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# PROCESS OPTIMIZATION AND GUIDANCE THROUGH MACHINE LEARNING

## Coagulation for Drinking Water and Industrial Source Water

*Dave Rutowski, Claros Process Management – Great Lakes  
Matthew Gray PE, Claros Optimization Engineering Team*

# AGENDA

- Description of monitoring tools for coagulation
- How they are implemented
- What it looks like
  - Additional technologies available
    - Components of concern
      - Manganese
      - Arsenic
      - Iron
    - Corrosion control / Phosphate dosing
    - Biological monitoring (Legionella, etc.)

# OUTCOMES

- Online monitoring for critical plant processes like coagulation Real time response to changes in water quality
- Systems that can see WQ changes or overfeeds in real time



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# COAGULATION

Upgrade plant performance

# COAGULATION BACKGROUND

- Coagulation is an essential process for the removal of suspended and colloidal material from raw water.
- The main difficulty is to determine the optimum coagulant dosage related to the influent of raw water. Excessive coagulant overdosing leads to increased treatment costs and public health concerns, while underdosing leads to a failure to meet the water quality targets and less efficient operation of the water treatment plan
- Process optimization and control is usually based on data from jar tests and simple flow-proportional dosing concepts
- no comprehensive or universally accepted mathematical description of the process has been developed so far
- In water treatment plants charge neutralization can be considered the predominant process, especially if the coagulant dose has been optimized.

# SURFACE WATER IS A COAGULATION CHALLENGE



Anyone else treating that nice Lake Erie water today?!

What's the highest NTU from your source water?!

We can go from  
**1 NTU to 1500 NTU**  
in under an hour at times!

Tyler Johnson  
-South Elgin, Ontario

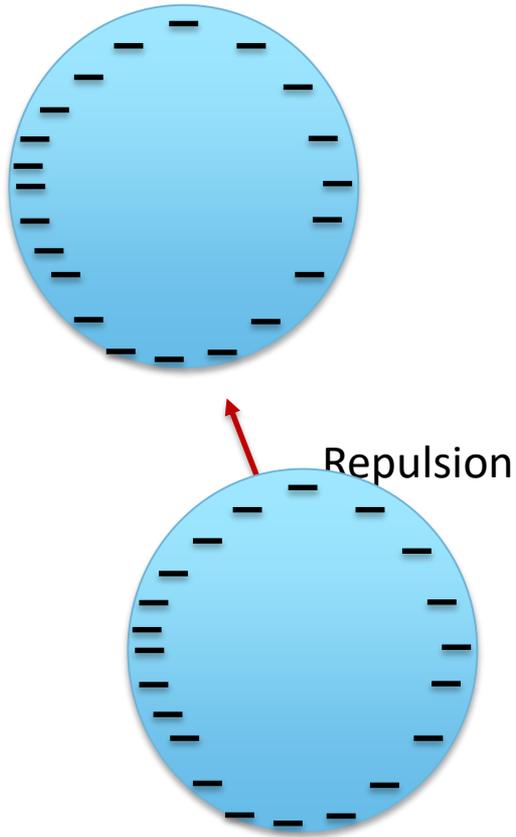
# COAGULATION, FLOCCULATION, AND SEDIMENTATION



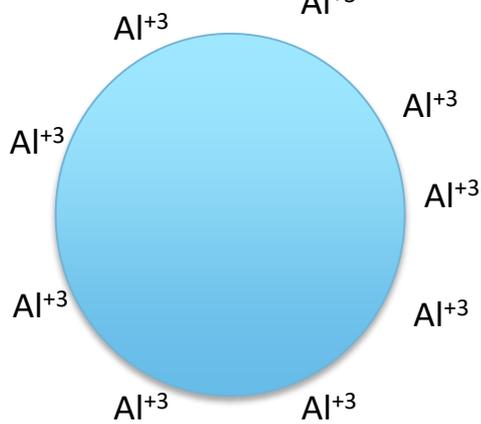
- The purpose of coagulation is to condition non-settleable solids and organics to clump together to form a floc
- The larger floc particles are then able to settle out
- Removal of suspended and colloidal substances from water is required for
  - Protecting Human Health
  - Regulatory Compliance
  - Aesthetics



# COAGULATION

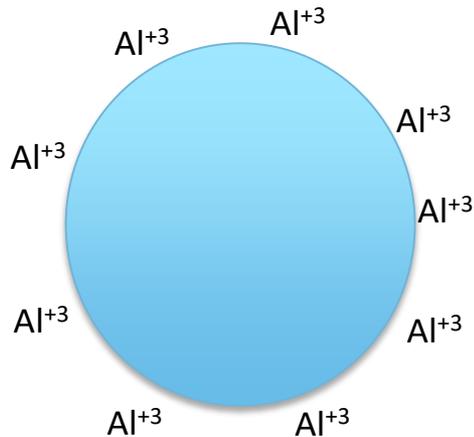


- Particles coming into a plant from surface water are generally negatively charged
- Those negative charges cause the particles to repel each other, in the same manner as the negative poles of 2 magnets push each apart



# COAGULATION

- Coagulation involves the destabilization of negatively charged colloidal particles by neutralizing charge with chemical coagulant
- Once the positively charged coagulant is added, it neutralizes the negative charges
- Then the particles can clump together to form a floc



# COAGULATION GOALS

- Chemical addition during coagulation is required for small colloidal particles due to slow settling velocities

Particle Size (mm)	Particle Size (microns)	Order of Size	Time Required to Settle (sg = 2.65)	Time Required to Settle (sg = 1.2)
10	10000	Gravel	0.4 sec	1.2 sec
1	1000	Coarse Sand	3.0 sec	9 sec
0.1	100	Fine Sand	34 sec	5 min
0.01	10	Silt	56 min	8 hours
0.001	1	Bacteria	4 days	32 days
0.0001	0.1	Colloidal	1 year	9 years
0.00001	0.01	Colloidal	> 50 years	> 50 years
0.000001	0.001	Colloidal	> 50 years	>50 years

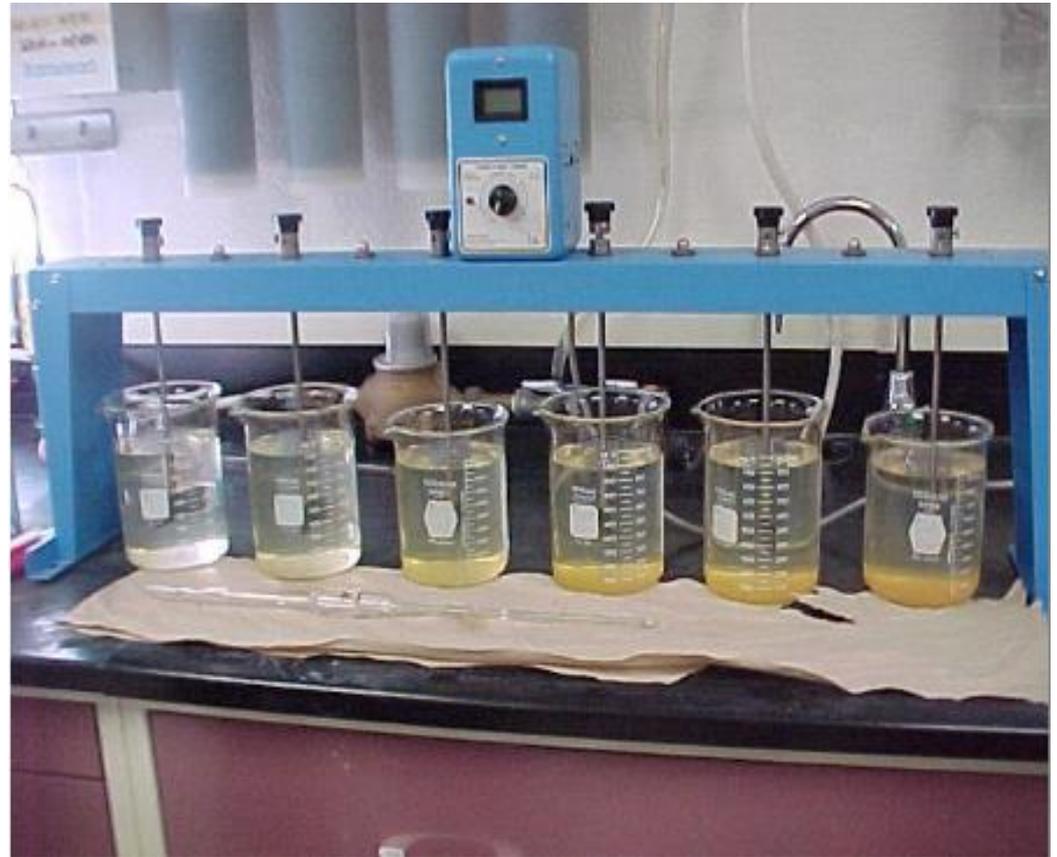
# COAGULATION MONITORING

## Factors that affect coagulation

- pH
- Temperature
- Coagulant type
- Mixing speed
- Alkalinity
- Turbidity
- Organic content

# COAGULATION MONITORING

- Proper coagulant dosing requires periodic jar testing
- Online instruments like streaming current can monitor the coagulation process
- Streaming current analysis can reduce the frequency of jar testing, but will not take its place



# COAGULATION MONITORING

- An east coast city recently budgeted over \$7 million for annual coagulant chemical costs
- That equates to about \$19K per day
- Unnecessary coagulant overdosing can be costly with little to no return on extra coagulant used
- Having a real time feed-forward and feedback response will help optimize coagulant dosing

# CONTINUOUS MONITORING PARAMETERS

## Raw water

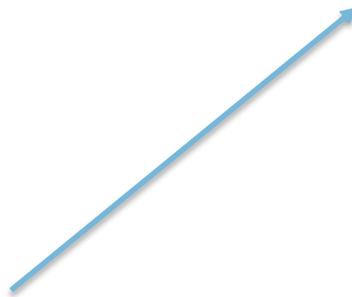
- Turbidity
- pH
- Flow
- Organic content, UV254
- Streaming Current



