Discrete Formulation for Multi-objective Optimal Design of Produced Water Treatment

Mariam Falahi, Vivek Dua, Eric S. Fraga

Sargent Centre for Process Systems Engineering, Department of Chemical Engineering, University College London (UCL), London, United Kingdom

e.fraga@ucl.ac.uk

Produced Water is naturally occurring water that is brought to the surface during the extraction of the oil and gas and it constitutes the largest waste stream in the oil and gas industry. In offshore platforms, the majority of the produced water is discharged into the ocean, threatening marine life. The treatment of produced water is attractive, not only to meet regulations but to secure a potential source of fresh water. The design of water treatment should consider economic, environmental, and social aspects.

This paper presents a discrete model for the evolution of oil droplet distribution due to breakage and coalescence phenomena. The discrete model combined with a superstructure representation for process design results in a mixed integer non-linear program which is solved using a nature-inspired meta-heuristic optimization method.

1. Introduction

Produced Water (PW) represents the largest waste stream associated with oil and gas production with a global estimated 3:1 volume to product ratio (Fakhru'l-Razi, Pendashteh, Abdullah, Biak, Madaeni, Abidin 2009). In 2022, the world generated more than 20 billion barrel of PW. The PW composition varies from one field to another. In general, it comprises of dissolved and dispersed oil compounds, dissolved formation minerals, production chemical compounds, production solids, and dissolved gases.

Currently, the majority of PW is treated in order to be discharged or re-injected. In offshore facilities, discharging is the most adopted practice. This option can result in polluting surface water in addition to creating a health hazard for both animals and plants (Jimenez , Mico , Arnaldos, Medina, Contreras 2018; Neff, Lee, DeBlois 2011). Treatment of the water to be discharged must be economical but also environmentally benign (Onishi, Ruiz-Femenia, Salcedo-Diaz, Carrero-Parreno, Reyes-Labarta, Caballero 2017) and socially acceptable. Therefore, there is a need to develop a methodology for designing a cost-efficient PW treatment system which addresses environmental impact simultaneously.

2. Produced water treatment

Produced water may be treated using physical, chemical, membrane and biological methods. The complex nature of PW and its varying composition makes it difficult to choose the most suitable treatment option that can meet the regulatory requirements for discharge, re-injection or reuse. Therefore PW is treated with multiple stages and multiple technologies as it is not possible for one technology to achieve the final destination requirements (Al-Ghouti, Al-Kaabi, Ashfaq, Da'na 2019). Typical technologies are listed here:

American Petroleum Institution Separator (API): The separation of the oil droplets is based on the rise rate or vertical velocity of the oil droplets to the separator surface due to the difference in density between phases according to Stokes's Law. Any oil droplets with rise rate greater than the surface loading rate, which is the flow rate divided by the separator surface area, will reach the surface of the separator within the processing residence time and will be removed. The API separator is a rectangular tank with two baffles to provide quiescent flow. The model of the API unit can be found in (Odiete and Agunwamba 2019; Api 1990).

Corrugated Plat Interceptors (CPI): CPI is an improvement of API separator with a smaller volume and higher efficiency and a set of plates added to the separation tank. The aim of the plates is to increase the coalescence between the oil droplets which increases their rise rate and hence the separation efficiency. (Api 1990; Pangestu, Zahra, Sarwono, Suryawan 2021; Okam 2008; Boraey 2018).

Hydrocyclone (HC): HC is a separation device that uses inertia to remove droplets and particles from liquids. The rotating body of the HC creates a spiral vortex. The droplets and particles gain inertia. The larger and denser droplets/particles have higher inertia and, therefore, they cannot follow the high-speed spiral motion of the water. They hit the internal wall of the HC body and move down to the collection point where they leave the stream. The smaller droplets/particles on the other hand, follow the vortex due to their smaller inertia and move upward in the same direction as the clean feed that leaves the device (Coker 2007).

Induced Gas Flotation (IGF): Similar to API and CPI, IGF separation is based on the difference in density between phases. In this process, the difference is increased by inducing gas bubbles to the unit. The bubbles attach to the oil droplets and solids. The new agglomerate has a lower density than oil and hence rise faster to the surface, where they are skimmed off (Selvam 2018).

PW treatment traditionally has four main stages: primary, secondary, polishing (optional) and tertiary treatment. The purpose of the primary treatment is to remove small oil droplets and suspended solids and is usually performed through API, parallel plate's interceptors or skim tanks. In the following stage, secondary treatment, technologies such as flotation, hydro-cyclone and centrifuge are used to remove smaller oil droplets and solids. In the polishing step, dispersed oil and ultra-small droplets and particles are removed. The tertiary step is used to remove dissolved solids and gas. Nevertheless, for purposes of conceptual design and to reduce a priori assumptions that restrict the design options, all units can be considered for each stage and the number of treatment steps is left open.

