Productivity Prediction of Sea Water Reverse Osmosis Desalination Plant Using Robust Regression

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Abstract

Multiple Linear Regression (MLR) is utilized to correlate the process parameters to the output permeate flow rate for a Seawater Reverse Osmosis (SWRO) desalination plant. Thorough residual analysis robust regression provided alternative methods to predict the response with higher accuracy compared to basic MLR analysis. Robust regression methods are developed in this study to predict the productivity of a seawater reverse osmosis plant based on key empirical correlations. The robust regression methodology considers important input operating parameters such as feed flow rate, feed pressure, outlet pressure of the multi-media filter, inlet and outlet cartridge filter pressures, outlet pressure of the high-pressure pump, and inlet seawater flow rate to pressure exchanger and correlates them to the permeate flow rate. The robust regression models are capable of accurately predicting response for any input operating parameters for the reverse osmosis plant. The regression models demonstrated strong statistical goodness-of-fit measures using Huber's method in terms of three-way interactions with a high R^2 of approximately 0.99 and a mean absolute percentage error of 2.4%. Furthermore, the robust regression results have been validated experimentally and the results showed very good agreement with measured values, with an error of approximately 0.8%.

Keywords
Desalination, Reverse Osmosis, Robust Regression, and Statistical Modeling.

1. Introduction
Drought is one of the "most dangerous" far-reaching of all-natural disasters on earth, according to the United Nations (UN, 2018) (Haile et al. 2020). Water scarcities have emerged as a result of population growth, rising living standards, and rapid development while more than 97% of the earth's water cannot be used for direct human consumption (e.g., drinking water) due to its high salinity (Bashitialshaaer 2020). According to the World Bank's data on renewable, internal freshwater resources per capita have decreased by half in the last 50 years, from 12,000 m^3 in 1967 to 5732 m^3 in 2017. Furthermore, there are more than 2.8 billion people which representing more than 40% of the world's population, living within 100 kilometers of the coast, and therefore, desalination is often used to solve freshwater scarcity in several parts of the world (Zapata-Sierra et al. 2022). Seawater desalination is an innovative technology that can provide sustainable solutions to water crises leading to rapidly increasing global desalination capacity, from 8000 m^3/day in 1970 to about 92.2 million m^3/day in 2020 (Bashitialshaaer 2020). More than 300 million people rely on water produced by 18,426 desalination plants in 150 countries, which provide more than 86.8 million m^3/day, according to the International Desalination Association (IDA) 2015 (Baawain et al. 2015). Egypt's water gaps are rapidly expanding due to rapid population growth and limited water resources where the total renewable water resources per capita are 584.2 m^3 /year with a 98.26 % water dependency ratio, according to (AQUASTAT*, 2018). In addition to the increasing need for water among the upper Nile Basin countries may result in a water shortage, as the Grand Ethiopian Renaissance Dam (GERD) represents a real threat to Egypt's share of the river's water (Abd Ellah 2020). An amount of 27.91 Billion Cubic Meters (BCM) of Egypt's water resources is expected to be lost as a result of the GERD (El-Nashar et al. 2018). According to the National Water-Food (NWF)

*AQUASTAT is the FAO global information system on water resources and agricultural water management.

Model, Egypt's desalination water resources in 2013 were 0.23 BCM per year. Egypt is increasingly investing in seawater desalination projects, which will potentially increase the country's water resources and minimize the negative impact of the GRED (Abdelkader et al. 2018).
The aim of this study is to compare the effectiveness of different regression methods and to develop a robust regression model that can predict accurately the permeate flow rate of the SWRO desalination plant under varying operating conditions. The structure of this paper is as follows: the literature review outlines the background of the desalination process, as well as statistical and empirical modelling in the SWRO system. Section 3 demonstrates the data collection and processing and regression methods used in this case study. The results of the regression models and validation are shown in section 4 after that. Finally, we conclude section 5.

2. Literature Review

2.1. Desalination Process

Desalination is the process of removing salts from brackish or seawater to produce fresh water. There are several methods to desalinate water which can be classified into three basic categories: evaporation-condensation, filtration, and crystallization, as represented in Figure 1. Evaporation-condensation is the traditional method of desalination where thermal involves vaporization, cooling condensation of saline water, leaving behind highly concentrated saline water (brine). Membrane-based technologies are the most common techniques of filtration methods which depend on the passage of water through a semipermeable membrane under pressure (Yadav et al. 2021). Whereas, crystallization is a solid-liquid phase separation technology that involves the formation of crystalline solid from a supersaturated solution (Yadav et al. 2022). Currently, there are two technologies with more desalination capacity in the world, multi-stage flash distillation and reverse osmosis (Alkaisi et al. 2017).