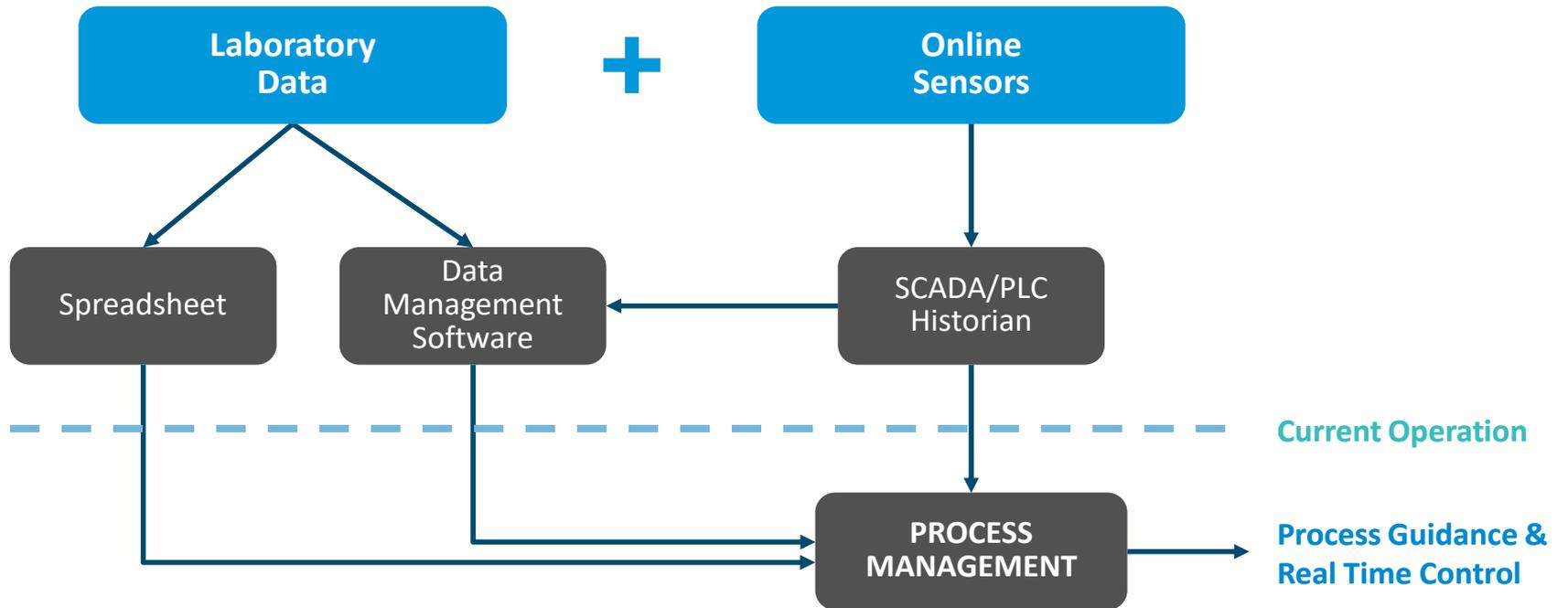
Coagulant dose

## Post sedimentation

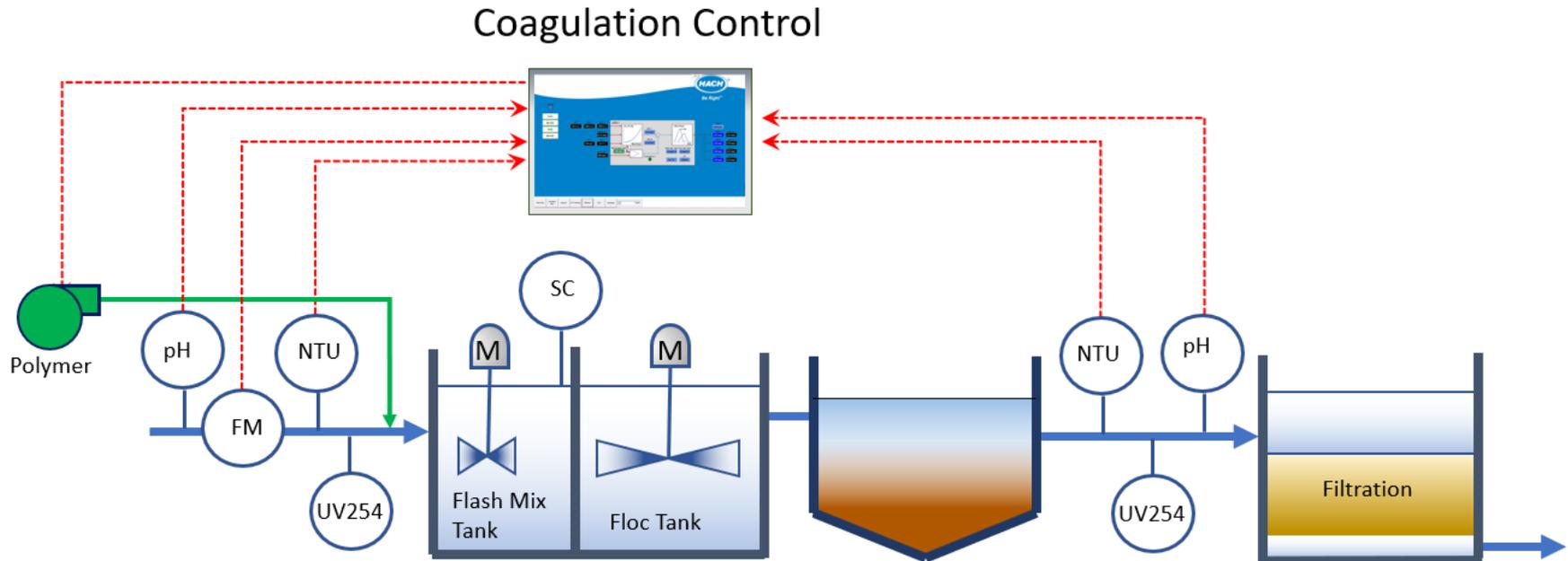
- Turbidity
- pH
- Organic content, UV254



# DATA SOURCES



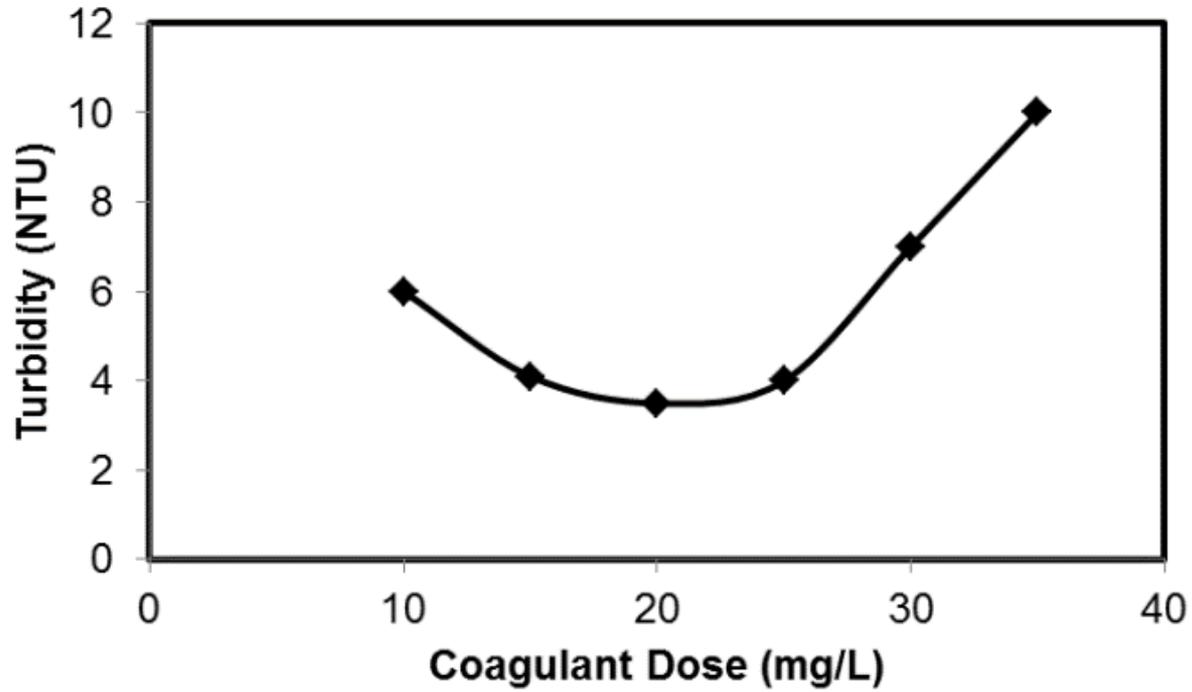
# COAGULATION(RTC – COAG)



The following benefits can be expected after implementation of the RTC-COAG system:

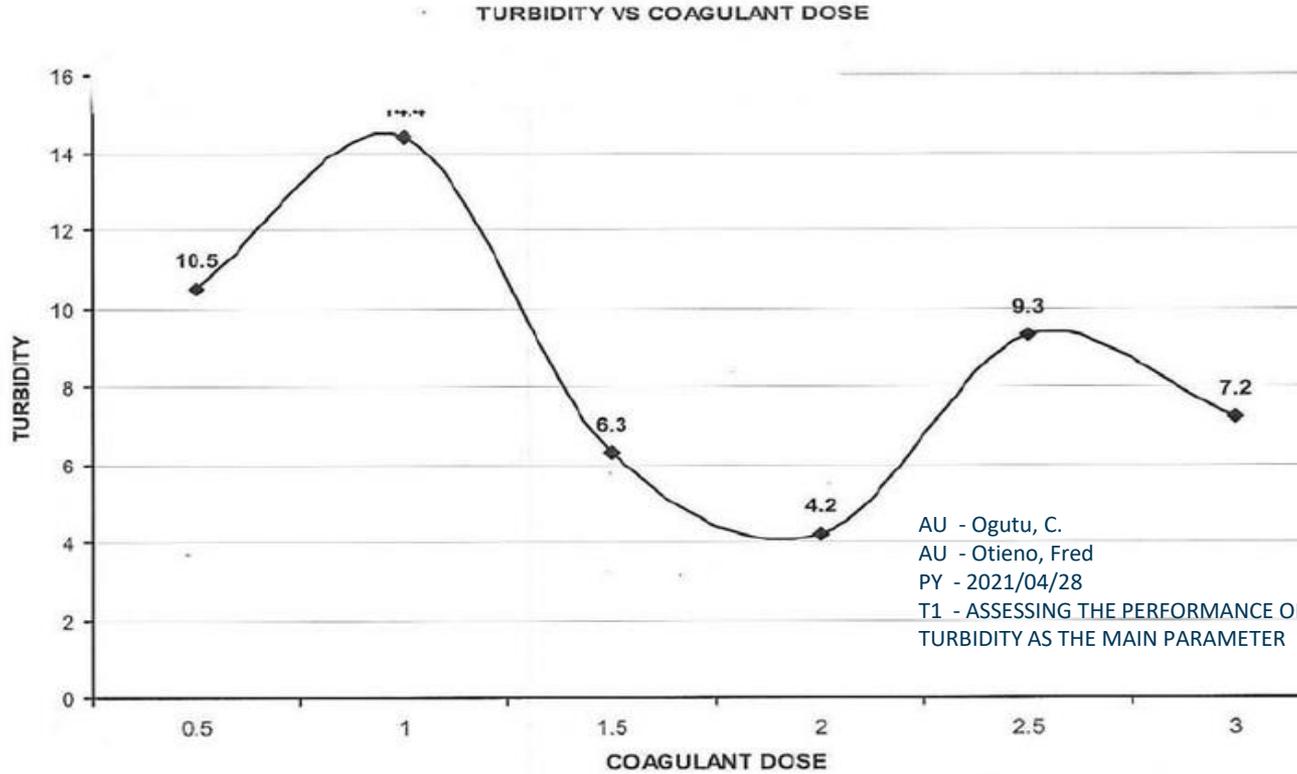
- Optimization of coagulation/ flocculation water treatment process
- Achieve savings on coagulant usage
- Improve solids and natural organic matter removal

# COAGULATION CURVE



CHEGG.COM

# COAGULATION CURVES



AU - Ogotu, C.  
AU - Otieno, Fred  
PY - 2021/04/28  
T1 - ASSESSING THE PERFORMANCE OF DRINKING WATER TREATMENT PLANT USING  
TURBIDITY AS THE MAIN PARAMETER

# RECAP



Coagulation relies on correct chemical dosing for a variety of parameters



Dosing coagulant based only on jar tests and seasonal adjustments may miss some raw water changes



Coagulant overdosing can be costly and provide little benefit



Coagulant underdosing results in diminished flocculation and sedimentation efficiency and shorter filter run times



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# WESTERN BERKS OPTIMIZATION CONCEPTS

# AGENDA

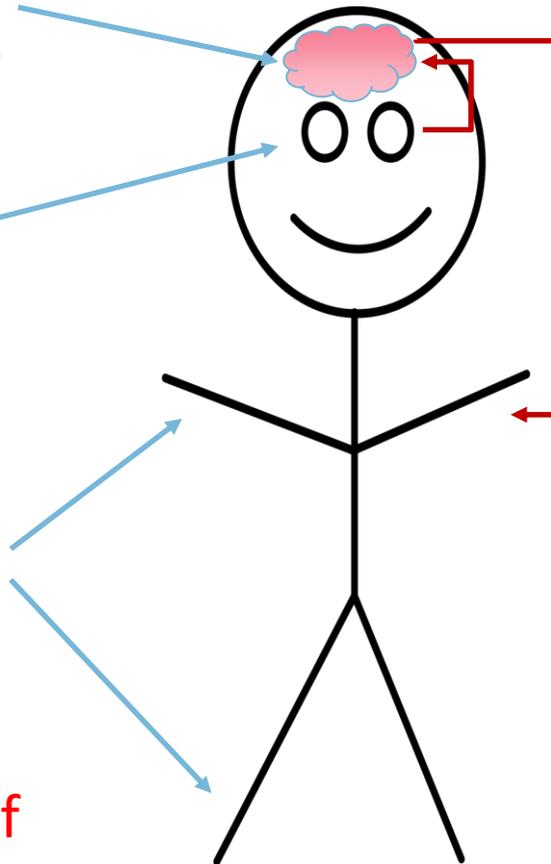
- Data
  - Sources
  - Validation
- Western Berks Water Authority
  - Background and Treatment Process Overview
  - Goals of Optimization of Mn and Coagulation Process
  - Concept
  - Results

# WHY IS DATA IMPORTANT?

Decision Making Process  
(Operator or Control System)

