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When does commercial software fail in predicting scaling tendency in reverse osmosis and what can we do better?

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ABSTRACT

Avoiding chemical scaling by sparingly soluble salts is a critical design component in desalination applications based on reverse osmosis. If not prevented, scaling can rapidly reduce membrane lifespan and performance while considerably increasing desalinated water production costs. Therefore, an important part of reverse osmosis process design is the calculation of scaling tendency of the concentrated rejected solution. For this purpose, commercial software packages developed by membrane manufacturers or suppliers of antiscalant chemicals are commonly used. Nevertheless, the ability of commercial software to produce realistic predictions of scaling tendency was scarcely studied. Here the performances of three prominent computer programs, one from a large membrane manufacturer and two from prominent antiscalant suppliers, are systematically tested by comparing their predictions to simulation results made by WATRO (weak acid transport in reverse osmosis) - an experimentally validated mechanistic model recently developed by the author. Three different cases were examined: 1st pass seawater reverse osmosis, brackish water reverse osmosis and 2nd pass of reverse-osmosis, treating seawater reverse-osmosis permeate. In many cases, it was found that the predictions made by the commercial programs were unrealistic, resulting in unnecessarily high recommended doses of antiscalants chemicals to the feed. The unrealistic predictions are mainly due to the incompetence of the tested commercial software in modeling the change in pH, developing in the concentrate upon increasing the permeate recovery ratio. Using the WATRO code, it was revealed that retentate pH calculations made by the commercial software is likely based on CO_2 permeation as the sole mechanism, together with ad-hoc modifications. However, this mechanism is often not the dominant one, while other dominant phenomena controlling acid-base dynamics in the retentate during reverse osmosis are unaccounted for or improperly treated, giving rise to unrealistic predictions. Specifically, the influence of background ions on proton dissociation constants and the cross-membrane transport of hydronium and hydroxide ions should be accounted for in order to improve commercial software predictions. Fortunately, the WATRO code provides a suitable framework for expanding the predicting capacity of currently available design tools, thus promoting a more optimal design.

Keywords: Reverse osmosis; Modeling and simulation; Antiscalants; pH evolution; Acid-base equilibrium; Solution-diffusion

I. Introduction

Chemical scaling is a persistent challenge in reverse osmosis (RO) desalination, often tackled by the addition of antiscalants and/or feed pH modification. Although accurate predictions of scaling tendency could significantly improve process economics, such reliable assessments for varying operational conditions and feed compositions remained thus far elusive. Inaccurate predictions may result in several adversative outcomes. For example, over-estimation of scaling propensity would result in over-dosing of antiscalant, thus increasing both the cost of desalinated

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water and the environmental impact associated with these chemicals. Moreover, it was demonstrated that over-dosing of antiscalants to RO feed may boost biofouling [1]. On the other hand, under-estimation of the scaling propensity may result in process design which unintentionally promote chemical scaling at high recovery ratios, potentially hindering membrane performance and lifespan.

For achieving accurate predictions of scaling propensity, it is imperative to accurately predict the pH developing in the retentate as permeate recovery increases. The pH value is significant for the precipitation and crystallization of most commonly encountered scale-forming minerals. Prominent examples are $CaCO_3$ and iron-oxides/hydroxides [2] for almost all RO applications, $Mg(OH)_2$ for high pH RO such as the boron removal 2nd pass after SWRO (seawater reverse osmosis), silica and aluminosilicates in BWRO (brackish water reverse osmosis) and high recovery RO for pure water production and various calcium-phosphate minerals in WWRO (wastewater reverse osmosis) for unlimited reuse. Modeling pH evolution during membrane filtration is challenging, since complex and interdependent phenomena are involved [3–5] .

The mechanisms underlying the evolution of pH with the increasing amount of extracted permeate can be divided in two groups: (1) changes in the relative composition of acid-base species due to different cross-membrane transport rates; and (2) changes in the apparent acid dissociation constants due to an increase in background solute concentration [6]. Regarding the first, a prominent example is the high permeance of neutral, acidic species (e.g. dissolved CO_2) to the permeate side versus the high retention of negatively charged, basic species (e.g. bicarbonate). This transport phenomenon induces a pH increase in the retentate with increasing recovery. Another transport phenomenon, which was recently found significant is the cross-membrane transfer of H^+ and OH^- via diffusion-electromigration [7]. For polyamide negatively charged membranes, this phenomenon was shown to induce a decrease in retentate pH. Regarding the second mechanism, typically the apparent proton-dissociation constants are shifted to lower values since basic species of environmentally abundant weak-acid systems are typically with higher ionic charge (with few exceptions e.g. ammonia). Upon increasing the concentration of background ions in the retentate, the activity of charged, basic species decrease due to (1) non-specific Debye-Huckel interactions with the ionic background (determined by the ionic strength); (2) ion complexation and ion-pairing, the most significant of which typically involves higher valence metal cation M^{a+} (e.g Ca^{2+}, Mg^{2+}) and a basic anion X^{b-}, forming a new solute MX^{a-b} with an equilibrium coefficient $k = [MX^{a-b}]/[M^{a+}][X^{b-}]$; (3) Specific interactions which are not ion-pairing, such as Pitzer-type interactions [8]. When the activity of a basic species decreases, equilibrium is disrupted, triggering proton dissociation reactions to restore equilibrium, thus reducing the pH. The Same effect of pH decrease is observed upon evaporation of seawater or other natural waters dominated by the carbonate weak-acid system [9]. It is the interplay between these phenomena which determines pH evolution in RO and thus scaling propensity.

