



A Systematic Review of WAVE Water Treatment Design Software and Related Technologies

Rishen Roopchand^{1*}, Jerome Andrew² and Bruce Sithole²

¹Department of Chemical Engineering, University of Johannesburg, Johannesburg, South Africa

²Biorefinery Industry Development Facility, Council for Scientific and Industrial Research, Durban, South Africa

Abstract.

The water treatment industry needs customized solutions. Despite the advancement of water treatment technologies, proposed designs must pass pilot trials before industrial implementation. Technology piloting is costly and time-consuming. Water treatment software tools can optimize processes through simulation to meet the industry's need for rapid process solutions, thus saving time and money. However, not many studies demonstrate the requirements and capabilities of water treatment design software. Hence, this study aims to demonstrate the ability of the Water Application Value Engine (WAVE) software to design a demineralized water production plant for a Biorefinery process. The feedwater data was input in WAVE. The ultrafiltration (UF) and reverse osmosis (RO) process operations were specified, and the required water output was specified. WAVE simulated the process and provided the water quality exiting each process operation. The UF reduced the total suspended solids in the feedwater, while the RO lowered the total dissolved solids, thus reducing the ions by 98.56%. This ion removal ensures that the process equipment is protected from corrosion while yielding a high-quality product in the biorefinery process. Several design warnings were issued, analyzed, and mitigated. The study concluded that WAVE could effectively design and simulate new water treatment processes. Additionally, WAVE can serve as a diagnostic tool to optimize existing water treatment plants. The findings implied that Engineers and Academics could use WAVE to meet the industry's demand for rapid and accurate process solutions. The reported methodology can serve as an empirical guideline for WAVE and similar software tools.

Keywords: water treatment plant design, software simulation, water application value engine software, process optimization, software diagnostic tool

1. Introduction

Effective water treatment for chemical processes is crucial for high-quality products and for preventing process equipment corrosion (Liu et al., 2019). While demineralized water is easily procured for laboratory-scale, water treatment plants must be developed to produce demineralized (process) water for industrial processes.



A steady demineralized water supply was required to upscale a novel cellulose nanocrystals production process. Hence, a water treatment plant was required to treat municipal water to demineralized water standards. The previous studies of Niemi & Palosaari (1994) and Cardona et al. (2005) showed that water treatment design entailed precise and lengthy programming. In this study, a relatively new software, Water Application Value Engine (WAVE), was employed to design the water treatment plant within a short period. The input requirements, simulation methodology, and software results undergo analysis and discussion with respect to the literature. Furthermore, the software was reviewed according to the following evaluation criteria: simplicity of the user interface, ease of use, quick, accurate and reliable simulation outputs, and cost effectiveness.

This study aims to review WAVE as a prospective water treatment design tool with respect to other design tools identified in the literature. Discernment regarding the efficacy of the software can aid the design and optimization of industrial water treatment plants to supply process water. The hypothesis put forth was that WAVE can output a technically and economically efficient water treatment plant design.

