Class and Home Problems (CHP) present scenarios that enhance the teaching of chemical engineering at the undergraduate or graduate level. Submissions must have clear learning objectives. CHP papers present new applications or adaptations that facilitate learning in specific ChE courses. Submit CHP papers through journals.flvc.org/cee, include CHP in the title, and specify CHP as the article type.

COMPUTATIONAL REVERSE OSMOSIS PROJECTS FOR UNDERGRADUATE CHEMICAL ENGINEERING EDUCATION

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INTRODUCTION

Traditional instruction is primarily instructor-directed, and assessment of student performance is heavily based on graded exams and homework assignments. The inclusion of team-based, industrially relevant projects promotes student-centered learning and a more comprehensive evaluation of student learning outcomes. Project-based learning (PBL) is an instructional pedagogy that enables students to apply and integrate knowledge through engaging projects that are set around contemporary, real-world challenges.[1] By actively participating in these projects, students not only gain problem-solving experience, but also gain skills in critical thinking, leadership, life-long learning, and the ability to communicate and collaborate. Moreover, they grasp the connection between theory and practice, enhancing their learning. Ultimately, they build their engineering capacity and workforce competency. Many successful stories of PBL in chemical engineering courses have been reported, ranging from first-year experience to capstone design.[2,3]

It is imperative for instructors to develop projects that are both intriguing and enlightening. The author chose reverse osmosis (RO) water desalination for two reasons. First, water scarcity is a global challenge.[4] In California, water shortage is a longstanding problem exacerbated by climate change, which calls for transformative solutions to water sustainability and resilience. This also opens opportunities for internship and full-time employment. However, there is no standalone water treatment course in the chemical engineering curriculum in the author's department. By enriching chemical engineering courses with content related to water treatment, the author hopes to equip the students with necessary knowledge and skill sets so they may tackle real-world problems after graduation. Second, key chemical engineering concepts (such as fully developed flow, dimensionless number, concentration polarization, residence time distribution, step response, and optimal control) are exemplified in these projects. It is worth mentioning that the University of Arizona has developed a unique hands-on course on membrane separation that encompasses bench-scale activities, operation of engineering-scale modules, and computer simulations that has greatly helped students understand the application of theoretical concepts on this subject matter.[5]

Over the past decade, the author has developed multiple course projects based on his research in membrane separation that have been implemented in several chemical engineering courses to enhance student success. The activities begin with field trips to local water desalination facilities, progressing to transport phenomena in RO, and culminating in design and control of emerging cyclic processes. A few examples of computational RO projects are discussed in the next section. A link is provided near the end of the paper for interested readers to download these projects and solutions.

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EXAMPLES OF COMPUTATIONAL RO PROJECTS

Project 1: Modeling of an Industrial Two-Stage RO Process Using an Ordinary Differential Equation (ODE) Model

This project is developed from operation data collected at a local municipal desalination facility (shown in Figure 1).

Figure 1. *Four RO trains employing spiral wound membrane modules in Chino I Desalter (Chino, California).*

Based on assumptions and simplifications including (1) 100% membrane salt rejection, (2) Darcy's law for flux, (3) approximate quadratic relation between retentate pressure drop and cross velocity (or feed velocity tangential to the membrane surface), and (4) constant temperature, the author proposed the following coupled ODE model to describe retentate flow and transmembrane pressure in a RO stage:[6]

$$\frac{dQ(x)}{dx} = -A_m L_p \left(\Delta P - \frac{Q_0}{Q} \pi_0 \right) \tag{1a}$$

$$\frac{d(\Delta P(x))}{dx} = -kQ^2 \tag{1b}$$

$$Q(x) = Q_0 \ @x = 0 \tag{1c}$$

$$\Delta P(x) = \ \Delta P_0 \ @x = 0 \tag{1d}$$

where Q, P, and π stand for retentate flow (gpm) hydraulic pressure (psi), and osmotic pressure (psi), respectively. x is the dimensionless location, or distance from the entrance divided by the length of one RO stage. In other words, 0-1 means the first stage, and 1-2 means the second stage, respectively. A_m is the membrane area in each stage (ft^2). L_p is membrane permeability (gpm/ft^2/psi). k is the pressure drop parameter (psi/gpm^2). Δ represents transmembrane properties. For example, ΔP is the difference between the retentate pressure and the permeate pressure. Subscript 0 represents the inlet conditions. L_p and k are calibrated by nonlinear regression of plant data [6] and are made available to the students. The system uses a 2:1 RO array (i.e., the number of pressure vessels in the first stage is twice of that in the second stage), therefore A_m and k in the second stage are different from those in the first stage.