Accounting for the above-mentioned coupled membrane transport-chemical equilibrium phenomena requires a more comprehensive modelling approach and advanced simulation tools. Such coupled simulation program - 'WATRO' (weak acid transport in reverse osmosis) - was recently developed In our previous study [10]. WATRO automatically couples the solution-diffusion-film membrane-transport model to elaborated chemical-equilibrium models. pH, species distribution, permeate concentrations, saturation indices (SI) and precipitation potentials (PP) are resolved with respect to recovery ratio. This numerical model was tested using different commercial spiral wound RO modules, for a range of feed pH values, using real seawater and synthetic SWRO permeate as feed. It is the only model shown to accurately predict all the parameters required for a full characterization of acid-base properties developing in all streams, namely pH, alkalinity and boron concentration in the retentate and permeate as a function of recovery. Therefore, WATRO is currently the best-available model and will be considered as benchmark in this work. Here, WATRO is compared with three commercial computer programs, one provided by a membrane manufacturer and two provided by antiscalants suppliers, in predicting scaling tendency. Three different feed water types are considered: (1) seawater; (2) brackish water; (3) SWRO permeate. It is shown that these commercial computer programs are limited in their ability to predict retentate pH values and as a result scaling tendency. The implications of inaccurate predictions are discussed also in terms of recommended antiscalants doses.

2. Methods

Commercial computer programs were obtained from two prominent antiscalant suppliers and one prominent membrane manufacturer. These programs will be referred here as Ass(a) and Ass(b) for the antiscalant suppliers and MM for the membrane manufacturer. These programs are used to project the pH of the brine (for all three) and the recommended antiscalant dose (for Ass(a) and Ass(b)) following RO treatment. The input to the programs includes feed composition and pH, recovery ratio and membrane element. The latter was only required for the membrane manufacturer software and had negligible or no effect on retentate pH evolution. Typical SWRO element was chosen for the seawater projection from the manufacturer element library, which is included in the commercial software. Similarly, typical BWRO element was chosen for the brackish water and low salinity permeate projections. Projections by the commercial programs were compared to simulation results made using the WATRO code [10] developed by the author. In the WATRO Python code, the solution-diffusion-film membrane transport model is closely coupled to elaborated chemical equilibrium calculation using the PHREEQC [11] numerical engine and the self-consistent Pitzer database [12]. Feed compositions used in the simulations are given in Table 1. Typical composition of the Mediterranean Sea was used for the seawater model. For the brackish water model, the feed composition of a brackish aquifer in Israel 'Mashabei-Sade' was adopted from [13]. RO permeate composition was taken from the SWRO projection done by the membrane manufacturer software (pH 8). 20 ppb's of dissolved iron were considered in the simulations performed using the software provided by the antiscalants suppliers.

Table 1
Feed compositions used in the simulations

Component	Na^+	Mg^{2+}	Ca^{2+}	K^+	F_{eT}	Cl^-	SO_4^{2-}	C_T	B_T
	mg/l	mg/l	mg/l	mg/l	mg/l as Fe	mg/l	mg/l	mg/l as HCO_3^-	mg/l as B
Seawater	11,453	1400	412	396	0.02	20,337	3241	165	5
Brackish	579	83	167	16	0.02	971	409	292	1
RO permeate	89	2.25	0.66	3.8	0.02	143	5.66	2.9	1.1

Table 2
Membrane parameters used in the WATRO simulation

Parameter:	Water permeability (μm/s/bar)	Salt permeability (μm/s)	Boron permeability (μm/s)	Salt mass-transfer coefficient (μm/s)	Boron mass-transfer coefficient (μm/s)
SWRO	0.58	0.0195	1.875	23.2	100
BWRO	1.2	0.094	2.78	9.4	16.2

Saturation indices and precipitation potentials in the brine as a function of pH were calculated directly in PHREEQC, assuming total rejection of salt, while the inorganic carbon concentration was taken from the relevant WATRO simulation. The membrane characteristic parameters used in the WATRO simulation are listed in Table 2. These parameters are typical to SWRO and BWRO membranes and were determined experimentally as described in a previous work by the author [10]. The Saturation Index (SI) used in this work was defined as follows,

$$SI = log\left(\frac{IAP}{K_{sp}}\right) \tag{1}$$

where IAP is the ion activity product and K_{sp} is the thermodynamic equilibrium constant for the dissolution reaction of the solid. The calcium carbonate precipitation potential (CCPP) or precipitation potential of brucite – i.e. the amount of solid that would precipitate from 1 L of solution until reaching equilibrium – was calculated numerically using PHREEQC .

