

*Keynote Lecture Paper***Clean Water and Clean Energy Production: Simulation Using Finite Element Method**

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One Dimensional Finite Element Method (FEM) is used to develop an analysis model for Pressure Retarded Osmosis (PRO), Direct Forward Osmosis (FO) and Reverse Osmosis (RO). A 1 D FEM model is developed and simulated on MATLAB. The predictions of the present method are compared with those available in literature, both numerical and experimental. In addition, for the first time in literature, the variation of concentration of solute on the feed and draw side as well as the variation of water permeate flux along the length using the variable mass transfer coefficient is predicted. There is a need to introduce new non-dimensional parameters to make the  $\epsilon$ -MTU model a more generalised model (applicable to FO, PRO and RO) and to aid the design of the mass exchangers.

**Keywords:** Pressure Retarded Osmosis (PRO); Forward Osmosis (FO); Reverse Osmosis (RO); Concentration Polarisation; Finite Element Method (FEM); Salt flux; Non-dimensional parameters

**Introduction**

Two of the biggest challenges man-kind is facing today is ENERGY and WATER SCARCITY. Non-renewable energy sources are no more abundant to satisfy our growing needs. The depleting quality and quantity of fresh water has given rise to water scarcity. A reliable alternate solution has to be put to action immediately. The concept of obtaining Clean Energy and Clean Water through simple osmotic processes can provide solutions to the problems at hand.

Osmosis is the spontaneous net movement of solvent molecules through a partially permeable membrane into a region of higher solute concentration, the direction that tends to equalize the solute concentrations on the two sides i.e. the feed and the draw side respectively of the mass exchanger.

Osmosis can be classified into Forward Osmosis (FO) or Reverse Osmosis (RO) depending on the direction of the movement of solvent molecules across the semi permeable membrane. Pressure Retarded Osmosis (PRO) is also in the same direction as the FO, where the osmotic pressure overcomes an applied

pressure (hydraulic pressure) to aid permeate flow.

PRO aids in clean energy production whereas RO in obtaining clean water. FO process helps in efficient RO process in cleaning water in particular the sewage water which contains foulants.

Owing to varied applications of osmotic processes and the need to develop an efficient design tool for analysis numerous analytical and numerical models are being developed worldwide. Sharqawy *et al.*, 2013 non-dimensionalised their analytical results and proposed  $\epsilon$ -MTU model, which can be used as a design tool for PRO systems using a linearized osmotic pressure function and ideal membrane characteristics. Straub *et al.*, 2014 propose their model for the module scale osmotic systems. Phillip *et al.*, 2010 developed a model that describes the reverse permeation of draw solution across an asymmetric membrane in FO operation. Recently, Tan and Ng, 2008 investigated the impact of External Concentration Polarization (ECP) and Internal Concentration Polarization (ICP) on the FO process and developed a model to predict the flux of FO process considering these effects. They used mass transfer coefficient calculated by the

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boundary layer concept to analyse ECP layer. Similar to the PRO  $\varepsilon$ -MTU model, an  $\varepsilon$ -MTU model for RO mass exchanger has been developed by Banchik *et al.*, 2014.

With the objective to find a simple yet effective tool to analyse and design mass exchangers, the authors propose a 1D FEM model applied to Osmotic processes.

### 1D FEM Model

FEM is a numerical method used to determine the approximate solution of various physical problems in engineering. The idealization of the physical problem to a mathematical model requires certain assumptions that together lead to differential equations governing that mathematical model. The FEM solves this mathematical model. Finite Element Modelling involves discretizing a region under consideration into a number of elements and then using an interpolation function to represent the variation of the field variable over an element. Solving the differential equation in FEM usually involves using variational or weighted residual method. Galerkin's weighted residual method is used in this investigation to solve the differential equations. In the Galerkin's method the weights used are the shape functions themselves.

