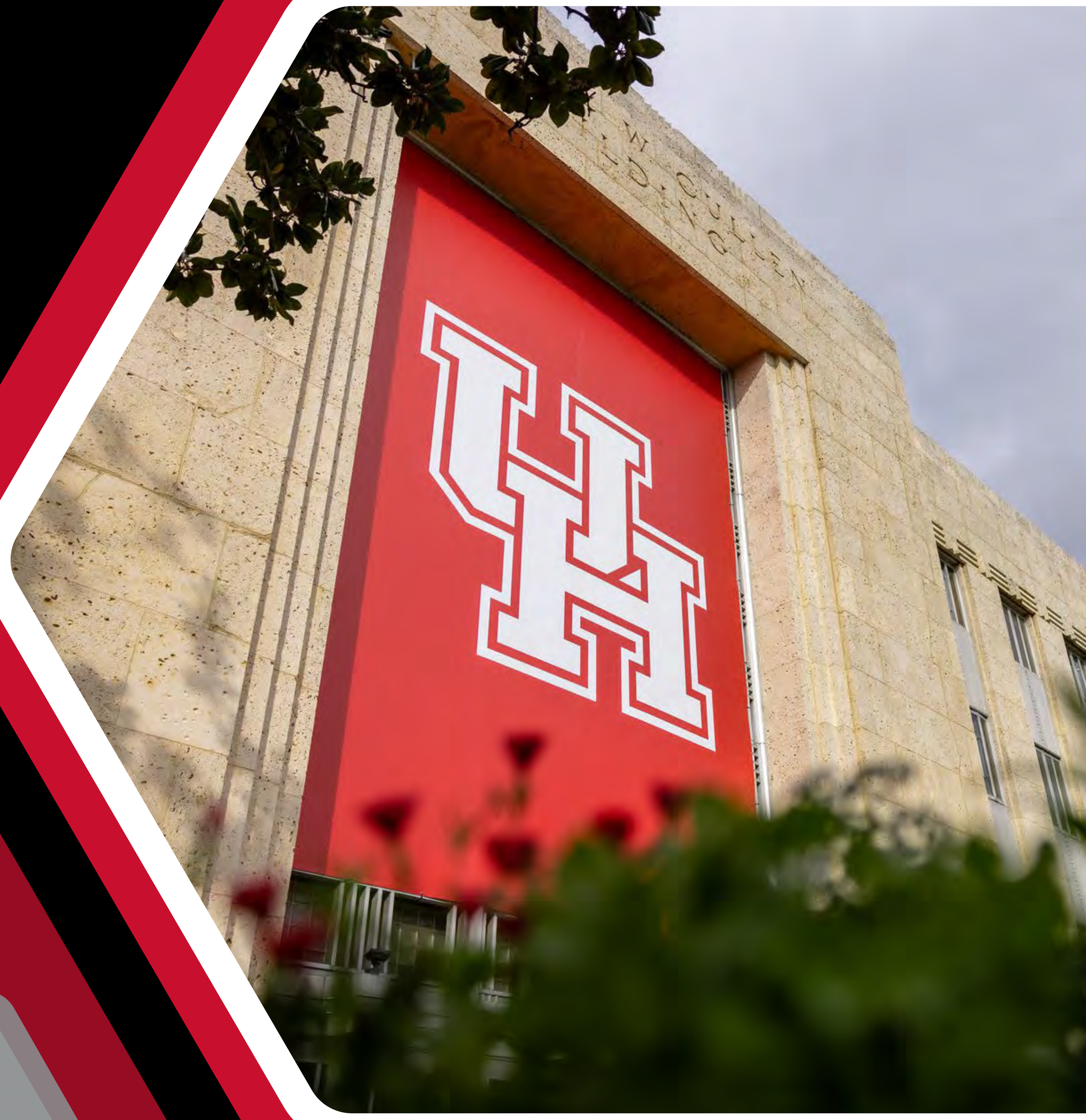
UH Energy
UNIVERSITY OF HOUSTON

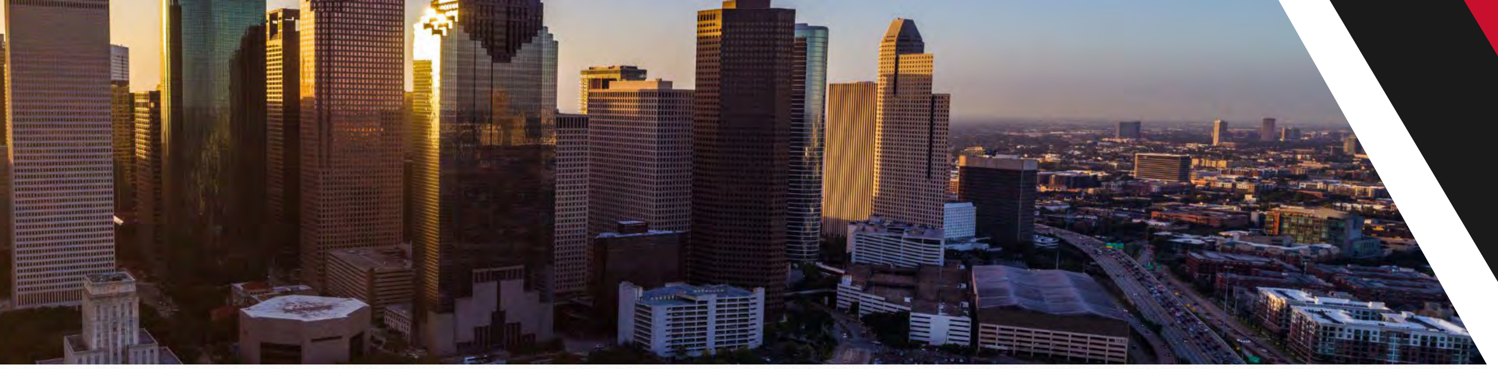
SOUTH TEXAS SECTION OF THE AMERICAN INSTITUTE OF CHEMICAL ENGINEERS

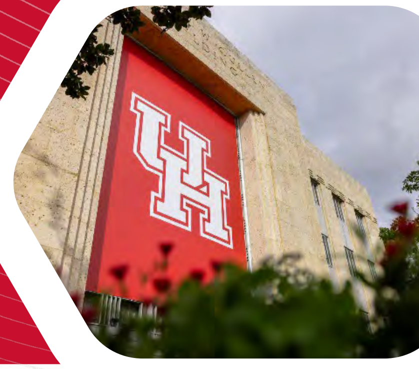
16th STS-AIChE Southwest Process Technology Conference

Sept 22-23, 2025

University of Houston







Experiences with process modeling of municipal and industrial wastewater treatment facilities

Andrew R. Shaw, Ph.D., P.E., ENV SP, BCEE – Global Practice & Technology Leader

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Black & Veatch, Houston TX

What to Expect

- Evolution of Process Design
- Why Modelling?
- Process Modelling Application: Examples
- Benefits of Using Models
- Takeaway Message

Evolution of Process Design

"Rule of Thumb" Approach

Empirical Approach

Kinetic Equation Approach

Modelling Approach

“Rule of Thumb” Approach

- E.g. TCEQ Guidelines or Ten States Standards

Table F.1. - Design Organic Loading Rates for Sizing Aeration Basins Based on Traditional Design Methods

Process	Applicable Permit Effluent Sets *Concentration milligrams per liter (mg/l)*			Maximum Organic Loading Rate *Pounds BOD_5/day/1,000 cubic feet (lbs/day/1,000cf)*
	Five-day Biochemical Oxygen Demand (BOD_5)	Total Suspended Solids (TSS)	Ammonia Nitrogen	
Conventional activated sludge process without nitrification	10	15	NA	45
	20	20	NA	
Conventional activated sludge process with nitrification when reactor temperatures exceed 15° C	10	15	3, 2, or 1	35

- Process should work well below a certain loading rate.
- Loadings established based on many years of experience.
- “Tried and true” rules of thumb.

Empirical Data Approach

- Design Curves
- - E.g. Trickling Filter Removal Rates

- Data points are actual performance values for several plants
- Gray area shows range of expected performance