Data

Pumps, Process



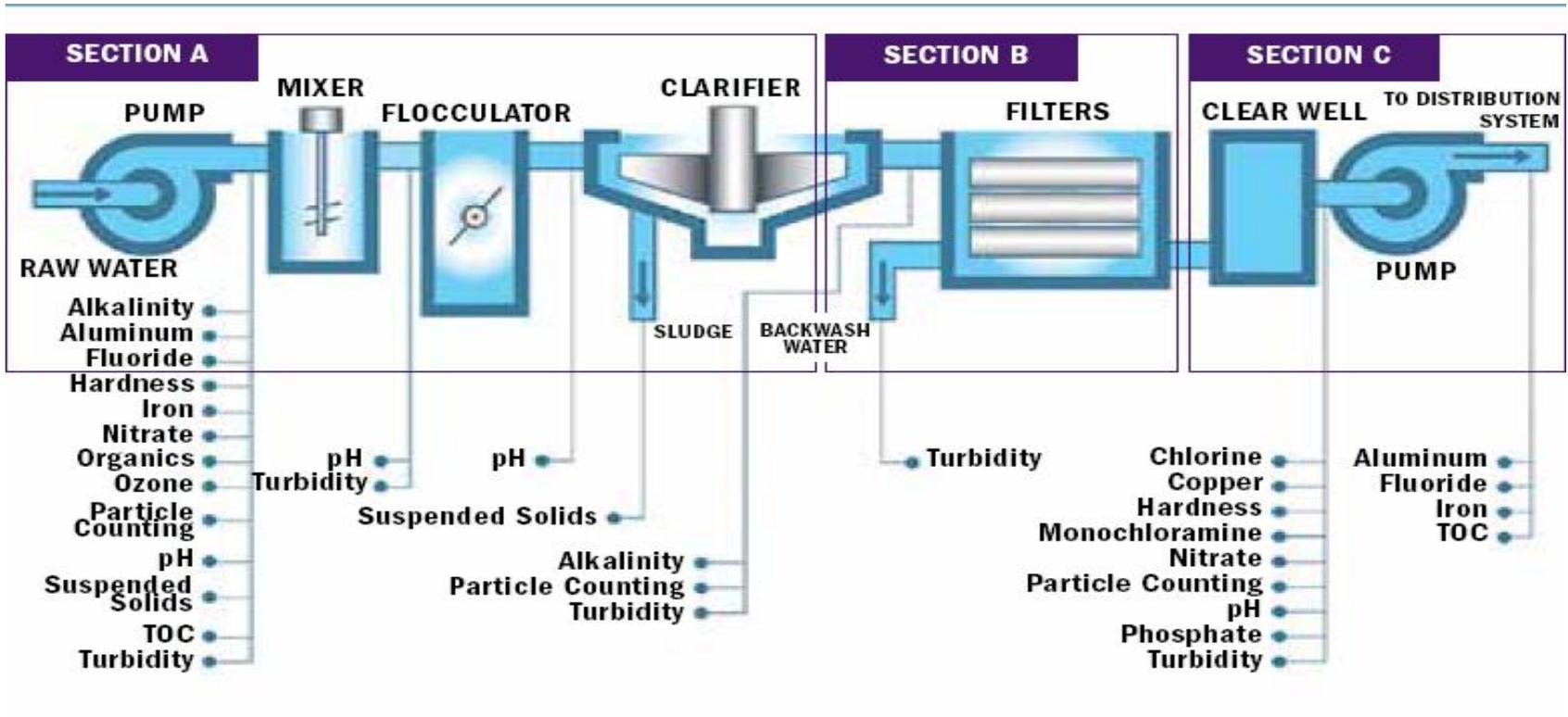
The more data that you have that is of good quality the better decisions you will make.

# DATA SOURCE

On-Line Sensors & meters

Laboratory

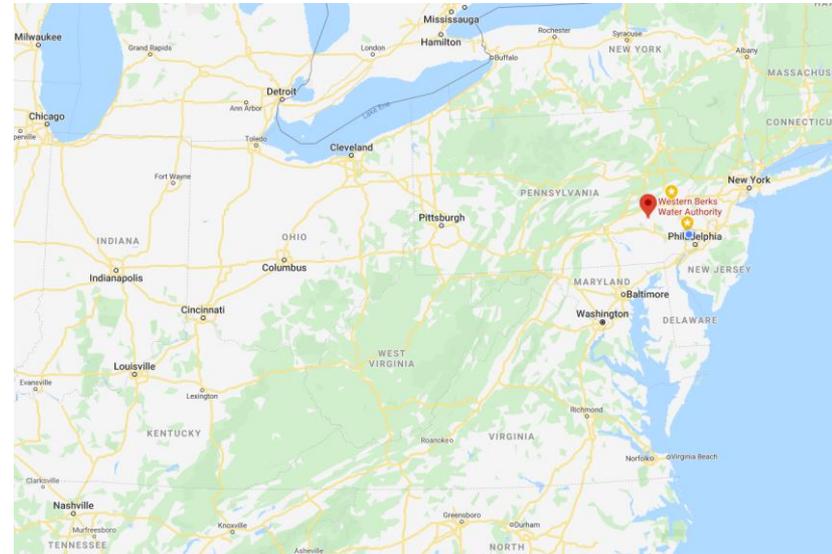
Historians (Database, Excel, SCADA, HACH WIMS)



# WESTERN BERKS WATER AUTHORITY OVERVIEW



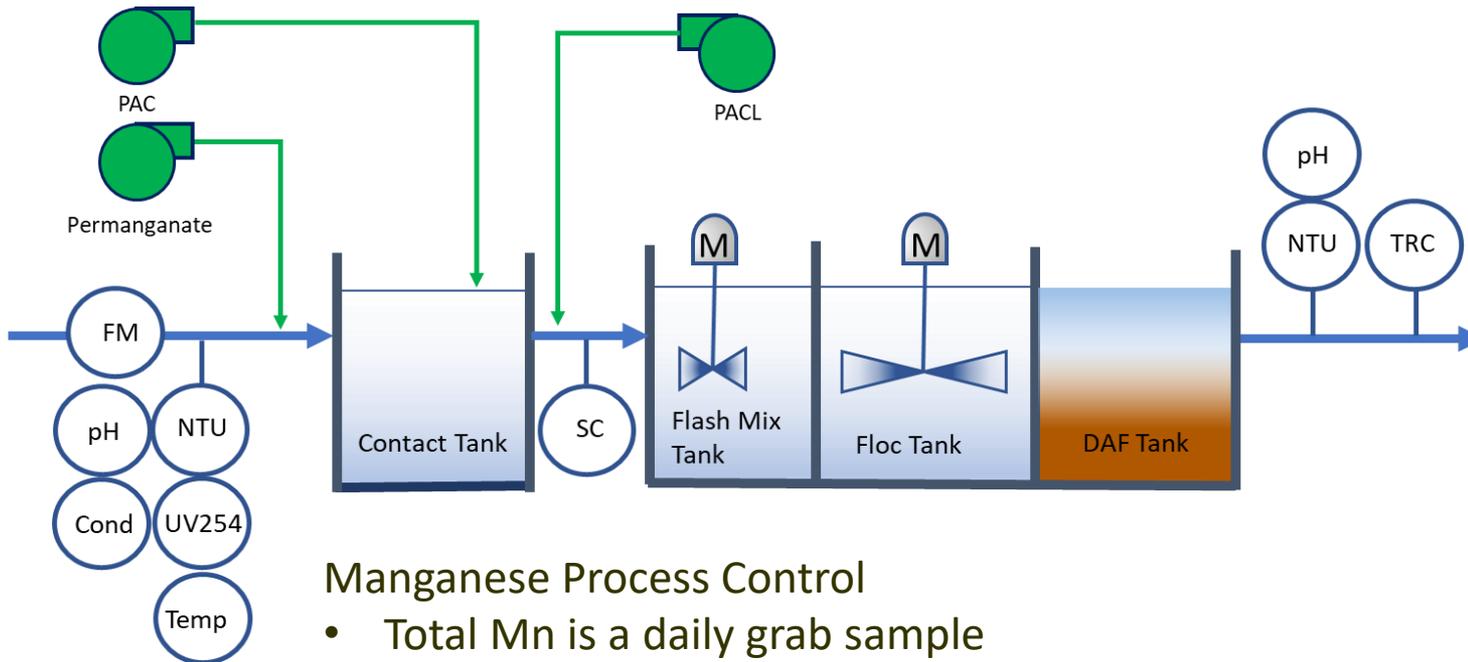
Blue Marsh Lake



- Produces 3.5 to 4.5 MGD of high quality water for 9 municipalities around Reading PA Area.
- The WBWA draws its water from an intake along the Tulpehocken Creek downstream of the Blue Marsh Dam.
- Will have the ability to draw water directly from the Reservoir in the near future.

# WESTERN BERKS WATER AUTHORITY OVERVIEW

Existing treatment process prior to filtration.....



## Manganese Process Control

- Total Mn is a daily grab sample
- Permanganate is manual adjusted based on Lab results

## Coagulation Process Control

- Manual Jar Tests vary based on water quality
- PACL is set by jar testing and adjusted by Streaming Current feedback control

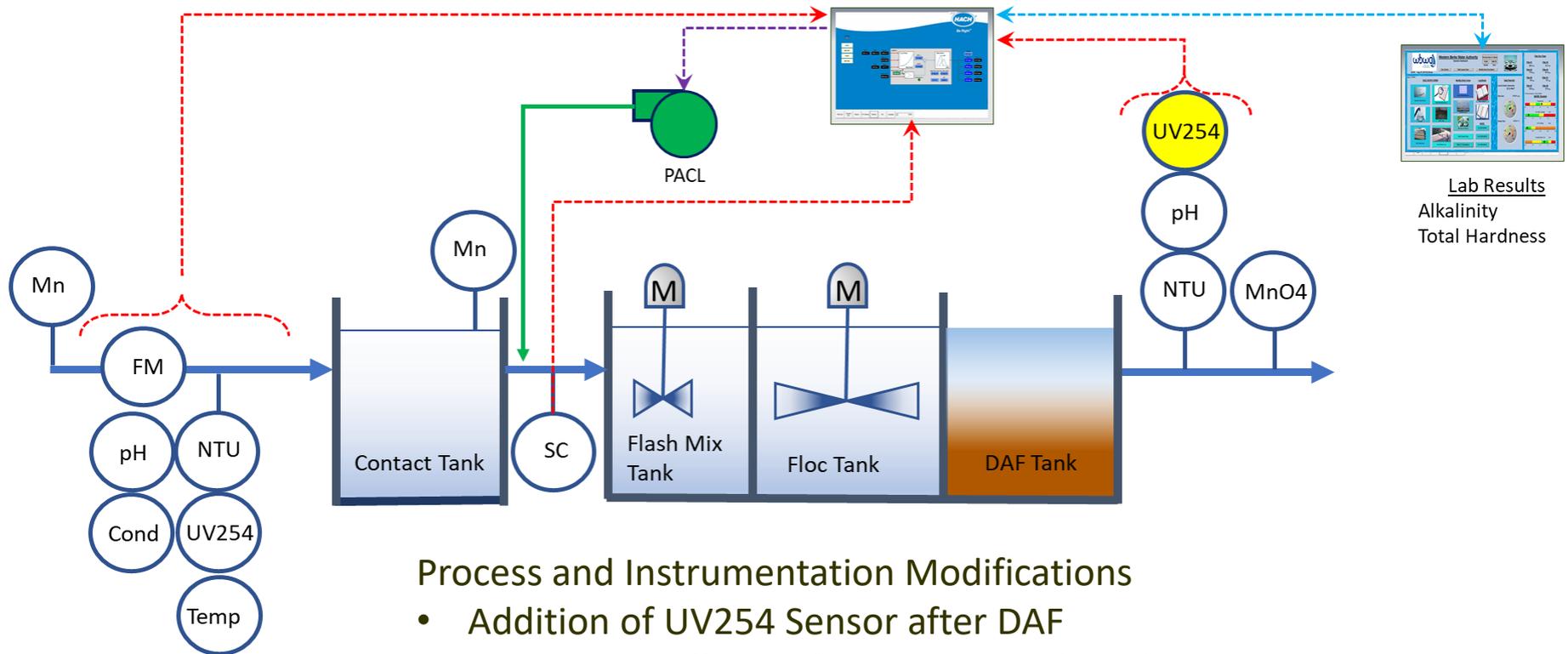
# WESTERN BERKS WATER AUTHORITY OVERVIEW

How could the existing Coagulation process control be improved.....