3. Results and discussion

Projections of retentate pH by three different commercial computer programs were compared to predictions made by WATRO, an experimentally validated code for predicting acid-base dynamics in reverse osmosis applications. Four different initial pH values were evaluated for each case, representing a range of typical and less typical operational conditions. The results for the first SWRO (seawater reverse osmosis) step, in which the feed is pretreated seawater, are shown in Fig. 1. The recovery ratio was 50% in this case whereas the feed pH values considered were 7, 7.5, 8 and 8.5. As the simulations made with the WATRO code show, the evolution of pH in the 1st step is significantly influenced by the pH of the feed. When feed pH is adjusted to 7.0, pH slightly increases with the recovery, mainly due to cross-membrane transport of CO_2, overshadowing other acid-base processes at this pH range (where CO_2 concentration is relatively high). The trend generally agrees with the commercial software used (excluding the decrease at low recovery predicted by Ass(b)), however, for higher feed pH values the trends predicted by the commercial software differ from the ones predicted by the more realistic and experimentally validated WATRO code. As seen in Fig. 1, the deviations increase for higher pH. To better understand the source of these discrepancies, additional WATRO simulations were performed, in which other significant acid-base processes i.e. pKa shift due to salt concentration and H^+/OH^- transport were disabled. The results, seen in Fig. 1d, more closely resemble the predictions made by commercial software, suggesting that this is the only mechanism considered by these programs. Nevertheless, at higher feed pH values, the concentration of CO_2 decreases and the concentrations of bicarbonate and carbonate increase, resulting in a weaker effect of CO_2 transport and a stronger effect of salt induced pKa shift (caused by reduction in the activity coefficient of bicarbonate, carbonate and borate). At feed pH of 7.5, these two mechanisms seem to balance each-other, thus the pH remain almost constant with increasing recovery. Most importantly, when the feed pH is 8.0 or higher, as commonly applied today, pH in the retentate decrease with increasing recovery, as predicted here by WATRO and was previously shown in full-scale [6,14] and pilot scale [10,15]. Interestingly, Ass(a) and MM programs attempt to tackle this discrepancy by artificially decreasing the retentate pH at low recovery. This Ad-hoc modification somewhat improves the accuracy of projections at high feed pH, however at low pH accuracy is hindered for Ass(a).

The deviations in pH evolution seen in Fig. 1 have significant implications on the scaling tendency of $CaCO_3$ and on the recommended antiscalant dose as shown in Fig. 2. This is especially true for the high end of predicted retentate pH, where errors in prediction are the largest. When feed pH was 8.5, as was previously applied on a full scale for single-pass boron removal [14], inaccurate assessment of retentate pH (8.5 instead of 8.25) resulted in ~40% overestimation in CCPP and ~15% overestimation in SI, which is on a logarithmic scale. While for Ass(b) the implications on the recommended antiscalant dose were low, the recom-