This project has three assignments. First, students are asked to solve for the retentate flow and transmembrane pressure along the process and the overall water recovery ($Y = 1 - Q_2/Q_0$) with given inlet conditions (Q_0, ΔP_0 and π_0) and process parameters in each stage (A_m, L_p, and k). Equation 1 is already in the standard form of a coupled ODE system, and any ODE solver (e.g., `ode45` in MATLAB®) may be used for numerical integration. After Eq. 1 is solved for the first stage, the final values of Q and ΔP are used as initial values for the second stage. The modeling results and plant data (Y = 81%) are shown in Figures 2a and 2b. The permeate rate Q_p is calculated as the difference between the feed rate Q_0 and the brine rate Q_2.

Next, students are asked to solve for the ΔP_0 that would be required for a set of recoveries in the range of 78-96% if the permeate production is kept constant. This problem is inverse to the previous one and may involve trial and error, but it can be handled by iterative algorithms (e.g., `fsolve` in MATLAB). Students then plot the specific energy consumption (SEC) as a function of recovery. The SEC, which stands for pump energy consumption per unit permeate rate, is an important term in the RO literature.[7] The model-predicted hydraulic NSEC (SEC normalized by feed osmotic pressure) at different recoveries is shown in Figure 2c. By observing the shape of the curve, the students may gain an in-depth understanding of friction loss in brackish water RO. Since the intake flow is inversely proportional to the recovery rate for a fixed permeate production, as it reduces, so does the friction loss in the membrane channel. This leads to a higher transmembrane pressure, which in turn results in a higher recovery rate (up to 92% in this case) and a lower energy consumption. However, as the recovery goes beyond 92%, the effect of osmotic pressure becomes dominant, and the required pump pressure and energy consumption start to skyrocket. Therefore, the recovery rate in RO desalination can never reach 100%. In inland areas, the RO brine is considered as a non-reclaimable industrial waste and must be properly treated and discharged in accordance with the local ordinances.[8]

Finally, students are asked to derive the dimensionless equation below (Eq. 2) if the friction loss can be ignored (a reasonable assumption for seawater RO due to its high osmotic pressure), or $\Delta P(x)$ is a constant in Eq. 1: [9,10]

$$\gamma = \alpha \left[Y + \alpha \ln \frac{1 - \alpha}{1 - Y - \alpha} \right] \tag{2}$$