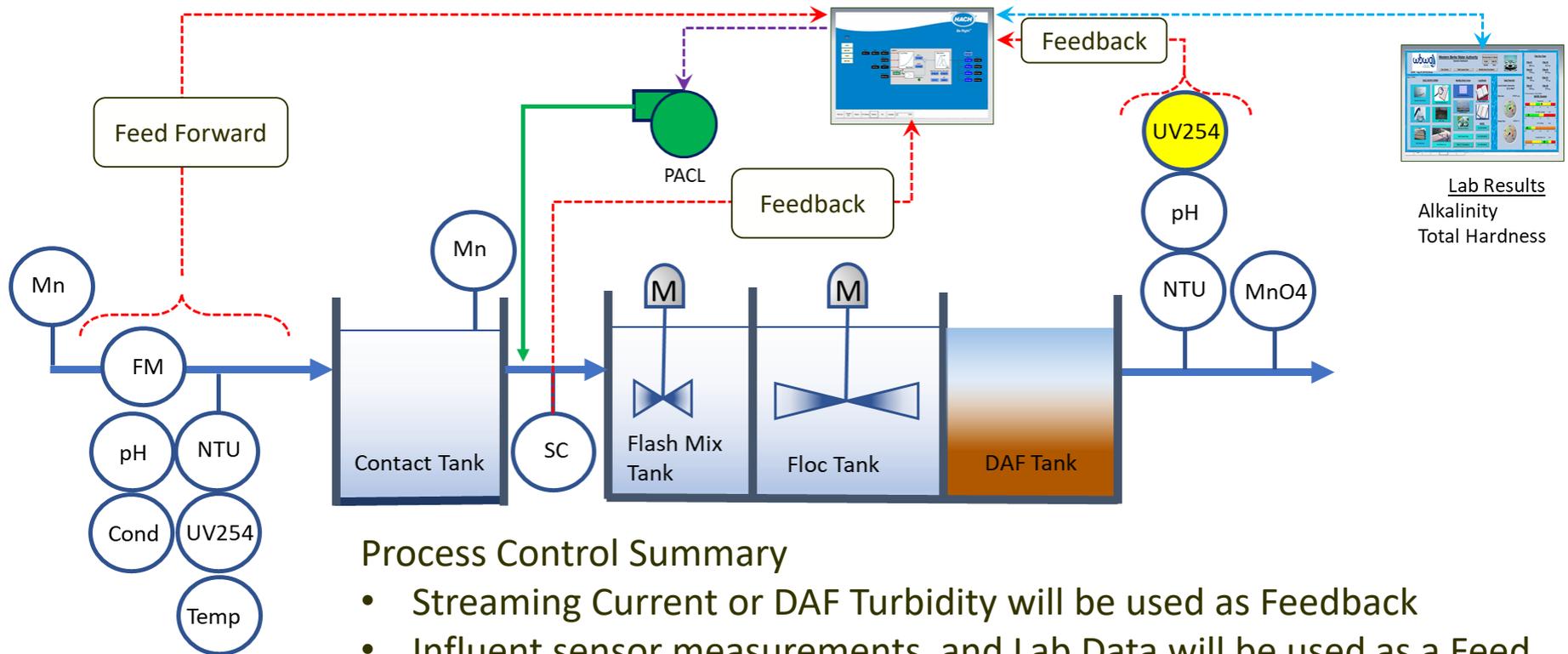
## Coagulation Process Control

- Manual Jar Tests vary based on water quality
- PACL is set by jar testing and adjusted by Streaming Current feedback control
  - Use historical instrumentation, operational, and laboratory data to build a feedforward model to predict the optimal PACL Dosage

# WESTERN BERKS WATER AUTHORITY COAGULATION PROCESS CONTROL



# WESTERN BERKS WATER AUTHORITY COAGULATION PROCESS CONTROL



## Process Control Summary

- Streaming Current or DAF Turbidity will be used as Feedback
- Influent sensor measurements, and Lab Data will be used as a Feed Forward Model
  - Ratio Control
  - Single Variable Regression
  - Multiple Variable Regression



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# DATA COLLECTION FOR FEED FORWARD MODEL

# DATA COLLECTION – SOURCES

Data from: January 1, 2018 – July 30, 2019 (>200,000 Data Points)

Online Sensor : 1 hour intervals

Laboratory : 1 day intervals

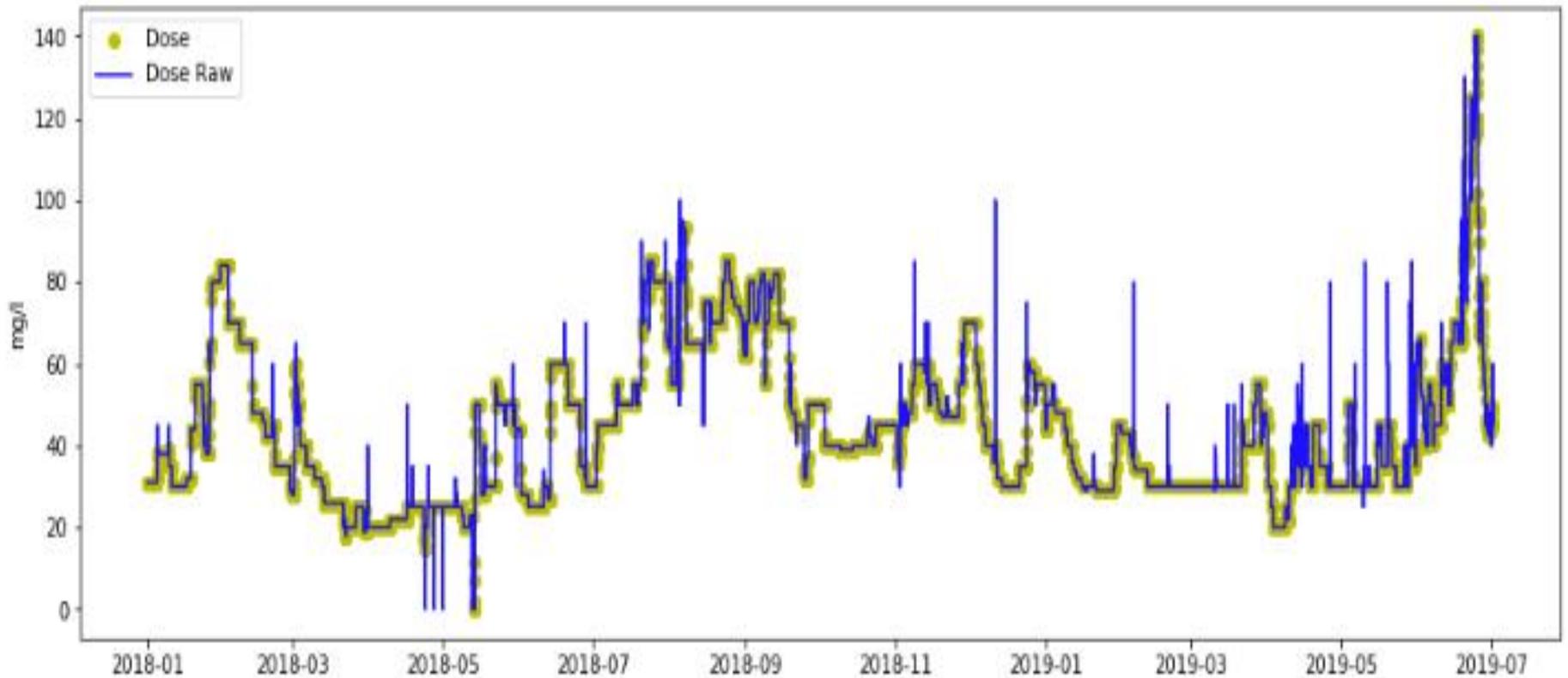
Collected from Output Report from WIMS

	Raw_Turb	Raw_pH	Raw_Cond	Raw_Temp	Flow	PACL_Dose	Pfilt_pH	Pfilt_Turb	Raw_Alk	Raw_TH	Raw_TMn	Eff_TMn	Eff_Alk	Eff_TH
<b>count</b>	13128.000000	13128.000000	13128.000000	13128.000000	13128.000000	13128.000000	13128.000000	13128.000000	13128.000000	13128.000000	13128.000000	13128.000000	13128.000000	13128.000000
<b>mean</b>	13.971130	7.862095	342.794251	10.424287	2334.323140	44.094759	7.446748	0.388629	126.179631	171.764279	0.082386	0.032642	119.080782	168.210452
<b>std</b>	10.015116	0.469533	40.021375	6.760251	184.528473	18.049994	0.201452	0.151020	9.657321	19.437813	0.021652	0.006079	10.248892	19.192033
<b>min</b>	3.473362	6.920001	244.710704	0.000000	1802.944912	0.000012	6.960919	0.163016	104.583333	136.000000	0.040506	0.009048	94.000000	135.607143
<b>25%</b>	8.238257	7.639926	314.876273	3.963647	2204.683353	30.000000	7.309732	0.269280	119.149489	156.187539	0.065238	0.030000	111.760695	153.747619
<b>50%</b>	10.906446	7.849878	340.905583	10.344263	2334.691480	40.000000	7.429535	0.377448	126.000000	168.216780	0.078661	0.030000	119.185958	165.523896
<b>75%</b>	15.985808	8.040000	364.137573	16.951030	2405.831587	54.963435	7.590000	0.466025	131.040931	184.000000	0.100000	0.037202	124.883185	177.523810
<b>max</b>	99.257054	9.414332	477.746375	22.137974	3203.894149	139.997547	8.213072	1.557340	157.785905	227.940476	0.140000	0.050000	149.685417	224.190476

# DATA VALIDATION

## Data Filters

- Hampel Filter to remove Outliers
- Low Pass Filter to average out smaller noise





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# FEED FORWARD COAGULATION MODEL CONCEPTS

# FEED FORWARD COAGULATION MODEL CONCEPTS

Dosage based on Ratio Control

- Raw turbidity verses actual dosage of PACL
- Raw UV Transmittance verses actual dosage of PACL

Machine Learning - Regression

- Single variable regression using raw UV Transmittance
- Multi-variable regression using all raw online and laboratory measurements

# MACHINE LEARNING ?



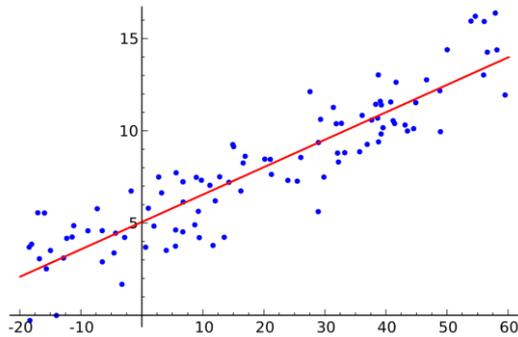
*“Machine learning is a method of data analysis that automates analytical model building. It is a branch of artificial intelligence based on the idea that systems can **learn from data, identify patterns and make decisions** with minimal human intervention.”*

## Steps Involved In Machine Learning :

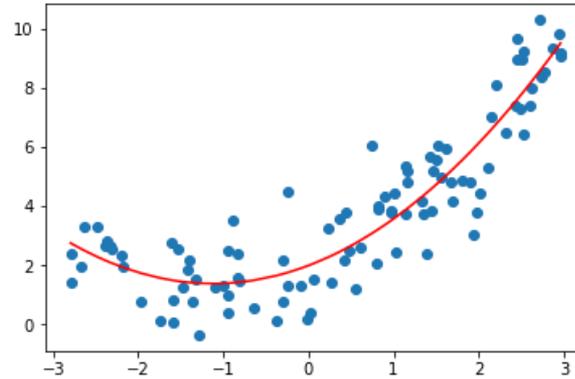
There are 5 basic steps used to perform a machine learning task:

- 1.Data Gathering
- 2.Data Cleaning and Preparation
- 3.Training a model.
- 4.Evaluating the model
- 5.Improving the performance.