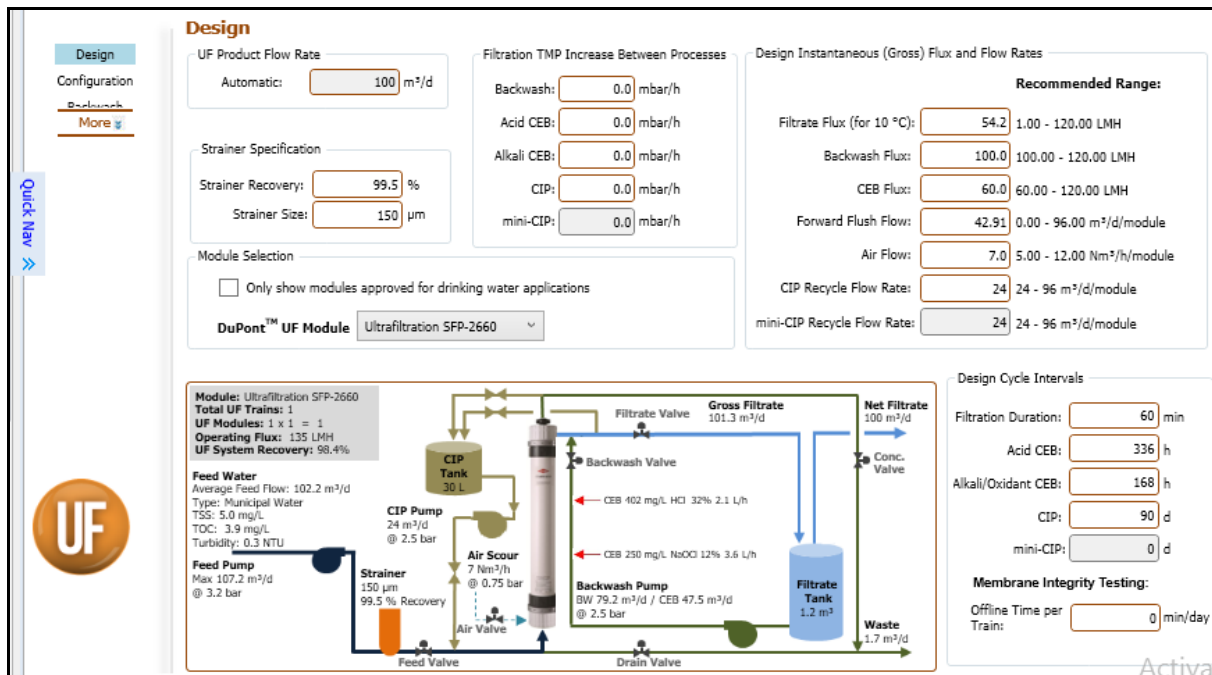
2. Methodology

WAVE is free software established by DuPont Water Solutions with extensive water treatment applications. WAVE modeled the ultrafiltration (UF) and reverse osmosis (RO) unit operations. Considering that Gauteng (South Africa) was selected as the plant location, the Ekurhuleni and Johannesburg Metro Municipal water analyses were sourced from Rand Water's data repository. The data was subsequently averaged for the input analysis. The water treatment flowsheet was configured by specifying the unit operation sequence. No pre-filtration step was envisaged as the turbidity of municipal water is lower compared to raw water sources, including river or rainwater.

The first unit operation specified was the Ultrafiltration (UF) unit. Thereafter, the second stage to be specified in the water treatment process was the reverse osmosis (RO) operation. Traditionally, a final polishing stage proceeding RO is employed to eliminate residual ions in the RO permeate. However, polishing operations were not selected in this design for two reasons. Firstly, the product water can conform to the process water quality standards with sufficient maintenance of the UF and RO units. Secondly, the plant's operational and capital costs will increase. After specifying the plant configuration, the municipal water type was selected, and 75 m³/day of product water was specified.

The municipal water quality was specified by inputting the source water data. A 20°C design temperature was used, while a temperature range between 10°C to 40°C was defined. Considering that the input values were estimates with missing source data and unbalanced averages, WAVE then automatically balanced the ions. Thereafter, the UF stage's configuration and layout were automatically specified. The strainer specification, product flowrate, feed pumps, module selection, design cycle intervals, and chemical dosing details are shown (Fig. 1).