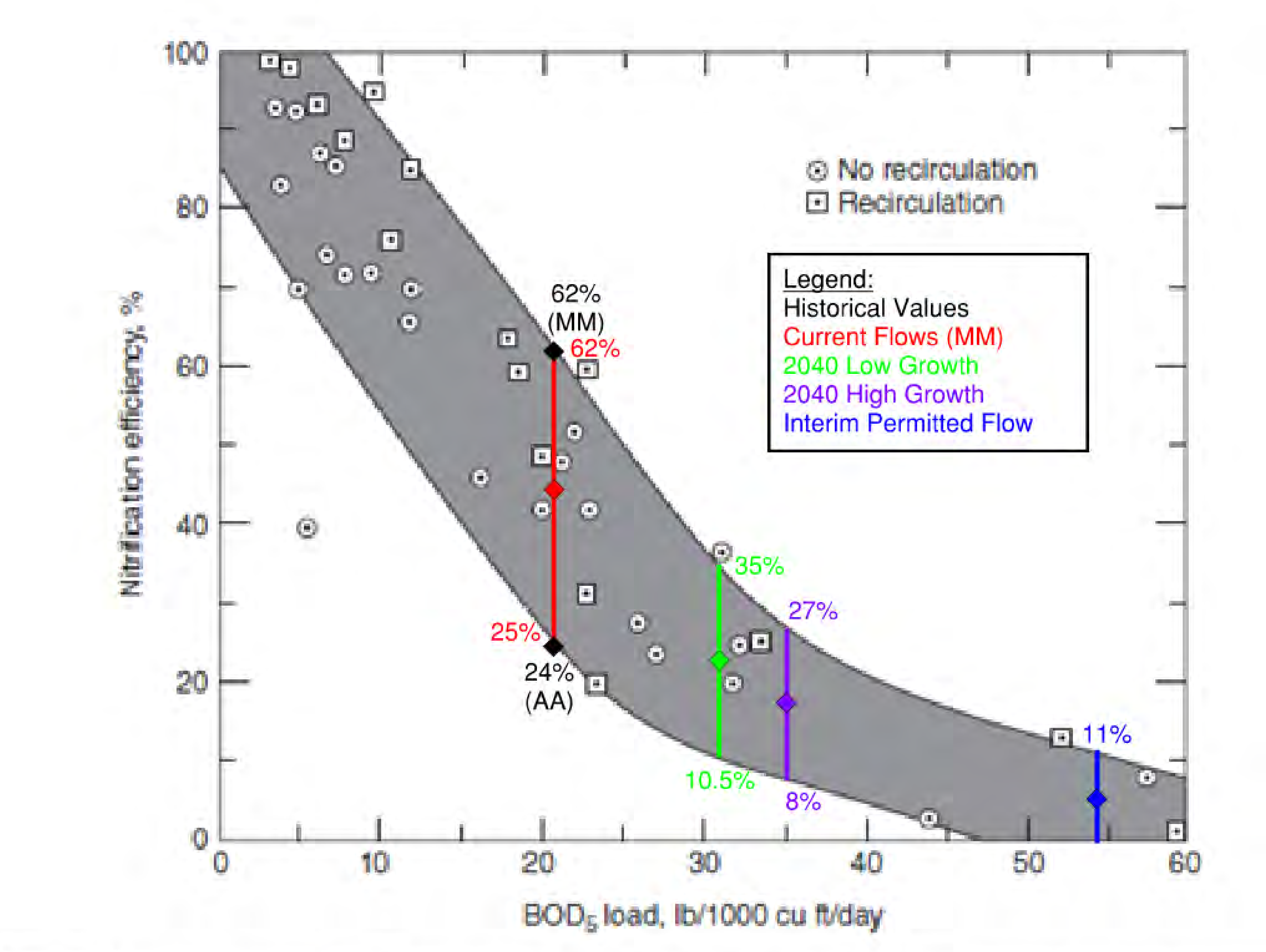


Figure 11.63 Effect of organic load on nitrification efficiency of rock trickling filters (lb/d/1000 cu ft × 0.016 02 = kg/m^3·d).