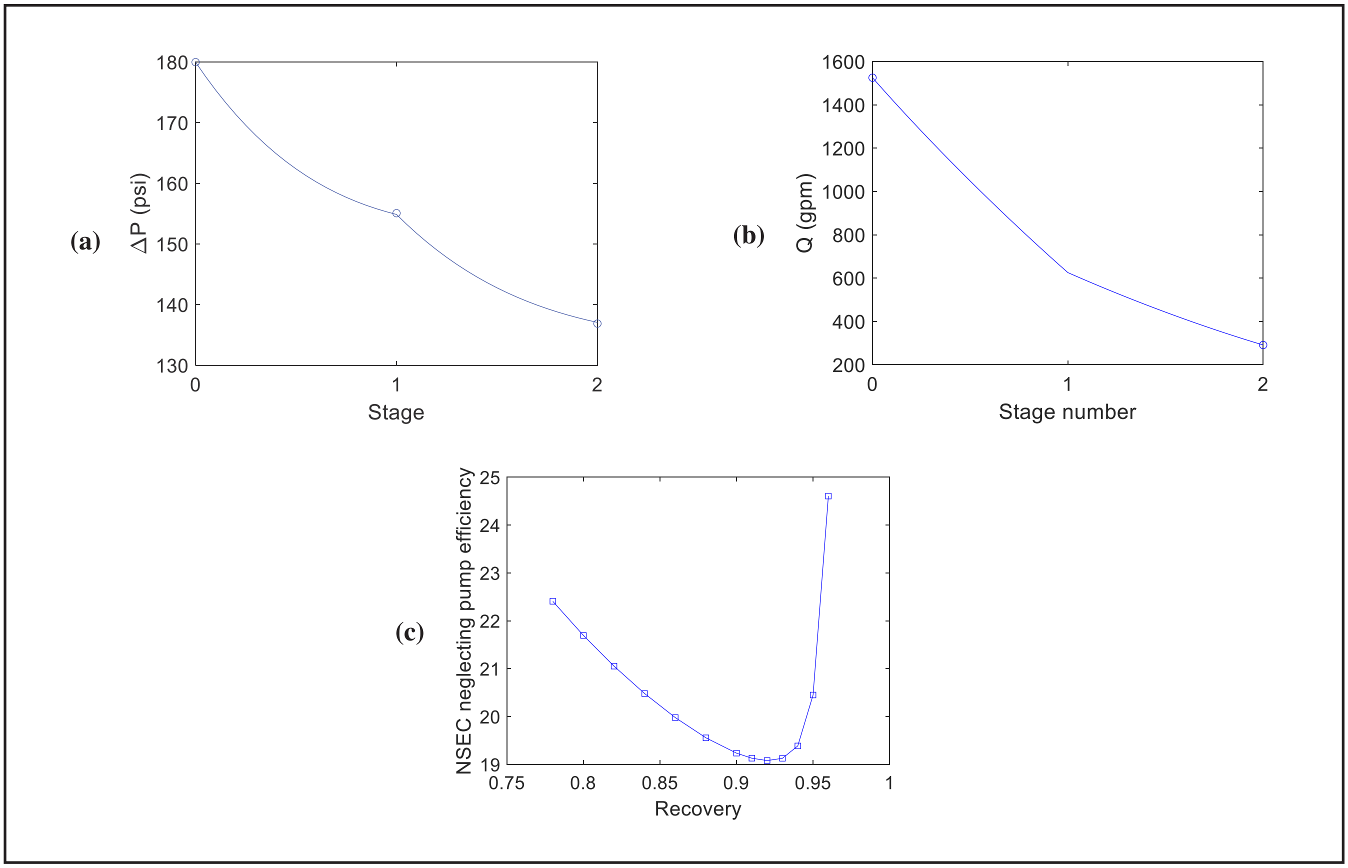

Figure 2. *Modeling results. (a) Transmembrane pressure (plant measurements are represented by symbols). (b) Retentate flow (plant measurements are represented by symbols). (c) NSEC at different recoveries.*

where $\alpha = \dfrac{\pi_0}{\Delta P}$, $Y = \dfrac{Q_p}{Q_0}$, and $\gamma = \frac{A_m L_p \pi_0}{Q_0}$. They are also required to explain the physical significance of each dimensionless number in Eq. 2. For example, α is the osmotic to hydraulic pressure ratio, and γ is the membrane capacity to intake ratio. In this assignment, students have an opportunity to refine their calculus and analytical integration skills. Moreover, dimensional analysis and dimensionless numbers are discussed at length in Transport Phenomena, a cornerstone course in the chemical engineering curriculum. For example, in momentum transport, the Fanning friction coefficient in a conduit is correlated as a function of the Reynolds number and the relative roughness.[11] In heat and mass transfer equipment, the effectiveness is found to be a function of the number of transfer units (NTU).[12] In this project, students extend the dimensionless parameters to the field of RO desalination, where the water recovery, Y, is implicitly correlated to the dimensionless pressure, α, and the membrane capacity/intake ratio, γ. Students are then referred to the literature for a 3D plot of Eq. 2.[9] For seawater RO the NSEC is strongly dependent on γ.[9,10] For brackish RO friction loss also affects the NSEC to a great extent.

Project 2: Modeling of an Industrial Two-Stage RO Process Using an Enhanced Differential Algebraic Equation (DAE) Model

In this project, the empirical model developed in Project 1 is enhanced using knowledge obtained from three-dimensional Computational Fluid Dynamic (CFD) simulations.[13] In spiral wound RO membranes, the feed channel is partially filled with net-type spacers, and, as a result, the relationship between friction loss and cross velocity is nonlinear even under laminar flow conditions. Using CFD, it is shown that the pressure drop per unit length of the commercial DuPont membrane of interest (i.e., FilmTec™ BW30-400) is proportional to the cross velocity with a power index of 1.67.[13] Moreover, because the semipermeable membrane allows water to permeate through it while the transport of salt is blocked, the balance between transverse convection and diffusion in the mass transfer boundary layer causes the salt concentration on the membrane surface to be higher than the bulk concentration. This phenomenon is known as concentration polarization. An enhanced system-level model accounting for these hydrodynamic and mass transfer characteristics is formulated in a DAE model:[13]

$$\frac{dQ(x)}{dx} = -J_w A_m, \ @x = 0, Q = Q_0 \quad (3a)$$

$$\frac{d(\Delta P(x))}{dx} = -k_f Q^{1.67}, \ @x = 0, \Delta P = \Delta P_0 \quad (3b)$$

$$J_w = L_p[\Delta P - \pi \exp\left(J_w/(k_m Q^{0.40})\right)] \quad (3c)$$

$$\pi = Q_0 \pi_0 / Q \quad (3d)$$

where J_w is water flux that varies spatially, k_f and k_m are pressure drop and mass transfer parameters determined from CFD simulations, respectively, and slightly modified by plant data.[13] The term $\exp\left(J_w/(k_m Q^{0.40})\right)$ represents the concentration polarization factor. Under typical industrial conditions, it is about 1.05 to 1.15.[14]