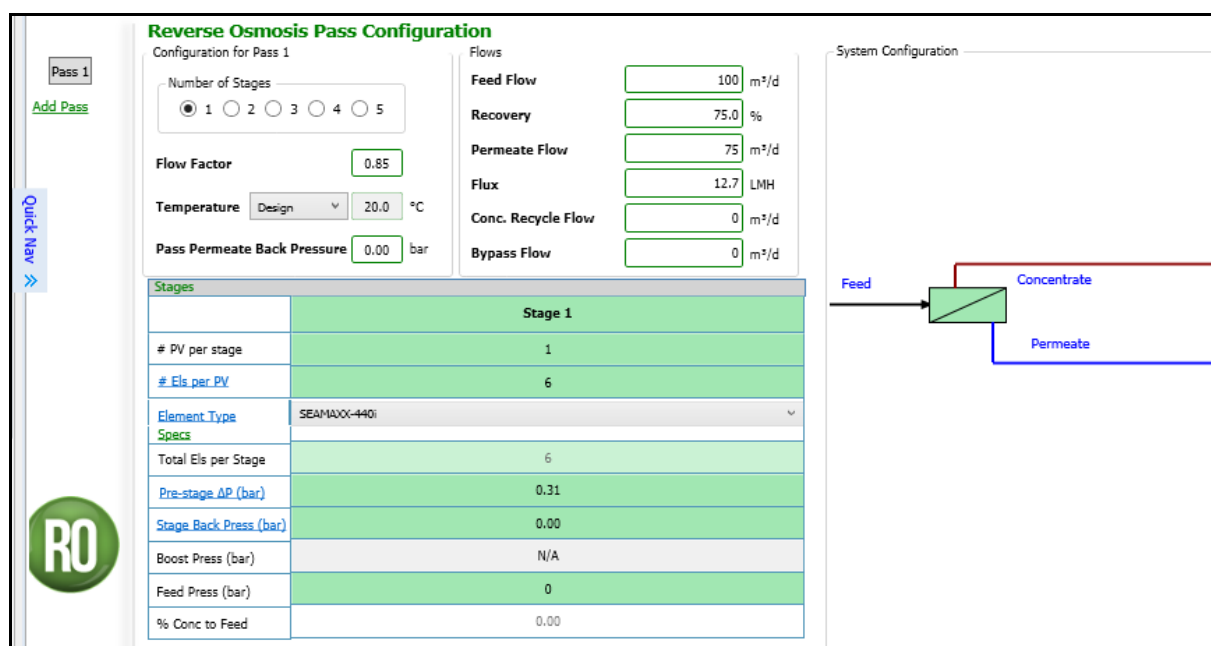
Figure 1: Specification of the Ultrafiltration stage



The UF design summary report was then produced (Results, Fig. 3). It was noteworthy that WAVE specified the reverse process details. These reverse process details included the backwash, chemically enhanced backwash, and clean-in-place procedures because the operational efficiency decreases with the acculation of suspended solids on the surface of the membrane. The backwash procedure pumps water through the membrane opposite the forward operation in regular intervals. The backwash dislodges the accumulated suspended solids from the membrane surface. However, backwashes lose their potency over time. Hence, regular chemically enhanced backwash procedures are required to sustain the membrane's performance.

Additionally, regular clean-in-place procedures are performed more frequently. The clean-in-place procedure is more thorough in relation to the chemically enhanced backwash. A single RO stage was allocated to reduce the plant's capital expense and footprint. WAVE recommended the RO element type. WAVE performed the RO design based on this specification and the UF results (Fig. 2).

Figure 2: Design Stage Schematic- Reverse Osmosis (RO)



3. Literature Review

UF and RO membrane technologies have been extensively researched over the last two decades. Rautenbach et al. (1996) piloted membrane technologies (RO, nanofiltration, and crystallization) for the treatment of dumpsite leachate. The permeate recovery rate of 97% indicated the membrane technology's feasibility in water treatment applications. The 8.3 kWh/m³ permeate power consumption was deemed relatively low and therefore feasible compared to evaporation. Notably, membranes were considered "modern wastewater treatment" technologies (Rautenbach et al., 1996). At that time, UF and RO were optimized for reduced energy, capital and operational investment costs, better recoveries, and zero discharge (Rautenbach et al., 1996). These focal points were addressed in further studies (Clever et al., 2000; Lorain et al., 2007; Knops et al., 2007; Sun et al., 2015; Loganathan et al., 2015; Ho et al., 2015).