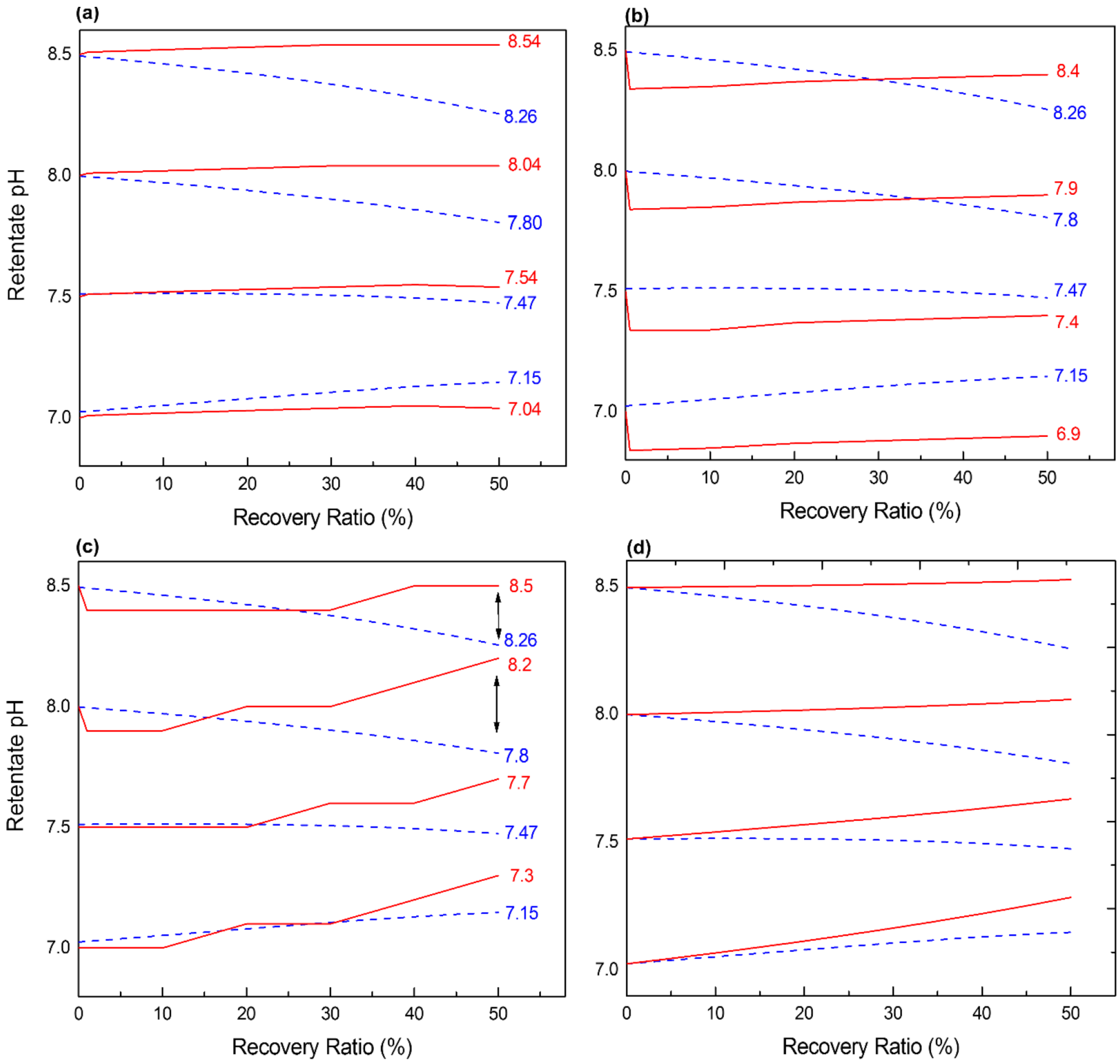

Fig. 1. pH evolution predictions for SWRO 1st pass. Blue dashed lines: WATRO, Red lines: (a) and (b) antiscalant suppliers Ass(a) and Ass(b) respectively, (c) membrane manufacturer, (d) WATRO not considering shift in pKa values and H+/OH- cross-membrane transport.

mended dose by Ass(a) increased sharply at the high pH range, potentially resulting in an antiscalant overdose by 5-fold. At the low pH range, $CaCO_3$ precipitation is thermodynamically or kinetically restricted, however accurate predictions of pH evolution are still important for assessing iron scaling rate. Iron typically precipitates initially as ferric-hydroxide ($Fe(OH)_3$) at a rate determined by the oxidation rate of ferrous-iron (the preliminary product of metal-iron corrosion) to ferric-iron. This oxidation rate is known to be a strong function of pH at the operationally relevant pH range [16]. Notably, both antiscalant suppliers recommend adding antiscalant to the feed even when scaling indices are negative in the retentate and precipitation is thermodynamically restricted. Practically, when indices are lower than those appearing in ambient seawater for aragonite (SI = 0.54, CCPP = 24.6), precipitation should still not occur due to kinetic limitations.

As shown above, the relatively constant composition of seawater and the widely used typical operational conditions applied in SWRO enable commercial process modeling software to compensate for unaccounted, however important, acid-base mechanisms via heuristic modifications in its code, thus reducing the inaccuracy in the predicted pH. In contrast, brackish water composition is highly variable and therefore, experience-based ad-hoc modifications do not always work, potentially leading to larger discrepancies. The higher recovery ratios applied in BWRO also contribute to the increased error in the pH value predicted for the final brine solution. As seen in Fig. 3 all three commercial programs predicted similar increasing trends in retentate

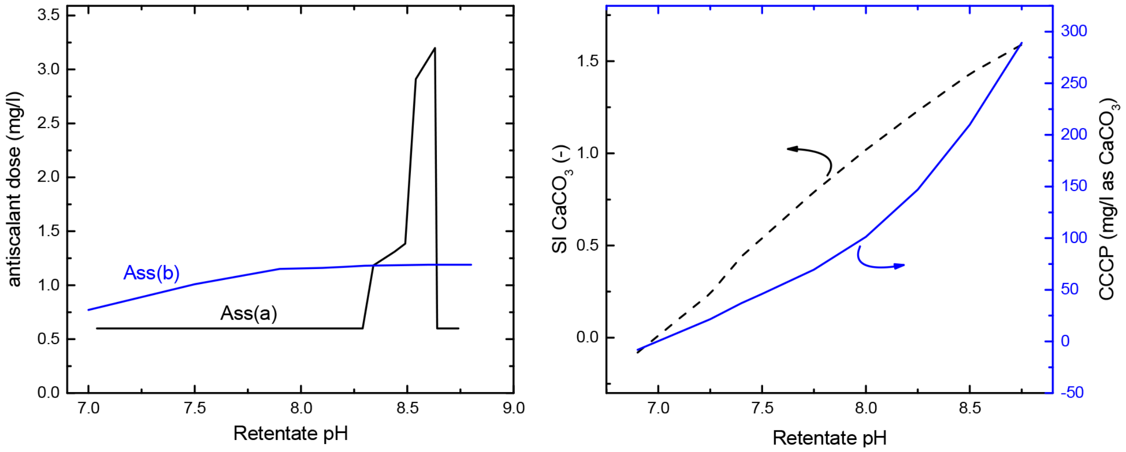

Fig. 2. Left hand side: recommended dose of antiscalant to SWRO 1st pass feed as a function of retentate pH (at 50% recovery ratio) by two different antiscalant suppliers for the feed composition given in Table 1 (Seawater). Right hand side: Saturation Index (SI) and calcium carbonate precipitation potential (CCPP) as a function of retentate pH. The CaCO$_3$ phase considered was aragonite. Feed composition and recovery are as stated above.