1D FEM has been used successfully in the past by Ravikumaur *et al.*, 1988 to analyse heat transfer on heat exchangers. Here the differential equation governing the heat transfer for the hot fluid in a given 1D element is

$$C_h dT = -U(T_h - T_c) dA \quad (1)$$

and that for the cold fluid is given by

$$C_c dT = U(T_h - T_c) dA \quad (2)$$

In Eq. (1) and Eq. (2)  $C_h$  and  $C_c$  represent the heat capacity rates of hot and cold fluid in the element,  $T_h$  and  $T_c$  represent their respective temperatures,  $dA$  refers to the incremental areas in their flow directions. Ravikumaur *et al.*, 1988 use linear isoparametric elements to approximate the field variables and the area. Finally using weighted residuals the Equations are solved and the heat exchangers are analysed.

Similarly, in this investigation the whole mass exchanger is discretised into a number of elements along the flow. Basic mass conservation, solute

conservation and the permeate flow equations are applied to obtain differential equations governing the permeate flow in each element. Galerkin's method is then applied to the differential equations to obtain a set of algebraic equations on which the boundary conditions are applied.

Osmotic pressure difference is the crucial driving force in the process of osmosis. The osmotic pressure is usually related to concentration of solution using the Van't Hoff's law. Van't Hoff's co-efficient assumes a linear relation with concentration and Osmotic pressure. The linear relation is valid only for dilute solutions and the approximation fails for concentrated solutions.

Van't Hoff's Law is given by eq. (3), where  $c^l$  is the Van't Hoff's co-efficient.

$$\pi = c^l w \quad (3)$$

However, to ensure that concentrative solution can also be included into the model, modified Van't Hoff's co-efficients are used. Many researchers (Tan and Ng, 2008), give the relation between osmotic pressure and concentration of a solution. Using this function  $f(w)$  which relates concentration ( $w$ ) to osmotic pressure the modified Van't Hoff's coefficient ( $c$ ) is defined as,

$$c = \frac{f(w)}{w} \quad (4)$$

For the purpose of illustration a counter flow PRO mass exchanger is shown in Fig. 1, where  $\dot{m}_d$  and  $\dot{m}_f$  are mass flow rates of draw and feed side.

On an arbitrary element under consideration we apply conservation of mass, conservation of species and take permeate flow ( $\dot{m}_p$ ) to be proportionate to net pressure difference. Also, to make the model

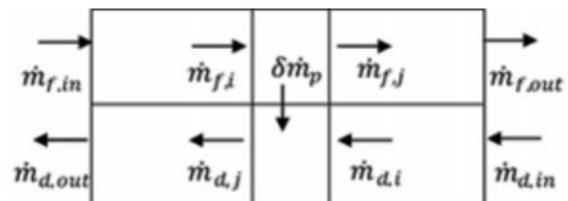


Fig. 1: Elemental discretization of a counter flow mass exchanger

realistic salt flux and concentration polarization effects are taken into account. Upon simplification of these equations and making suitable approximations like bulk concentration in each flow to be same as concentration at membrane we obtain the final set of differential equations obtained are the analogous osmotic process differential equations when compared to the heat transfer equations provided by Ravikumaur *et al.*, 1988.

On applying Galerkin's weighted residual approach to the differential equations we obtain the stiffness matrix and Force vector which defines the physics of the problem at each element. Using the stiffness matrix and force vector for each element and assembling all the elements we solve this problem on a MATLAB software. The model is verified with established experimental and analytical works. PRO 1D FEM model is verified with experimental work of Song *et al.*, 2013 as shown in Fig. 2. FO 1D FEM model is verified with experimental results of Phillip *et al.*, 2010. RO 1D FEM model is verified with analytical work of Banchik *et al.*, 2014. Excellent comparison has been obtained with the experimental and analytical values. The model can also take into account variation of mass transfer coefficient and Van't Hoff's coefficient along the length. The model gives useful results like variation of concentration, permeate flow and power density (for PRO system) along the length of the Osmotic system.

## Results and Discussion

The 1D FEM model serves as an excellent tool to analyse Osmotic processes. Due to its accuracy and simplicity in usage this simulation tool can be used for design of osmotic processes. Unlike many other analytical methods this model accounts for all real time conditions that one encounters in an osmotic process like concentration polarisation, reverse solute flux and variation of mass transfer coefficient. The mass transfer coefficient can also be modified to account for spacers using the experimental data. Since the analysis is elemental the simulation results of the 1D FEM model gives output (power density/water flux) along the length of the osmotic system. Here, water flux variation along a length of a FO system is predicted by the 1D FEM model in Fig. 5.