The students are asked to re-do the calculations in Project 1 using the enhanced model. The key challenge is that the local water flux, J_w, in Eq. 3c is in an implicit form that must be solved at each spatial step before Q and ΔP are integrated for one step. J_w at the new location is then solved and the integration is executed for another step. These are repeated until the end of the RO channel is reached. A comparison between both models and high-recovery experiments in the plant is shown in Figure 3. It appears that incorporating detailed friction loss and mass transfer characteristics in the system-level model slightly improves accuracy. It is interesting to note that the pump head remains fairly flat in the recovery range of 78-90%.

Additionally, students are asked to conduct a literature survey to explain why the water recovery in brackish RO plants in Southern California is limited to 85% or less even though Figure 3 shows that a 90% recovery may consume less energy relative to an 80-85% recovery. This is because the presence of sparingly soluble salts and minerals in the feed water (particularly silica, gypsum, and calcite).[15] If their solubility limits exceed saturation levels, crystal precipitation may occur, leading to permeation flux decline and even

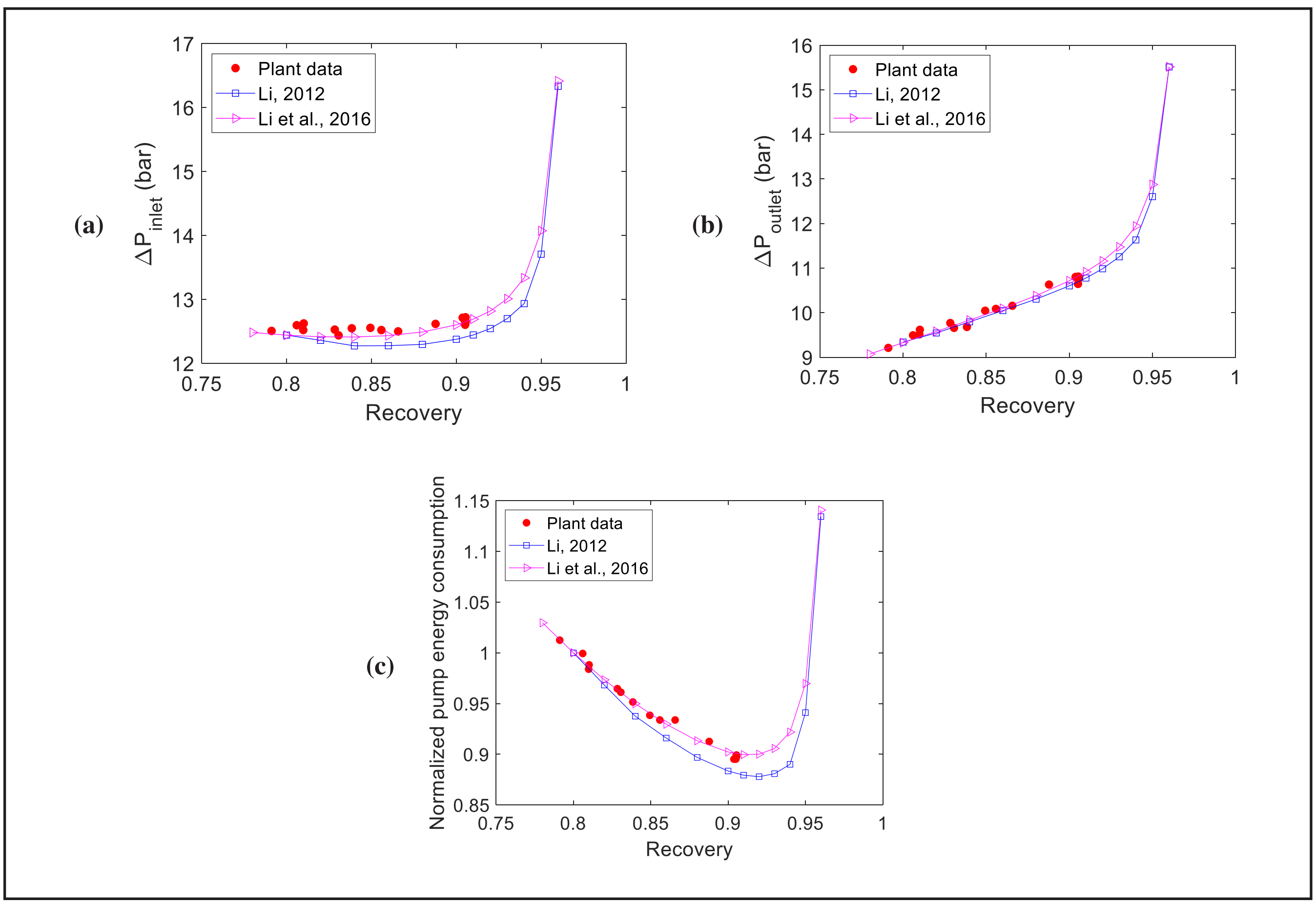

Figure 3. *Comparison between plant experimental data*[8] *and model predictions.*[6,13] *(a) transmembrane pressure at RO inlet. (b) transmembrane pressure at RO outlet. (c) pump energy consumption normalized by its value at an 80% recovery.*

membrane failure. Even though pretreatment is ubiquitously used in RO plants, it does have limitations. For example, the threshold inhibitors only slow the process of precipitation by interfering with the formation of crystals; they do not stop it.[16] Figure 4 shows precipitation in a brine line at the Chino I facility after 13 years in service. Moreover, a 90% recovery would require three or even four RO stages to prevent membrane elements from being overfluxed.[17] Interstage pumps may also be necessary to balance flux across multiple stages.[18] The coupling of multiple units brings about operational complexities.

Figure 4. *Precipitation in a brine line after 13 years in service at the Chino I Desalter.[16]*

Project 3: Residence Time Distribution in a Narrow Channel Under Laminar Flow Conditions

