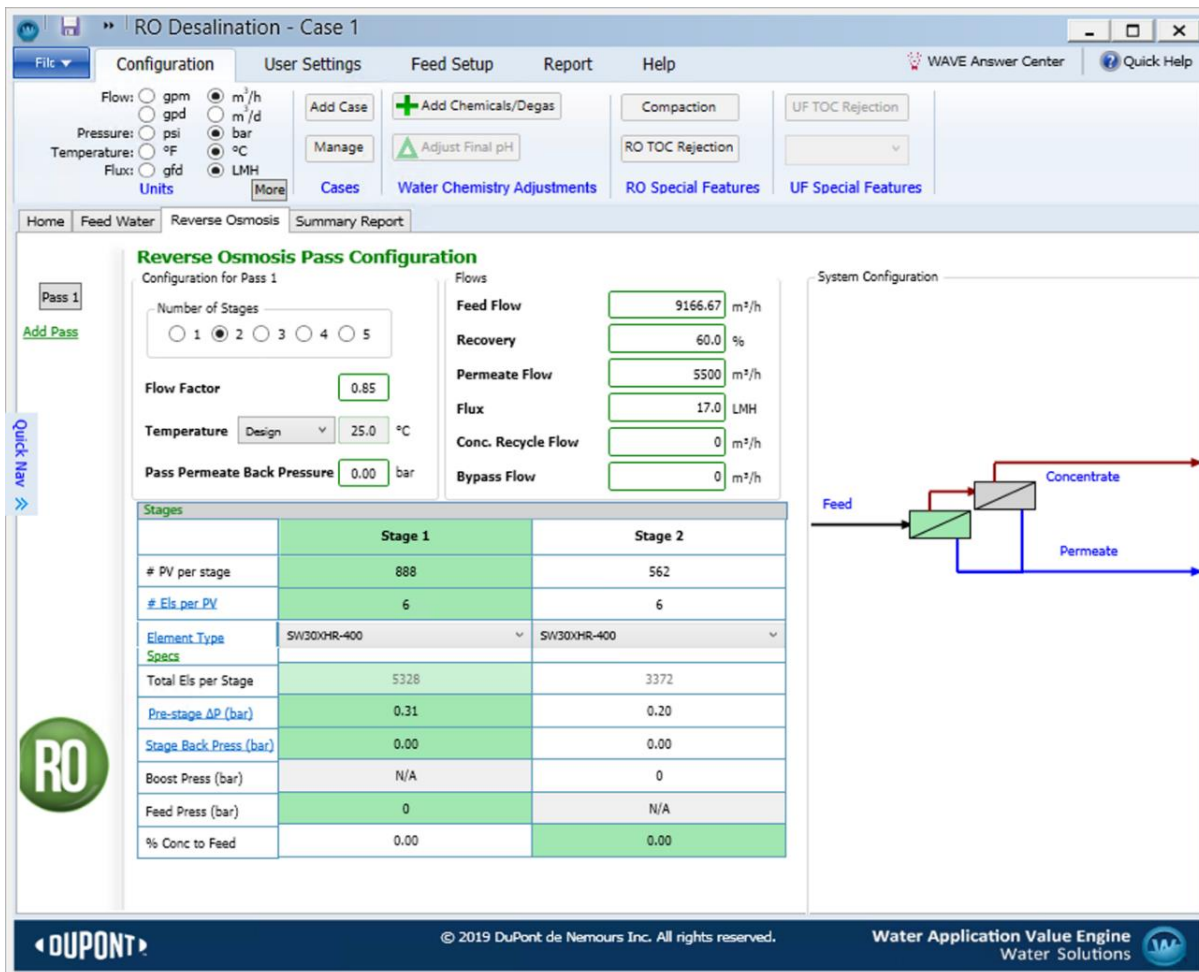


Figure 4.10: The RO design implemented in WAVE.

## 4.5 Interpreting the RO Results

When you are ready to proceed, ensure you are on the *Summary Report* tab, provided that your simulation converges. Information on the performance of the system will be shown, including flow rates in each stream, pressures, recoveries, calculated ion concentrations, and results from each stage or pass. Let us work through the results in the report:

- Summary Table.** The first table (right below the process diagram) summarizes the flow conditions in the RO system, as seen in *Figure 4.11*. Note that the RO feed from the first pass is 9,166 m<sup>3</sup>/h with 36,071 mg/L of dissolved solids (and at 78.6 bar), of which only 5,500 m<sup>3</sup>/h leaves in the permeate product stream (TDS 140.1 mg/L)! On the other hand, the concentrate stream leaving the RO system has a flow rate of 3,686 m<sup>3</sup>/h with a very high TDS of 89,479 mg/L. With this information we can analyze the performance of the system by calculating the salt rejection using the following formula:

#	Description	Flow (m <sup>3</sup> /h)	TDS (mg/L)	Pressure (bar)
1	Raw Feed to RO System	9,199	35,946	0.0
2	Net Feed to Pass 1	9,166	36,071	78.6
4	Total Concentrate from Pass 1	3,686	89,479	75.3
6	Net Product from RO System	5,500	140.1	0.0

**Figure 4.11:** Summary table for the RO process.

$$\text{salt rejection}(\%) = \left[ 1 - \left( \frac{\text{permeate salt concentration}}{\text{feed salt concentration}} \right) \right] \times 100\% \quad (4.7)$$

$$\text{salt rejection}(\%) = \left[ 1 - \left( \frac{140.1 \text{ mg/L}}{36,071 \text{ mg/L}} \right) \right] \times 100\% = 99.6\%$$

Therefore, the salt rejection is 99.6%. We are producing 5,500 m<sup>3</sup>/h in treated water (59.8% overall recovery). The rest of the water (RO concentrate) must be purified via other technologies or be disposed of. In our case we can either use an evaporation pond or return the concentrated brine back into the ocean. The handling of the RO concentrate will be discussed in further detail later in this chapter.

- **RO System Overview.** WAVE gives a summary of the design, configuration, and performance of the system in this table. Note a couple of key values: the recovery of the RO system is set (fixed) at 59.8%, the total active membrane area is 323,303 m<sup>2</sup>, and the specific energy to treat this feed stream is calculated as 4.58 kWh/m<sup>3</sup>.

? Can you see how this value for the specific energy would be useful in designing this system?

- **RO Flow Table (Stage Level).** WAVE summarizes a variety of flow/concentration parameters for each stage. You can use this table to determine if the design of each stage is adequate.
- **RO Solute Concentrations.** This table summarizes the concentration of each dissolved ion as a function of the stage, pass and stream. The table is reproduced in **Figure 4.12**. Note that in the concentrate streams, the ion concentrations increase with subsequent stages; as permeate water is filtered through the membranes, the less permeable salt ions remain behind in the concentrate streams. Similarly, the concentration of ions in the permeate streams also increases with subsequent stages due to the greater concentration driving force (*i.e.* osmotic gradient) between the highly-enriched concentrate stream and dilute permeate stream. However, it should be noted that the RO system rejects the majority of the ions, leaving a well-purified permeate stream, as seen in the “Total” column of the permeate results.

RO Solute Concentrations - Pass 1

Concentrations (mg/L as ion)						
	Feed	Concentrate		Permeate		
		Stage1	Stage2	Stage1	Stage2	Total
NH <sub>4</sub> <sup>+</sup>	0.00	0.00	0.00	0.00	0.00	0.00
K <sup>+</sup>	408.4	830.3	1,016	1.30	6.55	2.10
Na <sup>+</sup>	11,033	22,433	27,455	31.00	151.4	49.26
Mg <sup>+2</sup>	1,314	2,674	3,276	0.86	4.02	1.34
Ca <sup>+2</sup>	421.7	858.4	1,052	0.27	1.28	0.42
Sr <sup>+2</sup>	8.14	16.56	20.29	0.01	0.02	0.01
Ba <sup>+2</sup>	0.00	0.00	0.00	0.00	0.00	0.00
CO <sub>3</sub> <sup>+2</sup>	17.24	36.94	44.36	0.00	0.00	0.00
HCO <sub>3</sub> <sup>-</sup>	104.7	209.7	256.9	0.47	1.98	0.69
NO <sub>3</sub> <sup>-</sup>	0.00	0.00	0.00	0.00	0.00	0.00
Cl <sup>-</sup>	19,835	40,335	49,369	51.18	249.8	81.30
F <sup>-</sup>	1.33	2.70	3.31	0.00	0.02	0.01
SO <sub>4</sub> <sup>+2</sup>	2,776	5,651	6,924	0.73	3.36	1.13
SiO <sub>2</sub>	1.00	2.03	2.49	0.00	0.02	0.01
Boron	4.59	8.87	10.46	0.47	1.80	0.67
CO <sub>2</sub>	0.42	1.09	1.46	0.54	1.06	0.62
TDS*	35,946	73,100	89,479	88.51	428.8	140.1
pH	8.1	8.1	8.2	6.1	6.4	6.2

**Figure 4.12:** Calculated concentrations of dissolved species in each stage/stream of the RO system.

Note the relative concentrations of the species in the table—before and after the RO process. Some species are rejected to a higher degree (*i.e.* better retained in the concentrate) than others. Why do you think that this is the case?

