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Simulation and optimisation of a two-stage/two-pass reverse osmosis system for improved removal of chlorophenol from wastewater

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ABSTRACT

Reverse osmosis (RO) has become a common method for treating wastewater and removing several harmful organic compounds because of its relative ease of use and reduced costs. Chlorophenol is a toxic compound for humans and can readily be found in the wastewater of a wide range of industries. Previous research in this area of work has already provided promising results in respect of the performance of an individual spiral wound RO process for removing chlorophenol from wastewater, but the associated removal rates have stayed stubbornly low. The literature has so far confirmed that the efficiency of eliminating chlorophenol from wastewater using a pilot-scale of an individual spiral wound RO process is around 83%, compared to 97% for dimethylphenol. This paper explores the potential of an alternative configuration of two-stage/two-pass RO process for improving such low chlorophenol rejection rates via simulation and optimisation. The operational optimisation carried out is enhanced by constraining the total recovery rate to a realistic value by varying the system operating parameters according to the allowable limits of the process. The results indicate that the proposed configuration has the potential to increase the rejection of chlorophenol by 12.4% while achieving 40% total water recovery at an energy consumption of 1.949 kWh/m^3.

1. Introduction

Development of novel and diverse water treatment technologies are continuously evolving due to strict water quality regulations with emphasis on trace contaminants [1]. Effluents of many industrial applications contain a variety of micro-pollutants, which are released into a variety of water resources. Such micro-pollutants not only disrupt the biological ecosystem, but they also pose real threat to public health. They include phenol and phenolic compounds, which are colorless (at room temperature) crystalline substances, consisting of hydroxyl and aromatic hydrocarbon group. They are highly toxic even in the small amounts that they can be in the effluents from various industries including refineries, and fertiliser, pesticide, chemical, petrochemical, wood, and paint industries [2,3,4]. More importantly, the existence of a stable benzene ring in phenol and phenolic derivatives has increased their resistance to biological decomposition. Much recent research has focused on the removal of chlorophenol (suspected carcinogen), which is formed following the release of phenol into the environment (especially water). This is because it undergoes an active reaction with chlorine to form chlorophenol, which is more persistent than phenol and have a higher toxicity level [5]. The World Health Organization (WHO) and the U.S. Environmental Protection Agency (US EPA) have set the phenol concentration to 1 $\mu g/l$ in drinking water [6,7]. The Agency of Toxic Substances and Disease Registry (ATSDR) limited the concentration of dimethylphenol to a maximum of 0.05 ppm in surface water [8]. Also, the Japan Environmental Governing Standards constrained phenol concentration to 5 mg/l in water sources [9].

To resolve this problem, there has been several attempts to degrade the phenol and phenolic compounds from water using different treatment methods such as distillation processes, activated carbon adsorption, ion exchange, solvent extraction, chlorine dioxide, ozonation, UV/H_2O_2, catalyst wet air oxidation, biological methods, and membrane technology [1,10]. Interestingly, the UV/H_2O_2 is considered as the most used technology for achieving the restricted limits of phenol required. However, this technology not only consumes a lot of energy, but it also potentially increases the carbon concentration in re-used water [11]. However, due to continuous improvement in design and fabrication of membranes [12,13], amongst all these treatment processes, the RO process (energy saving process) are being widely used for removing organic compounds, such as sulphate, copper, cadmium, nickel,

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Nomenclature

A	Effective area of the membrane (m^2)
A_w	Solvent transport coefficient (m/atm s)
b	Feed and permeate channels friction parameter (atm s/m^4)
B_s	Solute transport coefficient (m/s)
C_b	The bulk feed solute concentrations at the feed channel (kmol/m^3)
C_f	The inlet feed solute concentrations at the feed channel (kmol/m^3)
$C_{f\,(plant)}$	The inlet chlorophenol concentration of the plant (kmol/m^3)
C_m	The dimensionless solute concentration in Eq. (5) (dimensionless)
C_p	The permeate solute concentration at the permeate channel (kmol/m^3)
C_w	The solute concentration on the membrane surface at the feed channel (kmol/m^3)
D_b	The solute diffusion coefficient of feed at the feed channel (m^2/s)
D_p	The solute diffusion coefficient of feed at the permeate channel (m^2/s)
de_b	The equivalent diameters of the feed channel (m)
de_p	The equivalent diameters of the permeate channel (m)
E	The specific energy consumption of high pressure pump of each module (kW h/m^3)
$E_{(Total)}$	Total energy consumption of the plant (kW h/m^3)
J_s	The solute molar flux through the membrane (kmol/m^2 s)
J_w	The permeate flux (m/s)
k	The mass transfer coefficient at the feed channel (m/s)
L	The length of the membrane (m)
m_f	Parameter in eqs. (10) and (11)
$P_{f\,(in)}$	The inlet feed pressure (atm)
$P_{f\,(out)}$	The outlet feed pressure (atm)
$P_{f\,(plant)}$	Plant feed pressure (atm)
P_p	The permeate channel pressure (atm)
Q_b	The bulk feed flow rate at the feed channel (m^3/s)
Q_f	The inlet feed flow rate at the feed channel (m^3/s)
$Q_{f\,(plant)}$	Plant feed flow rate (m^3/s)
Q_p	The permeate flow rate at the permeate channel (m^3/s)
Q_r	The retentate flow rate at the feed channel (m^3/s)
R	The gas low constant (R = 0.082 atm m^3/K kmol)
Re_b	The Reynold number at the feed channel (dimensionless)
Rec	Total permeate recovery (dimensionless)
$Rec_{(Total)}$	Total water recovery rate of the plant (dimensionless)
Rej	The solute rejection coefficient (dimensionless)
$Rej_{(Total)}$	Total chlorophenol rejection of the plant (dimensionless)
Re_p	The Reynold number at the permeate channel (dimensionless)
T	The feed temperature (°C)
$T_{(plant)}$	Plant feed temperature (°C)
t_f	Height of feed channel (m)
t_p	Height of permeate channel (m)
U_b	The bulk feed velocity at the feed channel (m/s)
W	The membrane width (m)