Typically, UF is used as a pretreatment operation for RO (Clever et al., 2000; Lorain et al., 2007; Knops et al., 2007; Sun et al., 2015; Ho et al., 2015; Loganathan et al., 2015). The research of Rosberg (1997) focused on UF as a pretreatment for RO and nanofiltration. UF was an expensive emerging technology at that time, and sand-filtration was preferred. Recent studies show that reduced UF costs made it the favoured RO pretreatment (Lorain et al., 2007; Sun et al., 2015). RO problems include precipitation, adsorption of organic fouling, colloidal dust deposition, and biofouling (Rosberg, 1997). UF pretreatment can eliminate these

problems. Hence, it is notable that the study of Rosberg (1997) perceived UF to be the ideal preliminary treatment for RO.

The study of Clever et al. (2000) used pre-filtration, UF, and RO to treat river water to yield process water. The pre-filtration removed suspended matter to prevent clogging of the UF membranes. The results demonstrated high availability and definitive plant operation. The system reduced microbes and suspended particles from river water, providing high-quality permeate (< 0.05 NTU). Considering these results, a commercial plant was implemented for a steel company. The operational insights based on the pilot plant study were used in the industrial plant.

The study of Knops et al. (2007) provided an economic validation of the UF-RO configuration for seawater treatment. The higher UF operating cost was previously viewed as an obstacle. Hence, the study recommended a new UF membrane to reduce operating costs by 2-7%. The UF operating costs, UF membrane investment amortization, increased output, and operating cost reduction revealed the economic aspects of the recommended system. WAVE automatically provides cost analyses of proposed designs, enabling rapid monitoring. If the budget is exceeded by the cost, the design can be adjusted to achieve cost effectiveness.

Like the study of Knops et al. (2007), the study of Lorain et al. (2007) determined the pretreatment benefits of membrane technologies in seawater treatment. To prevent membrane fouling, the RO silt density index must be less than 3 (Lorain et al., 2007). The study used a pilot unit to combine sand filtration, UF (pretreatments) and RO. The silt density index of the seawater ranged between 6.1 and 6.4. After UF, the silt density index ranged between 1.2 and 2, compared to 5.8 to 5.9 for sand filtration. Using sand filtration, the RO permeability decreased by 28% over 30 days, and the chemical cleaning interval occurred every 12 to 18 days. Using UF, the RO operated for 20 days in the absence of chemical cleaning. Based on these results, UF was experimentally supported as an effective pretreatment for RO.

In the study of Loganathan et al. (2015) the combined UF-RO arrangement was examined for the treatment of basal aquifer water to produce synthetic oil. The study aimed to attain zero-liquid discharge by incorporating evaporation and crystallization operations. The evaporation-crystallization unit effected evaporation of water within the RO reject flow, causing salt crystallization. According to laboratory-scale and pilot-scale tests, feed softening was required in the evaporator to eliminate scaling. Overall, the zero-liquid discharge approach effectively produced freshwater and minimized brine discharges. Although crystallization is recommended in water treatment plants, WAVE does not enable crystallization simulations.

Hybrid systems use coagulants and flocculants to aid pretreatment. Ho et al. (2015) piloted inline coagulation-UF. The study is novel as most pretreatments employ a strainer before the UF. To clump and remove dissolved organic matter from the treated water, coagulants such as ferric chloride, polyaluminium chloride, and aluminium chlorohydrate are used. Specifically, ferric chloride yielded the greatest removal of dissolved organic carbon (approximately 60%) and the highest phosphate (99%) and silica removals (14%). Similar to the research of Ho et al. (2015), the investigation of Sun et al. (2015) combined various pretreatments, including dual-stage sand filtration, UF, and ferric chloride flocculation. The UF effectiveness was evaluated by the membrane-specific flux. Combining ferric chloride flocculation with UF decreased the specific flux throughout a chemically enhanced backwash. Additionally, ferric chloride flocculation/dual-stage sand filtration/UF steadied the specific flux throughout a

chemically enhanced backwash compared to ferric chloride flocculation/UF only. Despite the advantages of hybrid technologies, designers are limited as WAVE cannot simulate them.