- RO Design Warnings.** The system should operate within the design guidelines. The guidelines outline the maximum recovery, the maximum permeate flow rate, the minimum concentrate flow rate, and the maximum feed flow rate per element. These design guidelines are based on the feed water and will be some of the common design warnings you encounter. WAVE issues design warnings when one or more calculated parameter (*e.g.* flow rate) is outside of the design guidelines. For example, we have a design warning, seen in **Figure 4.13**, indicating the maximum permeate flow per element has been exceeded in stage one of element one. We will address this issue soon.
- RO Flow Table (Element Level).** Like the table at the “stage level”, WAVE summarizes the flow/concentration results for each element in the system.
- RO Solubility Warnings.** Because RO systems tend to concentrate ions in the aptly named “concentrate” stream, in some cases the ion concentrations can exceed the solubility limits of the species. WAVE attempts to warn the user here if that is the case. As seen in **Figure 4.14**, we have three warnings associated with exceeding the calcium fluoride (CaF<sub>2</sub>) limit. One such warning tells us that the saturation of CaF<sub>2</sub> is above 100%. In concentrations above their solubility limit, ions can deposit on the membrane surfaces and cause mineral scaling, which decreases the membrane flux over time. We will address this issue soon.



**? What techniques can we use to prevent, mitigate or treat scaling?**

**RO Design Warnings**

Design Warning	Limit	Value	Pass	Stage	Element	Product
Permeate Flow Rate > Maximum Limit (m <sup>3</sup> /h)	1.20	1.25	1	1	1	SW30XHR-400

**Figure 4.13:** A design warning issued by WAVE.

**RO Solubility Warnings**

Warning	Pass No
Stiff & Davis Stability Index > 0	1
CaF <sub>2</sub> (% saturation) > 100	1
Anti-scalants may be required. Consult your anti-scalant manufacturer for dosing and maximum allowable system recovery.	1

**Figure 4.14:** A solubility warning issued by WAVE.

- RO Chemical Adjustments.** If any chemicals such as pH adjusters (acids, bases), anti-scalants, or dechlorinators are added, this table summarizes their effects on the system—positive or negative. Now, notice that the CaF<sub>2</sub> row is highlighted in red. This is WAVE’s way of telling us that perhaps some chemical addition would help mitigate the effects of the supersaturated calcium fluoride ions. Perhaps more interestingly, the calcium fluoride ions were at 17.2% of the saturation limit before the RO system; this value increases to 204% in the concentrate.

**Addressing RO Warning Messages.** Now that we have perused the RO summary report, let us address the two warnings that WAVE has issued: the permeate flow from element one in stage one exceeds the design guidelines maximum limit and the supersaturation of CaF<sub>2</sub> in the concentrate. Return to the *Reverse Osmosis* project tab, and consider the following actions:

The design warning observed in the summary report suggests that the maximum permeate flow per element has been exceeded for element one in stage one; the maximum permeate flow for this element is 1.20 m<sup>3</sup>/h while the simulated permeate flow is 1.25 m<sup>3</sup>/h. To increase the maximum permeate flow constraint that we currently violate, the system guidelines suggest we increase the active area per element. This can be observed in Table 22 of DuPont’s Tech Manual Excerpt titled “Membrane System Design Guidelines for 8-inch FilmTec™ Elements”: <https://www.dupont.com/content/dam/dupont/amer/us/en/water-solutions/public/documents/en/45-D01504-en.pdf>

The guidelines provide the maximum recovery, the maximum permeate flow rate, the minimum concentrate flow rate and the maximum feed flow rate per element. These design guidelines are based on the feed water and built into WAVE. A design warning will appear if the guidelines are not met. These will be some of the most common design warnings you may encounter.

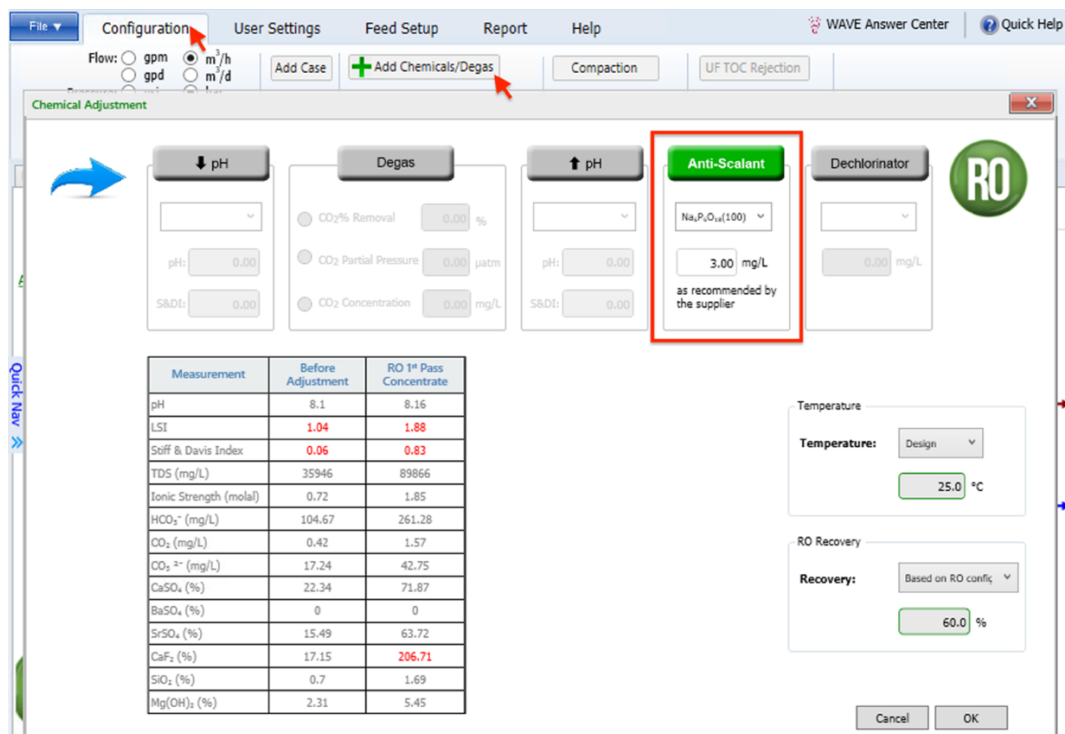
It is observed that for our feed water (seawater with open intake and generic conventional pre-treatment), elements with 400 ft<sup>2</sup> active area have a maximum permeate flow of 1.20 m<sup>3</sup>/h

while elements with 440 ft<sup>2</sup> active area have a maximum permeate flow of 1.33 m<sup>3</sup>/h. Therefore, we can replace the existing stage one and stage two elements to be SW30XHR-440 to ensure our system operates within the design guidelines. Navigate back to the *Reverse Osmosis* tab and select the new element type for stage one and two. Then, click on the *Summary Report* tab – you will notice that the design warning has been dismissed.

**?** Using a module with a larger membrane area is one solution. Can you think of others?

Now we will address the RO solubility warning: the calcium fluoride can precipitate and deposit on the RO elements. This is one way by which mineral scaling can occur. The scaling covers the membrane surface and prevents the permeation of water which negatively affects membrane performance. To address the solubility warning, we can modify the pH to increase the solubility of the species or add an anti-scaling chemical. For now, we will add an antiscalant to fix the solubility warning. Under the *Configuration* tab, click the “+Add Chemicals/Degas” button to open the “Chemical Adjustment” window, as seen in *Figure 4.15*. Click on the “Anti-Scalant” button to confirm that you are adding an antiscalant to the RO feed. Select sodium hexametaphosphate (Na<sub>6</sub>P<sub>6</sub>O<sub>18</sub>) from the drop-down menu, and use the manufacturer’s recommended dose of 3 mg/L. Click OK when you are finished.

Different antiscalants harness different mechanisms to prevent scale formation. Sodium hexametaphosphate, for example, inhibits the crystal growth process by acting as a dispersant to disrupt the boundary layer of the fluoride ions.



**Figure 4.15:** Chemicals can be added to the RO feed water to adjust the water chemistry. Here, we add sodium hexametaphosphate as an antiscalant.

Return to the *Summary Report* tab and review the solubility warnings. You will notice that the antiscalant warning did not go away. Note here that the warning does not go away because the calculation engine may not model the effect of the antiscalant. It might mitigate the scaling, but the software still warns us anyways that scaling could occur. At this time, we will ignore the saturation warning.



Want to learn more about the different antiscalants for RO systems? Check out the article titled “Antiscalants in RO membrane scaling control” written by Wei Yu, Di Song, Wei Chen, and Hu Yangthis. Refer to Table 3 for a full list of different antiscalants outlining the active ingredient and mechanism. The article can be found here: <https://doi.org/10.1016/j.watres.2020.115985>



If the design you proposed met all of the design requirements, would you recommend building this design at full scale? What would be the next steps to consider? What else should you consider when designing a system?

## 4.6 Addressing RO Concentrate Streams

Recall from Chapter 3 that, in some cases, most of the cost of treating water is handling the concentrate stream. Therefore, although we have completed our design and addressed the design warnings, we are not done. Disposal and treatment of the concentrate stream is difficult and costly because RO systems generate large amounts of very concentrated water – from the results in *Figure 4.11*, our process would fill over 35 Olympic size swimming pools *per day* with salt water that is 2.5 times more concentrated than seawater! We want to treat the concentrate stream further when it is of value or when it is hazardous. Thus, cost effective and efficient methods of treatment and disposal for RO concentrate are an area of active research. This section of the chapter will provide insight to the current and novel methods to treat and dispose of concentrate streams.

In some cases, the concentrate stream may be valuable, like in the dairy industry. When a milk-based substance is passed through a RO system, permeate water is produced and the concentrate can be used for dry/evaporated milk products. Generally, RO processes in the dairy industry are used for concentration or volume reduction of the milk product. In this specific case, both the concentrate and permeate are of value and can be used: the concentrate is a product and the permeate water can be used elsewhere in the process for purposes such as cleaning.