Residence time distribution (RTD) is an important concept in reactor engineering.[19] It is also critical in transient and cyclic operation of RO, which is an emerging research topic in water desalination.[20,21] For example, the closed-circuit RO (CCRO) by DuPont/Desalitech can attain a recovery up to 98% with a small footprint.[22] The CCRO is also relatively resistant to fouling compared to conventional steady-state designs, probably because the cycle time is shorter than the crystallization induction time of most sparingly soluble salts.

In this project, students are asked to obtain the RTD in a 2D plane rectangular channel (shown in Figure 5) under laminar flow conditions using COMSOL Multiphysics®. A spacer-filled RO channel may also be used for this project; however, it requires time-consuming 3D simulations.[23]

The COMSOL simulation is done in two steps. The first step is to obtain the flow field by solving the steady-state Navier-Stokes equation. The fully developed velocity profile [11] shown in Eq. 4 may be specified at the inlet to accelerate convergence:

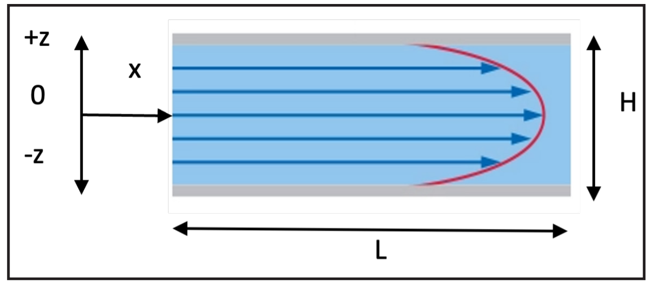

Figure 5*. Geometry of the 2D plane channel.*

$$v_x(z) = \frac{3}{2} v_{ave} \left[1 - \left(\frac{2z}{H}\right)^2\right] \quad (4)$$

where $v_x(z)$ is the axial velocity at location z measured from the center plane of the channel. v_{ave} is the average velocity. H is the channel height. The recommended values for the simulation are $H = 0.0008$ m, $L = 0.02$ m, and $v_{ave} = 0.1$ m/s.

Next, a virtual tracer [24] is introduced at the inlet (e.g., c_{in} = 100 mol/m^3), and the transient convection-diffusion equation is solved by "freezing" the flow field. The salt concentration at the outlet plane $c_{out}(z,t)$ is recorded, and the cumulative RTD function is calculated as shown in Eq. 5:

$$F(t) = \frac{\int_{out} c_{out}(z,t) v_x dz}{c_{in} v_{ave}} \quad (5)$$

The derivative of $F(t)$ is the RTD, $E(t)$. The RTD and cumulative RTD are analogous to the impulse and step responses in dynamic systems, respectively.[25]

In addition to the numerical solutions from transient CFD simulations, students are asked to derive the analytical solutions based on definitions given in a typical reactor engineering textbook:[23]

$$E(\theta) = \frac{1}{3\theta^3}\left(1 - \frac{2}{3\theta}\right)^{-\frac{1}{2}} \quad (6a)$$

$$F(\theta) = \left(1 + \frac{1}{3\theta}\right)\left(1 - \frac{2}{3\theta}\right)^{\frac{1}{2}} \quad (6b)$$

where θ is t divided by the space time, τ. A comparison of CFD and analytical solutions is shown in Figure 6 where they match closely.