The 1D FEM model is non-dimensionalised to analyse the effects of various parameters. The non-dimensional parameters are derived from the  $\varepsilon$ -MTU model (Sharqawy *et al.*, 2013; Banchik *et al.*, 2014). MTU in the  $\varepsilon$ -MTU model stands for mass transfer

unit given by  $\frac{A_m A \Delta P}{\dot{m}_{f,in}}$ , where  $A_m$ ,  $A$  and  $\Delta P$  denote membrane area, water permeability coefficient and Hydraulic pressure difference respectively. MTU is analogous to NTU of Heat Exchanger analysis.

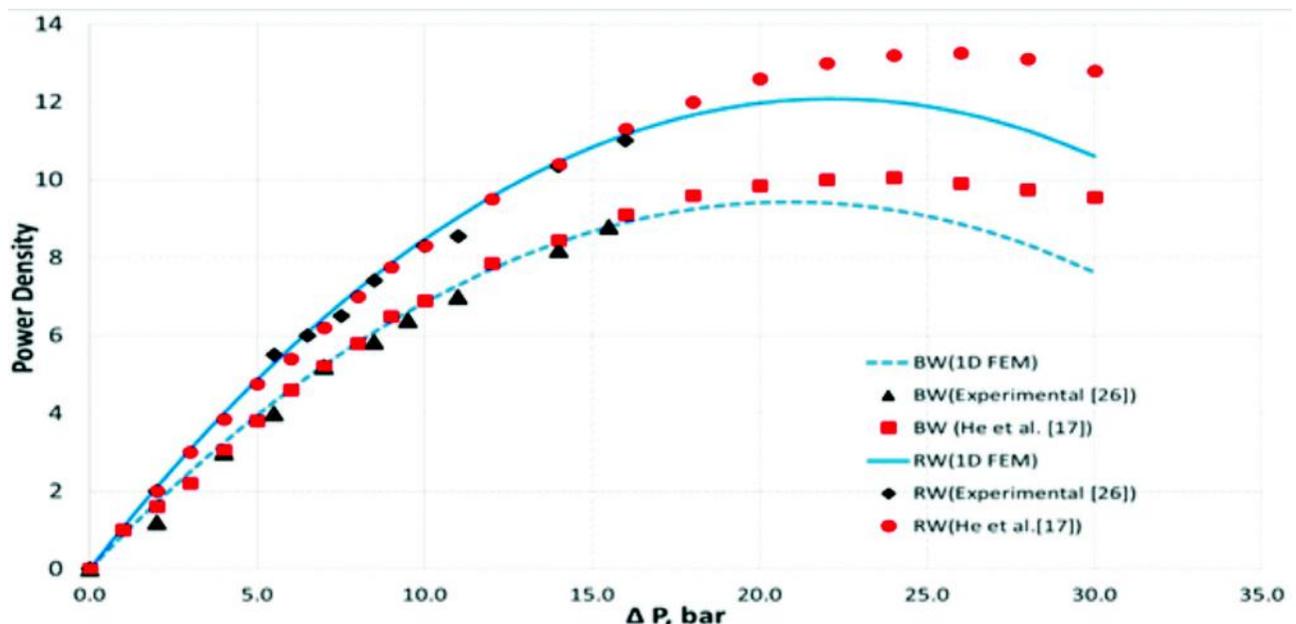


Fig. 2: Comparison and verification of the power density graph using 1 D Fem model for PRO system