3. Droplets Size Distribution

Oil exists in water in form of droplets that range from 0.5 to 500 micron in diameter. The droplets size distribution (DSD) has a significant influence on the performance of the separation unit. A distribution is typically described by a continuous function. However, for design, we consider a discrete formulation based on a logarithmic based discretization of the space (droplet volume). The continuous distribution is mapped to discrete space by the number of droplets present for any volume class size.

The DSD does not remain constant during the treatment process due to breakage and coalescence phenomena. Coalescence is a favorable phenomenon as it improves the efficiency of the separation process. API and CPI units are designed to increase the coalescence frequency between the oil droplets as that results in larger oil droplets and hence a higher rise velocity. Coalescence takes place in laminar flow condition only. The coalescence frequency between the oil droplets is a function of the collision frequency $h(d_i, d_j)$ and coalescence efficiency $\lambda(d_i, d_j)$:

$$\Omega(d_i, d_j) = h(d_i, d_j)\,\lambda(d_i, d_j) \tag{1}$$

The frequency is calculated using the Prince and Blanch model (Prince and Blanch 1990) while the efficiency is modelled based on the film drainage theory: for the coalescence to take place, the contact time between two droplets is equal to or higher than the time needed for the film between the droplets to drain (Li and Huang 2017).Unlike coalescence, breakage makes the separation more difficult as it results in smaller oil droplets which affects the rise rate negatively, leading to the requirement of more processing to achieve the desired quality of the output. In a liquid-liquid dispersion, breakage takes place due to the different forces applied to the droplet. In turbulent flow, the stress from the continuous phase destroys the droplets while the surface stress of the droplets and the viscous stress of the fluid inside it retain its form. The breakage frequency of a droplet of volume v is calculated using

$$\Omega(v) = C_1 \frac{\varepsilon^{1/3}}{(1 + \alpha_d)\, d^{2/3}} \, exp\left[-\frac{C_2\sigma(1 + \alpha_d)^2}{\rho_d \varepsilon^{2/3} d^{5/3}} - \frac{C_3\mu_d(1 + \alpha_d)}{\rho_d \varepsilon^{1/3} d^{4/3}}\right] \tag{2}$$

The conservation of the total volume of droplets is modelled with discrete population balance equations. These equations capture the exchange of the volume between the discrete classes using birth and death rate equations, corresponding to the breakage and coalescence phenomena described above. Due to the discrete nature of the representation, the number of new droplets, n, of a given volume, v, are distributed to two neighbouring volume classes, v_i and v_{i+1}, where $v \in [v_i, v_{i+1}]$, to ensure that the total volume overall remains constant:

$$n_i + n_{i+1} = n \tag{4}$$

where i is the class of drops with volume v_i and number n_i. This mapping to discrete space applies to new droplets generated by either coalescence or breakage. It is assumed that droplets in the largest volume class, $i = n_{\text{class}}$, do not coalesce and there is no breakage for droplets in the smallest class size, $i = 1$.

The evolution of the DSD over time is modelled using ordinary differential equations for each technology listed in the previous section. Each processing step is simulated for the residence time of each processing unit. The residence time is a function of units' design variables.

4. Case study

Produced water from an offshore facility of an oil and gas industry is treated in order to meet discharge requirements. The main contaminants to be removed from the feed stream are oil and grease (O&G) and total suspended solids (TSS). The initial concentrations of these contaminants and their desired values are shown in Table (1).

Table 1: Target contaminations and their desired values

Contamination	Initial Value (mg L^{-1})	Desired Value (mg L^{-1})
O&G	1500-2200	40
TSS	189	30

The aim of the design problem is to determine the sequence of treatment technologies along with the values of the design variables for each technology. The superstructure allows for up to 4 stages of processing. The objectivess are to minimize both the total system cost and the environmental impact. The total cost consists of the capital cost, cost of building and constructing the system, annualised assuming a plant life of 1 year (which can be changed), and the annual operating cost including the cost of chemicals, energy, and sludge handling (Bagheri, Roshandel, Shayegan 2018). The environmental impact is represented by an estimate of the total CO_2 emission due to energy consumption. Other criteria could be used.

The inlet DSD of O&G and TSS follows a normal distribution and is represented by the discrete mapping shown in Table (2) using 10 discrete classes for illustration. The values of log_{Vmin} and log_{Vmax} are chosen to be 11 and 16 respectively which result in droplets/particles diameters ranging from 5.7 to 267.3 μm for O&G and TSS.