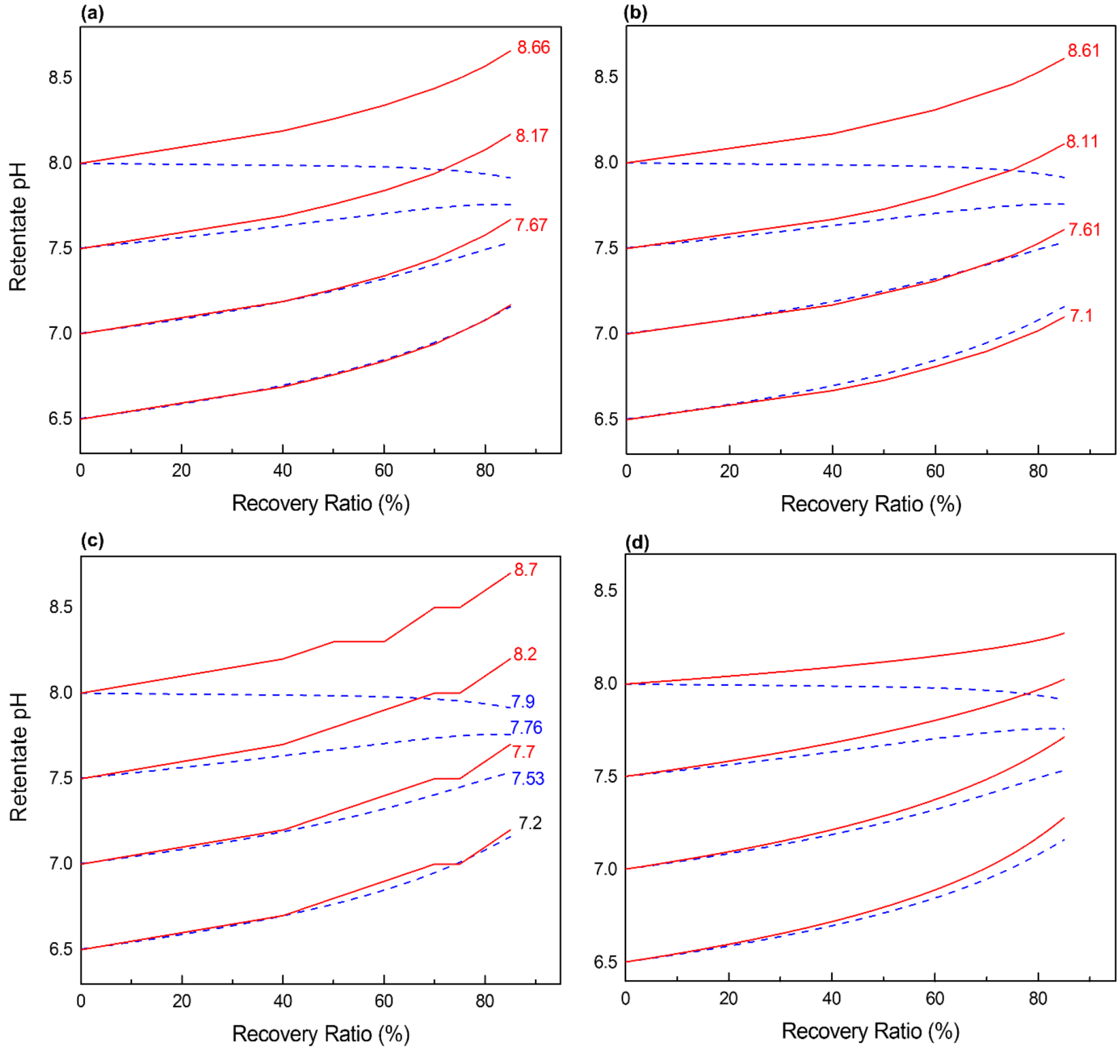

Fig. 3. pH evolution predictions for BWRO. Blue dashed lines: WATRO, Red lines: (a) and (b) antiscalant suppliers, (c) membrane manufacturer, (d) WATRO not considering shift in pKa values and H+/OH- cross-membrane transport.