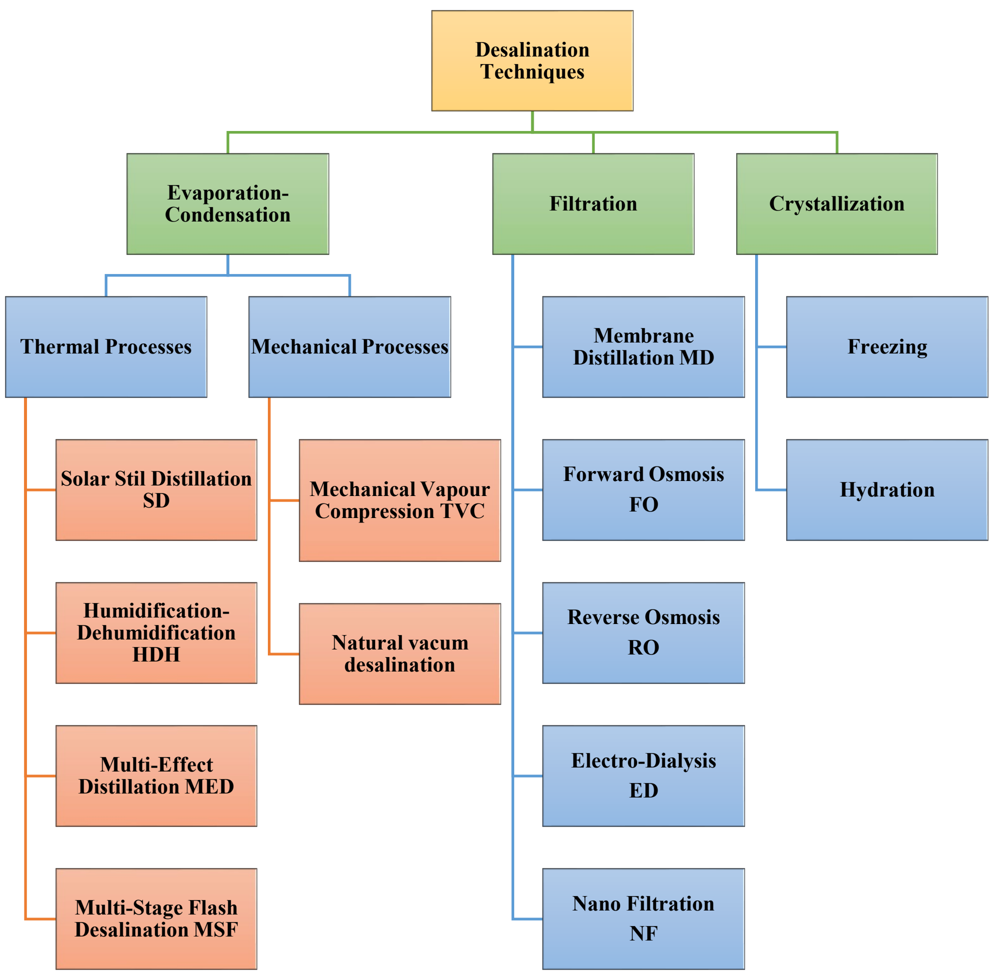


Figure 1. Classification of various desalination processes (Alkaisi et al. 2017)

2.2. Reverse Osmosis (RO) Technology

There is no doubt that reverse osmosis (RO) is an emerging technology in the water desalination field as it is easily adaptable to local conditions, plant size can be adjusted to meet short-term increases in demand and expanded incrementally as needed, and they have a significant cost advantage over treating brackish groundwater. The RO technology currently accounted for a major share of desalinated water production, with a capacity of more than 62% of the world's water production which is illustrated in Figure 2 (Alkaisi et al. 2017). Furthermore, the capital cost is approximately 25% less than that of thermal alternatives. The installed capacity of desalination plants using seawater as feed increased by 813 percent globally over the last three decades (from 1990 to 2019) (Eke et al. 2020).