Kinetic Equation Approach

- Metcalf & Eddy – Example using biokinetic equations

Table 8–10

Summary of equations used in the analysis of suspended growth processes

Application	Equation	Eq. No.
Temperature	$k_T = k_{20}\theta^{(T-20)}$	1–44
Rate of sCOD Utilization	$r_{su} = \frac{kXS}{K_s + S}$	7–12
	$\mu_{max} = Yk$	7–16
Rate of NH_4-N Oxidation	$r_{NH_4} = \left(\frac{\mu_{max,AOB}}{Y_{AOB}}\right)\left(\frac{S_{NH_4}}{S_{NH_4} + K_{NH_4}}\right)\left(\frac{S_o}{S_o + K_{o,AOB}}\right)X_{AOB}$	7–101
Rate of NO_3-N Utilization	$r_{NO_3} = \left(\frac{1 - 1.42Y_H}{2.86}\right)\left[\frac{\mu_{H,max}S_s}{Y_H(K_s + S_s)}\right]\left(\frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}}\right)\left(\frac{K'_o}{K'_o + S_o}\right)(\eta)X$	7–133
Specific Growth Rate and SRT	$\mu_{AOB} = \mu_{max,AOB}\left(\frac{S_{NH_4}}{S_{NH_4} + K_{NH_4}}\right)\left(\frac{S_o}{S_o + K_{o,AOB}}\right) - b_{AOB}$	7–94
	$SRT = \frac{1}{\mu_{AOB}}$	7–98
	$SF = SRT_{des}/SRT_{min}$	7–73
Biomass Production, Heterotrophs (VSS)	$P_{X,bio} = \frac{QY_H(S_o - S)}{1 + b_H(SRT)} + \frac{(f_d)(b_H)QY_H(S_o - S)SRT}{1 + b_H(SRT)}$	8–20 (A + B)
Sludge Production ($P_{x,VSS}$)	$P_{x,VSS} = P_{X,bio} + \frac{QY_n(NO_x)}{1 + b_n(SRT)} + Q(nbVSS)$	8–20
Sludge Production ($P_{x,TSS}$)	$P_{x,TSS} = \frac{P_{X,bio}}{0.85} + \frac{QY_n(NO_x)}{0.85[1 + b_n(SRT)]} + Q(nbVSS) + Q(TSS_o - VSS_o)$	8–21
Reactor Mass and Volume	$Mass = X_{VSS}(V) = (P_{X,VSS})SRT$	7–56
	$Mass = X_{TSS}(V) = (P_{X,TSS})SRT$	7–57
SRT	$SRT = \frac{VX}{(Q - Q_w)X_e + Q_wX_R}$	8–27
	$SRT = \frac{V}{Q_w}$	8–31
	$SRT = \frac{\left(\frac{R}{1 + R}\right)V_A + V_M}{Q_w}$	8–36
CMAS Effluent bsCOD	$S = \frac{K_s(1 + b_H SRT)}{SR\ldots}$	7–46
CMAS Biomass	$X = (\ldots$	
CMAS Oxygen Req'd	$R_o = \ldots$	
Ammonia oxidized	$NO_x = \ldots$	
Stage Reactor Oxygen Req'd	$R_{o,i} = \ldots$	
Food to Mass Ratio	$F/M = \ldots$	
Organic Loading	$L_{org} = \frac{\ldots}{(V)}$	7–69

9. Design MLSS X_{TSS} concentration = 3000 g/m³; values of 2000 to 3000 g/m³ can be considered
10. Peak to average TKN loading rate ratio = 1.5

Solution, Part A—BOD removal without nitrification

1. Develop the wastewater characteristics needed for design.
   a. Find bCOD.

   bCOD = 1.6 (BOD) = 1.6 (140 g/m³) = 224 g/m³

   b. Find nbCOD using Eq. (8–12).

   nbCOD = COD − bCOD = (300 − 224) g/m³ = 76 g/m³

   c. Find effluent nonbiodegradable sCOD ($nbsCOD_e$).

   $nbsCOD_e$ = sCOD − 1.6 sBOD
   = (132 g/m³) − (1.6)(70 g/m³) = 20 g/m³

   d. Find nbVSS using Eq. (8–7, 8–8 and 8–9).

   nbpCOD = TCOD − bCOD − nbsCODe

   nbpCOD = (300 − 224 − 20) g/m³ = 56 g/m³

   $$VSS_{COD} = \frac{TCOD - sCOD}{VSS}$$

   $$VSS_{COD} = \frac{(300 - 132)\text{g/m}^3}{60\text{ g/m}^3} = 2.8\text{ g COD/g VSS}$$

   $$nbVSS = \frac{nbpCOD}{VSS_{COD}}$$

   $$nbVSS = \frac{56\text{ g COD/m}^3}{2.8\text{ g COD/g VSS}} = 20.0\text{ g nbVSS/m}^3$$

   e. Find the iTSS.

…emoval only.
…(8–20) in Table 8–10.