In other cases, the concentrate is waste and disposal is the only option. There are many factors to consider when choosing a method of disposal. The article titled “Reverse Osmosis Concentrate Disposal in the UK” by Deborah Squire outlines a list of import considerations when choosing the disposal option. For example, a consideration is the site location and its accessibility to concentrate handling and disposal methods.

The article “Reverse Osmosis Concentrate Disposal in the UK” by Deborah Squire can be found here: [https://doi.org/10.1016/S0011-9164\(00\)00134-X](https://doi.org/10.1016/S0011-9164(00)00134-X)

A common disposal method is discharging the concentrate directly into surface water such as the ocean. As you can see in the *Summary Report* generated by WAVE, the flow rate is 3,686 m<sup>3</sup>/h and the TDS is 89,455 mg/L; this is almost three times more concentrated than the feed water! Discharging high volumetric flows of highly-concentrated brine into surface water can have undesirable, negative environmental effects. In some cases, the concentrate may even contain contaminants that are harmful to the environment and human health. Therefore, even in cases where the concentrate is waste, additional treatment may be required to dispose of the concentrate responsibly and ethically. The article titled, “Novel Technologies for Reverse Osmosis Concentrate Treatment: A Review” by Sung Hee Joo and Berrin Tansel discusses emerging contaminants in RO concentrate, the currently available technologies, and future areas of research.



To read more about emerging contaminants in RO concentrate the article titled “Novel technologies for reverse osmosis concentrate treatment: A review” by Sung Hee Joo and Berrin Tansel can be found here: <https://doi.org/10.1016/j.jenvman.2014.10.027>

Another common method of disposal is to use an evaporation pond. An evaporation pond can be constructed as a basin which holds the concentrate and allows the sun to evaporate the water from the concentrate, leaving behind the salts. A visual representation of an evaporation pond created by LENNTECH can be seen in **Figure 4.16**. This method may be useful when there is sufficient land available. Additionally, the climate must be suitable to facilitate evaporation of the remaining water in the concentrate.

Many technologies may be utilized to treat the RO concentrate. The article titled, “Treatment Technologies for Reverse Osmosis Concentrate Volume Minimization: A Review” by Arun Subramani and Joseph G. Jacangelo discusses multiple technologies used to treat RO concentrate. The methods are reviewed based on the mechanism of separation: membrane-based or thermal-based. The article also discusses emerging technologies such as forward osmosis and eutectic freeze crystallization.

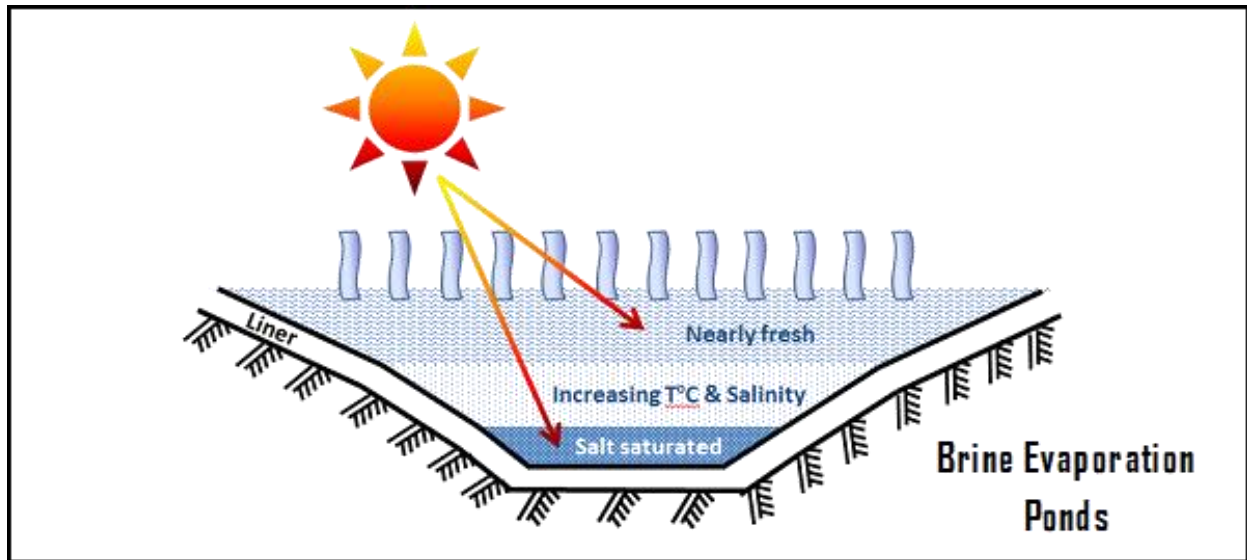


The article titled “Treatment Technologies for Reverse Osmosis Concentrate Volume Minimization: A Review” by Arun Subramani and Joseph G. Jacangelo can be found here: <https://doi.org/10.1016/j.seppur.2013.12.004>

In some cases, we may choose to have the concentrate pass through a second RO system, thus recovering more water and concentrating the brine solution further. This may occur when the concentrate contains environmental contaminants and so the WWTP must pay *per volume* to have the concentrate trucked away. We can simulate this in WAVE by taking the concentrate from the first RO process to be the feed stream for a second RO process. The flowsheet on WAVE allows you to place technologies in a linear fashion, allowing the permeate of one technology to be the feed to the next technology. A new file must be made to simulate treating the concentrate from the initial RO process. All the information for the concentrate stream can be obtained from the “Summary Report” tab in WAVE.

Give it a try yourself and design/simulate a second RO system to treat the concentrate stream. Do you think this is a good option to handle the RO concentrate?

Overall, when designing a RO system, it is necessary to consider how the RO concentrate is handled to ensure it is properly disposed or treated. When deciding the best method to handle the RO concentrate, there are many factors to determine the best method of either disposal or treatment.



**Figure 4.16:** A representation of a brine evaporation pond from LENNTECH. Image Source: <https://www.lenntech.com/processes/brine-evaporation-ponds.htm>

## 4.7 Chapter Questions

### Question 1.

Part 1. It is important to keep in mind that in reality the feed conditions may vary outside the parameters values or ranges. For example, temperature may vary due to seasonal changes. Consider how a change in feed temperature will affect the salt rejection of the system. Hypothesize what will happen to the salt rejection if the temperature is increased and decreased, with constant flux.

Part 2. Analyze the performance of the system we designed in the chapter. Calculate the current salt rejection when the temperature is set to the design temperature of 25°C. Now, re-run the simulation to calculate the salt rejection when the temperature ranges from 10°C to 35°C using 5°C increments. Was your hypothesis correct from the Part 1? Take this opportunity to discuss the results with your colleagues or classmates. Consider and indicate what other factors may affect the performance of the system.

### Question 2.

Part 1. You are tasked with designing/simulating a new RO system to treat seawater for potable water use in a small city (you can use the standard seawater reference). Keep in mind that further treatment may be required to meet drinking water requirements, but we will just focus on designing the RO system for now. The small city requires a volumetric flow rate of 1000 m<sup>3</sup>/h of treated water and you can assume a 60% recovery. Simulate the system using WAVE and explain how you address any design warnings; sometimes there may be many ways to address an issue.

Part 2. You now find out that the standard reference seawater is not an accurate representation of the source water as the TDS is approximately 40,000 mg/L. Now change the feed water type to be “Seawater – Salinity = 40000” from the water library. Check the summary report. Do you notice any new design warnings? Address these design warnings giving reasons to your course of action.

*-End of Chapter-*

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**Chemical Engineering 4M03:  
Industrial Separations Processes  
Introduction to the WAVE Design Software**

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**Custom Courseware – Chapter 5**



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*Revision: R3*



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## 5. Integrating Ultrafiltration and Reverse Osmosis Processes

**Chapter #5 will introduce the following information:**

- Simulation of ultrafiltration and reverse osmosis systems
- Analyzing the results of the ultrafiltration and reverse osmosis simulation
- Addressing simulation warning messages
- Optimizing UF/RO systems

In the previous chapters we looked at ultrafiltration and reverse osmosis individually and simulated them separately on WAVE. In this chapter we will simulate UF and RO on WAVE and understand the advantages of using them in series to accomplish the design goals of the scenario in this chapter.

**!** It is highly recommended to complete the previous chapters before beginning this one, as it is less guided and assumes a basic understanding of UF/RO processes and the WAVE software.

### 5.1 Problem Definition

In *Section 2.3* we investigated a short case study on treating brackish mine wastewater. Due to more stringent wastewater discharge regulations you are tasked with using the available technologies to remove the salt ions from the wastewater.

Recall that currently, the mining operation must deal with an average of 350 m<sup>3</sup>/h of brackish wastewater drawn from a tailings pond which has an average composition summarized in *Table 5.1* (*i.e.* Table 2.1 in Section 2.3) below.

By the end of this chapter we want to address the following questions:

- What effluent quality (*i.e.* composition) can be achieved using UF/RO processes?
- What UF/RO technologies are needed for this preliminary design?
- What operating considerations are there?

To address the company's questions and concerns, we will use WAVE to determine the effectiveness and feasibility of using UF/RO membrane processes in treating the wastewater. The following chapters will be structured to focus on the design of UF system first, followed by the design of the RO system.

**Table 5.1:** Water quality analysis (WQA) of the effluent water stream from the actual iron mine. The valuable iron has been removed in previous steps.