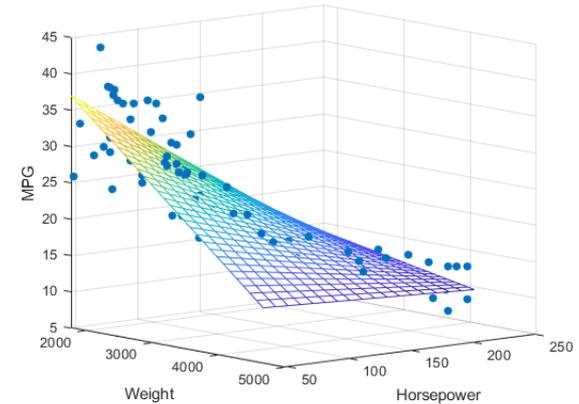
# REGRESSIONS – SIMPLE MACHINE LEARNING



Linear (Ratio)  
 $Y = A + X * B$



Single Variable  
Polynomial Regression  
 $Y = A + X^n * B$

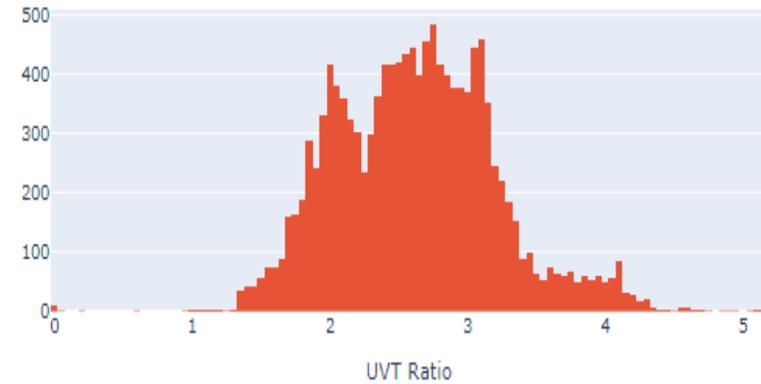
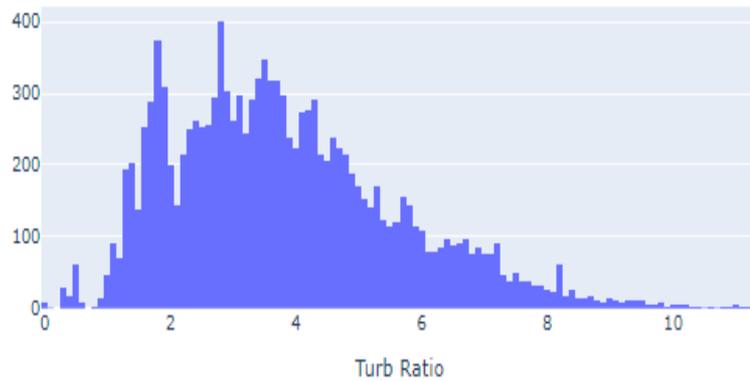


Multiple Variable Polynomial  
Regression  
 $Y = A + X1^n * B1 + X2^n * B2 \dots$

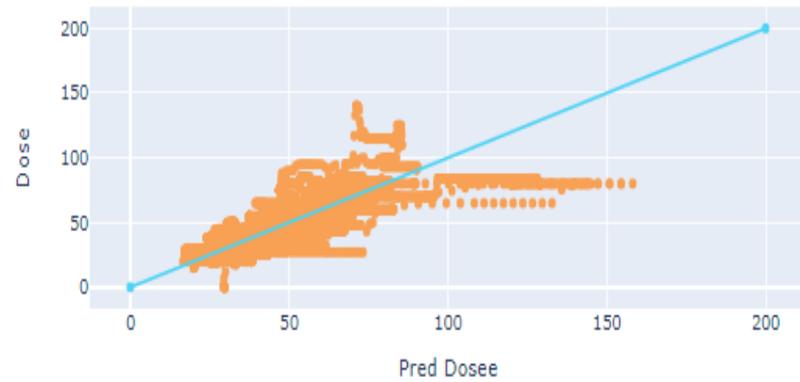
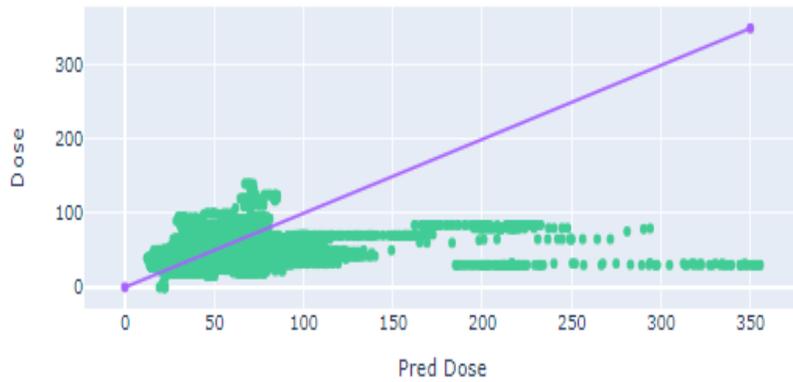
2/3 of the data is used to calculate Equation Coeff. (A,B.....)

1/3 of the data is to verify the Data

# COAGULATION CONTROL BASED ON RATIO



- Turb Ratio
- UVT Ratio
- Turb Ratio
- 100% Fit
- UVT Ratio
- 100% Fit



# FEED FORWARD COAGULATION MODEL CONCEPTS

## Dosage based on Ratio Control

- Raw turbidity verses actual dosage of PACL
  - Median Ratio of 3.6 PACL Dose (mg/l) per Raw Turbidity (NTU)
  - The Ratio span of 1.4 to 7.2 (5<sup>th</sup> to 95<sup>th</sup> Percentile)
  - Use the median ratio to predict PACI Dosage
    - Poor results
    - R<sup>2</sup> of -2.6
    - With error range of -31 to 56mg/l (Actual Avg Dose of 44 mg/l)
- Raw UV Transmittance verses actual dosage of PACL
  - Median Ratio of 2.6 PACL Dose (mg/l) per UV Transmittance
  - The Ratio span of 1.7 to 3.7
  - Use the median ratio to predict PACI Dosage
    - OK results
    - R<sup>2</sup> of 0.6
    - With error range of -15 to 17mg/l (Actual Avg Dose of 44 mg/l)

# FEED FORWARD COAGULATION MODEL CONCEPTS

Dosage based on Regressions

- Single Variable Polynomial Regression  
(Raw UV Transmittance)
- Multiple Variable Polynomial Regression Median