Table 2: The initial droplets/particles size distribution of O&G and TSS in the PW inflow using 10 discrete volume classes

I	1	2	3	4	5	6	7	8	9	10
DSD	0.05	0.08	0.11	0.14	0.17	0.14	0.11	0.08	0.05	0.02

The resulting optimization problem was solved using a nature inspired meta-heuristic optimization procedure based on plant propagation (Salhi and Fraga 2011) with an implementation in Julia (Fraga 2021) and which has been previously used to solve dynamic optimization problems (Fraga 2019).

5. Results and discussion

Two non-dominated solutions are identified for the multi-objective design problem. Both solutions represent the same configuration but with different values of the design variables. The first solution costs 2,827,023 USD y^{-1} and its annual CO_2 emission is 718,993 kg CO_2e. The second solution reduced the emission by 159,486 kg CO_2e but increased the annual cost by 46,455 USD y^{-1}.

The optimal configuration of the system is the CPI as a primary treatment followed by HC and then IGF. API is not chosen since CPI is found to be better. CPI has a higher total separation surface compared to API for the same footprint. In both configurations, CPI was chosen as a primary unit to satisfy the inlet constraints of the secondary stage. IGF needs to have a pre-treatment as it cannot handle an inlet oil concentration of more than 1000 mg L^{-1}. Similarly, HC is not able to process an inlet with oil droplets larger than 200 μm.

The values of $D_{O\&G}^{CPI}$ and h^{CPI} determined by the optimization are close to their lower bounds, 40 μm and 0.012 m respectively. This value of the cut diameter allows the removal of approximately 65% of the oil and solid volumes at the first stage while the small distance between the plates in the CPI separator increases the coalescence between the droplets and hence improves their removal efficiency. The two solutions differ in the values of $D_{O\&G}^{CPI}$, 40 versus 40.3, h^{CPI}, 0.0127 versus 0.0129, and in the width of the plates, 6 m versus 5.4 m.
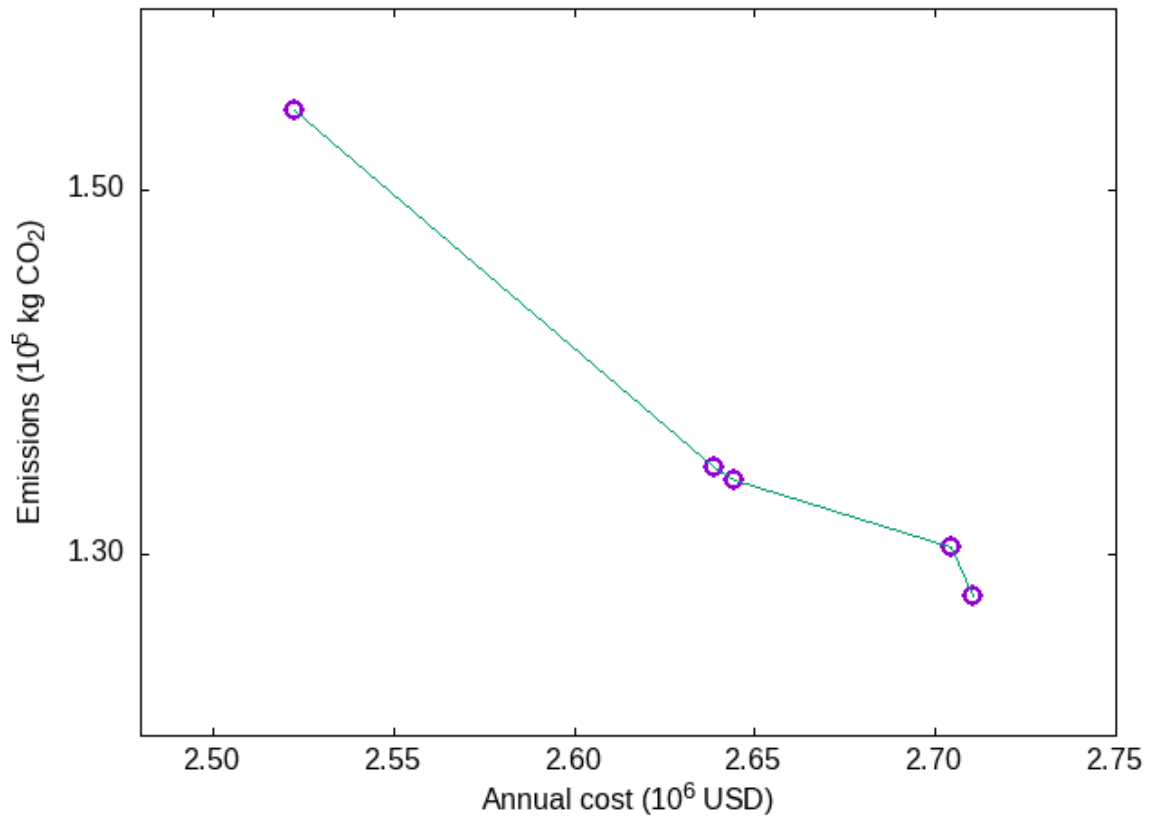
Figure 1 Pareto front of the PW treatment system annual cost and CO2 emission obtained by solving the multi-objective optimization problem for 25 classes