… − S)SRT
…RT)

Q = 22,500 m³/d

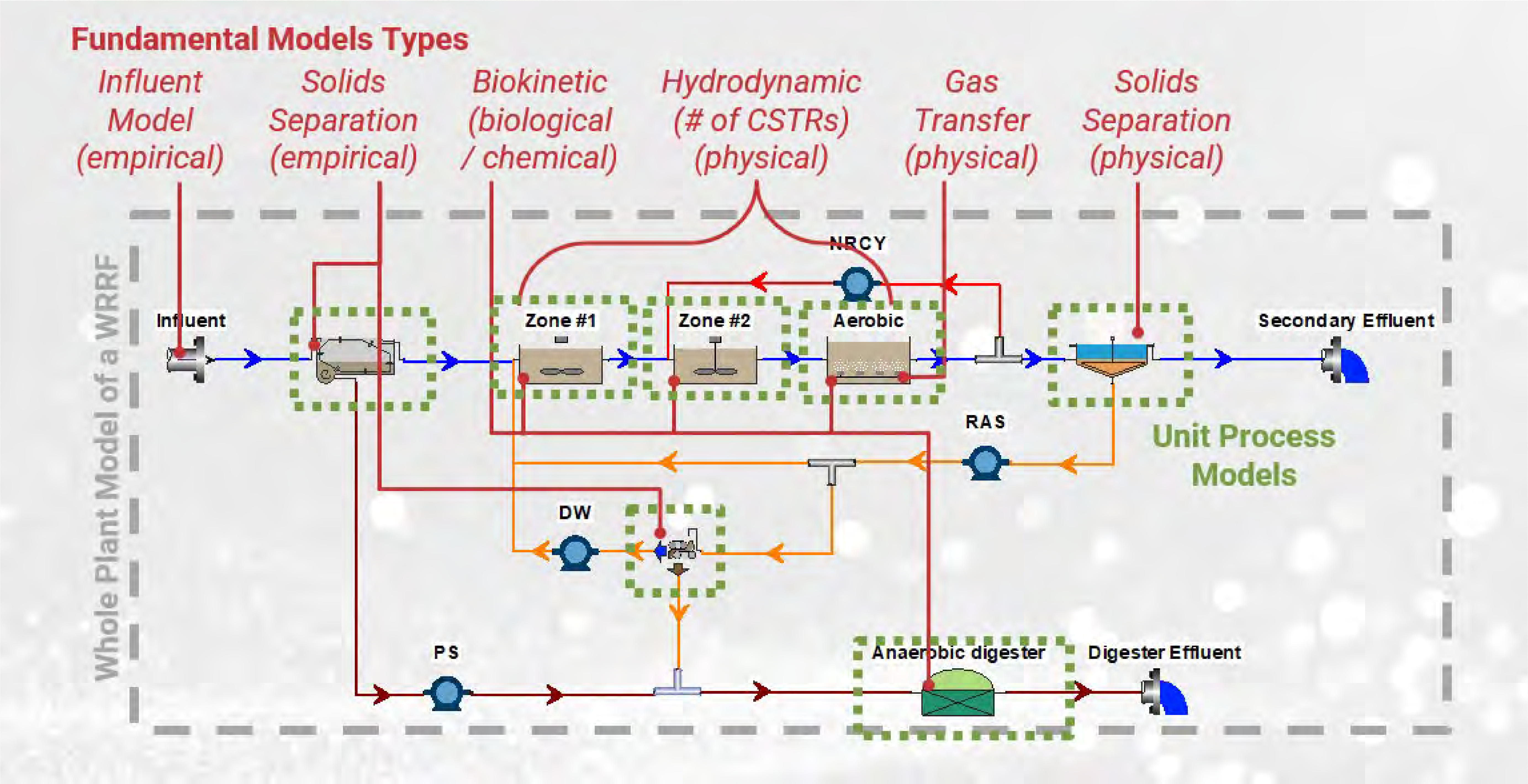
WAS Production

2. Design suspended growth system for BOD removal only.
   a. Determine biomass production using Eq. (8–20) in Table 8–10.

$$P_{X,Bio} = \frac{QY_H(S_o - S)}{1 + b_H(SRT)} + \frac{(f_d)(b_H)QY_H(S_o - S)SRT}{1 + b_H(SRT)}$$

Use of Process Models

- A sophisticated method combining both empirical and biokinetic equations



Why Modelling?

Why Modeling?

