# Introduction

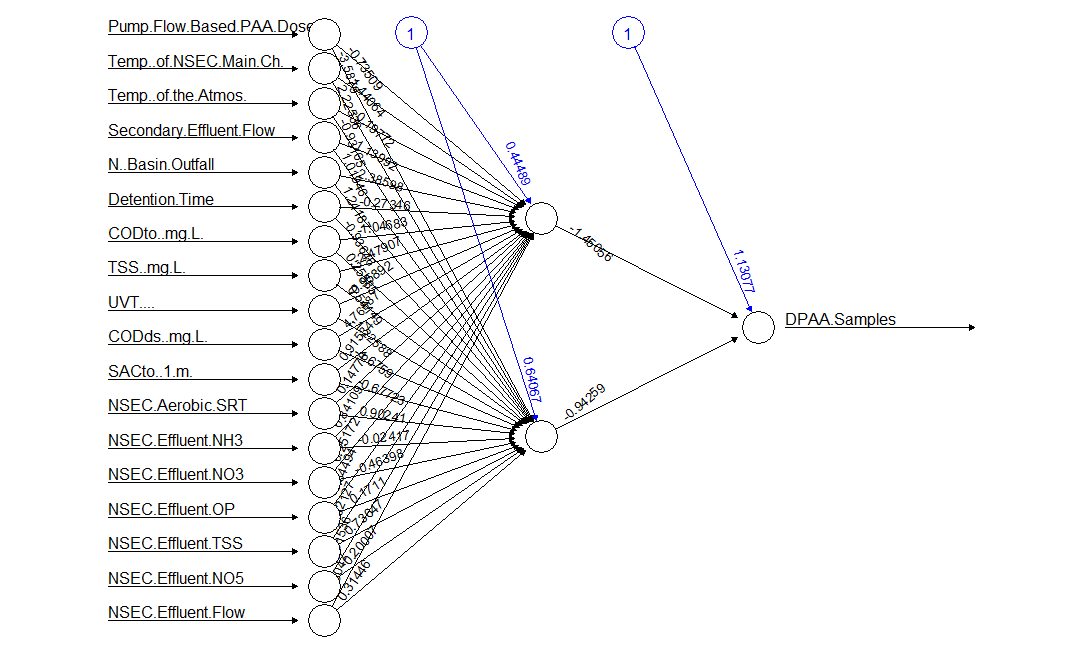
The goal of this work is to reduce the cost of disinfection using peracetic acid (PAA) at the Robert W. Hite Treatment Facility operated by the Metro Wastewater Reclamation District (MWRD) in Denver, CO. Due to differences between the initial PAA pilot and full-scale disinfection installation (e.g., geometry and residence time of disinfection basin, variable influent *E. coli* concentrations, variable PAA initial demand), MWRD experienced an instance of exceeding its *E. coli* discharge limit for a single day (252 MPN/100 mL based on a 7-day geometric mean, 126 MPN/100 mL based on a 30-day geometric mean) while operating in constant CT dosing mode. To ensure an exceedance does not occur and that proper dosing is achieved, MWRD is currently operating at a constant initial dose of PAA (1.2 mg/L PAA at the time of this report. This approach has increased PAA chemical costs substantially and has resulted in a re-evaluation of the PAA dosing strategy.

Manoli et al. (2019) proposed a novel CT-based PAA dosing strategy derived from first principals. A double-exponential model of microbial inactivation was solved given a first order model of PAA decay and an n-CSTR hydraulic model. The formulation predicted effluent fecal coliform concentrations given influent fecal coliform concentration and the integrated CT (ICT). ICT was solved given the initial concentration of PAA, the PAA decay constant, and the initial demand of PAA. The PAA decay constant was estimated by solving for various ICTs using Excel Solver and in for Manoli et al. ranged from 0.01-0.02 min-1. Given the average ICT for a given hour, fecal coliform samples were taken at the inlet and outlet to fit the microbial inactivation model. The fitted parameters (*β,* kd, m, kp) varied with each batch, which demonstrates that the first order model may not fully describe PAA demand and decay kinetics in a real water matrix, requiring four degrees of freedom to fit the model to the observed data.