It is seen from Figure 6 that the RTD of a plane channel is different from that of a plug flow reactor (PFR), which is a Dirac delta function.[19]

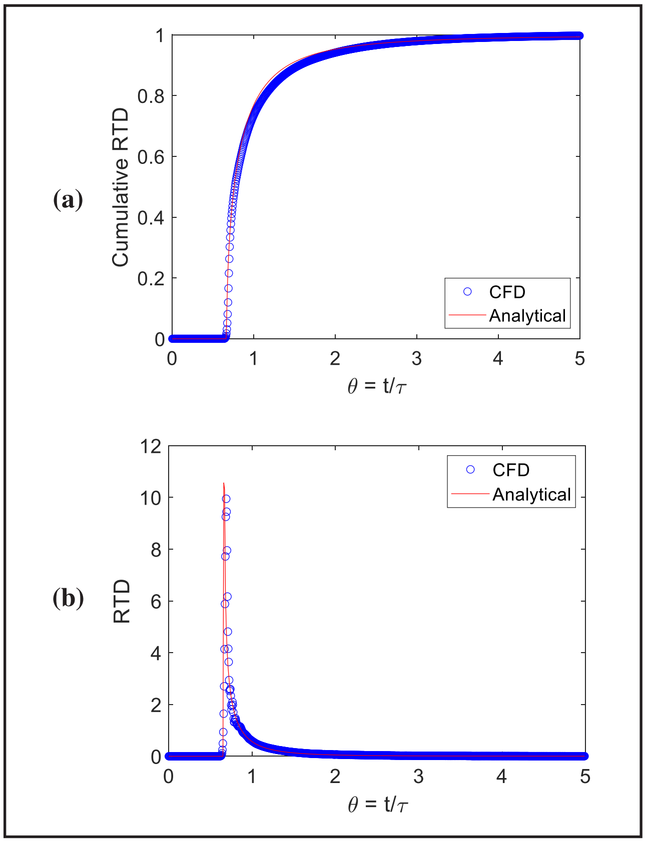

Figure 6. *Comparison of CFD results with analytical solutions. (a) Cumulative RTD. (b) RTD.*

Project 4: Optimal Trajectory of Applied Pressure in Filtration Step of Batch RO

The batch RO is based on transient and cyclic operation of a system consisting of a volume-varying cylinder and a spiral wound membrane unit. In the filtration step (shown in Figure 7), the brine is continuously recyled to the cylinder (to avoid excessive salt accumulation on the membrane surface), and the volume of the cylinder reduces. Because the salt concentration level in the system increases with respect to time, the applied pressure $P(t)$ must increase accordingly. Once a desired water recovery is reached, the membrane is flushed, and the cylinder is refilled before processing the next batch.

To a first approximation, consider the filtration step in an ideal batch RO process where friction loss, concentration polarization, and axial variation in salt concentration can be ignored. The system has an initial volume of V_0 and an osmotic pressure of π_0. We are interested in determining the optimal trajectory of $P(t)$ during the entire duration of operation from 0 to t_f (final time) so that the PV work [26] can be minimized for a specified initial volume, processing time, and water recovery. This can be formulated as an optimization problem in a dimensionless form:[20]

$$\min_{u(t^*)} NSEC = \frac{\int_0^1 u\gamma\left(u - \frac{1}{x}\right) dt^*}{Y} \tag{7a}$$

$$\frac{dx}{dt^*} = -\gamma\left(u - \frac{1}{x}\right) \tag{7b}$$

$$x(0) = 1 \tag{7c}$$

$$x(1) = 1 - Y \tag{7d}$$

where $NSEC = \frac{SEC}{\pi_0}$, $\gamma = \frac{A_m L_p \pi_0 t_f}{V_0}$, $u = \frac{P}{\pi_0}$, $x = \frac{V}{V_0}$, and $t^* = \frac{t}{t_f}$. The definition of γ in batch RO is similar to the one in continuous RO, except that V_0/t_f is replaced by Q_0 in the latter.

