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OPTIMISATION OF A LIQUID-LIQUID EXTRACTION BASED SUSTAINABLE WATER DESALINATION PROCESS

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Abstract

In this paper, a waste heat liquid-liquid extraction method is considered for the seawater desalination. The mathematical model is a result of mass and energy balances, phase behaviour and salt distribution in the two phases. Because of the high non-linearity of the phase behaviour and the salt distribution these are being approximated by the use of piecewise linear approximations methods and the solutions are presented. The results indicate that the quality of solution is not affected by the use of the approximation.

Keywords: Design; Optimization; Piecewise linearization; Solvent Extraction.

1. Introduction

Water is one of the most abundant resources on earth. Although, it covers almost 75% of the earth's surface, only 3% of this is fresh water. This small percentage can be found in ground water, lakes and rivers, while the remaining 97% can be found in the oceans. The water shortage problem could be potentially addressed with the use of a sustainable seawater desalination process.

Separating salt from water and obtaining potable water is usually performed by methods that require large amounts of energy and are costly. The conventional methods of desalination are divided in thermal and membrane processes. The dominant thermal desalination method is the multi-stage flash distillation that requires external steam supply at 100^OC, while the dominant membrane method is reverse osmosis and requires energy to power a pump that would increase the pressure up to 70bar. Multi-stage flash (MF) along with reverse osmosis (RO) account for 86% of the worldwide capacity of water desalination.

In this paper, a sustainable desalination method that uses waste heat is considered. This method is called the Puraq method and can produce fresh water by solvent extraction with a specially tailored liquid polymer solvent. These specially tailored polymers can pass from regions of complete miscibility into two phase separation when mixed with water. The Puraq process has two unique advantages over MF and RO because no membrane is necessary for the process and the temperature range is between $30 ^O$C and 60^OC. This makes the Puraq process a highly competitive process that is worthwhile being investigated.

2. Process Modeling

The process consists of a deaerator, a heat transfer contractor, a wash contractor and heat exchangers. In the deaerator, the dissolved gases are mechanically removed from

the feedwater. In the heat transfer contactor, the liquid-liquid extraction takes place where water and salt are transferred from the carrier to the solvent, followed by a centrifugation where more-dense components of the mixture migrate away from the axis of the centrifuge, resulting in potable water. In the wash contractor, the polymeric solvent is washed in order to remove the salt dissolved in it. Finally, the heat exchangers are used for heat recovery. A more detailed description of the flowsheet can be found in Lazare et al. In this paper, the liquid-liquid extraction (LLE) unit and the wash contractor, as shown in Figure 1, will be the main focus. In Figure 1, seawater (stream 5) mixes with the polymer stream (stream 4) within the LLE unit. During this step water and salt distribute to the polymeric phase based on the salt distribution coefficient correlation that was first described in Lazare (1992) and is given in equation 1.
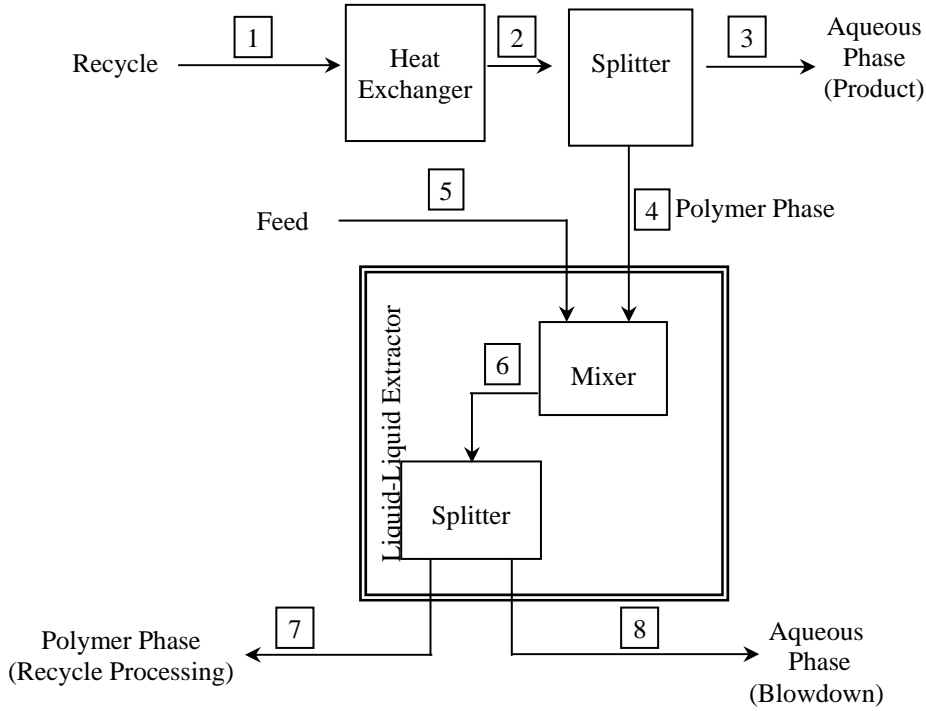