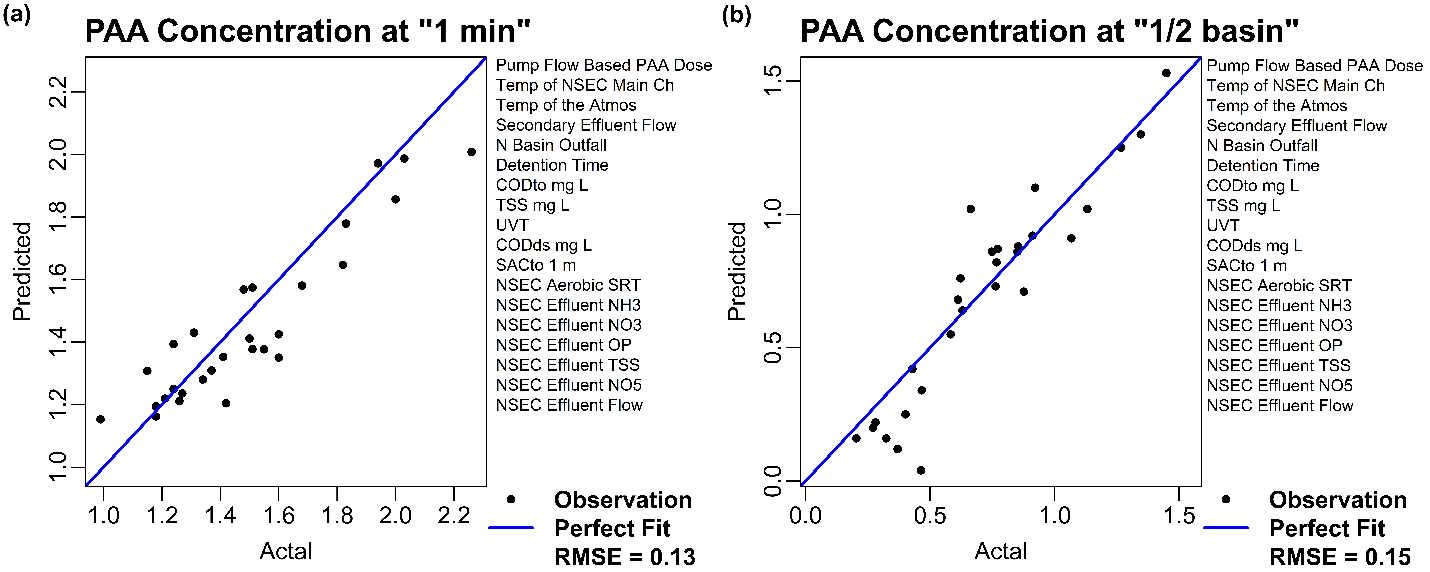
Manoli et al.’s approach assumes that there is in initial immediate consumption of PAA that occurs prior to exponential decay. From PAA concentration profiles of the disinfection basin at MWRD (Figure 1), this does not appear to be the case. If the initial demand were instantaneous, there would not be such a change in slope between 0-5 minutes and 5-60 minutes. A single exponential model fit for the two sampling campaigns in Figure 1 (excluding the initial dose at time 0) gives a coefficient of determination (R2) of 0.94, which is slightly less than the double exponential approach of 0.99. When integrated, the difference in CT is 0.4 mg/L\*min (24.8 mg/L\*min for single exponential and 25.2 mg/L\*min for double exponential when HRT is 60 minutes). However, the double exponential approach could not be fit in real time given the position of the current online analyzer. The difference between the time of sample collection and the exponential model prediction is approximately 10-13 minutes. However, this is just for one snapshot in time.

**Figure 1.** Exponential model fits of two PAA sampling events throughout the MWRD Hite North disinfection basin (observations in blue and orange, model fits in gray and yellow). Online PAA data collected by a Chemscan is plotted in green. The online PAA data is plotted at the sample collection time, not accounting for the accelerated degradation rate with exposure to the autosampler tubing itself, which is a better approximation of conditions at 16-20 minutes of hydraulic retention time as opposed to 5-8 minutes.

Historically, there has been a large difference in Alternatives to predicting PAA concentration using first order models are non-deterministic approaches, such as statistical models and neutral network models. Both approaches have the advantage of being able to consider the impact of multiple variables without a known relationship. However, water quality and operational parameters of a wastewater treatment system are too complex for many statistical models (e.g., linear regression, generalized linear models, random forest model, support vector machines). Therefore, neural networks were used to predict concentrations of PAA throughout the disinfection basin (Figures 2 and 3). Neural networks have the flexibility to incorporate many nonlinear relationships without the need to explicitly define them with first principals models.



**Figure 2.** Example neural network model structure to predict PAA concentration from 18 online process variables with two hidden nodes.



**Figure 3.** Neural network predictions of PAA concentration at the (a) “1 minute” and (b) “1/2 basin” grab sampling locations given the variables listed to the right of each parity plot.

To identify which variables are most important to the prediction of PAA concentration throughout the basin, combinations of different number of process variables (from Figure 2) and hidden nodes were used to train and test neural network predictions. The most frequently included variables in the models that were successfully able to predict the PAA concentration at the sampling location labeled “1-minute” include flow and water quality parameters of the North secondary effluent (i.e., disinfection basin influent) measured by nutrient sensors and a visual spectrum analyzer at the point of dosing.

|  |  |
| --- | --- |
| Variables | R2 |
| Pump.Flow.Based.PAA.Dose + Temp..of.NSEC.Main.Ch. + Temp..of.the.Atmos. + Secondary.Effluent.Flow + CODto..mg.L. + TSS..mg.L. + CODds..mg.L. + NSEC.Effluent.TSS + NSEC.Effluent.NO5 | 0.8245533 |
| Pump.Flow.Based.PAA.Dose + Temp..of.NSEC.Main.Ch. + Temp..of.the.Atmos. + Secondary.Effluent.Flow + NSEC.Effluent.OP + NSEC.Effluent.NO5 + NSEC.Effluent.Flow | 0.8239120 |
| Pump.Flow.Based.PAA.Dose + Temp..of.NSEC.Main.Ch. + Temp..of.the.Atmos. + Secondary.Effluent.Flow + CODds..mg.L. + NSEC.Aerobic.SRT + NSEC.Effluent.OP + NSEC.Effluent.NO5 | 0.8227897 |
| Pump.Flow.Based.PAA.Dose + Temp..of.NSEC.Main.Ch. + Secondary.Effluent.Flow + N..Basin.Outfall + CODto..mg.L. + NSEC.Effluent.OP + NSEC.Effluent.TSS + NSEC.Effluent.NO5 | 0.8220495 |
| Pump.Flow.Based.PAA.Dose + Temp..of.NSEC.Main.Ch. + Temp..of.the.Atmos. + Secondary.Effluent.Flow + NSEC.Effluent.OP + NSEC.Effluent.NO5 | 0.8200637 |
| Pump.Flow.Based.PAA.Dose + Temp..of.NSEC.Main.Ch. + Secondary.Effluent.Flow + NSEC.Effluent.NO3 + NSEC.Effluent.OP + NSEC.Effluent.NO5 | 0.8199546 |