## Laboratory

- Raw Total Hardness
- Raw Alkalinity

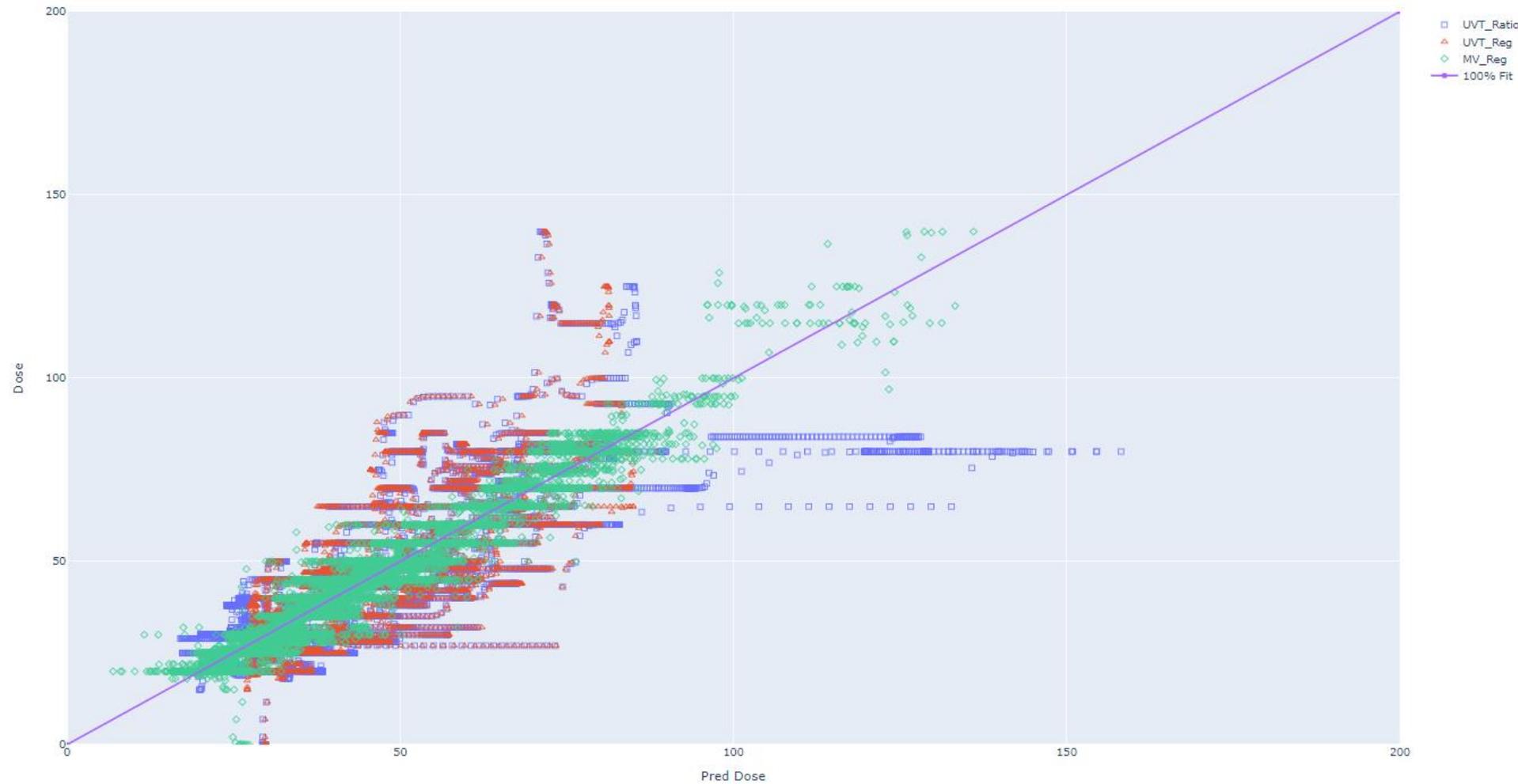
## Online Sensors

- Raw UVT
- Raw Turbidity
- Raw pH
- Raw Conductivity
- Flow
- Temperature

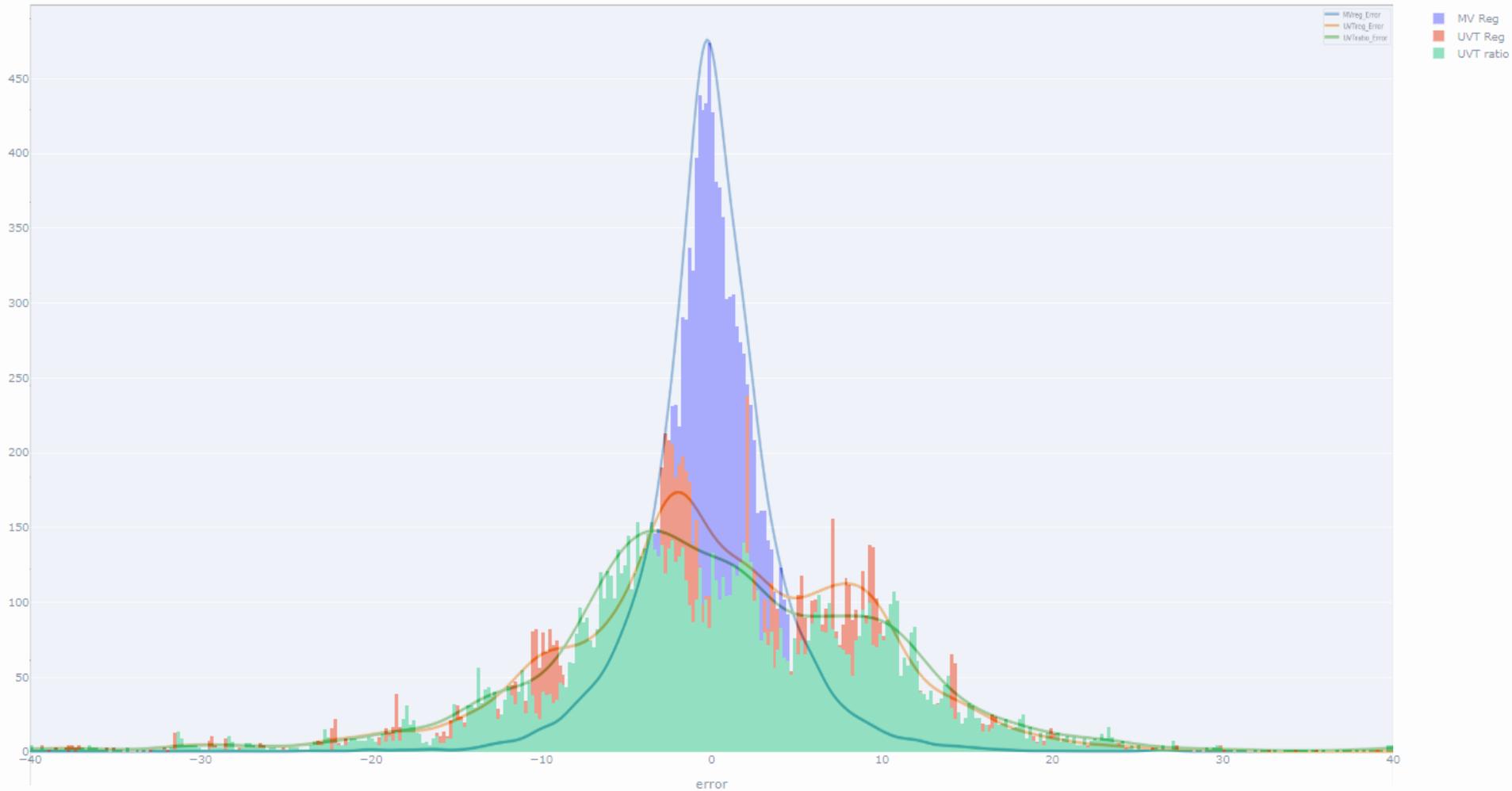
# PREDICTED VERSUS ACTUAL PACL DOSE



# PREDICTED VERSUS ACTUAL PACL DOSE



# PREDICTED VERSUS ACTUAL PACL DOSE - ERROR

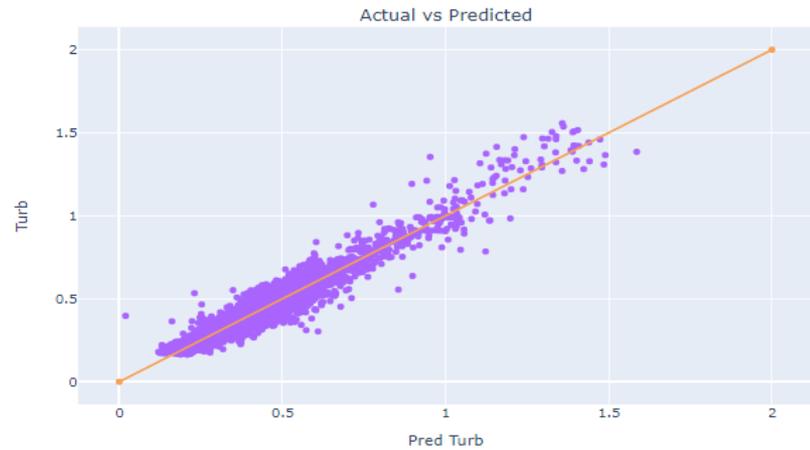
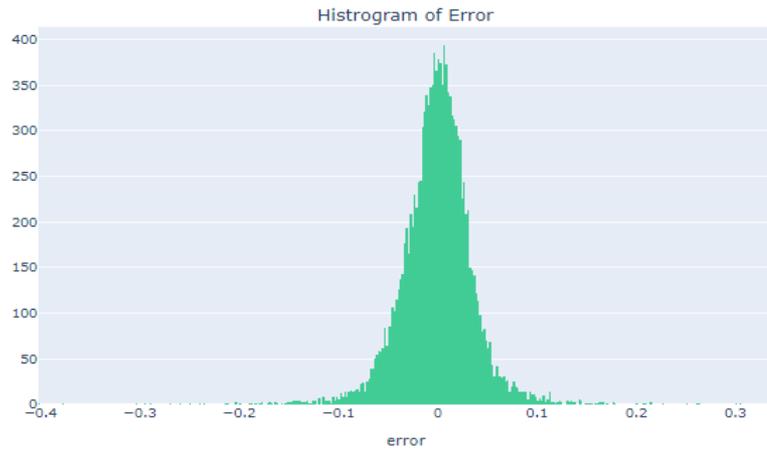


# FEED FORWARD COAGULATION MODEL CONCEPTS

- Single Variable Polynomial Regression (Raw UV Transmittance)  
Use the model to predict PACl Dosage
  - Good results
  - $R^2$  of 0.70
  - With error range of -15 to 13mg/l (Actual Avg Dose of 44 mg/l)
- Multiple Variable Polynomial Regression Median  
Use the model to predict PACl Dosage
  - Great results
  - $R^2$  of 0.95
  - With error range of -6.2 to 6.2mg/l (Actual Avg Dose of 44 mg/l)

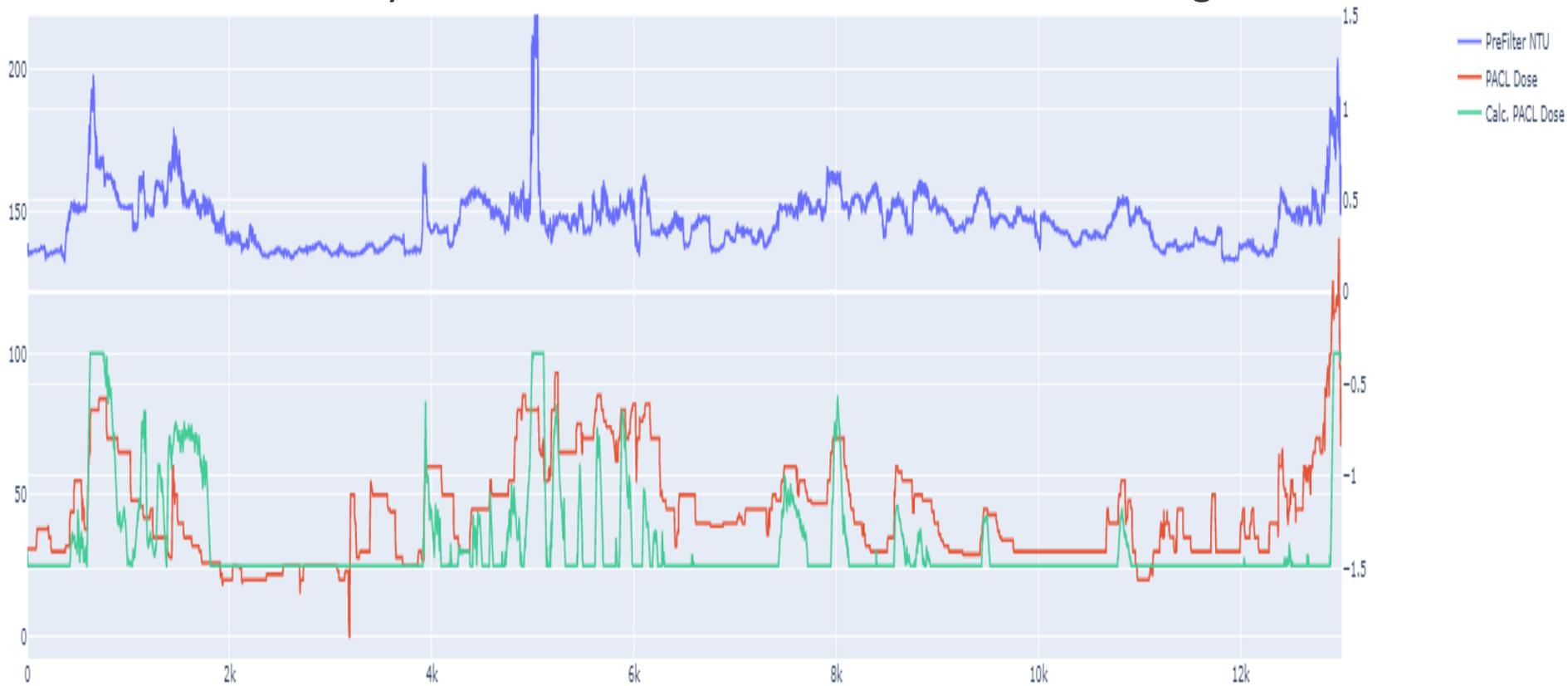
Can the Regression be use to predict Pre Filter Turbidity ?