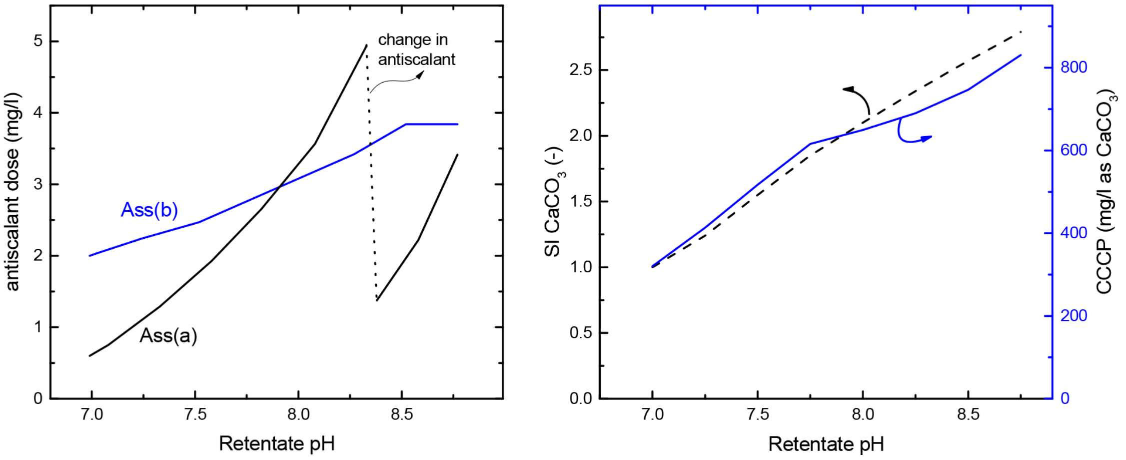

Fig. 4. *Left hand side:* recommended dose of antiscalant to BWRO feed as a function of retentate pH (at 80% recovery ratio) by two different antiscalant suppliers for the feed composition given in Table 1 (*Brackish*). *Right hand side:* Saturation Index (SI) and calcium carbonate precipitation potential (CCPP) as a function of retentate pH. The CaCO$_3$ phase considered was calcite. Feed composition and recovery are as stated above.

pH. Notably, the trend is perfectly identical for all four feed pH values tested, which is clearly unrealistic since pH evolution in the retentate is highly influenced by the feed pH.

The assumption that retentate pH always increases in the same manner is probably rooted in operational experience obtained for low feed pH. Historically, before the use of antiscalants became widespread, chemical scaling in RO desalination was controlled mainly by acidifying the feed, aiming typically for pH < 7. At this low pH, acid-base dynamics in the retentate are completely dominated by CO$_2$ transport and only weakly depend on ionic composition and inorganic carbon content, which might explain how the notion that pH evolution is similar in all cases could have been conceived. Indeed, when the feed pH was set to 6.5 the commercial software predictions accurately followed the WATRO simulation results as shown in Fig. 3. However, CO$_2$ transport became less dominant at higher feed pH values due to a decrease in its concentration, as supported by the simulation results presented on Fig. 3d, where only CO$_2$ transport was considered in WATRO. In addition, at higher pH the salinity induced pKa shift which pulls down the retentate pH is more dominant, since the concentrations of the negatively charged bicarbonate and carbonate increases. As a result, deviations from the mechanistic model WATRO increased with feed pH, while at the highest feed pH the trend was reversed, resulting in an overestimation of brine pH by 0.7–0.8 units.

The inaccuracies in predicting retentate pH have a significant influence on scaling tendency projections and recommended antiscalant dose also in the case of BWRO. At feed pH of 7, although overestimation is relatively small, (7.6–7.7 compared to 7.5), the increase in calcite SI and CCPP (Fig. 4) is sharp, leading to a >50% increase in antiscalant dose recommended by Ass(a). At the highest pH where discrepancies in the retentate pH are maximal, overdosing of 30% was recommended by Ass(b), while Ass(a) recommends using a different antiscalant above a certain supersaturation level. The leveling of Ass(b) dose at pH > 8.5 is either due to efficiency limit or to crystallization of the antiscalant itself. Clearly, more accurate predictions, also in this case, would result in a more suitable antiscalant dose, significant savings in chemicals consumption and the reduction in water cost.

The last case considered in the simulations was the high pH 2nd pass, commonly applied in SWRO desalination plants for boron removal. Unlike in seawater and brackish water, the inorganic carbon content in RO permeate (used as feed for the 2nd pass) is very low, resulting in low buffering capacity. Due to the low resistance to pH changes, predicting the retentate pH evolution is particularly challenging in this case. Nevertheless, the WATRO code was shown to reproduce experimental data at typical conditions with excellent accuracy [10]. In this case, a striking difference between WATRO simulations and the predictions made by commercial programs was found, as seen in Fig. 5. While all commercial programs predicted a strongly increasing trend, the WATRO code predicted an opposite, decreasing trend. It is noted that both Ass(a) and Ass(b) programs predicted almost the same pH (within 0.01 pH unit) for all pH and recovery ratio conditions tested and are thus plotted together. As in the SWRO and BWRO cases, when CO$_2$ transport was the sole acid-base mechanism considered in WATRO (see Fig. 5c), a sharp increase in retentate pH was projected, similar to the antiscalant commercial software. However, different from the previous cases, the main mechanism decreasing the retentate pH was not the salinity induced pKa shift. This is supported by the results which consider both CO$_2$ and pKa shift shown in Fig. 5c, showing the latter mechanism only slightly influenced the simulation results.