Sievers et al. (2017) recommended combining customized process technology to meet water treatment demands instead of standard solutions. Hence, the use of software to design water treatment plants is anticipated to facilitate quick customized solutions. This assertion supports the use of WAVE in this study to design the required water treatment plant. Furthermore, Sievers et al. (2017) outlined a vision for 2030 to overcome technology shortcomings. The most critical research target is “continuous optimization of production systems” to decrease pollution loads and water demand. Hence, water treatment design software can optimally design new plants and optimize existing plants for improved performance. WAVE can achieve both purposes.

Software simulations are expected to provide a virtual reality of processes in the fourth industrial revolution. This advancement can eradicate the requirement to implement pilot plants for commercial trial runs. In this review phase, simulated research was reviewed with respect to WAVE. The study of Niemi and Palosaari (1994) established a flowsheet to simulate UF and RO technologies. Although much research was performed on pilot plant studies during this time, this study was among the first to apply simulation. UF and RO membrane separation models were developed to calculate the membrane area, permeate flux, and solute rejection, while the UNICORN program simulated the stream matrix. Polynomial equations were fitted to experimental data, and mass transfer prototypes were used to determine the rejection and permeate flux. Although this flowsheet simulation approach was previously practical, mass transfer equations and parameter fitting tools are integrated into modern software packages. In addition, the study’s software tool required comprehensive input data, which is not needed by current simulation packages. Both advantages are offered by WAVE.

As with many studies in which UF is employed as a preliminary treatment stage to RO (Lorain et al., 2007; Sun et al., 2015), the study of Cardona et al. (2005) combined UF and a two-stage RO system to treat seawater. Excel was used to simulate the plant using Visual Basic macros. This simulation technique differed from WAVE in two ways. Firstly, WAVE enables specification of the pass numbers and stages for UF and RO configurations. Secondly, the preliminary treatment phase outlined in the study of Cardona et al. (2005) was designed on a different program to the primary simulation.

In contrast, WAVE automatically incorporates the pretreatment phase within the design configuration. The study of Cardona et al. (2005) perceived UF to be an energy efficient technology- which sharply contrasted the notion that UF is costly in the investigation of Rosberg (1997) conducted earlier. Considering this perception shift, the cost efficiency of membrane technologies in water treatment has improved over time.

RO membrane scaling is a widespread concern investigated in the research of Karabelas et al. (2020). The water industry is challenged by inadequate techniques to evaluate the potential for feedwater scaling, selection, improving scaling control strategies, and observing membrane scale-formation while the process is running (Karabelas et al., 2020). Hence, the study outlined RO scaling mechanisms, monitoring, and mitigation procedures. The scale deposition rate per unit membrane-surface-area was identified as the most suitable parameter to model and quantify infant scaling. The study recommended developing a predictive tool during the early design and optimization of RO-plants.

Furthermore, the study suggested combining membrane-scaling test results with module simulations. It is notable that WAVE can produce scaling design warnings. Aligned to the suggestions of Karabelas et al. (2020), the WAVE software can manipulate the initially specified parameters to yield improved operation outputs.

Despite the novelty of the information provided in the literature studies (pilot plants and simulations), no water treatment plant study has been demonstrated using recent software simulation and design tools. Furthermore, the trouble-shooting capabilities and analysis of design results have not been reported in previous research. Hence, this study aimed to design a water treatment process capable of producing process water for a new biorefinery process using WAVE as a case study.