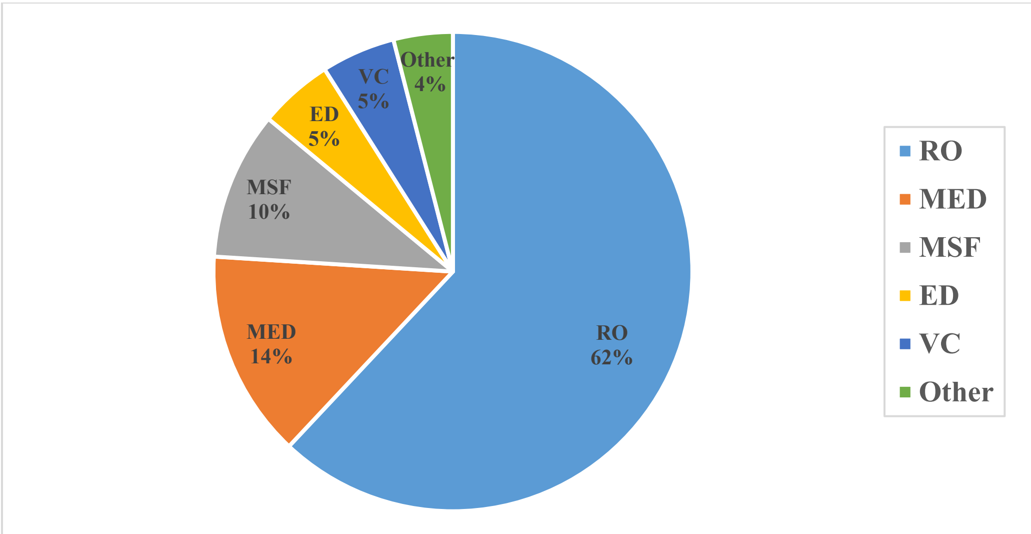


Figure 2. Contribution of desalination processes to world water production (Alkaisi et al. 2017)

Membrane-based desalination has been acknowledged as one of the promising approaches to resolving the water scarcities global challenges (Goh et al. 2018). Membranes for RO desalination come in multiple different modules: plate and frame, tubular, spiral wound, and hollow fiber (Qasim et al. 2019). Figure 3 shows the commonly employed membrane types in desalination technologies over the last 40 years. The spiral wound membrane type has been used to achieve 87% of global desalination capacity (Eke et al. 2020).

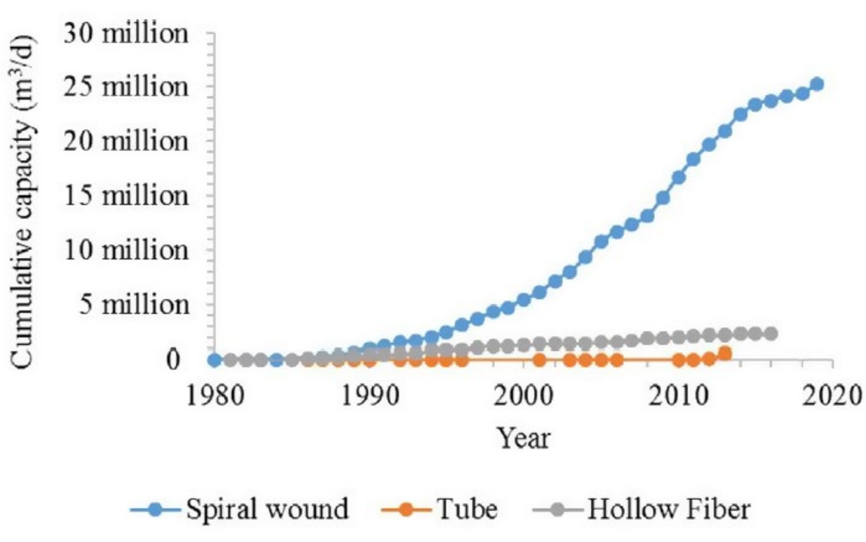


Figure 3. Membrane types are employed in desalination plants and their contributions (Eke et al. 2020)