Subscript

μ_b	The feed viscosity at the feed channel (kg/m s)
μ_p	The permeate viscosity at the permeate channel (kg/m s)
ρ_b	The feed density at the feed channel (kg/m^3)
ρ_p	The permeate density at the permeate channel (kg/m^3)
ρ_w	Molal density of water (55.56 kmol/m^3)
θ	Parameter in Eq. (24)
ΔP_{drop}	The pressure drop per each element (atm)

chromium, and phosphate, from water with very high efficiency of around 99% [14–18]. The efficiency of the RO process for removing organic compounds from water is highly dependent on the nature of the compound and molecular weight, the operating conditions, the pH of the feed (which controls the extent of organic dissociation in the solution), the matrix of the membrane and the solute-membrane polymer interaction. All these parameters affect the sorption of organic compounds through the membrane body. More importantly, the laboratory investigation of [19] confirms that the efficiency of eliminating chlorophenol from water using a pilot-scale of an individual spiral wound RO process is around 83%, compared to 97% for dimethylphenol [20]. The 83% chlorophenol rejection rate is obtained using 13.58 atm, 2.583×10^{-4} m^3/s and 31 °C of operating feed pressure, flow rate and temperature respectively, with 22% total water recovery at an energy consumption of 2.034 kWh/m^3. The relatively low chlorophenol rejection rate is probably attributed to its high hydrophobicity properties in water (easily dissolved in water) in addition to its high activity due to the presence of hydroxyl group, which makes it easily penetrable through the membrane. Existing literature shows that the experimental study of Sundaramoorthy et al. [19] is the only study that deals with the removal of chlorophenol from water using the spiral wound module of RO process but with only one membrane RO module.

This paper explores the feasibility of an alternative RO process configuration of two-stage/two-pass RO process instead of a single stage considered by Sundaramoorthy et al. [19] for improving the current low chlorophenol rejection via simulation and optimisation. The work of Hafez and E1-Manharawy [21] motivated this work who used a full-scale plant using several technologies such as pH-adjustment, addition of the polymer coagulant, chlorination, dechlorination, filtration including RO membrane separation of two-stage/two-pass design of medium pressure RO membrane (maximum 16 bar) process to remove chromium from tannery effluent. The results showed that the plant can remove 99.9% of chromium based on the combined technologies used.

2. Multi-stage RO process model

The successful lumped and distributed modelling of an individual spiral wound RO process for the removal of phenol and its derivatives from water has been achieved by Srinivasan et al. [22], Sundaramoorthy et al. [19], Srinivasan et al. [23], Srinivasan et al. [20], Al-Obaidi and Mujtaba [24], Al-Obaidi et al. [25], Al-Obaidi et al. [26], Al-Obaidi et al. [27] and Al-Obaidi et al. [28]. Nevertheless, the efficiency of the two-stage/two-pass design of multi-stage RO system considering the chlorophenol removal from wastewater has not been investigated yet. Therefore, this research elucidates the capacity of this design with implementing simulation and optimisation studies to maximise the rejection parameter at an official total recovery rate of 40% and acceptable limit of energy consumption. Recently, Al-Obaidi et al. [29] developed a specific steady state model based on the solution-diffusion model, which showed an acceptable agreement with experimental data of dimethylphenol removal from water. This same model will be calibrated for use in the two-stage/two-pass multi-stage RO process for the removal of chlorophenol. All model equations are presented in Table A1 of Appendix A, while Tables A2 and A3 show the degree of freedom analysis of the model for the convenience of the readers. The intended outcome of this research is to achieve a better RO network for removing chlorophenol from water than those used in the past. gPROMS Model Builder 4.0 [30] is used in this work for simulation and optimisation.