# MULTI – VARIABLE REGRESSION RESULTS TO PREDICT PRE FILTER TURBIDITY



# COAGULATION DOSE OPTIMIZATION

Pre-Filter Turbidity Goal : 0.3- 0.5 NTU : Potential PACL Savings: 11%

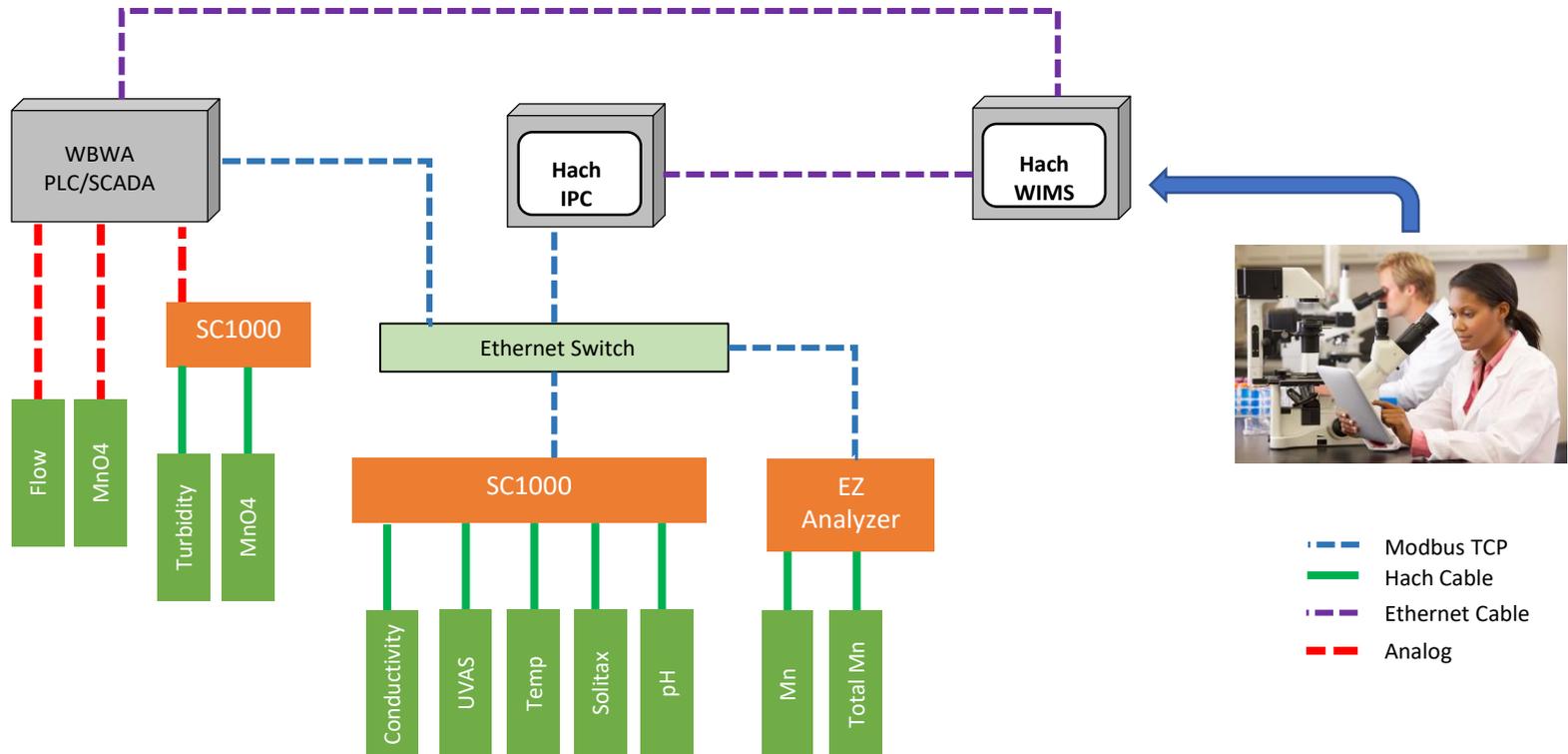




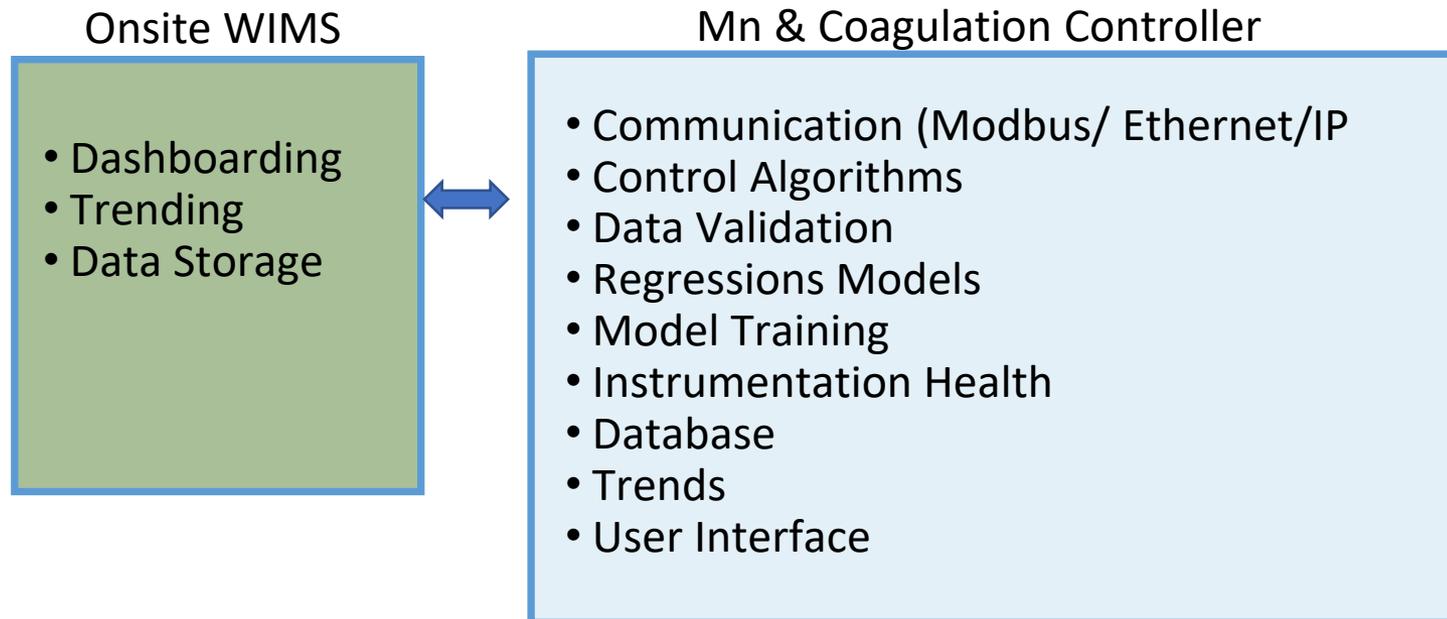
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# MN AND COAGULATION IMPLEMENTATION

# NETWORK OVERVIEW



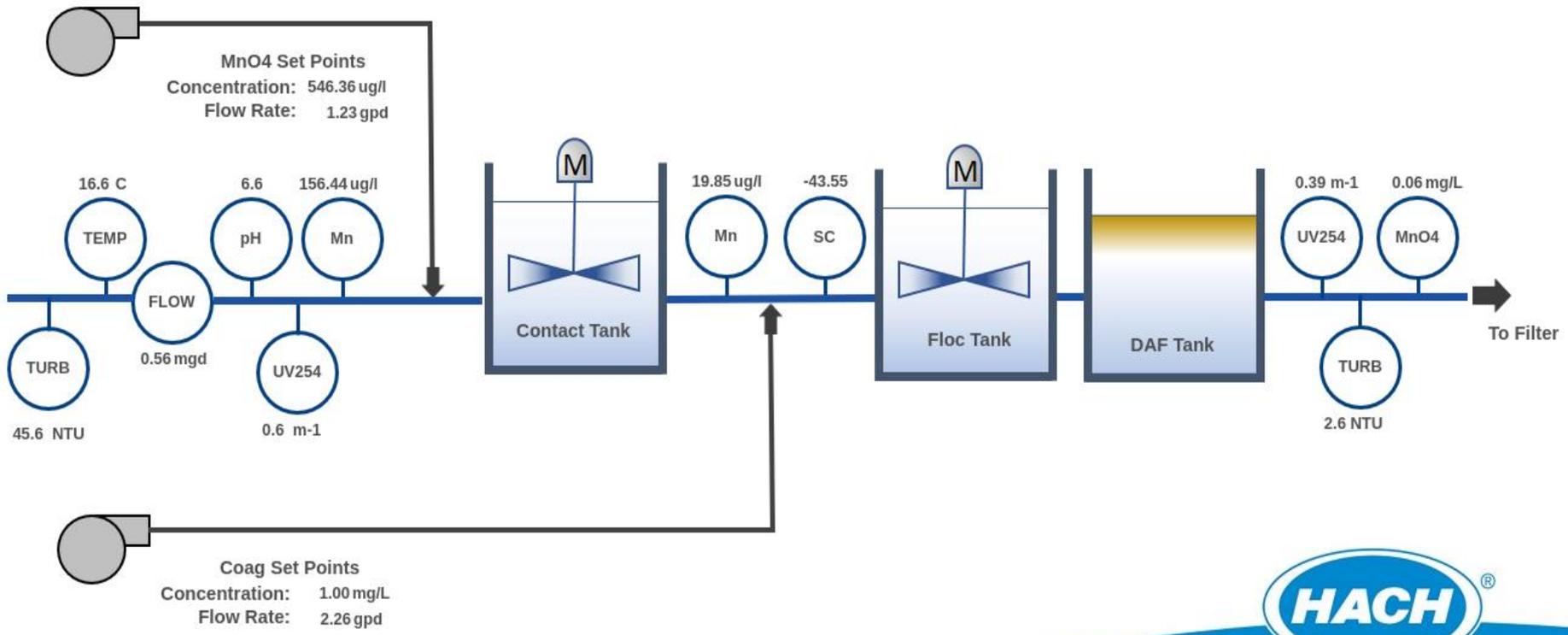
# CONTROLLER FRAMEWORK OVERVIEW



# USER INTERFACE OVERVIEW



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# NEXT STEPS

- Installation and Startup - Spring/Summer 2020 - Future
  - Validation of the Feed forward models
  - Tune MnO<sub>4</sub> Control
  - Confirmation of the intended goals have been achieved
    - Use of real time measurements to adjust Permanganate dosage
    - Use of historical instrumentation, operational, and laboratory data to build a feedforward model to predict the optimal PACL Dosage



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# QUESTIONS

# DATA COLLECTION – SOURCES

## Laboratory & Operations

- Raw & Prefilter Total Hardness
- Raw & Prefilter Total Alkalinity
- PACL Dosage
- Historical Total Mn
- Historical Sensor Data

## Online Sensors

- Raw & Prefilter UV254
- Raw & Prefilter Turbidity
- Raw & Post Mn
- Raw & Prefilter pH
- Streaming Current
- Raw Conductivity