2.3. Statistical and Empirical Modeling in Sea Water Reverse Osmosis (SWRO) Plants

2.3.1. Statistical Modeling

In order to investigate how operational parameters affect the response of the reverse osmosis membrane separation process, researchers usually use statistical approaches such as regression analysis and analysis of variance (ANOVA). Multiple regression analysis is used to predict the effect of changing different input parameters on the performance of SWRO such as the work of (Stillwell et al. 2016) who used a multiple linear regression model to predict the Specific Energy Consumption (SEC) of desalination and claimed that approximately 85 % of the variation in SEC can be explained by the inputs defined in their model. Also, SEC has been minimized using a regression-based predictive model; however, the effect of other input variables such as control of feed pressure and opening of reject valve was introduced which resulted in an improvement of the efficiency of the SWRO desalination process in terms of energy and cost (Joseph et al. 2021). Additionally, Avlonitis et al. (2012) developed an experimental study of the SEC and employed empirical fit of the data to select economic optimum operating points for pressure and recovery. Other researchers focused on different responses such as the assessment of SWRO critical flux (Jang et al. 2021). In other instances, regression was reported in the literature for purposes of validating the results of other models, such as comparing resulting correlations of regression analysis to Reverse Osmosis System Analysis (ROSA) such as the work of (M. Alahmad 2010) and (Jeong et al. 2019); furthermore, Joseph et al. (2019) developed a dynamic simulation of the RO desalination process and validated its results by comparing real data from an industrial seawater desalination process to the dynamic conditions predicted by the model based on R^2 analysis.

2.3.2. ANOVA and MNAOVA Methods

Analysis of variance (ANOVA) and Multivariate ANOVA are used to understand the effect of the interaction of the parameters on the output and also to investigate the most significant influencing factors on the response. Selvi et al. (2015) performed multiple regression modeling by correlating input operating parameters on the response water recovery ratio while ANOVA estimates were used to validate the model to be highly significant, as evidenced by R^2 analysis. ANOVA was also used to identify the significant factors that affect Computational Fluid Dynamics (CFD) in the desalination process (Venkatesan et al. 2015). Moreover, Maalouf et al. (2014) used a regression model for a simulation-optimization approach to design a system for the safe disposal of brine wastes, while a regression model was developed to relate the input and output parameters of the simulation model with a high coefficient of determination R^2 and ANOVA to validate the model results. Similarly, Kolluri et al. (2015) used Multivariate ANOVA to evaluate the performance and efficiencies of the pretreatment processes. Also, Subramani et al. (2014) applied a statistical analysis based on stream characteristic data (flow rate, concentration, and pH) over time while the significance of regression was evaluated based on Multivariate ANOVA and found that the permeate characteristics are dependent on feed stream flow rate.

2.3.3. Review Outcome

Multiple linear regression (MLR) is a widely used statistical analysis method to correlate input process parameters to required responses. This method yields an empirical correlation that can be utilized to predict the response for any input parameter values. Regression analysis provides appropriate solutions for quantitative comparisons between different model outcomes in terms of how much variance or goodness of fit R^2. In addition, Regression is also used to validate model outcomes by R^2 analysis. While ANOVA is used to assess the significance of regression models and the influence of parameters and their interactions on the output response.

3. Data Collection and Methods Applied

3.1. Plant Description

The Rumaila desalination site, situated in Marsa Matrouh Egypt, is designed with a capacity of 48,000 m^3/day. It consists of two plants. Each plant consists of six units which are designed according to the standard design of the large-scale SWRO process shown in Figure 4., The figure shows a seawater intake, pre-treatment, RO system, and post-treatment.

The desalination units produce water using the RO technique with a recovery ratio of 40%, with of seawater inlet capacity of 625 m^3/hr to produce 250 m^3/hr of permeate water, and 375 m^3/hr of rejected water being treated and discharged to the sea. A pressure exchanger (PX-Q300) is used as an energy recovery device (ERD).

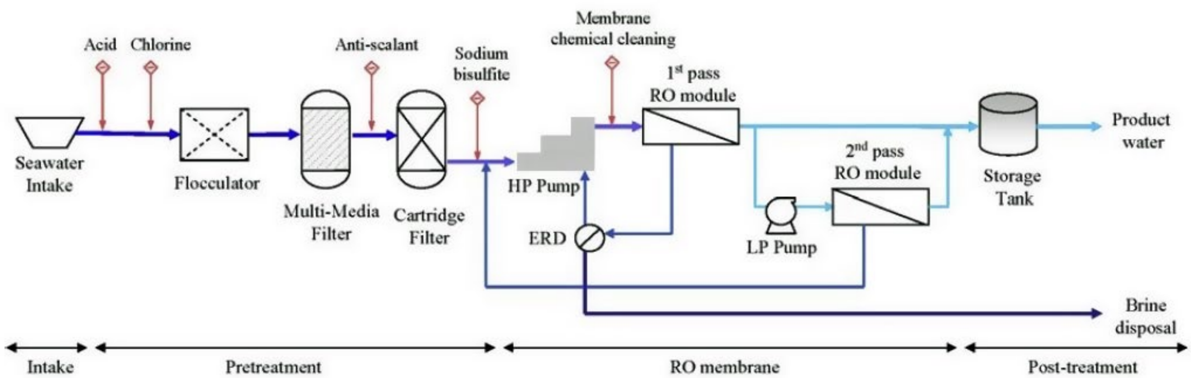


Figure 4. Schematic diagram of a typical SWRO desalination process (Kim et al. 2009)