Equation 7 is in the standard form of a typical optimal control problem with terminal value constraint, where x is the state variable and u is the manipulated variable.[27] By constructing the Hamiltonian, it is shown that solution to Eq. 7 can be determined by solving the ODEs in Eq. 8a and Eq. 8b: [20]

$$\frac{dx}{dt^*} = \frac{\gamma(1 - Y\lambda x)}{2x}, @t^* = 0, x = 1 \tag{8a}$$

$$\frac{d\lambda}{dt^*} = \frac{\gamma(Y\lambda x - 1)}{2Yx^3}, @t^* = 0, \lambda = \lambda_0 \tag{8b}$$

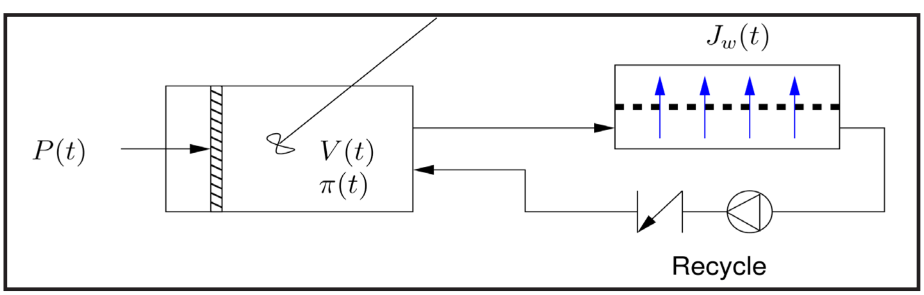

Figure 7*. Schematic of the filtration step in a batch RO employing a cross-flow spiral wound membrane element and a recirculation pump.*

where λ is called the costate variable, whose initial value λ_0 is unknown a priori. However, with an initial guess of λ_0, an integration of Eq. 8 from $t^* = 0$ to $t^* = 1$ should give the final values of x and λ, and $x(1)$ must satisfy $x(1) = 1 - Y$. This can be solved numerically (e.g., using the shooting method). In fact, an analytical solution to the optimal control problem is possible: [20]

$$x = 1 - Yt^* \tag{9a}$$

$$u = \frac{1}{1 - Yt^*} + \frac{Y}{\gamma} \tag{9b}$$

$$NSEC = -\frac{\ln(1-Y)}{Y} + \frac{Y}{\gamma} \tag{9c}$$

Students are asked to provide a comparision between numerical and analytical results (shown in Figure 8). It appears that the volume of the system should reduce linearly, or the flux should be time-invariant to minimize the PV work. In such a case, the batch RO mimics infinite continuous RO stages with inter-stage booster pumps.[20]

Next, the students are asked to comment on detrimental effects in batch RO operation. For example, because the RTD of RO differs from that of a PFR, a flushing period equivalent to one space time will not purge out all the brine. This leads to cycle-to-cycle buildup of salt before a cyclic steady state is reached.[21,28] Moreover, if permeation is turned off during flushing, the flux in the batch RO step must be elevated to maintain the designed cycle-average flux.

A cyclic process must be able to bring a system back to its original state at the end of every cycle so the process can be repeated. There are many thermodynamic cycles covered in the thermodynamics course.[26] In the last part of this project, students are asked to borrow ideas from the thermodynamics course as well as industrial examples (e.g., pressure swing adsorption used for gas separation) to come up with practical cyclic designs for the batch RO. Some designs were provided in the author's publications.[29, 30]

RESULTS AND CONCLUSIONS

These computational RO projects, together with other water-relevant projects, were deployed in several sophomore, junior, and senior level courses (Applied Mathematics, Transport I, Transport II, Unit Operations, and Process Control) at Cal Poly Pomona. Typically, students are divided into groups consisting of three to five members. The entire class elects a student manager who oversees the execution of the project. The student manager is also a member of a group. At the end of the project, each group turns in one technical report addressing questions asked in the project statement.