Property	Value
Average Temperature (°C)	15±7
Turbidity (NTU)	85.2
pH (@ 15 °C)	7.52
Total Suspended Solids (mg/L)	80.9
Total Organic Carbon (mg/L)	11.2
Cationic Species	Concentration (mg/L)
Ammonium	1.56
Barium	0.065
Calcium	101
Magnesium	133
Potassium	25.7
Sodium	95.3
Strontium	0.875
Anionic Species	Concentration (mg/L)
Bicarbonate	83
Chloride	209
Nitrate	1.7
Sulfate	700
Neutral Species	Concentration (mg/L)
Boron	0.08
Silica	3.06

### 5.1.1 Setting Up the Simulation

**?** For your reference, the following subsection (5.1.1) has been repeated, verbatim, from the second chapter of this course, *Section 2.3.1*. If you are confident in specifying the water quality and the water flow rate, you can skip forward to the next section of this chapter.

**Setting the Display Units.** To ensure that your results match the ones presented in these chapters, you must ensure that your units of measurements match the units in **Figure 5.1**. To configure the units, navigate to the *Configuration* tab in the top menu and click “More”. We will use metric units by default, and it is recommended that you choose “m<sup>3</sup>/h” to match the influent flow rate given in *Section 2.3*. Verify your simulation’s units match the units in **Figure 5.1**. Click “OK” when you are finished.

**Specifying the Feed Water Quality.** In *Section 2.3*, we were given a WQA for the brackish effluent stream from the mine (*i.e.* **Table 5.1**). Now, we will input the data that we have into WAVE. Begin by navigating to the *Feed Setup* tab in the top menu bar and then navigate to the *Feed Water* in the project settings tab, as seen in **Figure 5.2**.

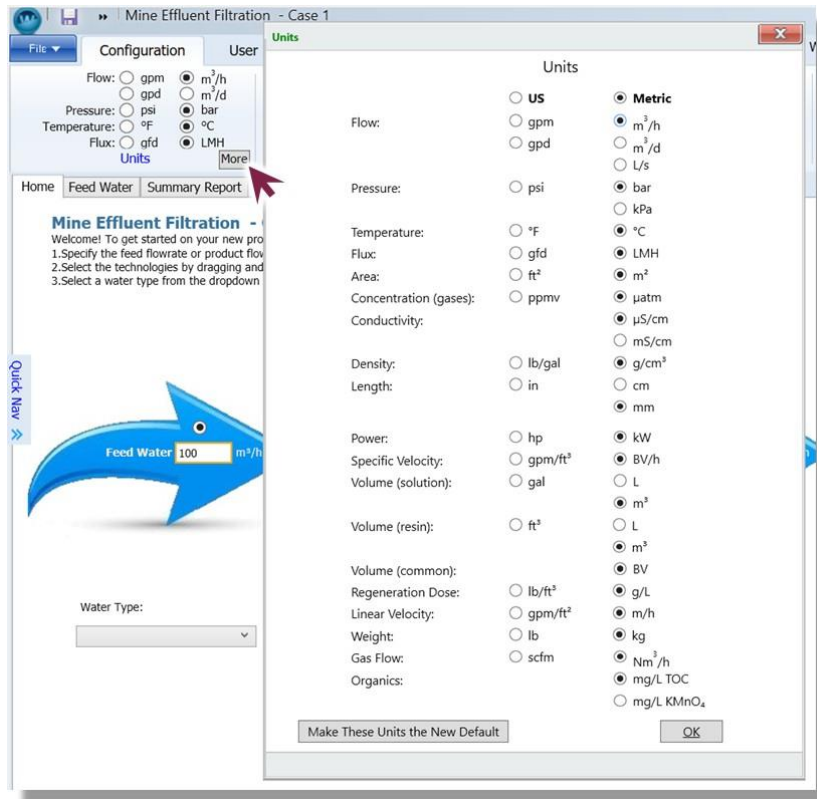


Figure 5.1: Setting the display unit preferences for the WAVE simulation.

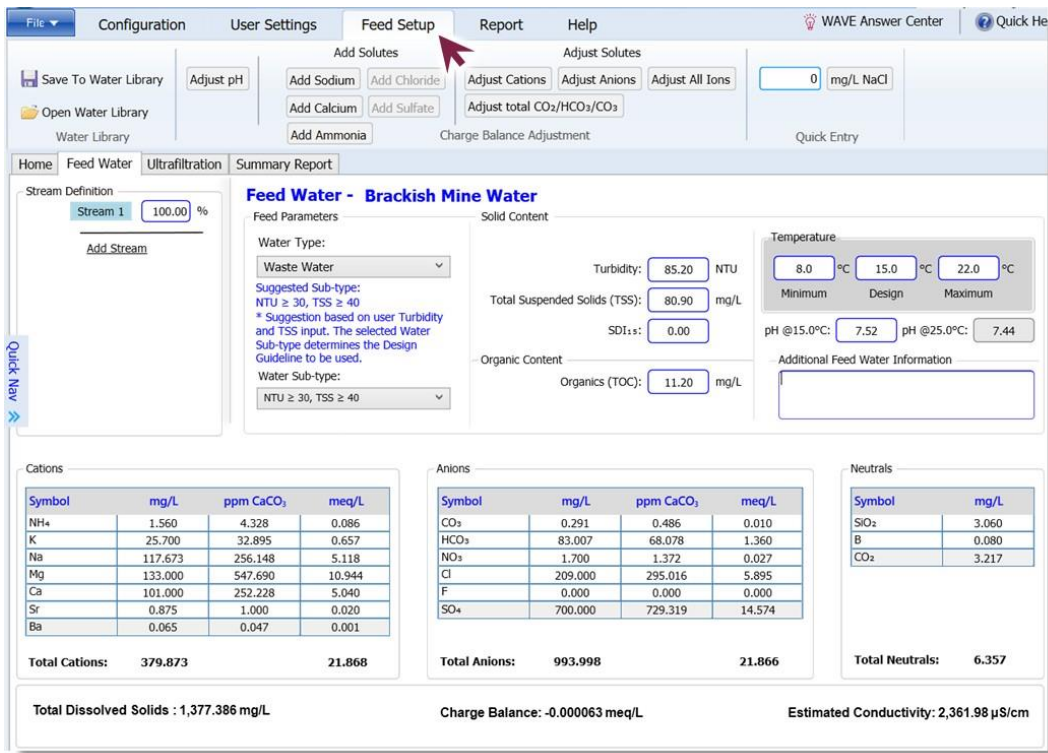


Figure 5.2: Assigning water quality parameters to the brackish feed stream.

- In the *Feed Parameters* panel, under the *Water Type* and *Water Subtype* drop-down menus, select the categories which *best describe your* water source with regards to total suspended solids (TSS) and *turbidity*<sup>1</sup>. Here, we will choose “Waste Water” and “NTU  $\geq$  30, TSS  $\geq$  40” to match our WQA. This guides WAVE in performing its calculations.
- In the *Solid Content* panel, we can specify the turbidity, TSS, Silt Density Index (SDI), and organics content (total organic carbon; TOC). Use the values from **Table 5.1** to fill in the *Solid Content* fields with exception to the SDI (*i.e.* the SDI value is 0 mg/L). All parameters in the *Solid Content* panel are *optional*.
- Beside the *Solid Content* parameters are fields to input the system temperature and pH. Fill in these values from **Table 5.1**. The “minimum” and “maximum” design temperatures are the bounds between which the system should operate. We can use the variation on the temperature (7°C) to populate these (albeit optional) fields.
- At the bottom of the screen, we can populate the tables of *Cations*, *Anions*, and *Neutrals* with values from **Table 5.1**. Be sure to use the columns with units of “mg/L”. If a species is not specified in our WQA, leave that row blank (*i.e.* 0 mg/L).

Notice that several values update as you fill in the fields. For example, WAVE sums the total dissolved solutes to estimate the solution conductivity. WAVE also sums the total cations, anions and neutral species to calculate the overall “concentration of charge” (units: meq/L).<sup>2</sup>

Even though we have not specified any carbon dioxide concentration, WAVE has calculated this field to be a non-zero value due to chemical equilibria that exist in the water (*e.g.* bicarbonate  $\rightleftharpoons$  carbon dioxide equilibrium) at the given pH and temperature.

① The calculations behind the water quality parameters (*e.g.* chemical equilibria) are quite complex; we will not delve into them in detail. Just be aware that WAVE performs calculations in the background based on thermodynamic models to ascertain which chemical species are present, and in what concentration/activity.

At the bottom of the *Feed Setup* screen, note the “*Charge Balance*” value of approximately -0.97 meq/L. What do you think that this means if you have  $\sim$  0.97 milli-equivalents of negative charge per liter? Think of the net “milli-equivalent” of charge as being a milli-molar excess of positive or negative ions. The interpretation of this value is that given the composition of salts/solids that we have specified (based on the WQA), the solution has an *overall (net) negative charge* equal to this value. Our WQA analysis may not have detected additional cations in solution (*e.g.* residual Fe, Ni, etc.) that would balance out the negative charge. We know that a solution cannot have a net charge: ions are always balanced by their counterions. As our solution has a net negative charge, we must “balance” it with more positive ions. In the software, we can do this by

<sup>1</sup> The turbidity or “cloudiness” of water is reported in the standard *Nephelometric Turbidity Units* (NTU).