4. Results and Discussion

4.1 Ultrafiltration Design

Figure 3: UF Design Summary

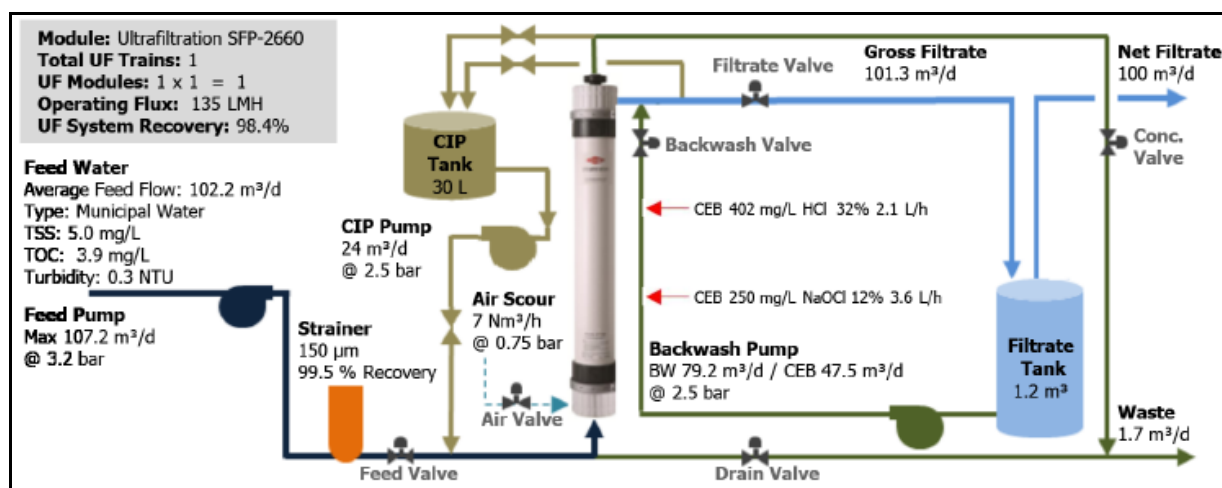


Table 1: Comparison of UF Input and Output Streams

Parameter	Feed	Permeate
Temperature (°C)	20.0	20.0
Turbidity (NTU)	0.3	< 0.1
Total suspended solids (mg/L)	5.0	0.0
Total organic carbon (mg/L)	3.9	3.5
Silt density index	0.2	< 2.5
Total dissolved solids (mg/L)	449	449
pH	8.1	8.1

Considering the absence of a pre-filtration stage, the WAVE software recommended a 150 micron strainer to remove suspended solids at a rate of 0.5 m³/day. If not removed, these suspended solids would obstruct the UF membranes. The UF detailed design report (Fig. 3) showed the forward and reverse operation cycles (backwash, chemically-enhanced backwash, and cleaning-in-place). The UF flowsheet also incorporated the suggested strainer. Additional UF parameters comprised the membrane pressure ratings, pump hydraulics, electrical costs,

and dimensions of the storage tank. It is notable that each specification is critical to implement the design.

The UF permeate and feed results (Tab. 1) demonstrated that the total suspended solids in the UF output stream were completely removed. Considering that the UF's purpose was to eliminate the source water's suspended solids, this result was anticipated. The decreased total suspended solids in turn reduced the turbidity by 67%. Although the total organic carbon was slightly decreased, the UF operation did not affect the source water's total dissolved solids. The total dissolved solids reduction was expected through the subsequent RO operation. WAVE issued two UF design warnings. According to the warnings, the trans-membrane pressure and filtration flux values were slightly above the design limits. However, considering that the backwash frequency and feed flowrate can be altered to eliminate the warnings, the mentioned result was not deemed a concern.