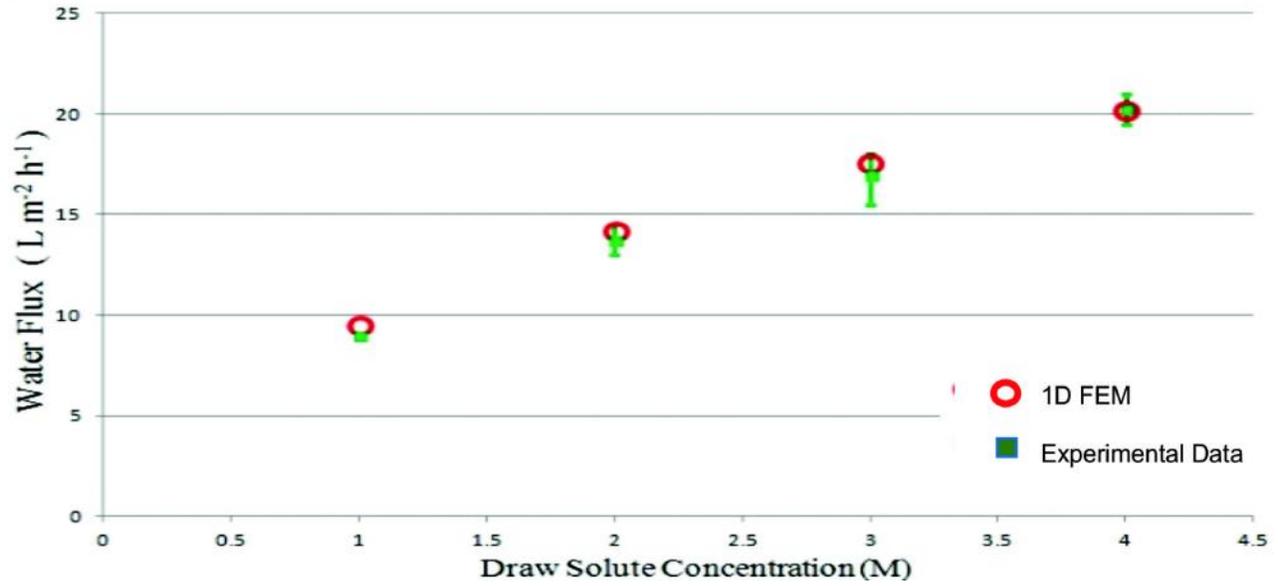


Fig. 3: Comparison of Experimental results (Phillip *et al.*, 2010) for water flux in the presence of polarisation effect and reverse salt flux, with 1D FEM model for FO system

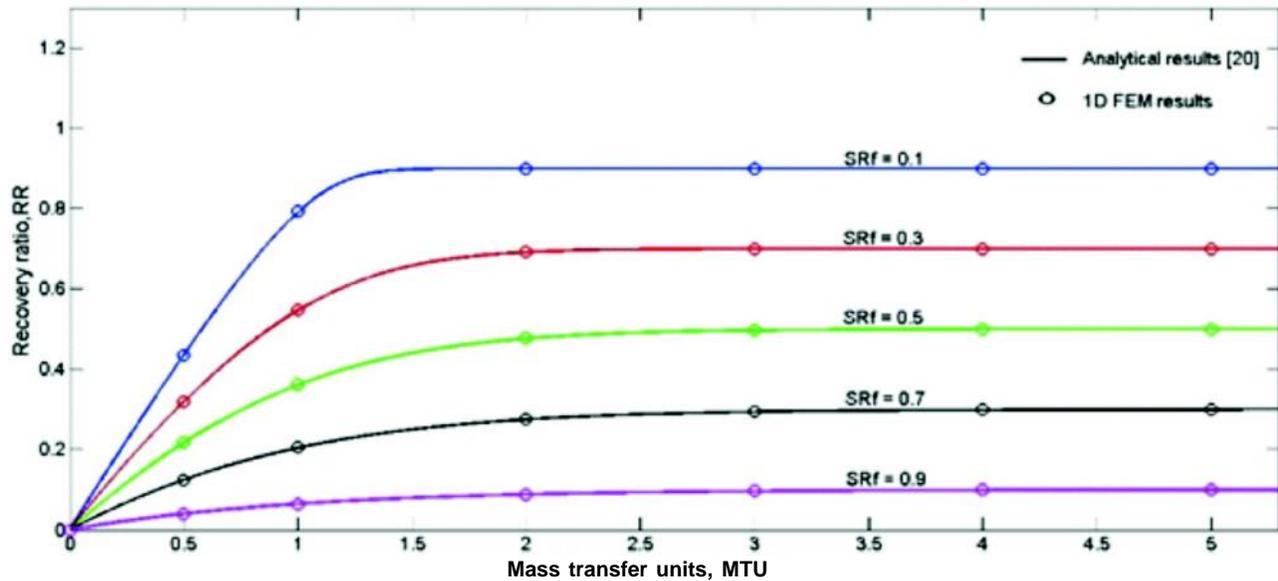


Fig. 4: Comparison of 1D FEM model for RO system with analytical results of Banchik *et al.*, 2014