In the HC model, a higher number of parallel hydrocyclones with smaller diameters (0.4m) were chosen as the smaller diameter cyclone has a higher separation ability than the larger ones.

The impact of the DSD on the process design was tested by varying the number of classes from 5 to 25. The problem with 5 class sizes resulted in a process design with two units only, CPI and IGF. This is because in case of 5 classes, the volume is distributed among fewer classes and hence the removal accuracy is compromised. In all other cases, using a finer discretization of the volume, 3 stages were required to meet the process specifications. As the number of classes increases, the oil and solid volumes are distributed more accurately among the classes and hence the separation efficiency is more sensitive to the cut diameter of the processing units. For 15-25 class sizes, two different configurations are identified: CPI → HC → IGF and CPI → IGF → HC. The computational effort grows as the square of the number of classes, requiring 24 minutes to solve the problem with 25 classes on an 8 core computer system.

Figure 1 shows the Pareto front obtained by solving the multi-objective problem for 25 classes. Using 25 classes resulted in two different configurations compared with just one obtained with 10 classes. The objective function values are lower for all solutions in the 25 classes. The cost of the most environmentally friendly solutions in case of the 25 classes is lower than that of the 10 classes by 6% (2,710,370 vs 2,873,479) while the emission is lower by 77% (127,655 vs 559,508). The significant change in the emission is due to the reduction of the IGF unit height from 5.7 to 0.5 m. The highest point to the left of the graph is the most cost effective solution with 2,522,537 USD y^{-1} and 154,444 kg CO_2e. The difference in the number of parallel hydrocyclones and their diameters and the height of the IGF are the main contributor to the cost and emission reductions in comparison. The values of the design variables of the main case (10 classes), shown in Table 3, are 8, 0.49 m and 7.4 m compared to 1, 0.9 m and 0.5 m in 25 classes.

Table 3 The optimal values of the units' design variables obtained from solving the multi-objectives optimization problem for 25 classes

Annual Cost ($USD y^{-1}$.)	CO_2 Emission ($kgCO_2e$)	Sequence	CPI				HC		IGF			
			D_{OnG}^{CPI}	L^{CPI}	w^{CPI}	h^{CPI}	n^{HC}	d^{HC}	n^{IGF}	r^{IGF}	h^{IGF}	Qg
			μm	m	m	m		m		m	m	$m^3 s^{-1}$
2,644,501	134,087	CPI, IGF, HC	45.7	3.5	1.9	0.015	7	0.51	4	1.7	0.5	0.00002
2,522,537	154,444	CPI, IGF, HC	49.3	4.3	5.1	0.012	1	0.90	2	1.5	0.5	0.00004
2,710,370	127,655	CPI, HC, IGF	49.5	3.6	2.6	0.012	11	0.45	4	1.5	0.5	0.00002
2,638,694	134,805	CPI, IGF, HC	46.0	3.5	2.0	0.015	7	0.51	4	1.7	0.5	0.00002
2,704,604	130,397	CPI, IGF, HC	45.9	3.6	2.6	0.0129	11	0.45	4	1.5	0.5	0.00002

6. Conclusion

The design of the process for produced water treatment has been formulated as a discrete nonlinear dynamic multi-objective optimization problem. This enables us to investigate the trade-off between economic and environmental criteria, specifically the total cost and CO_2 emissions. The discrete dynamic model has been solved for different class sizes, demonstrating that the discretization has an impact on the types of solutions obtained along with the values of the two objective functions.

The case study presented considers a droplet size distribution where all the drops are larger than 5 μm. However, in some cases, the smallest droplets may be as small as 0.5 μm. To address design problems considering droplets in this range of size will require using technologies with higher separation efficiencies, such as membranes, nutshell filters and centrifuge separators. The development and implementation of models for these technologies is now being considered and will be incorporated into the superstructure to enable solving a broader range of problems for produced water treatment. Furthermore, incorporating such units into the superstructure optimization procedure will enable the design of systems capable of meeting the requirements of other PW destinations such as re-injection and beneficial reuse.