Figure 1. Flowsheet of heat transfer contractor

$$K_s = 1.5 \cdot e^{0.00006914 \cdot x_s^3 - 0.01278 \cdot x_s^2 + 0.84114 \cdot x_s - 18.133} \tag{1}$$

Another key correlation is the phase equilibrium relationship that was also described by Lazare (1992) and is given in equation 2.

$$\frac{-7.612}{1 + \dfrac{3.25 \cdot (1 - x_s)}{x_s}} = \ln(1 - x_p) + \left(1 - \frac{1}{150}\right) \cdot x_p + \left(13.45 - \frac{4005.148}{T}\right) \cdot x_p^2 \tag{2}$$

Both equations are non-linear and can cause computational difficulties. In previous work done by our group, the phase equilibrium correlation was substituted by a linear equivalent as shown in equation 3.

$$x = 0.01T + 0.4 \qquad\qquad\qquad (3)$$

In this work, both correlations will be approximated using a piecewise linear approximation method as presented by Polykarpou et al. For all required linearizations, the approach presented in Natali et al. was employed in order to obtain the optimal points that approximate the relevant non-linear functions. In figures 2 and 3 the actual non-linear correlations are shown with the solid lines while the optimal piecewise linear approximations are denoted with the square points.
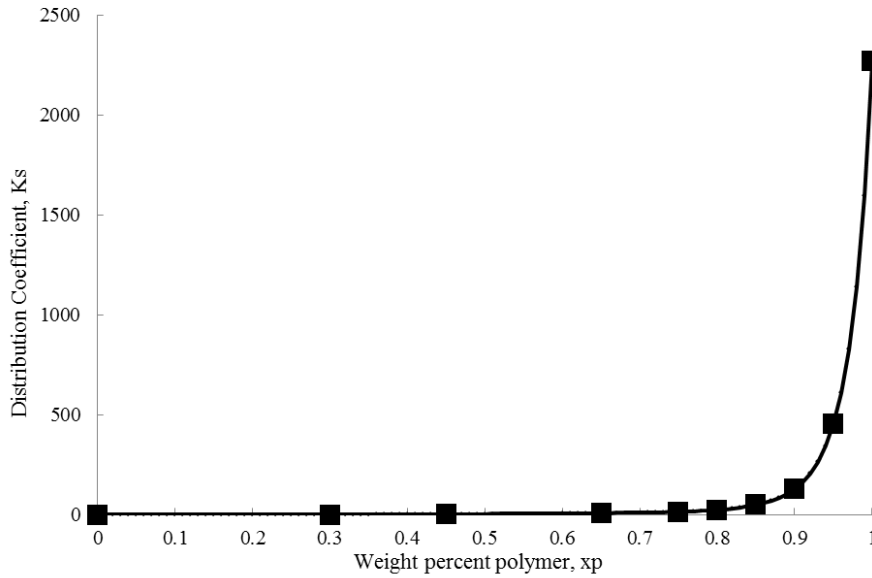

Figure 2. Distribution coefficient of salt

3. System Definition

The proposed mathematical model consists of an objective function, as presented in equation 4 and is defined by the energy balance related to the heat exchanger. The objective is to minimize the energy use.

$$Q = \sum_i (F2_i \cdot Cp_i) \cdot T2 - \sum_i (F1_i \cdot Cp_i) \cdot T1 \qquad\qquad (4)$$

where i refers to components: water, salt and polymer.

Equation 4 is subject to a number of constraints, described by the mass balances and the piecewise linearization equations. Equations 5-7 describe the salt distribution linearization.