In this investigation to account for varying Van't Hoff's Coefficient and the difference in Van't Hoff Coefficient on feed and draw side, a new non-dimensional parameter Van't Hoff Coefficient ratio

$C_{vr}$  is defined as  $C_{vr} = \frac{c_f}{c_d}$ . In the  $\epsilon$ -MTU model

Figs. 6-8, show various design graphs for different  $C_{vr}$  for a given Osmotic Pressure ratios  $SR_f$

$\left(\frac{\pi_{f,in}}{\Delta P}\right)$  and  $SR_d \left(\frac{\pi_{d,in}}{\Delta P}\right)$ . It can be seen that on

increasing  $C_{vr}$  the curves raise. However in Fig. 8 the graphs meet at a point and the curve with a greater

$MR \left(\frac{\dot{m}_{d,in}}{\dot{m}_{f,in}}\right)$  value which has a higher RR value

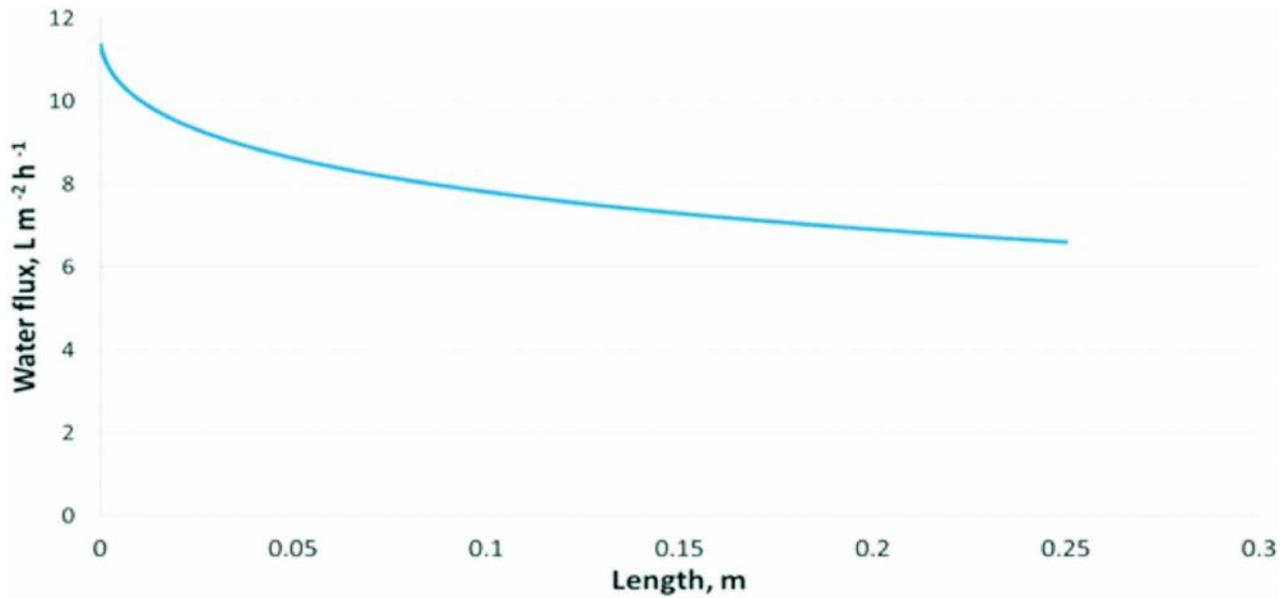


Fig. 5: Variation of water flux along length for volumetric flow rate of 2 l/min with feed concentration 0.5M ( $w_{f,in} = 0.0293$  Kg/Kg) and draw concentration 1M ( $w_{d,in} = 0.0585$  Kg/Kg) in FO system