Nomenclature

n	Number of droplets/particles	μ_d	viscosity of the dispersed phase, $kg\ m^{-1}s^{-1}$
d	Diameter of droplets/particles, μm	D_{OnG}^{CPI}	cut diameter of CPI for O&G droplets, μm
h	collision frequency	L^{CPI}	length of the CPI plate, m
λ	coalescence efficiency	w^{CPI}	width of the CPI plate, m
Ω_C	coalescence frequency between droplets/particles	h^{CPI}	distance between CPI plates, m
Ω_B	coalescence frequency	n^{HC}	number of the parallel Hydrocyclone
$C_{1,2,3}$	constants	d^{HC}	body diameter of the Hydrocyclone, m
ε	energy dissipation rate, $m^2 s^{-3}$	n^{IGF}	number of IGF cells
α_d	volume fraction of the dispersed phase	r^{IGF}	radius of IGF cells, m
σ	interfacial tension between oil and water, $kg\ s^{-2}$	h^{IGF}	high of IGF cells, m
ρ_d	density of oil, $kg\ m^{-3}$	Qg	gas flowrate into IGF cells, $m^3 s^{-1}$

References

Al-Ghouti M., Al-Kaabi M., Ashfaq M., Da'na D., 2019, Produced Water Characteristics, Treatment and Reuse: A Review, Journal of Water Process Engineering, 28, 222–39.

API, 1990, Monographs on Refinery Environmental Control-Management of Water Discharges. Design and Operation of Oil-Water Separators. American Petroleum Institute Publication, Publication 421.

Bagheri M., Roshandel R., Shayegan J., 2018, Optimal Selection of an Integrated Produced Water Treatment System in the Upstream of Oil Industry, Process Safety and Environmental Protection, 117, 67–81.

Boraey M., 2018, A Hydro-Kinematic Approach for the Design of Compact Corrugated Plate Interceptors for the de-Oiling of Produced Water, Chemical Engineering and Processing-Process Intensification, 130, 127–33.

Coker K., 2007, Ludwig's Applied Process Design for Chemical and Petrochemical Plants, Gulf Professional, 1.

Fakhru'l-Razi A., Pendashteh A., Abdullah L., Biak D., Madaeni S., Abidin Z., 2009, Review of Technologies for Oil and Gas Produced Water Treatment, Journal of Hazardous Materials, 170 (2), 530–51.

Fraga E.S., 2021, ericsfraga/Fresa.jl: First Public Release (R2021.06.30), Zenodo. Doi:10.5281/zenodo.5045812.

Fraga E.S., 2019, An example of multi-objective optimization for dynamic processes, Chemical Engineering Transactions, 74, 601-606.

Jimenez S., Mico M., Arnaldos M., Medina F., Contreras S., 2018, State of the Art of Produced Water Treatment, Chemosphere, 192, 186–208.

Li C., Huang Q., 2017, Analysis of Droplet Behavior in a de-Oiling Hydrocyclone. Journal of Dispersion Science and Technology, 38 (3), 317–27.

Neff J., Lee K., DeBlois E., 2011, Produced Water: Overview of Composition, Fates, and Effects, In Produced Water, Produced water: Environmental risks and advances in mitigation technologies, 3-54.

Odiete W., Agunwamba J., 2019, Novel Design Methods for Conventional Oil-Water Separators, Heliyon 5 (5): e01620.

Okam C., 2008, Investigation of Oily Wastewater Treatment Processes, Swansea University (United Kingdom).

Onishi V., Ruiz-Femenia R., Salcedo-Diaz R., Carrero-Parreno A., Reyes-Labarta J., Caballero J., 2017, Multi-Objective Optimization of Renewable Energy-Driven Desalination Systems, In Computer Aided Chemical Engineering, 40, 499–504. Elsevier.

Pangestu N., Zahra N., Sarwono A., Suryawan I., 2021, Produced Water Treatment Planning Using Corrugated Plate Interceptor and Ultra Filtration for Water Recycling, Jurnal Serambi Engineering 6 (4).

Selvam A., 2018, Removal of Dispersed Oil Drops by Induced Gas Flotation, Master's thesis, Norwegian University of Science and Technology.

Prince M., Blanch H., 1990, Bubble Coalescence and Break-up in Air-Sparged Bubble Columns, AIChE Journal 36 (10), 1485–99.

Salhi A., Fraga E.S., 2011, Nature-Inspired Optimisation Approaches and the New Plant Propagation Algorithm, 2011, the International Conference on Numerical Analysis and Optimization, K2,1–8.