3.2. Data Manipulation and Processing

For the first unit of the Rumaila 1 plant, designated as R1RO1, data collection and processing were done over four years, from 2017 to 2020 where all sensor values are saved hourly, and sensors are calibrated according to a regular maintenance plan. The data was collected from the sensors using a supervisory control and data acquisition (SCADA) system. The SCADA system's files were extracted and analyzed to determine the values of each sensor separately. The data were filtered based on operational experience and standard operating ranges. The data was analyzed based on the high-pressure and feed pumps capabilities. The outliers of operating ranges were removed since they lead to higher error when applying the regression analysis.

3.3. Methods

The most widely used statistical technique for estimating the relationships between independent variables and a dependent response variable (Y) is multiple regression analysis. The least-square errors are frequently used in multiple regression techniques. However, the least-squares regression can perform poorly when the data set involves outliers (Balding et al. 2006). One approach to overcome this problem is to remove the influential observations from the least-square fit (Hesamian et al. 2021). However, accurate residual analysis is time-consuming and requires extensive training. Robust regression provides an alternative to least squares regression that seeks to reduce the influence of observations that are apparently outliers and provides much better regression coefficient estimates (Jerry L. Hintze 2007). M-estimation is the most common general robust regression method (Huber 1981). NCSS[†] has been used to develop multiple regression analyses for the desalination unit using different regression methods to correlate operating parameters. Multiple regression analysis has been implemented to input independent variables (X's) namely; feed flow rate, feed pressure, outlet pressure of the multi-media filter, inlet and outlet cartridge filter pressures, outlet pressure of the high-pressure pump, and inlet seawater flow rate to pressure exchanger. The permeate flow rate (Y) is the dependent response variable also known as a predicted variable. Huber's method reduces the weight of observations with large residuals while Tukey's Biweight method completely down weights the observations with large outliers until their weight is set to zero. Both of the methods are based on M-Estimators and use iteratively reweighted least squares (Jerry L. Hintze 2007). The interactions of X's are used to generate more independent variables which are used to analyze the influence of these independent variables and generate strong correlations to the response. In the present study, the robust regression models were developed using two different levels of X's interactions. The first one is up to 2-way in terms of individual variables, two-way interactions, and squared numeric variables. The second one is up to 3-way. where all individual variables, two-way interactions, three-way interactions, squared numeric variables and cubed numeric variables are included in the model.

[†]NCSS.2021 v21.0.3 is a robust statistical and graphics program developed by NCSS, LLC for researchers, businesses, and academic institutions.

4. Results and Discussion

MLR analysis generates Y predictions based on a simple regression equation without interaction where the R^2 coefficient increased from 0.63 to 0.84 as a result of the data preprocessing.
Four different robust regression models have been applied to the same X's using Huber's and Tukey's Biweight method each in terms of two- and three-ways interactions.

4.1. Actual Versus Predicted Observations Developed by Regression Models

The actual and predicted values of the dependent response variable have been presented in a scatter plot which is considered as one of the most effective data visualization graphs that indicates the model effectiveness. The actual vs. predicted observation generated from multiple linear regression is shown in Figure 5. Figure 6 shows the actual versus predicted observation generated from the robust regression model developed by Huber's method in terms of 3-way interaction. For a strong fit, the points should be closer to the trend line, with narrow confidence bands. When comparing figures 5 and 6, it can be clearly seen that Figure 6 shows less scatter and points are closer to the trend line and have fewer outliers, with much higher R^2.