Additional indications in the design report included the backwash cycles and filtration mode. Additionally, the valve and pump conditions were outlined as functions of the UF action steps (backwash, chemically-enhanced backwash, and cleaning-in-place). Outlining such UF actions is advantageous for control and instrumentation engineering, which requires a comprehensive background regarding the interrelations between the valve and pump functions of each step. The utility and chemical costs (dosing chemicals, service water, and electricity) concluded the UF design report (Tab. 4). The recommended dosing chemicals maintain the water pH within desirable ranges to intercept the scaling of membranes. The daily chemical and utility costs were comparatively low (\$ 2.26) aligning to a specific water cost of \$ 0.023 per cubic meter.

4.2 Reverse Osmosis Design

Table 2: RO Stream Information

Stream	Description	Flow (m ³ /day)	Total dissolved solids (mg/L)	Pressure (bar)
1	Raw feed to RO system	100.0	444.2	0.0
2	Net feed to Pass 1	100.0	444.3	5.2
4	Total concentrate from Pass 1	25.0	1,755	4.6
6	Net product from RO system	75.0	3.05	0.0

Table 3: RO Ion Removal

Ion	Feed	Permeate	% Removal
Ammonium	0.63	0.02	96.83
Potassium	6.93	0.10	98.56
Sodium	25.46	0.33	98.70
Magnesium	17.97	0.08	99.55
Calcium	44.59	0.19	99.57
Strontium	17.18	0.07	99.59
Barium	4.91	0.02	99.59
Carbonate	3.22	0.00	100.00
Bicarbonate	313.3	2.16	99.31
Nitrate	0.05	0.01	80.00
Chloride	4.34	0.05	98.85
Fluoride	0.07	0.00	100.00
Sulfate	5.58	0.01	99.82
Total dissolved solids	444.2	3.05	98.56

Table 4: Cost Comparison between UF and RO

Parameter	Daily cost (\$)		Specific (per m ³)	
	UF	RO	UF	RO
Service water				
• Feed water	0.23	3.50	-	-
• Wastewater disposal	1.50	17.26	-	-
Electricity cost	0.86	1.6	-	-
Specific energy	-	-	0.10 kWh	0.24 kWh
Chemicals				
• Citric acid	0.01	-	-	-
• Sodium hypochlorite	0.01	-	-	-
Feed pump	-	1.63	-	-
Utility and chemical cost	2.26	22.4	-	-
Specific water cost	-	-	\$ 0.023	\$ 0.298

WAVE suggested one RO train. Generally, the train and pass numbers depend on the source water contamination in terms of solutes removal. The municipal water source was expected to contain fewer solutes than others, such as seawater (Cardona et al., 2005; Lorain et al., 2007; Knops et al., 2007; Sun et al., 2015). Therefore, the single train, single pass RO system output by WAVE was considered accurate.

Unlike the comprehensive flowsheet output for the UF configuration (Fig. 3), no corresponding RO output was produced. The RO stream information was specified in Tab. 2. Notably, the total permeate dissolved solids decreased from 443.2 mg/L to 3.05 mg/L (98.56% reduction). The notable total dissolved solids reduction in the permeate enables it to be used as deionized (process) water for industrial processes. Therefore, this result validated the single-pass specification that was initially input.

Considering the doubled capital cost that would arise from implementing a standby RO train, it was not suggested. The operational RO system is equipped with regeneration capabilities, such as regular backwashes, chemically enhanced backwashes, clean-in-place, and the (optional) dosing of antiscalants and anti-foulants. Hence, the no-standby recommendation was validated from a technical viewpoint. The total system recovery of 75% was deemed sufficient to supply deionized water to the Biorefinery production process in the required quantity.

WAVE issued two RO design warnings: the element recovery exceeded the maximum limits and the concentrate flowrate fell below the minimum limits. Similar to the UF design, these warnings outlined that the performance of the physical system would not completely conform to the simulated system. These warnings are concerned with the UF product volume

being passed through the RO. A holding tank is therefore proposed to store the UF permeate, thus ensuring that the RO system's booster pumps have sufficient water supply for the RO membranes. Consequently, the holding tank configuration will allow the RO system to meet the minimum element recovery limits and concentrate flowrate.