$$Ks = \sum_l \delta_l \cdot v_l \tag{5}$$

$$xp = \sum_l \gamma_l \cdot v_l \tag{6}$$

$$\sum_l v_l = 1 \tag{7}$$

where parameters δ_l and γ_l define the piecewise linear points used and v_l is a SOS2 variable, so that at most two of them can be non-zero at the same time.
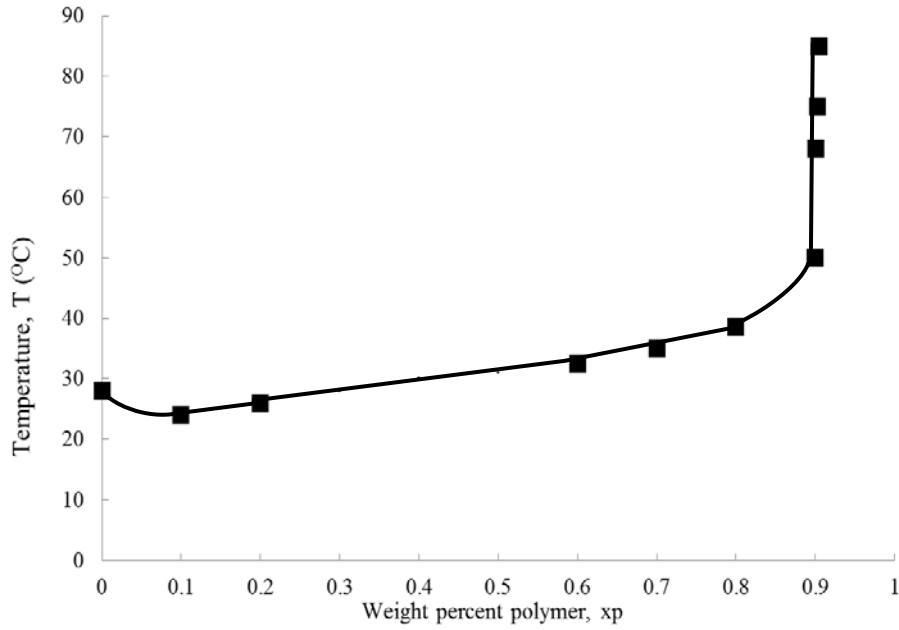

Figure 3. Phase diagram

Similarly, equations 8-10 describe the phase equilibrium relationship.

$$xp = \sum_{l'} \varepsilon_{l'} \cdot \mu_{l'} \tag{8}$$

$$T = \sum_{l'} \zeta_{l'} \cdot \mu_{l'} \tag{9}$$

$$\sum_{l'} \mu_{l'} = 1 \tag{10}$$

The overall problem is stated as follows:

Given: The seawater feed in terms of water and salt concentration;
Feed temperature;
Specific heat capacities;
Phase equilibrium correlation;
Salt distribution correlation;
Minimum percentage of salt in the product.

Minimise: Energy consumption.

The resulting model is a mixed integer non-linear programming (MINLP) mathematical model. It is mixed integer because we have SOS2 variables involved and remains non-linear, because in the energy balances as shown in equation 4, both temperature and flow are variables. Nonetheless, the approximation of the non-linear correlations can have a benefit when the overall flowsheet is implemented.

4. Results and Discussion

The model was implemented in GAMS on Dell Desktop Core i5 3.25GB RAM 3.16GHz machine. Moreover different MINLP solvers were used, with SBB being the most robust. In terms of model statistics, the resulting MINLP model consists of 37 constraints, 86 continuous variables and has a CPU time 0.05s.

In figure 4 the calculated flows of salt for both the aqueous and polymeric phase are presented. As expected, the blowdown stream F_7 has the highest content of salt, as this is the stream that is discarded back to the sea. Moreover the change over between the salt content before and after the liquid-liquid extractors represents the effect of the both the salt distribution and the phase equilibrium correlations.
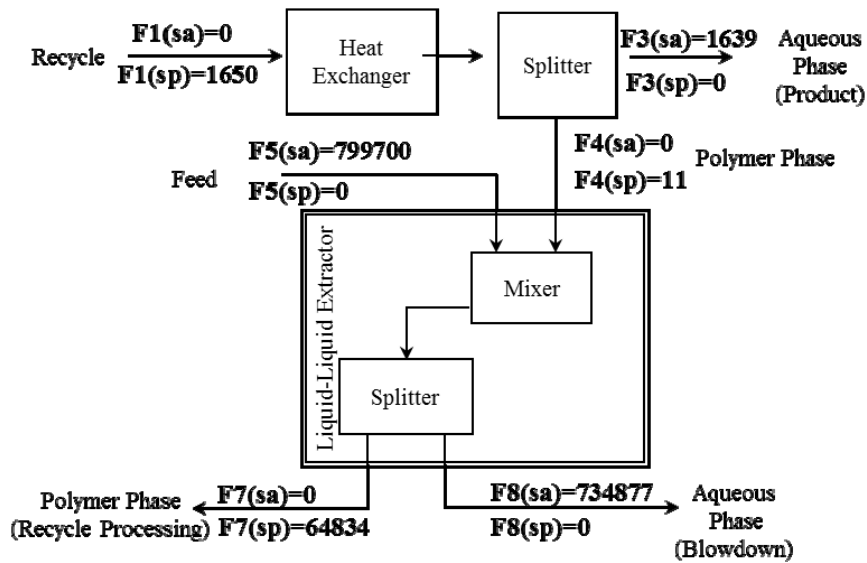

Figure 4. Salt flows for aqueous and polymer phase in lbs/hr

Finally, the use of piecewise linear approximation, does not affect the quality of the solution and as mentioned earlier provides the base for expanding the flowsheet and including heat integration as part of the optimization.

5. Concluding Remarks

In this paper an MINLP model for LLE water desalination process using piecewise linear approximation was presented. The linear approximation of non-linear correlation offers an advantage over using the original correlations. Current works involve implementing the overall flowsheet in order to determine how energy consumption can be further reduced.

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