<sup>2</sup> One mole of Na<sup>+</sup> ions produces one equivalent (+1 eq) of charge. One mole of Ca<sup>2+</sup> ions produces +2 eq of charge. One mole of Cl<sup>-</sup> ions produces -1 eq of charge.

either (a) adding sodium ions, (b) adding calcium ions, (c) adding ammonia (ammonium) ions, or (d) adjusting the pH (adding  $H^+$  ions).

In our example here, we will balance the net charge by adding sodium ions. Using more sodium is unlikely to change critical results (*e.g.* fouling) as sodium salts are generally soluble over a wide range of process conditions. However, additional  $Na^+$  ions may decrease the quality of the permeate water due to the small size and ability for these ions to cross RO membranes (as oppose to  $Ca^{2+}$ ). Under the *Feed Setup* menu bar tab, click “Add Sodium” to automatically balance the charge with sodium ions. The charge balance should now be a very small value (approximately  $-0.000063$  meq/L), which is essentially zero. The completed result is shown in **Figure 5.2**. We are ready to continue; return to the flowsheet by clicking on the *Home* project setting tab.



If you enter a water composition that is not charge-balanced, WAVE will not let you leave the *Feed Setup* screen until you make changes which set the net charge of the solution to zero.

**Specifying Desired Flow Rates.** WAVE requires the user to specify either the total flow rate of the influent or effluent so that it can perform its calculations. In our scenario in **Section 2.3**, we were told that the mine produces  $350$   $m^3/h$  of brackish wastewater. This is the influent flow rate to the treatment system. Return to the *Home* tab and ensure that the “*Feed Water*” radio box () is ticked and set the flow rate in the field below. Check that your units are correct! Your flowsheet should look like that shown in **Figure 5.3**. If we knew how much treated water that we needed to produce, we could set the flow rate of *Product Water* instead. We are now ready to add membrane processes to our system. Save your project before moving on.

## 5.2 Adjusting the Ultrafiltration Process Settings

One of our separation process design heuristics says to “separate out the easiest-to-remove species first”. Take another look at **Table 5.1** (*i.e.* Table 2.1 in Section 2.3) what sorts of species are present in the water? What are the easy-to-remove contaminants in this feed water? In membrane filtration, the largest particles tend to be the easiest to remove. In our system, this would be the suspended or colloidal species: that is, the total suspended solids (TSS) and the turbidity. These particles are generally greater than  $10$  nm in size and may even exist in the micron size range ( $\mu m$ ). According to the “filtration spectrum”, we could use a UF membrane in order to remove the colloidal matter first. This section will deal with the design and operation of UF membrane systems for the removal of suspended solids and turbidity.



**Figure 5.3:** Specifying the flow rate.

Once you have specified the feed chemistry it is time to add the UF technology to the flow sheet by dragging and dropping it from the technologies panel on the *Home* tab. As seen in **Figure 5.4**, the UF process is now applied to the flow sheet.

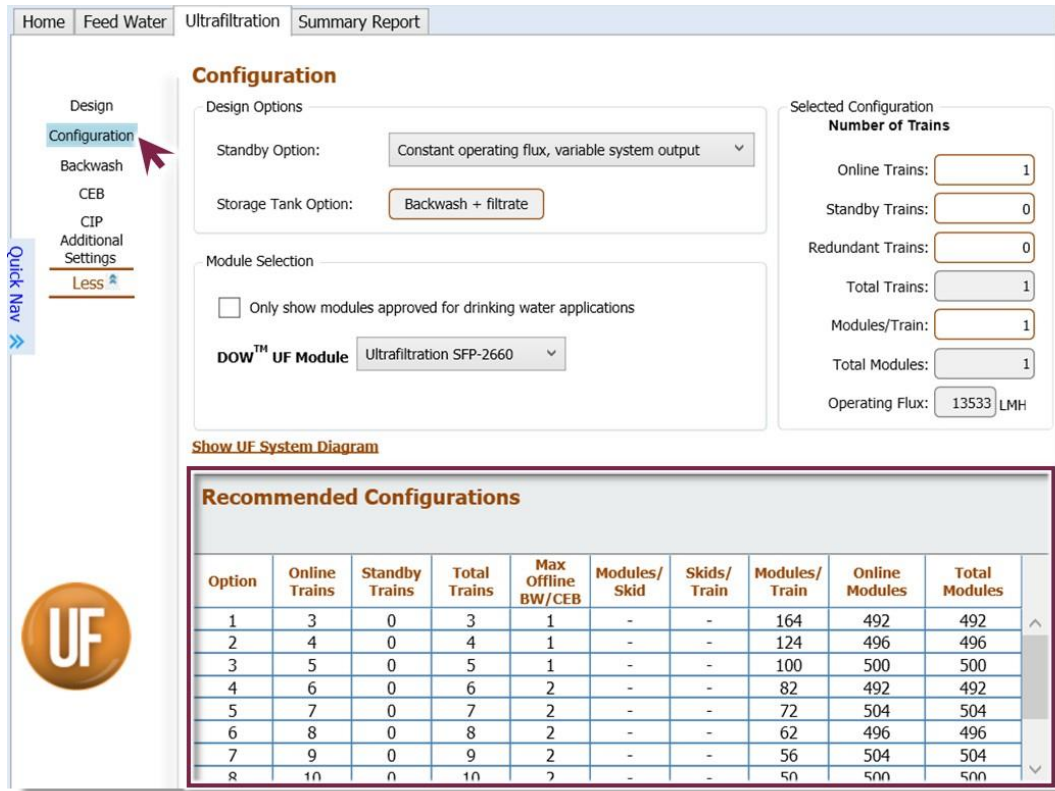
Navigate to the *Ultrafiltration* project tab – the default settings associated with the UF process for this example are found here, as seen in **Figure 5.5**. For now, we will leave the default values as-is, including the default membrane module as the SFP-2660 – more on this to come!

Recall that under the *Configuration* tab on the left side of the screen we can choose the exact layout of the membrane system with regards to number of modules and modules per train. As you can see, WAVE has given us recommendations of configurations. The recommended configurations are based on this scenario, considering the water quality and the required flow of our feed water, hence why they are different than the suggested configurations we saw in **Chapter 3**. The suggested options can be seen in **Figure 5.6**.



**Figure 5.4:** Adding a UF system to the flowsheet.

**Figure 5.5:** Default UF settings for the UF system which can be customized and adjusted.



**Figure 5.6:** Suggestions from WAVE of various configurations for treating brackish wastewater.

Now, we must select one of the recommended configurations. Recall the “default” option is to have only *one train* and *one module* and note the operating flux in the *Selected Configuration* panel is 13,533 LMH (L/m<sup>2</sup>/h). Similar to what we saw in *Chapter 3*, this flux is massive and unreasonable. We will select a reasonable middle ground option: Option 6, with 8 trains and 62 modules/train (496 total modules). Double-click on that row in the table to populate the *Selected Configuration* panel. Now the operating flux through a given membrane is 25 LMH—much more reasonable!

**?** Take a look at the design screen, and investigate the operating parameters that have been adjusted for our chosen configuration. What is the UF system recovery? Do you think there is opportunity to improve and optimize the system based on the values for the *Feed Water*, *Net Filtrate* and *Waste* streams? If so brainstorm some ideas to optimize the UF system. Save your ideas for later as we will attempt to optimize the system.

### 5.3 Interpreting the Ultrafiltration Report

Let us review the results from the simulation of the UF system. Navigate to the *Summary Report* tab in the project tabs.

**!** If WAVE displays an error that the simulation cannot converge, then ensure that your design parameters are as specified in the courseware. Restarting the software can help clear previous solutions and may enable convergence.



The lower section of the “UF Summary Report” is shown in **Figure 5.7**. Let us look at the last category to diagnose any issues associated with our design. Two design warnings are present:

1. “Forward Flush Flow < Min”: during the forward flushing membrane cleaning process, the flow rate (0.8 m<sup>3</sup>/h/module) is less than the recommended value (1.0 m<sup>3</sup>/h/module). We should increase the forward flushing flow rate manually.
2. “Fouled Membrane TMP @ TBW > Max”: the transmembrane pressure at the time of backwashing starts (2.6 bar) is higher than design guidelines (2.5 bar). We need to reduce the TMP during backwashing.

To fix these issues, return to the *Ultrafiltration* tab and change the value of the “*Forward Flush Flow*” to 1 m<sup>3</sup>/h/module on the *Design* view under the “*Design Instantaneous (Gross) Flux and Flow Rates*” panel to dismiss the first warning. To deal with the elevated pressure during backwashing, we can reduce the flux of backwash water through the membrane: change the value of the “*Backwash Flux*” to 110 LMH from 120 LMH on the *Design* view under the “*Design Instantaneous (Gross) Flux and Flow Rates*” panel. Return to the *UF Summary Report* and all warning messages should be gone.

Now, observe the UF Water Quality table seen in **Figure 5.8**:

- Turbidity has decreased from 85.2 NTU to less than 0.1 NTU.
- All the TSS has been removed.
- The TOC content has decreased from 11.2 mg/L to 10.1 mg/L. The remaining TOC is most likely a dissolved fraction that passed through the UF membranes.
- Notably, the dissolved content (salts, small organics, etc.) remains unchanged at 1,382 mg/L! There is a need for a subsequent treatment process to remove these components.