The prevailing mechanism driving pH evolution under SWRO 2nd pass conditions is the cross-membrane electro-migration of H$^+$ and OH$^-$ ions, driven by spontaneously arising electric potential gradient. The source of the electrical driving force is the difference in the permeation rates of anions versus cations. For the negatively charged polyamide membranes considered, anions permeate slower than cations, creating a positive electric field in the perme-

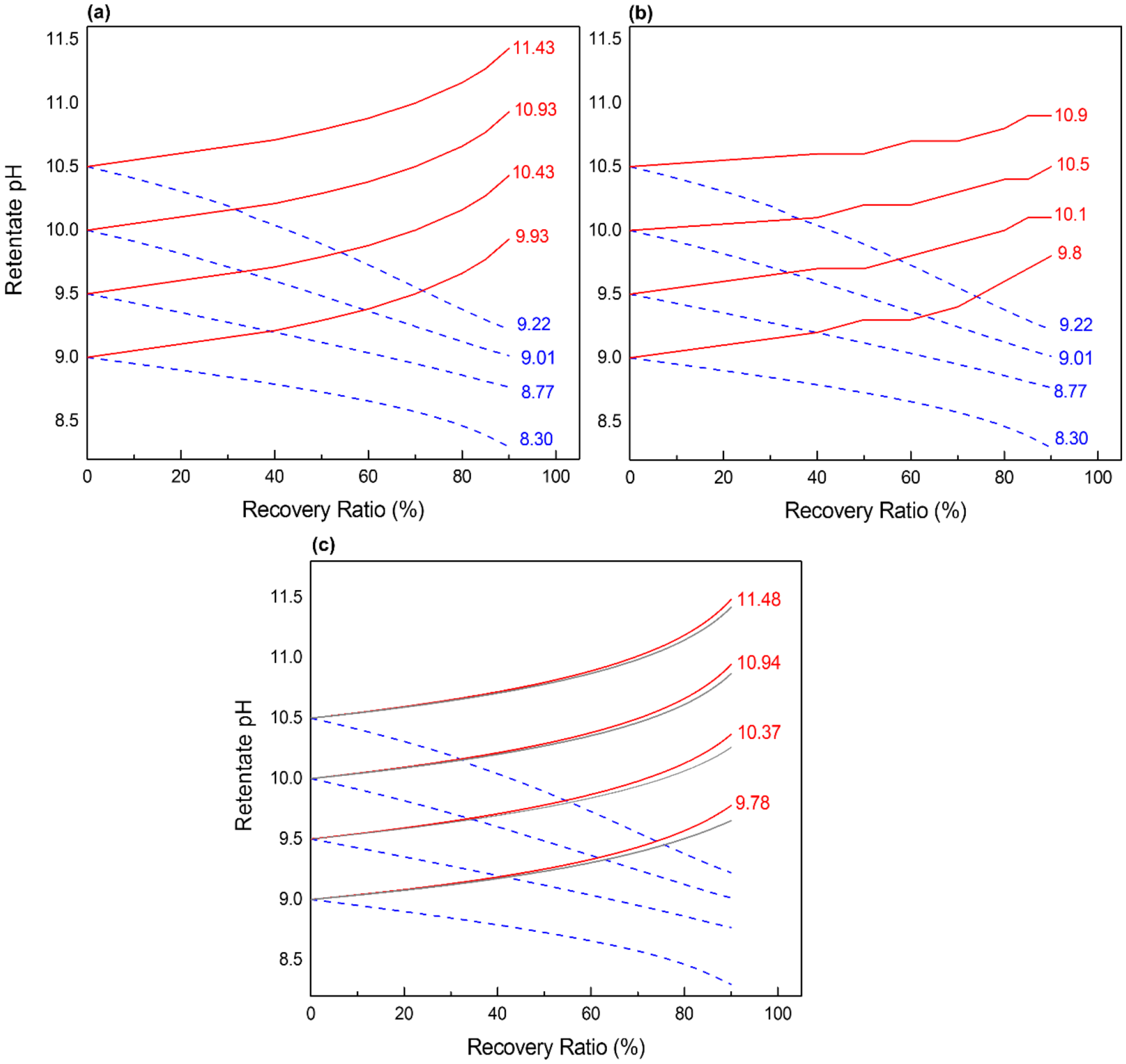

Fig. 5. pH evolution predictions for SWRO 2nd pass. Blue dashed lines: WATRO, Red lines: (a) antiscalant suppliers, (b) membrane manufacturer, (c) WATRO only considering CO_2 transport (red curves) and WATRO only considering CO_2 transport and pKa shift without H+/OH- cross-membrane transport (grey curves).

ate direction which drives OH^- ions towards the permeate and H^+ ions towards the retentate. The result is a net positive alkalinity flux from the retentate to the permeate (0.2–0.01 meq/l), significantly decreasing the pH in the poorly buffered RO retentate. This phenomenon was previously demonstrated [15] followed by a systematic study and the development of a mathematical model [7] which was later embedded in the WATRO code. As seen in Fig. 5, not considering this mechanism resulted in over estimations of the retentate pH by 1.5 to 2.1 pH units.