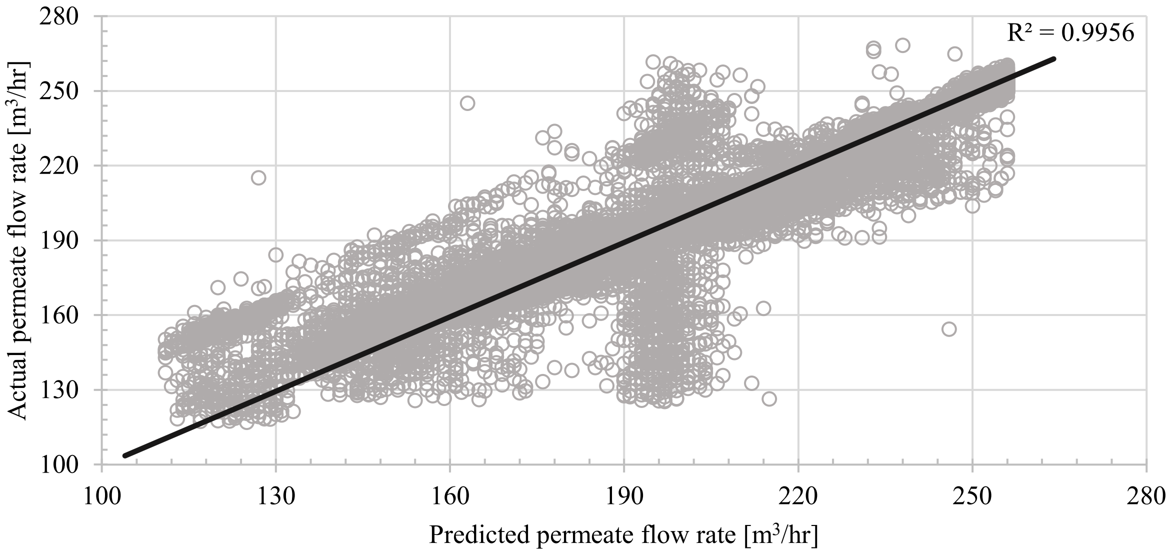


Figure 5. Multiple linear regression analysis predicted versus actual permeate flowrate [m^3/hr]

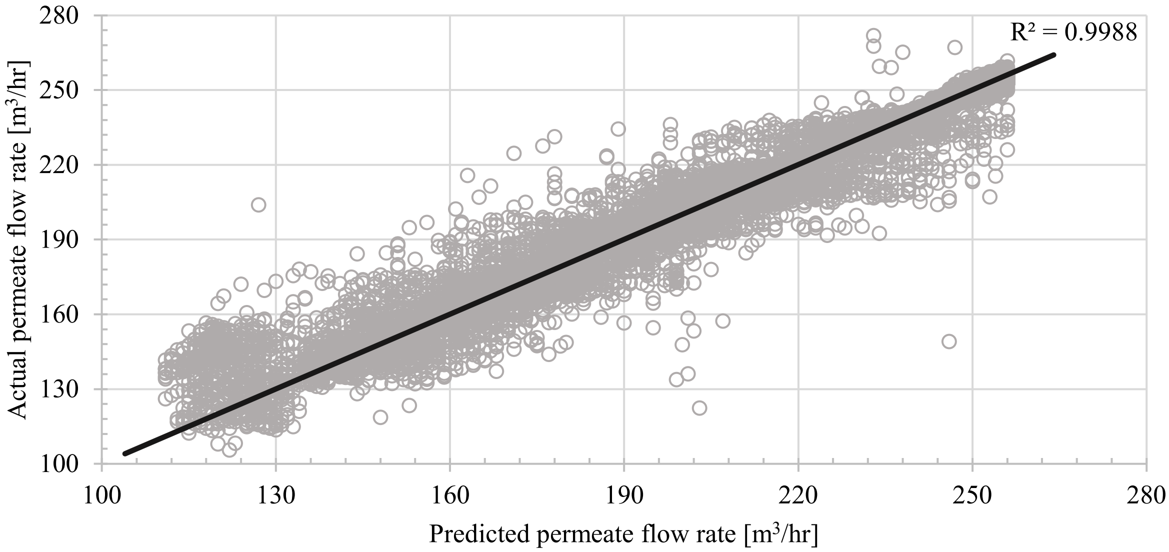
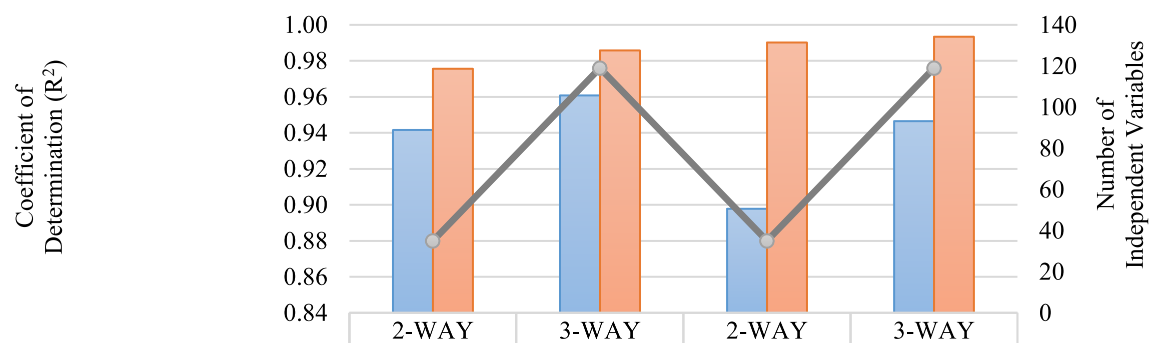