The screenshot shows a software interface with a navigation bar at the top containing 'Home', 'Feed Water', 'Ultrafiltration', and 'Summary Report'. A red arrow points to the 'Summary Report' tab. Below the navigation bar is a sub-header 'Ultrafiltration Report'. The main content area is titled 'UF Water Quality' and contains a table with the following data:

Stream Name		Stream 1	
Water Type		Waste Water (8.0 - 22.0 °C)	
		Feed	Expected UF Product Water Quality
Temperature	(°C)	15.0	15.0
Turbidity	(NTU)	85.2	≤ 0.1
TSS	(mg/L)	80.9	-
Organics (TOC)	(mg/L TOC)	11.2	10.1
TDS	(mg/L)	1382	1382
pH		7.5	7.5

Below the water quality table is a section titled 'UF Design Warnings' with a table containing two rows of warnings:

Design Warning	Limit	Estimate
Forward Flush Flow < Min (m <sup>3</sup> /h/mod)	1.0	0.8
Fouled Membrane TMP @ TBW > Max (bar)	2.5	2.6

**Figure 5.7:** A portion of the tabulated results for the simulation of the UF system, showing the provisional water quality results and design warnings.

**UF Water Quality**

Stream Name		Stream 1	
Water Type		Waste Water (8.0 - 22.0 °C)	
		Feed	Expected UF Product Water Quality
Temperature	(°C)	15.0	15.0
Turbidity	(NTU)	85.2	≤ 0.1
TSS	(mg/L)	80.9	-
Organics (TOC)	(mg/L TOC)	11.2	10.1
TDS	(mg/L)	1382	1382
pH		7.5	7.5

**Figure 5.8:** Water quality report for the UF system (DuPont SFP-2660) treating mining wastewater.

Also note the results in the *UF System Overview* and *UF Operating Conditions* tables. Overall, our system has 8 trains producing an average product water flux of 20 LMH at an average TMP of 0.18 bar (15°C) and a net recovery of 64.3%. Each train creates 29 m<sup>3</sup>/h of the total 223.9 m<sup>3</sup>/h of permeate water produced by the UF system.

☞ Let us modify our current process to see if we can optimize the system in any way. First save your current project as it is – we will be using it later on in the following sections.

## 5.4 Optimizing the Ultrafiltration System

On your own, consider the following open-ended scenarios in order to optimize the UF process. Each scenario builds upon the previous one. Attempt to mitigate any warning messages that WAVE produces.

1. In our ultrafiltration, example the permeate water recovery is low (< 70%). Does DuPont sell a UF membrane that would provide a better recovery? If so, replace the DuPont SFP-2660 with this membrane. Is the removal of turbidity/organics affected?
2. The current system configuration sees a constant flux forced through the membranes, but a variable total water output as modules are taken offline for cleaning due to fouling. Realistically, the mining company would prefer a water variable flux and a constant total water output, meaning that additional trains (“standby trains”) are put online to compensate for declining flux due to fouling and those taken offline due to cleaning. This can be changed by choosing the “*Constant System Output, Variable Operating Flux*” option in the *Configuration* view. Remember to select a configuration from the table! Note that there are now *Standby Trains* in the design: trains that are only sometimes operational to “make up” additional capacity as the other membranes are taken offline for preventive maintenance (*i.e.* cleaning).

- Does varying the total number of trains (including online plus standby trains) change the recovery of permeate water or the removal of solids?

☞ Also save your “optimized” treatment system as a *new file*. As everyone’s optimization process will be different, we will use the unoptimized version at the beginning of the next section for the sake of simplicity! You can come back to these optimized parameters after you have added subsequent RO system.

An example of one optimization scenario that was designed, two online trains (with one standby train) of IntegraFlux SFP-2880XP membrane modules were used, producing a system recovery of 67.96% and the TMP as designed was 0.2 bar at 15°C (see **Figure 5.9**). The permeate water contained  $\leq 0.1$  NTU of turbidity, 10.1 mg/L organics, and 1,382 mg/L of dissolved solids (see **Figure 5.10**).

#### UF System Overview

Module Type	IntegraFlux SFP-2880XP	
# Trains	Online = 2	Standby = 1
		Redundant = 0
# Modules	Per Train = 74	Total = 222
System Flow Rate (m <sup>3</sup> /h)	Gross Feed = 350.0	Net Product = 236.7
Train Flow Rate (m <sup>3</sup> /h)	Gross Feed = 175.0	Net Product = 118.3
UF System Recovery (%)	67.96	
TMP (bar)	0.25 @ 8.0 °C	
Utility Water	Forward Flush: Pretreated water	Backwash: UF filtrate water

**Figure 5.9:** The system overview of the optimized UF system.

#### UF Water Quality

Stream Name	Stream 1	
Water Type	Waste Water (8.0 - 22.0 °C)	
	Feed	Expected UF Product Water Quality
Temperature (°C)	15.0	15.0
Turbidity (NTU)	85.2	$\leq 0.1$
TSS (mg/L)	80.9	-
Organics (TOC) (mg/L TOC)	11.2	10.1
TDS (mg/L)	1382	1382
pH	7.5	7.5

**Figure 5.10:** The water quality of the optimized UF system.

## 5.5 Simulating Reverse Osmosis in Series with Ultrafiltration

In the previous sections, we “separated the easiest-to-remove species first” (the large colloidal species) through the use of UF membranes. If we look at the quality of the permeate water stream (see **Figure 5.8**), there is still significant amounts of solids left in the water, namely the *total dissolved solids* (TDS = 1,382 mg/L). In this chapter, we will use RO membranes in order to reject the smaller “dissolved” species and produce highly-purified product water.

Following our UF process that we designed in the previous section, we would like to install a RO system. That is, the *permeate water* from the UF process will feed into the RO system. To do this in the software, simply drag and drop the green “RO” icon onto the block-flow diagram (on the *Home* tab) right after the orange “UF” icon, as we did before. In this “default” configuration, WAVE assumes that the permeate water will flow into the next process as the feed. The results are shown in **Figure 5.11**.



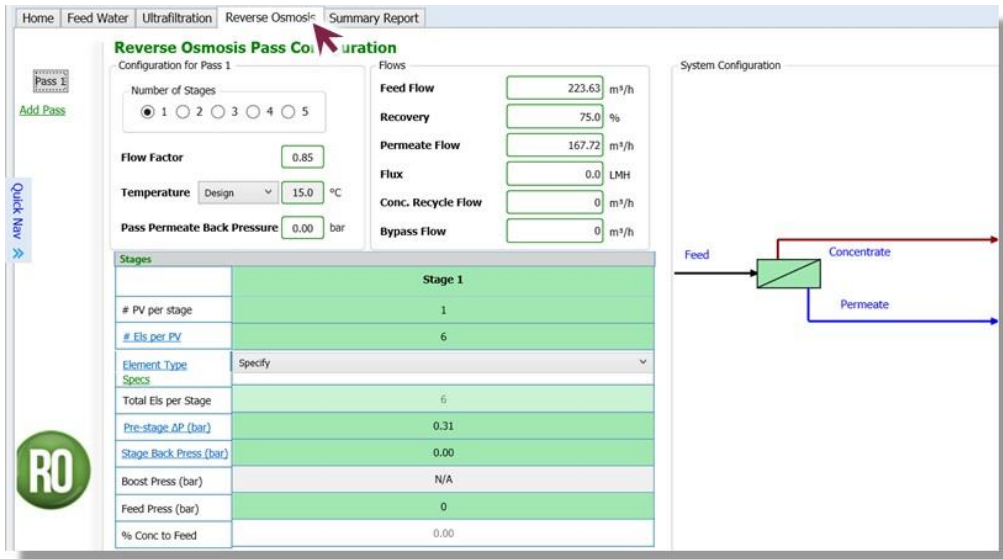
Note a limitation to the WAVE software, we cannot take the concentrate stream from the UF process and treat it within the original flow sheet. A new WAVE file would be required to simulate treating the concentrate stream.

Access the *Reverse Osmosis* tab to begin. **Figure 5.12** shows the initial screen whereby the user can adjust RO parameters. Recall that the default layout is for a single-stage, single-pass system. To improve this design, let us consider the system that we have:  $\sim 224 \text{ m}^3/\text{h}$  of permeate water containing mainly of dissolved solids (*i.e.* salts;  $\sim 1,400 \text{ mg/L}$ ). Assuming that the effluent discharge standards are not extremely strict, the “quality” of the permeate water is not too important. However, as we have a large volume of water to process and because we lost a significant fraction ( $\sim 30\%$ ) during the UF step, we should process as much of the feed to the RO system as possible. Thus two design goals can be made:

1. As a high rejection of solids is not necessary, a minimum number of passes is acceptable.
2. As a high recovery of water is necessary, using multiple stages is advisable.



**Figure 5.11:** Adding an RO system to the flowsheet following an UF system.



**Figure 5.12:** Editing the design parameters for RO systems.

① While we are only using one pass in this design, the same process applies to all additional passes. Click “Add Pass” on the far left panel of the screen to increase the number of passes in a subsequent design.

Begin by adding additional stages onto our first pass. Let us begin with *three* stages in the pass: Choose “3” stages in the *Configuration for Pass 1* panel. We can now specify which exact membranes that we would like within the modules. WAVE allows the designer to use a different membrane type in each stage! For our system, let us return to the “perform the easiest separation first” heuristic:

- For the first stage, let us choose a more permeable membrane in order to create as much permeate water as possible before the feed water becomes saturated with salt. WAVE offers nanofiltration membranes (*i.e.* NF-series membranes) in addition to reverse osmosis membranes in its RO model. So for the first stage, select the “NF90-400/34i” membrane from the *Element Type* drop-down menu. The datasheet for this element can be found here: <https://www.lenntech.com/Data-sheets/Dow-Filmtec-NF90-400-34i-L.PDF>.
- For the subsequent two stages, let us choose RO membranes with good performance. Select the “XLE-440” membranes for these stages. The datasheet for this element can be found here: <https://www.lenntech.com/Data-sheets/Dow-Filmtec-XLE-440.pdf>.