The large overestimations in the case of SWRO 2nd pass dramatically affect scaling tendencies and recommended antiscalant doses as shown in Fig. 6. For both potentially scale-forming minerals, calcite ($CaCO_3$) and brucite ($Mg(OH)_2$), a transition from under saturation to supersaturation occurs at pH > 9.22 which is the maximum pH value predicted by WATRO. As a result, for the specific SWRO permeate composition considered here, calcite and brucite formation is thermodynamically restricted therefore antiscalant may not be required (nevertheless antiscalant addition for controlling calcite scaling is still recommended under this pH by Ass(b)). Contrarily, for the high pH predicted by the commercial software (9.8–11.43) the brine is always supersaturated with respect to calcite, while supersaturation for brucite is reached at pH~10.3 and rises steeply at higher pH values. In this case, the rise in recommended antiscalant dose from pH 7 to pH 8.5 is attributed by Ass(a) to ferric-hydroxide, while at higher pH values the rise is attributed to $CaCO_3$ scaling. No specific recommendation were given to for brucite, despite supersaturation of this mineral. As seen in Fig. 6, the highest overestimation of pH (11.43 Vs. 9.22) resulted in 100% increase in the recommended antiscalant dose. Beyond scaling, the overestimation of pH in the retentate could limit the feed pH selected by process designers (aiming to avoid scaling) and consequently boron rejection would be hindered.

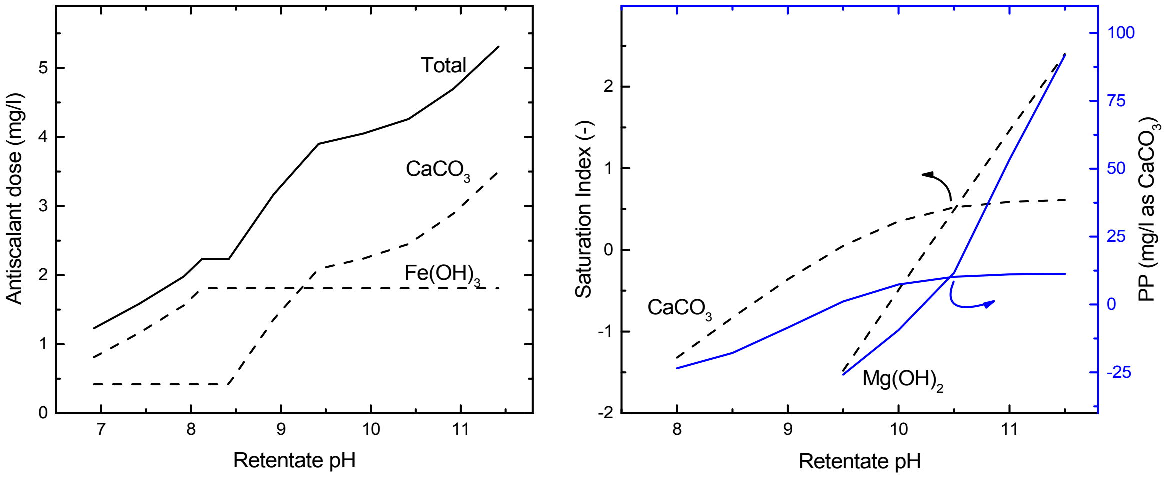

Fig. 6. Left hand side: recommended dose of antiscalant to SWRO 2nd pass feed as a function of retentate pH (at 85% recovery ratio) by antiscalant supplier (b) for the feed composition given in Table 1 (RO permeate). Dose due to ferric-hydroxide and $CaCO_3$ supersaturation is presented. Right hand side: Saturation Index (SI) and precipitation potential (PP) for calcite and brucite ($Mg(OH)_2$) as a function of retentate pH. Feed composition and recovery are as stated above.

5. Conclusions

In this work, the capacity of commonly used commercial programs for predicting pH evolution in reverse-osmosis retentate and the resulting scaling tendency was systematically tested against an experimentally validated mechanistic model. It was shown for three different typical RO feed compositions that significant deviations in retentate pH occurs, resulting in inaccurate assessment of scaling predictions and (mainly) over-estimation of the antiscalant dose required for scaling prevention. Currently available process design tools could be significantly improved if additional acid-base mechanisms will be incorporated in programs provided by antiscalants suppliers and membrane manufacturers. The open-source freely-available WATRO code could be adopted by programmers to improve commercial software predictions, as-well as by process designers and operators seeking a more reliable prediction of pH and scaling tendency. More realistic scaling predictions are thus feasible and could increase the cost-effectiveness of RO desalination processes and minimize potential environmental impact of antiscalants [17]. Future research is underway for expanding the model to reverse osmosis [18] and nano filtration of wastewater effluents [19,20].

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