Figure 6. Huber's robust regression predicted versus actual permeate flowrate [m^3/hr]

4.2. Performance of Robust Regression Models

The coefficient of determination R^2 is one of the important performance measures which shows the proportion of variation in the dependent variable that can be predicted by the independent variables. Robust regression analysis generates robust weights for each observation ranging from zero to one, whereas the higher bias observations contribute with a low weight to minimize their contributions to the determination of the regression coefficients. the robust regression analysis can develop higher R^2 when increasing the terms of interaction as shown in Figure 7. Moreover; the adjusted R^2 values equal R^2 which indicates the corrected goodness-of-fit.



	2-WAY	3-WAY	2-WAY	3-WAY
	Huber's Method		Tukey's Biweight Method	
R^2	0.94	0.96	0.90	0.95
R^2 after Robust Weighting	0.976	0.986	0.990	0.993
Number of Ind. Variables	35	119	35	119

Robust Regression Methods

Figure 7. Coefficient of determination of robust models and the interaction levels

Well-known model performance metrics including Mean Absolute Error, (MAE) estimated using equation (1), Root Mean Squared Error, (RMSE), estimated using equation (2), and Mean Absolute Percentage Error, (MAPE) estimated using equation (3) has been shown in Figure 8.

Figure 8. Comparative error analysis for different regression models

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|Ai - Fi| \tag{1}$$

$$RMSE = \sqrt{\frac{(Ai - Fi)^2}{n}} \tag{2}$$

$$MAPE = \frac{1}{n}\sum_{i=1}^{n}\frac{|Ai - Fi|}{Ai} * 100\% \tag{3}$$

Where; A_i: actual observations, F_i: Predicted observations, and n: number of observations.

4.3. Model Validation

4.3.1. ANOVA Analysis

The ANOVA analysis reports of robust methods up to 3-way terms are demonstrated in Table 1. The ANOVA results show a low relative error for both methods, with 0.986 and 0.993 R^2 after robust weighting for Huber's and Tukey's Biweight methods, respectively, and both using (up to 3-way) interactions terms.

Table 1. Analysis of variance report developed by NCSS

Robust Regression Method	Source	Degrees of Freedom (DF)	R^2	Sum Squares (SS)	Mean Square (MS)	F-Ratio
Huber's	Intercept	1	6.94E+08	6.94E+08		
	Model	119	0.9858	1.99E+07	166937	11141.3
	Error	19157	0.0142	287040.4	14.98358	
	Total (Adjusted)	19276	1	2.02E+07	1045.473	

Tukey's Biweight	Intercept	1	6.55E+08	6.55E+08		
	Model	119	0.9934	1.78E+07	149479	24331.1
	Error	19157	0.0066	117691.6	6.143529	
	Total (Adjusted)	19276	1	1.79E+07	928.9112	

In the ANOVA Table Source stands for the source of variation while the variance estimates are computed using sums of squares. Two mean squares are formed, one for model and the other for error, using the Sum of squares previously computed after robust weighting for the ANOVA. The F-Ratio was used in testing the equality of the model and estimated using equation (9).

The *Degrees of Freedom (DF)* are estimated using:

$$N = \sum n_i \tag{4}$$

$$DF_M = K - 1 \tag{5}$$

$$DF_E = N - k \tag{6}$$

Where the subscript *M* refers to model, *E* refers to error, *K*: the number of independent variables, and *N*: number of observations.
The *mean squares* are estimated using:

$$MS_M = \frac{SS_M}{DF_M} \tag{7}$$

$$MS_E = \frac{SS_E}{DF_E} \tag{8}$$

The *F-Ratio* is estimated using:

$$F - Ratio = \frac{MS_M}{MS_E} \tag{9}$$

The ANOVA analysis shows that Tukey's Biweight method has lower values in F-Ratio and Sum of Squares Error (SS_E).