WAVE also allows the user to specify each individual element type within the pressure vessel. This is referred to as an internally staged design (ISD). This configuration is patented by The Dow Chemical Company and aims to reduce uneven flux distribution across elements. We will not implement an ISD in this scenario but for future reference the user can create an internally staged design by specifying it on the stage parameters table on the *Reverse Osmosis* tab. To do so, click on the element drop down menu and choose the “ISD (internally staged design option)”. A new window will appear called “Element Configuration – Internally Staged Design”. In this window the user has the ability to choose each element type for the individual elements in the PV

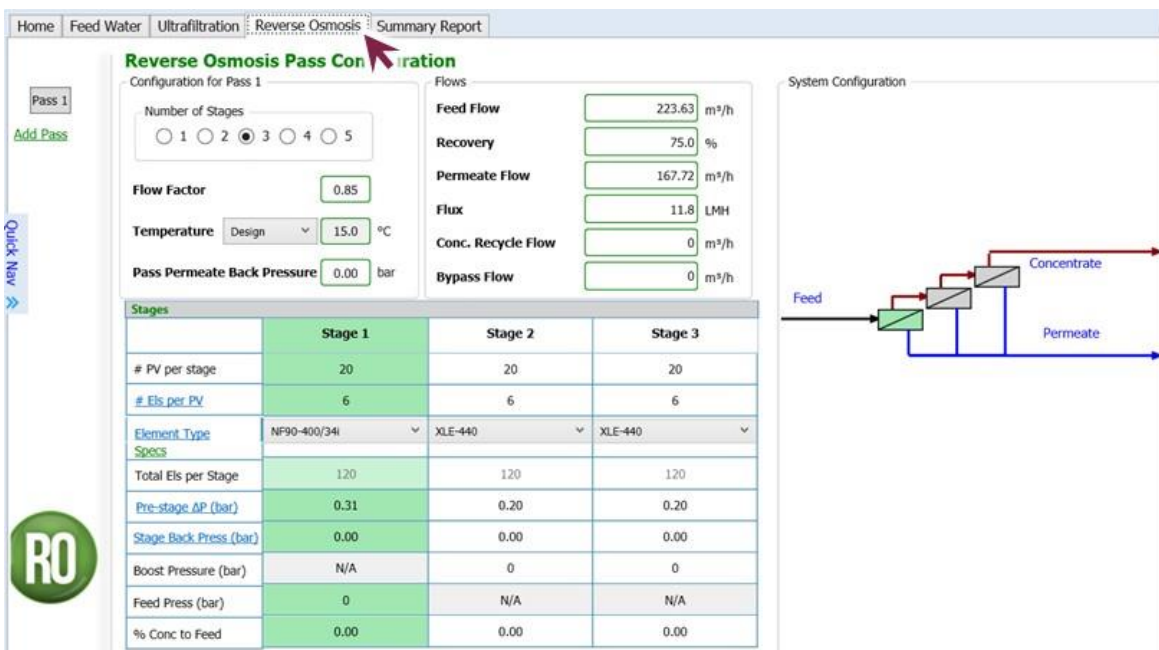
and clicking “OK” will implement the design. To edit the design later click “Edit ISD” under the element type drop down menu in the stages parameter table.

To learn more about the advantages of an ISD check out this article here: <https://www.waterworld.com/international/desalination/article/16200586/internally-staged-designs-key-to-cost-cutting-in-desalination>

Having selected our membrane types, we must tell WAVE how many pressure vessels (PVs) that we wish to have in each stage. In a real UF/RO system, the number of PVs per stage would be the result of a complex optimization problem involving values such as water recoveries, operating costs, and plant footprint. For now, assign 20 PVs in each stage by typing the number into the “# PVs per stage” field in each stage. With 20 PVs in each of the 3 stages, and 6 elements per PV, the plant would have  $20 \times 6 \times 3 = 360$  total RO elements. The number of elements per PV is also assignable ( $\leq 8$ ), but we will leave these values as default (6) for now. Check back to **Figure 5.13** for the design parameters of our RO system.

! Note we are not using the membrane design steps from the Chapter 4 for the sake of simplicity. In this chapter finding any given solution in this case is sufficient.

Let us now run the simulation to determine the performance of our combined UF/RO system. Be sure that you check your parameters before you continue. WAVE’s calculations often fail to converge—especially with RO systems—if there are incorrect parameters.



**Figure 5.13:** The chosen design parameters for our three-stage, single-pass system.

## 5.6 Reverse Osmosis System Simulation Results

Click on the *Summary Report* tab. Provided that your simulation converges, select the new *Reverse Osmosis Report* tab below. Let us analyze and work through the results in the report:

**Summary Table.** In the first table (right below the process diagram), we have a summary of the flow conditions in the RO system, seen in *Figure 5.14*. Note that the RO feed from the UF trains enters the first pass at 223.8 m<sup>3</sup>/h and 1,378 mg/L of dissolved solids (and at 5.3 bar), of which only 167.9 m<sup>3</sup>/h leaves in the product stream (final TDS ~60 mg/L)! The concentrate stream leaving the RO system on the other hand has a flow rate of 56 m<sup>3</sup>/h with a very high TDS of ~5,323 mg/L. Even though we are feeding 350 m<sup>3</sup>/h of influent to the entire system, we are only producing 167.9 m<sup>3</sup>/h in treated water (48% *overall* recovery). The rest of the water (UF, RO concentrate) must be purified via other technologies, or would be sent back to the tailings pond.

☞ Verify that the average membrane flux in the RO system is equal to 11.8 LMH, the value in the RO System Overview table.

**RO Design Warnings.** Like with the UF system, we have several design warnings, as seen at the top of *Figure 5.15*. Here, we can see that the flow rates of the concentrate streams in the second and third stages of the design are lower than the system limits. We will address this issue soon.

**RO Solubility Warnings.** As is seen at the bottom of *Figure 5.15*, we have three warnings associated with exceeding the barium solubility limit (as barium sulfate). One such warning tells us that the saturation of barium sulfate (BaSO<sub>4</sub>) is above 100%. Barium is a notable problem in RO systems and even in tiny concentrations, it can cause problems as precipitated barium salts can deposit on the surface of the membranes and cause mineral scaling, which decreases the membrane flux over time. We will also address this issue soon.

**RO Chemical Adjustments.** Notice that the BaSO<sub>4</sub> row is highlighted in red. This is WAVE's way of telling us that perhaps some chemical addition would help mitigate the effects of the supersaturated barium sulfate ions. Perhaps more interestingly, the barium ions were at ~770% of the saturation limit even before the RO system. This value skyrockets to almost 4,000% in the concentrate from the first pass!

**Addressing RO Warning Messages** Now that we have analyzed the RO summary report, let us address the two warnings that WAVE has issued: the low concentrate flow rate in the second and third stages, and the supersaturation of barium sulfate in the feed/concentrates. Return to the *Reverse Osmosis* project tab, and consider the following actions:

#	Description	Flow (m <sup>3</sup> /h)	TDS (mg/L)	Pressure (bar)
1	Raw Feed to RO System	223.9	1,377	0.0
2	Net Feed to Pass 1	223.8	1,378	5.3
4	Total Concentrate from Pass 1	56.0	5,323	2.5
6	Net Product from RO System	167.9	60.69	0.0

**Figure 5.14:** Summary table for the RO process.

### RO Design Warnings

Design Warning	Limit	Value	Pass	Stage	Element	Product
Concentrate Flow Rate < Minimum Limit (m <sup>3</sup> /h)	4.09	3.84	1	2	6	XLE-440
Concentrate Flow Rate < Minimum Limit (m <sup>3</sup> /h)	4.09	3.60	1	3	1	XLE-440
Concentrate Flow Rate < Minimum Limit (m <sup>3</sup> /h)	4.09	3.39	1	3	2	XLE-440
Concentrate Flow Rate < Minimum Limit (m <sup>3</sup> /h)	4.09	3.21	1	3	3	XLE-440
Concentrate Flow Rate < Minimum Limit (m <sup>3</sup> /h)	4.09	3.05	1	3	4	XLE-440
Concentrate Flow Rate < Minimum Limit (m <sup>3</sup> /h)	4.09	2.92	1	3	5	XLE-440
Concentrate Flow Rate < Minimum Limit (m <sup>3</sup> /h)	4.09	2.80	1	3	6	XLE-440

### RO Solubility Warnings

Warning	Pass No
Langelier Saturation Index > 0	1
BaSO <sub>4</sub> (% saturation) > 100	1
Anti-scalants may be required. Consult your anti-scalant manufacturer for dosing and maximum allowable system recovery.	1

**Figure 5.15:** Warnings issued due to design and solubility violations in the RO system.

- The concentrate flow rate is too low in many of the later pressure vessels. This can cause a problem because scaling or fouling is often mitigated by keeping the flow rate of water in the modules high. A high flow rate produces a high water velocity, which can “lift” scalant particles off the membrane’s surface. One common way of increasing the concentrate flow rate (and water velocity) in RO systems is to actually recycle some of the final concentrate back to the feed of the RO system. This increases the flow rate of water over all the stages, but also increases the TDS concentration due to the concentrated recycled salt solution! To recycle the concentrate stream back to the feed in WAVE, click any field in the *Flows* panel and set the “*Conc. Recycle*” field to be 35.00%, a value which should increase the concentrate flow rates in the modules just enough to suppress the warnings. The physical interpretation is that 35% of the final concentrate stream will be returned to the feed inlet, as seen in **Figure 5.16**. Make sure that the concentrate is recycled “to the head of Pass 1”. Type “Enter” and then click “OK” when you are finished.