Additionally, WAVE showed solubility warnings that are linked to the dissolved solids' possible scaling of the RO membranes. WAVE recommended dosing antiscalants into the water supplied to the RO membranes to counteract these warnings. The antiscalants are recommended for direct dosage into the proposed UF holding tank to mitigate the simulation warnings in question. Considering that the simulation warnings allows for mitigation factors to be implemented, this strategy can be categorized as predictive maintenance.

The feed and permeate solute concentrations are indicated in Tab. 3. The last column shows the percentage reduction caused by the RO operation. As anticipated, RO caused a substantial solute reduction (exceeding 97%). The ions reduction in turn reduced the total dissolved solids by 98.56%.

The costs of the UF and RO were equated (Tab. 4). The daily RO chemical and utility costs summed to \$ 22.4, which was approximately ten times the corresponding UF chemical and utility costs. Considering the greater power requirement to reach the sizeable differential pressure across the RO to eradicate the dissolved solids, this steep cost difference is justified. As a result, the projected specific cost per cubic meter of RO water was \$ 0.298. Additionally, the wastewater disposal cost exceeded that of the UF system because the salt reject stream requires treatment prior to release into the environment. As recommended in the study of Loganathan et al. (2015), crystallization can be used to achieve these zero liquid effluent discharges.

This study perceived two major shortfalls concerning the WAVE software. Firstly, the software lacks the capability to simulate hybrid pretreatment methods (Sun et al., 2015; Ho et al., 2015). Hence, hybrid pretreatment methods cannot be simulated within the main water treatment design. Secondly, the WAVE software cannot model crystallization processes to treat the salt reject streams. Again, separate simulations will be required outside WAVE if crystallization is required.

In spite of these shortfalls, the WAVE software enabled the comprehensive design of the water treatment plant to supply deionized (process) water to the Biorefinery plant. A cost effective and simplistic design methodology using the WAVE software was performed, which validated the study's hypothesis. Contrasting the earlier simulation models found in the studies of Niemi & Palosaari (1994) and Cardona et al. (2005), the WAVE simulations are possible without too many inputs being required. There are no limitations or assumptions to achieve the presented results. Overall, WAVE performed well according to the established evaluation criteria relating to user efficiency, cost efficiency, and results reliability.

5. Conclusions

Considering that water treatment plants can be simulated using design software such as WAVE, this eliminates the reliance on pilot plant trials to gain insights about a process prior to commercial implementation. This finding implies that time and money can be saved for stakeholders such as Engineers and Academics. Each WAVE simulation presents a unique water treatment design specific to the problem being addressed. This degree of customization

addresses Sievers' et al. (2017) concern regarding the infeasibility of water treatment designs that are not customized to individual requirements.

WAVE enables the 2030 water treatment industry goal of Sievers et al. (2017) concerning the ongoing improvement water treatment designs. In addition, the WAVE software predicted design issues, enabling effective mitigation measures. Hence, the hypothesis was validated regarding WAVE's ability to undertake the process water production plant to supply deionized water to the new Biorefinery production process.

There are two main practical implications of this study. Firstly, the efficient design of new water treatment processes can be done using the WAVE software. If there are no actual source water analyses, the designer can employ historic water quality analyses. Secondly, WAVE can be used as a diagnostic tool by implementing mitigation measures in response to design warnings to optimize existing water treatment plants.

The detailed design steps outlined in this study form a practical guideline for stakeholders to undertake effective and practical design studies using WAVE. The mitigation factors and analysis of the design results further guide the logic applied when designing new water treatment plants or optimizing existing ones. It is recommended that other water treatment plant simulation software be demonstrated for future research. In addition, crystallization technology must undergo development to simulate zero liquid effluent discharge scenarios.

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