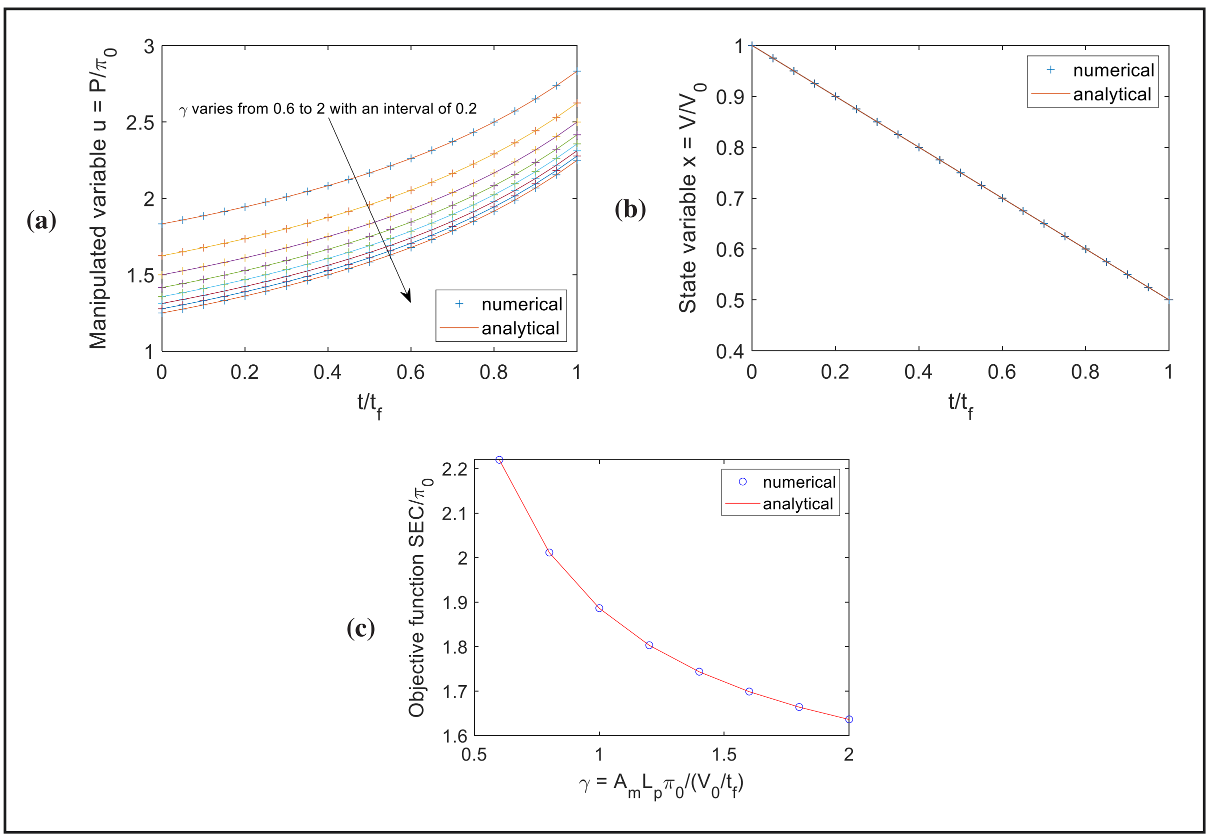

Figure 8. *Optimal solution to the batch RO. (a) Trajectory of manipulated variable. (b) Trajectory of state variable, (c) NSEC. γ varies from 0.6 to 2 with an interval of 0.2.*

Sometimes students also present their work that is peer-evaluated. These projects were shown to help enhance the student learning experience. For example, Applied Mathematics is a bottleneck sophomore course in the chemical engineering curriculum that had a drop, fail, and withdrawal (DFW) rate as high as 40%. The DFW rate was reduced to less than 10% in four semesters after implementing team projects (including the first RO example), along with several other active and adaptive learning activities (paired learning with junior students, online quizzes with unlimited attempts on basic math concepts, supplemental modules on applied mathematics, and Process Oriented Guided Inquiry Learning (POGIL®) sessions[30] where students developed their own problem-solving skills with the aid of the instructor). Mastering these computational projects helped students digest course material better; the class average of exam scores increased by 26%. Moreover, some students secured jobs in water/wastewater treatment in water districts and chemical companies as well as ultrapure water production in semiconductor and pharmaceutical industries.

For instructors who are interested in adopting these computational projects in their courses, project statements, programming codes and/or student reports can be downloaded via the permanent link below: https://drive.google.com/file/d/10OY3UfnMMKKHLpS_TeJbxEFMhEai6cds. A summary of recommended courses for deployment and concepts covered in each project is listed in Table 1.

ACKNOWLEDGMENTS

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TABLE 1
Summary of Computational RO Projects and Concepts Covered

Project	Recommended Courses	ChE Concepts	Computing Tools and Concepts
1	Applied Mathematics, Fluid Mechanics	Friction loss, Darcy's law, dimensionless number, SEC	ODEs, nonlinear equations, analytical and numerical integrations
2	Fluid Mechanics, Mass Transfer, Separation Processes	Friction loss, pump head, mass transfer, flux, concentration polarization, SEC, scaling, and fouling	DAEs, nonlinear equations, numerical integration
3	Reactor Engineering, Separation Processes, Process Dynamics and Control	Fully developed flow, Navier-Stokes equation, mass transfer, transient diffusion-convection equation, space time, process dynamics, step response, impulse response, RTD	CFD
4	Process Dynamics and Control, Process Design	PV work, process dynamics, optimal control, cyclic steady state, cyclic design	ODEs, analytical and numerical integrations, shooting method

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