🔗 What capital and operating cost implications are there if you recycle 35% of the final concentrate stream back to the feed of the RO system?

Implementing a concentrate recycle is also a good strategy in terms of operation costs, specifically electricity. Recycling the water around increases pumping costs but overall is cheaper than other options.

- The warning associated with the barium ions reflects the fact that barium ions and sulfate ions—of which we have a high concentration—react (almost) irreversibly to form insoluble barium sulfate which can scale the RO membranes. This scale is very difficult to remove. As such, we would like to minimize the scaling or decrease the barium saturation. Two potential solutions are to modify the pH of the RO feed to increase the solubility of the offending species, or by adding an anti-scaling chemical. For now, we will try the latter option. Under the *Configuration* tab, click the “+ Add Chemicals/Degas” button. Click on the “Anti-Scalant” button to confirm that you are adding an antiscalant to the RO feed; select sodium hexametaphosphate (Na<sub>6</sub>P<sub>6</sub>O<sub>18</sub>) from the drop-down menu, and use the



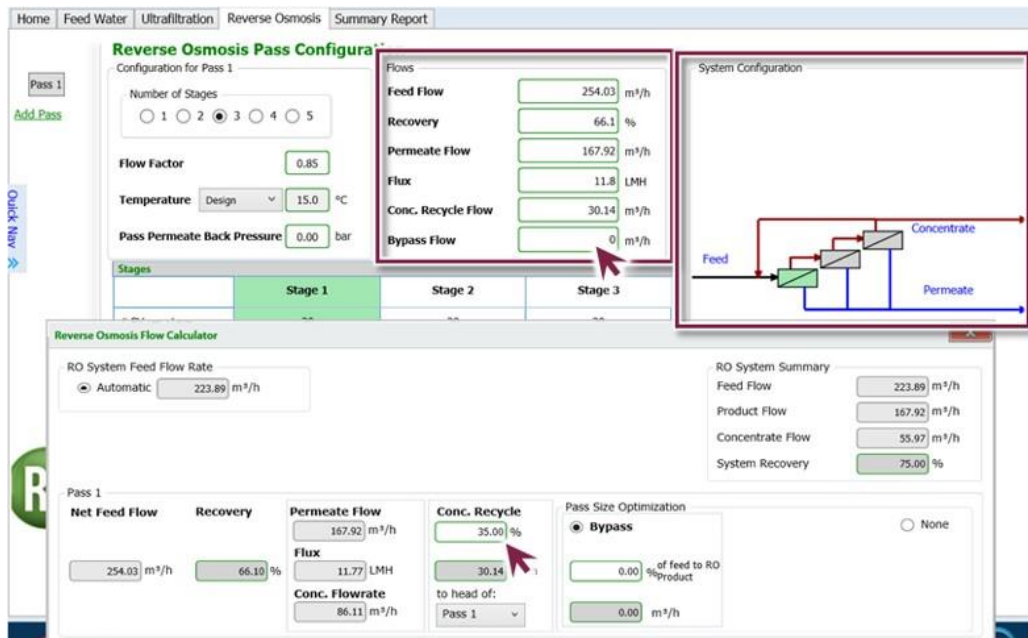
“manufacturer’s recommended dose” of 3 mg/L. This can be seen in **Figure 5.17**. Click “OK” when you are finished.

? Consider the cost of adding the antiscalant given that we add 3 mg/L of sodium hexametaphosphate ( $\text{Na}_6\text{P}_6\text{O}_{18}$ ). Calculate the total amount, in kilograms, of antiscalant per day based on the feed to the RO system.

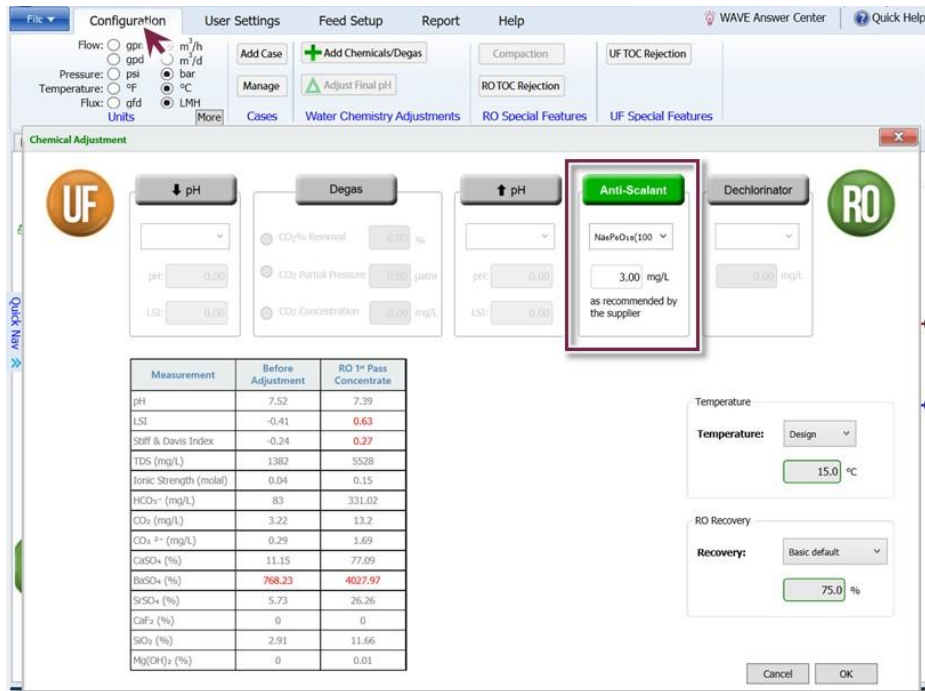
The amount of antiscalant adds up and may be costly in many cases. But it may be costlier to deal with the consequences of scale such as frequent chemical cleanings and even replacement of elements.

Return to the *Reverse Osmosis Report* and check the *RO Design Warnings* and *Solubility Warnings*. You will notice that the concentrate recycle eliminated the design warnings, however the addition of the antiscalant did not change the solubility warning. The water chemistry reactions that occur are often highly complex and the calculation engine may not accurately model what is going on between the barium and antiscalant. Keep this in mind when analyzing the results, perhaps the antiscalant works or does not. A pilot scale study can be used to observe the effects of the antiscalant. Barium is a persistent scalant, and even in the low concentrations that we see in this particular system, it can still cause issues. In some cases, feedwaters with barium may require a chemical precipitation step before using any RO membranes, or a cation exchange resin may also be used. At this time, we will ignore the barium saturation warning with the realization that other technologies may be needed to prevent or mitigate barium sulfate scaling.

i WAVE can model a cationic exchange resin to remove barium ions, but that is beyond the scope of this chapter.



**Figure 5.16:** Recycling a fraction of the final concentrate stream back to the feed to the RO system.



**Figure 5.17:** Chemicals can be added to the RO feed water to adjust the water chemistry. Here, we add sodium hexametaphosphate as an antiscalant.

## 5.7 Optimizing the Ultrafiltration & Reverse Osmosis System

On your own consider the following open-ended scenarios which will lead you in optimizing the combined UF/RO process. Each scenario can build upon the previous one; do not return to the original scenario with each question. Again, attempt to address any warning messages that WAVE produces. Remember that the WAVE software has a tendency of not being able to converge its calculations, especially when simulating RO systems. As a tip, when you make a change to system parameters and it works, save the system immediately. If a subsequent change makes a calculation fail to converge, but you undo that change, WAVE will sometimes fail to converge again! (WAVE may be using the non-convergent solution as an initial condition.) In this case, restart the software and return to the saved file. When in doubt, restarting the software clears previous values from the memory—especially those pesky non-convergent “solutions”!

1. Previously in **Section 5.4**, you optimized your UF system. We returned to the unoptimized version so we all would be using the same results. Re-optimize the UF system. In particular, we want to engage the *standby trains* so that the UF process has a constant system output, but variable operating flux. Recall that this option is found in the *Configuration* view. You may need to adjust your RO settings to compensate for the increased flow rate (*e.g.* the number of PVs per stage).
2. By changing the membrane element type, can you improve the quality of the permeate stream, with all else equal?

3. What is the effect of adding or removing a stage on the separation (*e.g.* the permeate quality, recovery, number of PVs/elements, etc.)?
4. Similarly, what happens if you add an additional *pass*? You can assume that the second pass is identical to the first, with the same number of stages, the same elements in each stage, the same number of PVs per stage, and so on.
5. In the simulation up until this point, we have used WAVE's default RO total recovery value (75%)—the fraction of the feed to the RO system that is recovered in the permeate stream. With your current system, can you increase the recovery percentage? What parameters do you have to modify to address any design warnings? Hint: the recovery can be adjusted by clicking on any field in the RO *Flows* panel, then adjusting the *System Recovery* value in the *RO System Summary* panel. What are the implications of increasing the system recovery on the subsequent treatment of the discharged RO concentrate stream?
6. Can you reduce capital costs reducing the number of PVs required in each stage?
7. Just like we added an antiscalant, add pH-adjusting chemicals to see if a different pH (higher or lower) can prevent the barium saturation warning.

-End of Chapter-