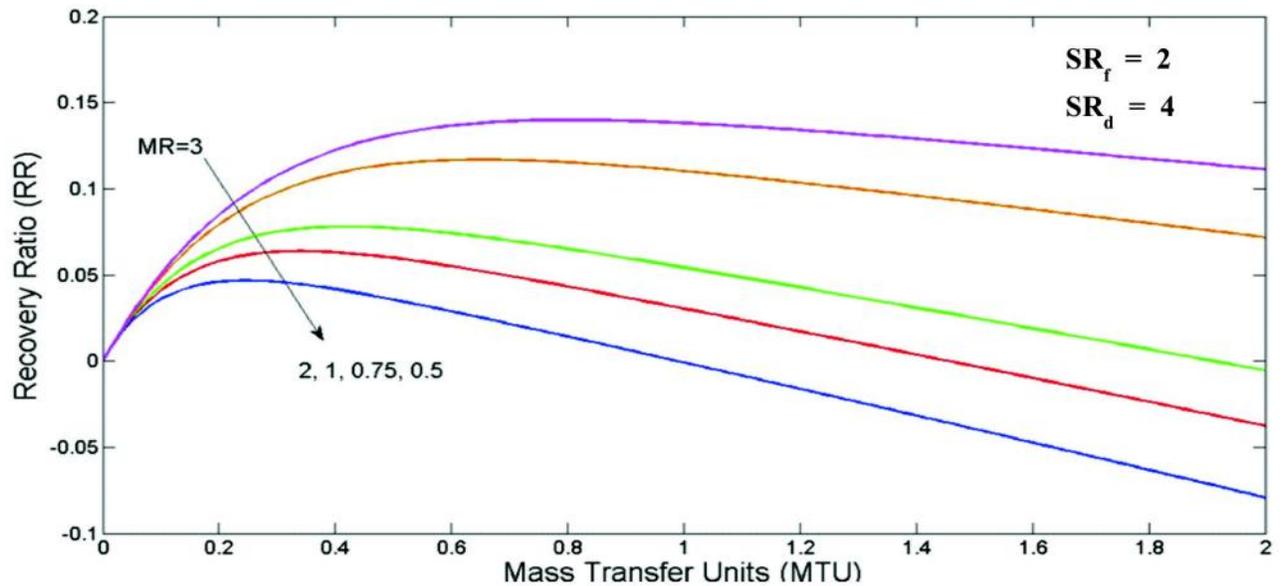


Fig. 6: Graph of RR v/s MTU for  $C_{vr} = 0.9$  for a PRO process

before the point of intersection has a lower RR value for a point beyond the point of intersection. This indicates that with different  $C_{vr}$  ratio the behavior varies significantly and the effect cannot be ignored.

**Conclusion**

In the present investigation, Pressure Retarded Osmosis (PRO), Forward osmosis (FO) and Reverse

Osmosis (RO) is analysed using 1D Finite Element Method (FEM). The model is simple to use and MATLAB takes only a few seconds to give the simulation results. 1D FEM model predicts the water flux and concentration variation along length of the PRO, FO and RO systems. This model is realistic as concentration polarisation effects and reverse solute flux is taken into account. Also, new non-