## 15 Total Sources of Data

- Raw Water 7
- Post Treatment 7
- Operation 1

# UV % REGRESSION

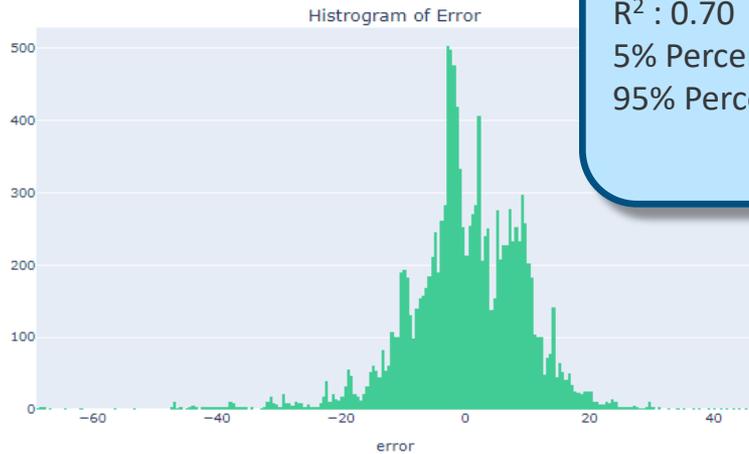


## UV % Regression Results:

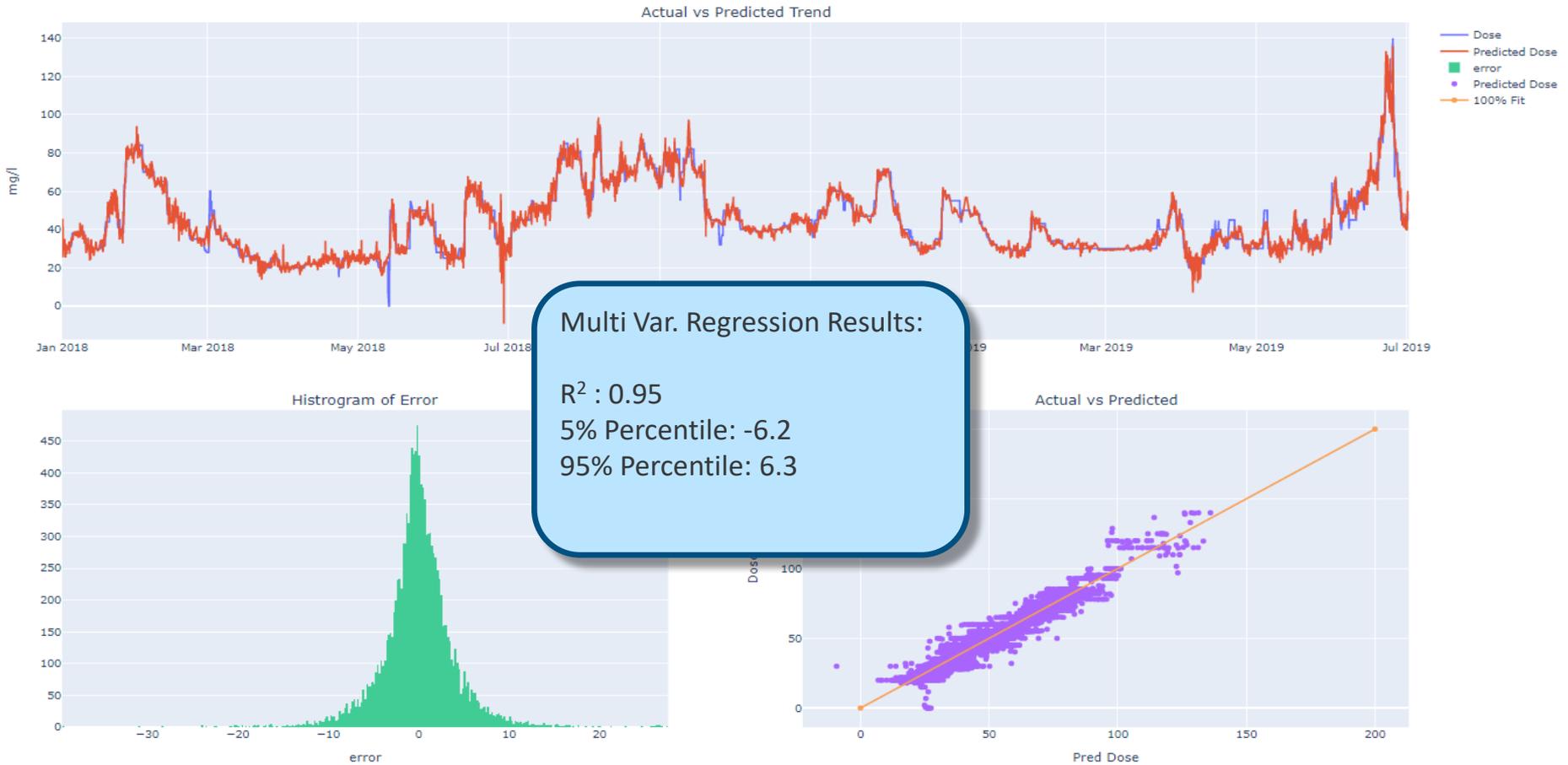
$R^2 : 0.70$

5% Percentile: -15

95% Percentile: 14



# MULTI – VARIABLE REGRESSION RESULTS



# RAW TURBIDITY AND UV TRANSMITTANCE PACL DOSAGE RATIO

## Ratio Results:

### Turbidity

Median Ratio: 3.6

$R^2$  : -2.6

5% Percentile: -31

95% Percentile: 56

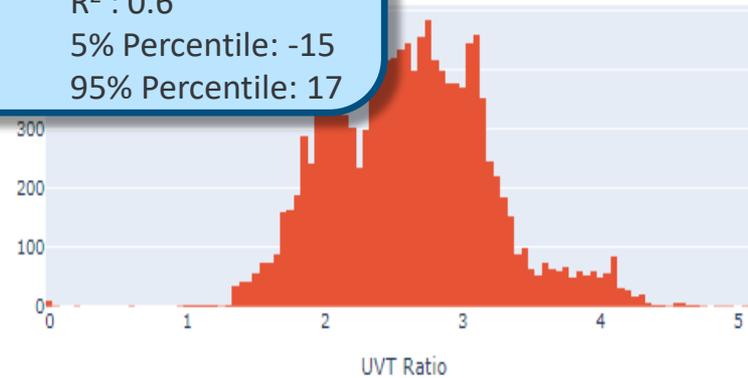
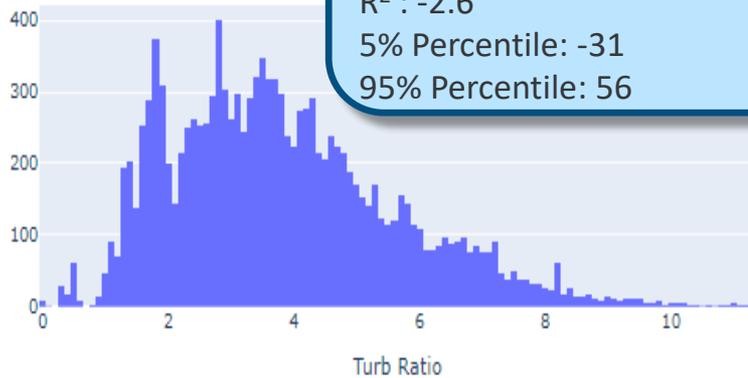
### UV Transmittance

Median Ratio: 2.6

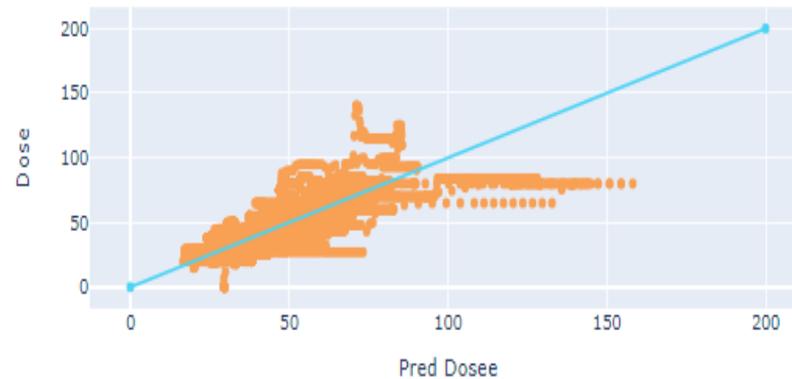
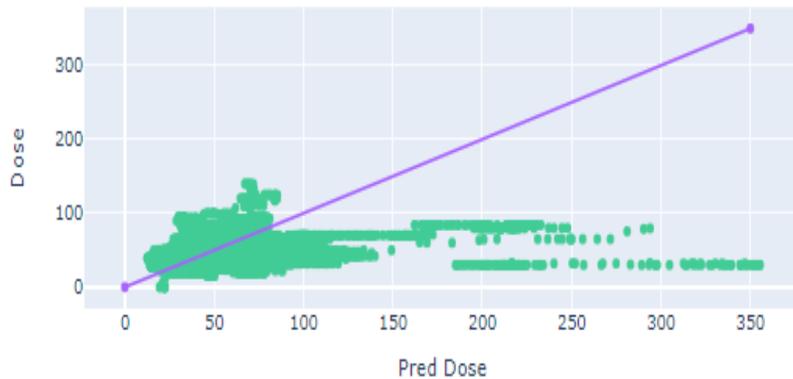
$R^2$  : 0.6

5% Percentile: -15

95% Percentile: 17



- Turb Ratio
- UVT Ratio
- Turb Ratio
- 100% Fit
- UVT Ratio
- 100% Fit



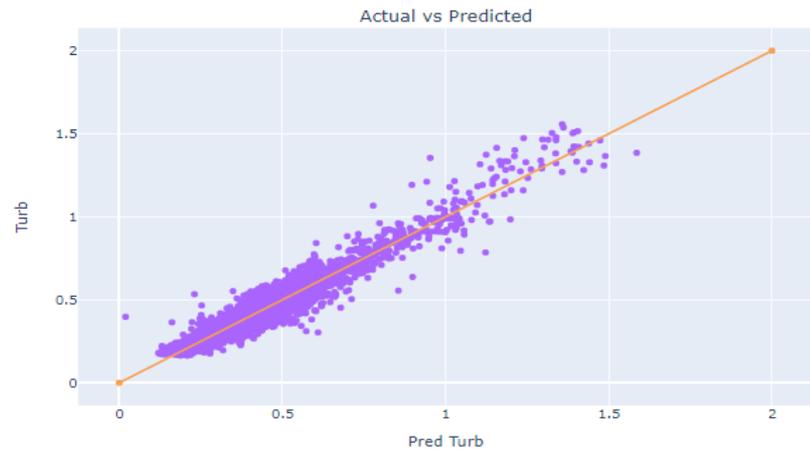
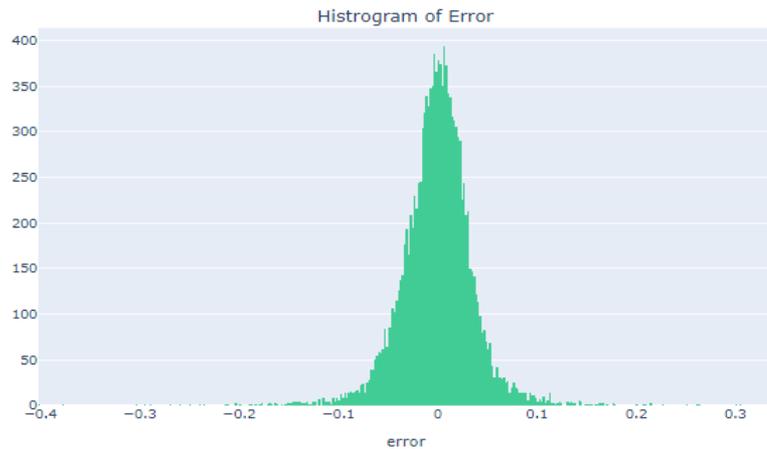
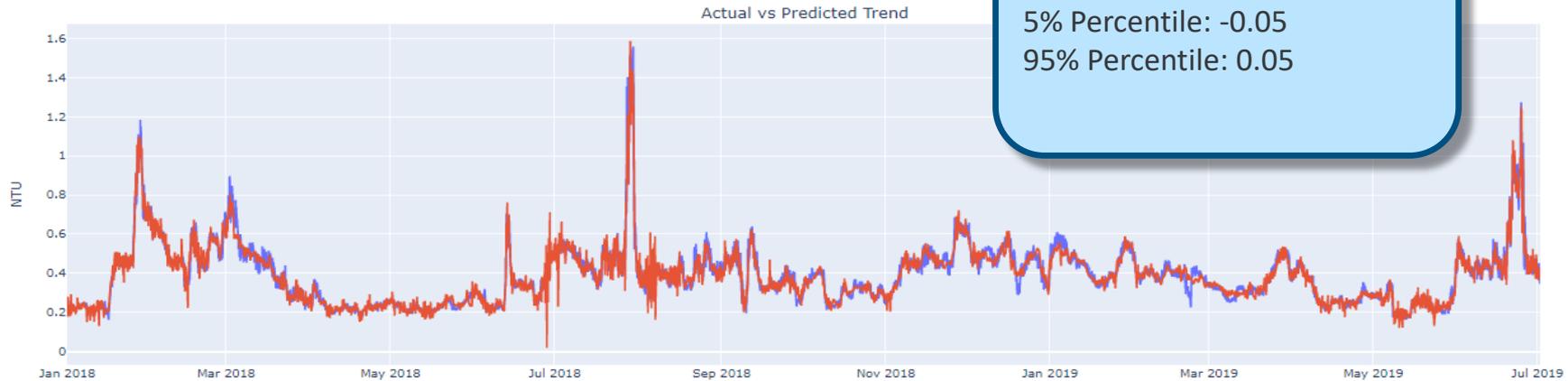
# MULTI – VARIABLE REGRESSION RESULTS TO PREDICT PRE FILTER TURBIDITY

Multi Var. Regression Results:

$R^2 : 0.92$

5% Percentile: -0.05

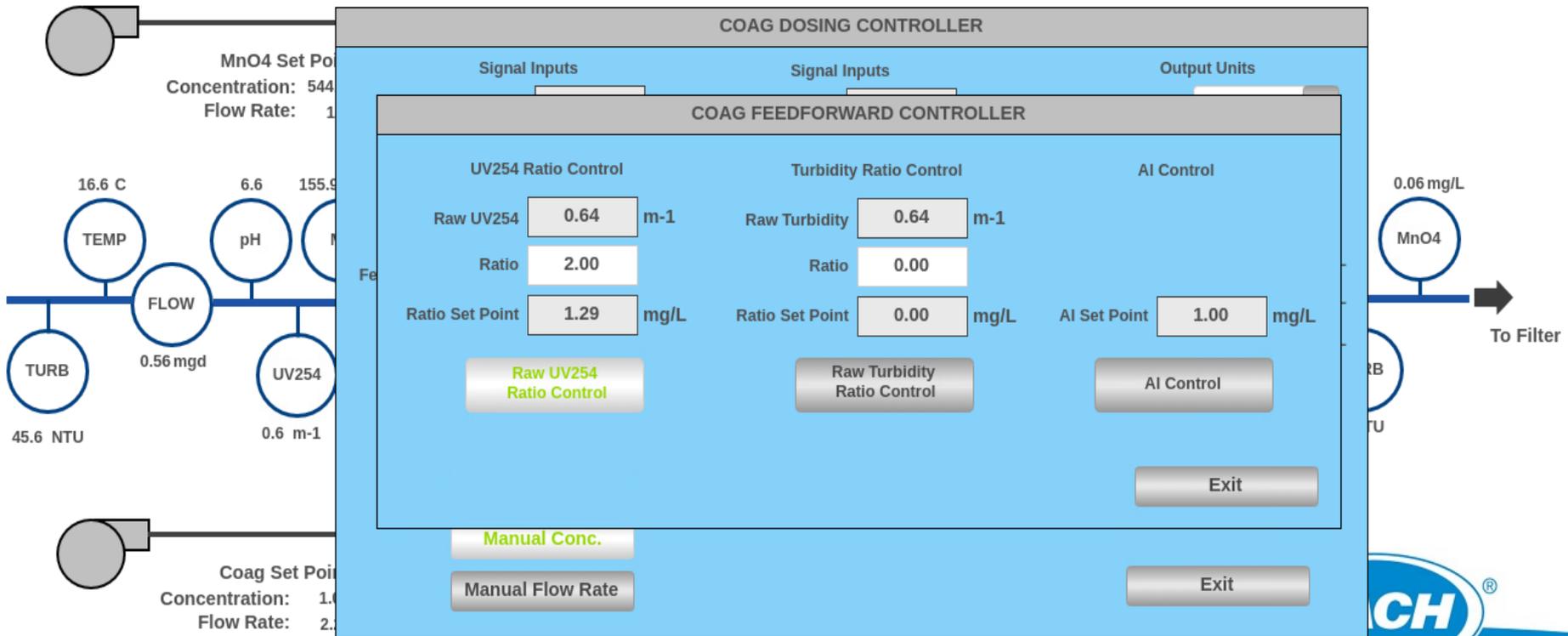
95% Percentile: 0.05



# USER INTERFACE OVERVIEW



WESTERN BERKS WATER AUTHORITY



# SUMMARY

- Managnese
  - Equipment Install
  - Integration with existing Scada
- Coagulation
  - Tuning of the feedback loops
  - Validation of the Feed forward models
  - Confirmation of the intended goals have been achieved
    - Use of real time measurements to adjust Permanganate dosage
    - Use historical instrumentation, operational, and laboratory data to build a feedforward model to predict the optimal PACL Dosage