4.3.2. Experimental Validation

Huber's method in terms of three-way interaction was validated experimentally demonstrated in Table 2 by collecting plant sensor measurements and substituted in the robust equation to estimate the permeate flow rate. When comparing real to robust results, a low error of 0.8 % was found, proving its validity.

Table 2. Experimental validation of Huber's robust regression method

Method	X_1	X_2	X_3	X_4	X_5	X_6	X_7	Y	Predicted Response	Absolute Bias	Error%
Huber's	4.1	3.1	2.8	2.4	62.2	493	348	145	143.8	1.2	0.8
Tukey's Biweight	4.1	3.1	2.8	2.4	62.2	493	348	145	163.2	18.2	12.5

Where independent variables refer to numeric x's as follows feed pressure (X_1), outlet pressure of the multi-media filter (X_2), inlet pressure of the cartridge filter (X_3), outlet pressure of the cartridge filter (X_4), outlet pressure of the high-pressure pump (X_5), feedwater flowrate (X_6), inlet seawater flow rate to pressure exchanger (X_7), and the permeate flow rate is the dependent response variable refers as (Y).
While Tukey's Biweight method has higher R^2 and F-Ratio in ANOVA, Huber's method develops higher accuracy in experimental validation because robust weighting as Huber's method considers down weights of residual analysis while Tukey's Biweight method considers zero weighting for outliers, evidenced by the comparative error analysis shown in Figure 8.

5. Conclusions

Robust regression provides an alternative approach to basic multiple linear regression that works through a robust residual analysis to minimize the influence of outliers. In addition, more independent variables are generated as a result of the interactions of the input variables, which are analyzed to generate strong statistical correlations using robust methods. Four different robust regression models have been developed using Huber's and Tukey's Biweight methods. Their performance was evaluated in terms of R^2, mean square error, root mean square error, and mean absolute percentage error.

From the statistical analysis carried out in this study, the following could be concluded:
1. Multiple linear regression performs poorly without input data preprocessing.
2. Three-ways interactions have a higher accuracy performance, as expected.
3. In terms of up to three-way interactions, Tukey's Biweight method provides the highest R^2 after robust weighting.
4. Huber's method correlations have higher accuracy which generates correlations that describe the real physical behavior of the system. This was confirmed by experimental validation even though Tukey's Biweight develops a higher F-Ratio in ANOVA.
5. Huber's method provides higher performance in terms of error metrics and the Huber's robust equation has been experimentally validated yielding a very low relative error.
6. The data preprocessing and robust regression improved the fitting R^2 coefficient from 0.63 (before preprocessing) to approximately 0.99 with an improvement of approximately 57%.

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Biographies

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Yehia M. Youssef is a Professor of Material Engineering at the Department of Chemical and Petrochemical Engineering at the AASTMT. He graduated from Alexandria University- Faculty of Engineering, Chemical Engineering Department in 1992. He obtained his Ph.D. degree in Materials Science and Engineering from the Department of Materials, Imperial College London-UK in 2003. Prof. Youssef has many years of Industrial experience in the steel industry. He has more than twenty years of experience in the industrial and research fields. He worked as a Research Associate at Imperial College London for three years. He is currently a Professor of Materials Engineering at the Department of Chemical and Petrochemical Engineering at the AASTMT. His research interests include several areas covering structure-property relationships, investigating the microstructural properties of superalloys and advanced materials, and manufacturing techniques for advanced materials such as additive manufacturing. In addition, he is active in several research areas related to water and wastewater treatment.

Khaled S. El-Kilany is a Professor of Industrial Engineering at the Department of Industrial and Management Engineering at the AASTMT, which is accredited by the Engineering Accreditation Commission of ABET since 2010. The department offers both B.Sc. and M.Sc. degrees in Industrial and Management Engineering. Prof. El-Kilany is currently the head of the department since February 2009. He is also Dean of Industry Service Complex at the AASTMT. He is a senior member of the IISE and is a reviewer of several journals, conferences, and textbooks. He has received his Ph.D. in Mechanical and Manufacturing Engineering from Dublin City University, Ireland; where his research work included modeling and simulation of the automated material handling system of Intel's wafer fabrication facility Fab24, which was the second wafer fabrication facility in the world that produces 300mm wafers. His research interests lie in the analysis and improvement of manufacturing systems performance; specifically, material flow, production planning and scheduling, and WIP management using discrete-event systems simulation and optimization techniques.