Modeling Contaminant Rejection by Nanofiltration Membranes using a Phenomenological Model
Kevin Ohm1,2, Kara Mihalik2,3, Erica Clevenger2,3, Christopher Bellona, PhD2,3
1Humboldt State University, 2ReNUWIt, 3Colorado School of Mines

Introduction
To meet standards for drinking water and potable reuse, treatment facilities may employ nanofiltration (NF) membranes or reverse osmosis membranes to remove dissolved contaminants, bacteria, and viruses in the water. Prior to the installation of a full-scale membrane system, it is useful to know how effective it will be at removing certain contaminants to ensure the requirements will be met. As new contaminants of concern are identified, understanding the effectiveness of a membrane system at removal of these contaminants is beneficial to utilities and regulators.

However, pilot scale systems are expensive and bench scale systems do not provide accurate representations of the full-scale systems. To solve this problem, models have been developed to prediction rejection at the full scale prior to installation. This analysis used a phenomenological model with parameters obtained from bench-scale experiments to predict rejection of various contaminants. The objectives of this analysis were to develop a model to predict the performance of a full-scale membrane system and determine if parameters obtained at the bench-scale can predict rejection at the full-scale.

Methods
In 2011, bench-scale testing was performed to measure rejection of 19 contaminants by an NF membrane (NF270, Filmtec). Data collected from these experiments were used to determine parameters needed to predict contaminant rejection by the membrane. These parameters are specific to the system, the membrane, and the contaminant. In addition, pilot-scale experiments were performed to determine rejection of the same contaminants at various recoveries. The pilot-scale data was also used to determine parameters for use in the model.

In the summer of 2012, a code was developed using the phenomenological model to predict rejection at the pilot-scale based on the parameters obtained at the bench-scale. This code used the parameters for one contaminant along with hydraulic pressures associated with different recoveries at the pilot scale to predict rejection from the model. As this code was developed in an older version of MATLAB, and had become partially corrupted, it had to be updated to work with the current version of MATLAB. The code was updated in the summer of 2020 to predict contaminant rejection and recovery for each contaminant data was collected for. These results were used to plot rejection and recovery found from the bench-scale model and pilot-scale experiment to determine accuracy of models compared to the pilot-scale data. Finally, a code was developed to adjust the permeability coefficient and contaminant permeability of each contaminant until the model more closely matched the experimental data.
Results
For some of the contaminants, such as gemfibrozil, the model was found to predict rejection at the pilot scale with a high degree of accuracy. However, for other contaminants, such as triclocarban, the bench-scale parameters caused the model to predict rejection that varied significantly from what was measured in the pilot-scale experiment (Figure 1).

![Graph showing rejection rates for different compounds](image)

For most of the contaminants tested, when the difference between pilot-scale and bench-scale model was noticeable, such as atenolol, the bench-scale parameters underestimated the rejection of the contaminant. However, when the pilot-scale data showed low contaminant rejection, the bench-scale model significantly overestimated rejection, as shown with triclocarban (Figure 1).

Possible sources of error include contaminant measurement and sample contamination. Errors in contaminant measurement are supported by the experimental data for caffeine. Rejection would be expected to decrease as recovery increases, but this trend is not observed in these data.

Conclusion and Recommendation
Parameters obtained from the bench-scale generally caused the model to underpredict rejection at the pilot-scale. The model overestimated rejection when the pilot-scale rejection was lower. These parameters could be altered to make the model more accurately predict pilot-scale rejection.

These data were collected in 2011 and contaminant analysis and membrane systems have improved since then. Due to this, this experiment should be run again with current analytical technology to get more accurate concentration values. In addition, this should be run with a modern membrane to ensure the results are applicable to current technology. Finally, if the model still does not accurately predict rejection, it should be determined why bench-scale parameters do not accurately predict rejection at the pilot-scale.
**References**