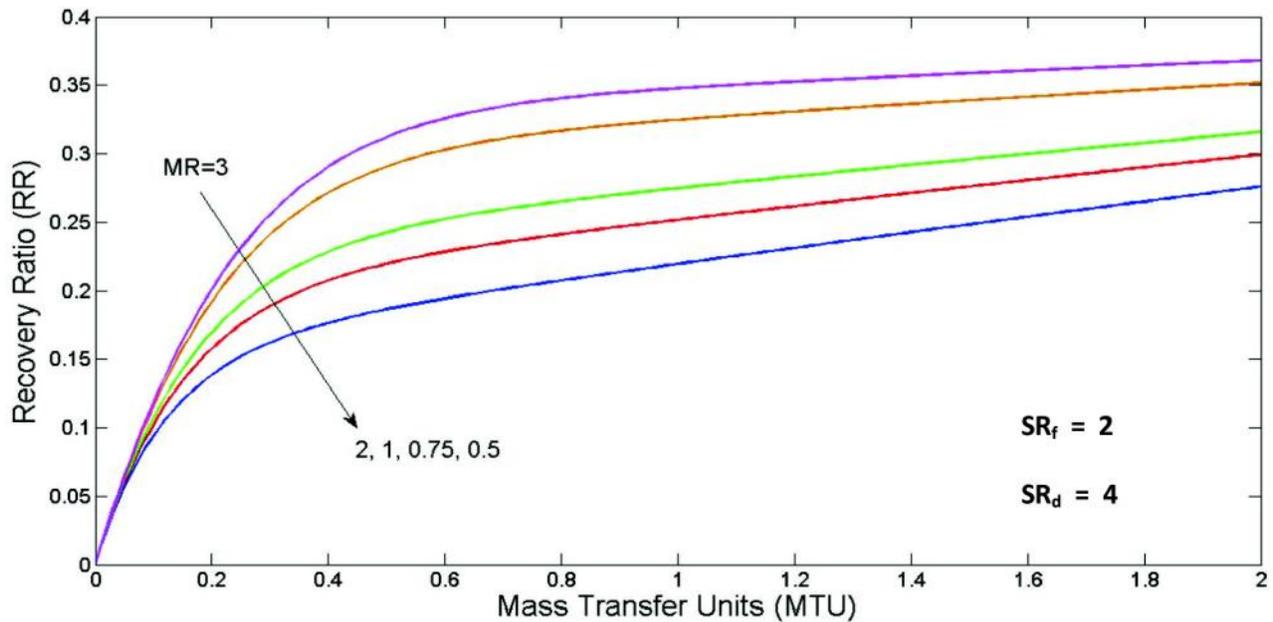


Fig. 7: Graph of RR v/s MTU for  $C_{vr} = 1.1$  for a PRO process

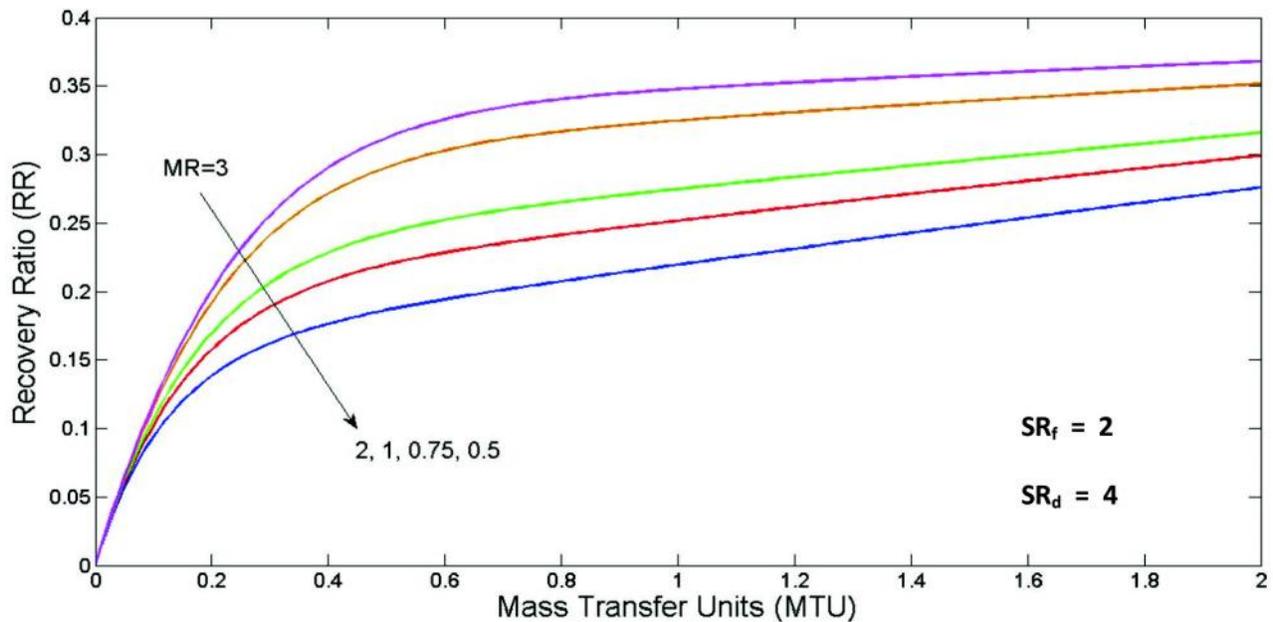


Fig. 8: Graph of RR v/s MTU for  $C_{vr} = 1.5$  for a PRO process

dimensionalised units are presented to aid in design of the Osmotic processes.

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