Title

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Initial note for technical report

This technical report represents a sanitized version of a report submitted for the NAWI project, with all references to protected data or results removed. This technical report is still useful as a summary of the approach and methods used, which should be applicable to similar problems in the future.

We also note here that the software referred to here as "ProteusLib" has been renamed and refactored under the name "WaterTAP" in the project going forward.

Purpose of report

This report satisfied a data validation team milestone for *initial validation of reverse osmosis water treatment priority unit modules (i.e., digital twin) in ProteusLib*. It specifically describes the process and results for developing a digital twin of the Charles Meyer Desalination Plant in Santa Barbara (hence, "SB desal plant").

Overview

A *digital twin* is a computer model that has sufficient breadth and fidelity to enable diagnostic and predictive analyses for outputs of interest. We have constructed a digital twin of the SB desal plant using the ProteusLib software developed for NAWI under task 4.2.2, and specifically the ProteusLib models of pumps, filters, mixers, splitters, and reverse osmosis units and a seawater property model. The steps needed to configure this digital twin with the real conditions of the SB desal plant are: (1) Data reconciliation, which is gathering the data and plant connectivity and ensure that all relevant values are present and in the correct units and validating the data using material and energy balances, and correct for errors, gaps, or deviations; (2) Parameter estimation, which is matching model parameters with data from previous step, filling missing parameters with initial estimates, then iteratively refining estimated values.

Once we completed the digital twin, we used the optimization capabilities of ProteusLib to compute outputs of interest over a chosen range of inputs. The primary output of interest to the owners of the plant is its specific energy consumption (kWh/acre-foot).

The remainder of this report will provide more detail on the data reconciliation, parameter estimation, and analyses we performed.

Data reconciliation

The data reconciliation combined over 200 files with varied types of specifications and measurements of the SB desal plant: simulations, calculations, bills, equipment drawings, equipment manuals, technical diagrams, inspection reports, technical reports, SCADA drawings, and operating data. The team reviewed all this information and placed it in a data catalog – a spreadsheet with source, type and description for each item – for future reference. This data and the accompanying catalog are available under a folder in the delivered archive.

In the process described above, we identified a subset of the data that was most relevant and useful for the analysis. This included the P&ID (piping and instrumentation, i.e., process flow) diagrams from plant designs and screenshots of the operational SCADA displays, daily and monthly averages for plant inputs and outputs, 5-minute samples of operating data from a "typical" day, and specification sheets for equipment – particularly the pumps.

The P&ID diagrams and SCADA screenshots allowed us to establish the connectivity of the major components of the plant for pretreatment, desalination, and post-treatment.

The daily data analysis allowed us to determine the plant efficiency on days with varying product water production and the monthly data analysis allowed us to understand relationships between temperature, salinity, and energy consumption. The 5-minute data from a typical day was critical for building the ProteusLib models.

Because pump energy consumption was identified as key factors in the overall plant energy consumption, the pump specifications were important for getting a more accurate estimate of pump efficiency at different observed flow rates.

The key findings from data reconciliation are available in the full report.

Parameter estimation

To move from diagnostic to predictive analysis with ProteusLib, the next step was to perform parameter estimation for the parameters in the ProteusLib unit operations. For the reverse osmosis (RO) units, we used data on the inlet flowrate, pressure, and electroconductivity, retentate flowrate and pressure, permeate flowrate and electroconductivity, and specifications of the membrane area. For the pressure exchanger, we used the operational data on the low-pressure side flowrate and inlet and outlet flowrate and pressure, and the high pressure side inlet flowrate and pressure. For the gravity sand filter, we used data on the filter inlet flowrate and outlet pressure, and pretreatment outlet flowrate; all water loss was attributed to the backwashing of the filter. Finally, for the cartridge filter, we used the data on the cartridge filter pressure drop.

The results of the parameter estimation are available in the full report.

Digital twin analysis

Once the parameters have been estimated for the unit models, we are ready to connect them to create the digital twin of the SB desal plant. The digital twin is a steady state model, which means that it models the behavior of the plant at a given point in time, using time-averaged parameters. This model spans seawater intake, pretreatment filtration, RO desalination, and product water. The baseline values for the model — seawater flowrate, RO inlet pressure, total membrane area, and RO recovery — were based on the one "typical" day of high-resolution data, in addition to (in the case of membrane area) the plant specifications. This model can calculate the specific energy consumption of the plant.

The estimated value given the baselines mentioned previously is available in the full report. Comparison with actual energy consumption allowed us to draw conclusions about processes excluded from the analysis such as chemical preparation, sludge treatment, and backwashing.

Using this model, we were able to estimate the sensitivity of the plant energy consumption to other values and draw conclusions about the dependence of energy consumption to both pump efficiency and key decision variables (seawater flow rate, RO inlet pressure, and membrane area), with more details in the full report. The equation-oriented modeling approach allowed us to use the same model to estimate, e.g., RO inlet pressure for a given water recovery.

Preliminary modes of operation optimization

For considering optimal design parameters, we can observe the trends in specific energy consumption as we optimize the inlet RO pressure and membrane area subjects to constraints on RO water flux. We also were able to estimate energy savings when replacing equipment that our data pointed to as a major contributor to energy usage at different recovery rates, with the results shown in the full report.

Summary

We have described how we gathered and reconciled highly diverse data on the SB desal plant, used that data for parameter estimation for unit operations, then connected these unit operations (using the ProteusLib software) to create a digital twin of the full treatment train. We then described how we used this digital twin, after fitting and correcting for low-production days, to perform sensitivity analyses. Finally, we showed some of the potential of the equation-oriented approach by optimizing for different parameters, and by evaluating quantitatively the impact of replacing the fixed drive seawater pump with a variable drive unit. These analyses provide useful answers to important questions for the managers and operators of the SB desal plant.

Acknowledgment

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