- Cost Benefits
- Modeling for Design and Operations
    - Simple applications
    - More complex applications
- Preferred Approach for Nutrient Removal

Cost Benefits

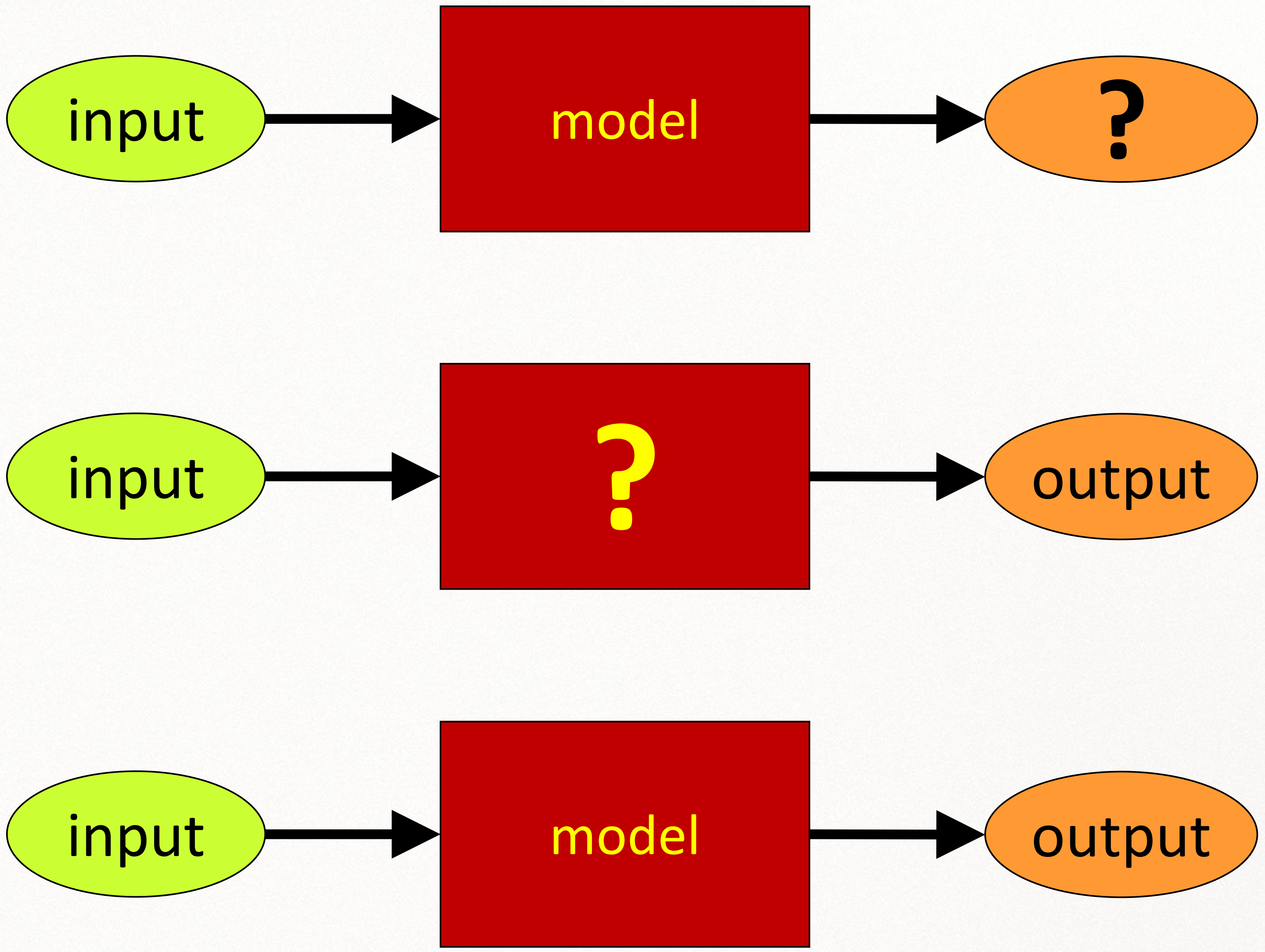
Photo by Celyn Kang on Unsplash

- Modeling is cheaper than piloting
- Modeling is much cheaper than full-scale
- Try things in *Virtual Space* before trying it in *Real Space*

$5k-$100k → $100k-$2M → $2M - ???

Model → Pilot → Full-scale

Modelling both Simple and Complex Scenarios



… predict

… understand

Can help bridge gaps in the data – useful for mass balancing.

… communicate

Preferred Approach for Nutrient Removal

- Plantwide Mass Balances
- BNR design
- Dynamic models give us max/min and averages
  - Blower sizing
  - Diffusers
  - Pumping
- Sensitivity analyses

United States Environmental Protection Agency | Office of Research and Development Washington, DC 20460 | EPA/600/R-10/100 August 2010

EPA

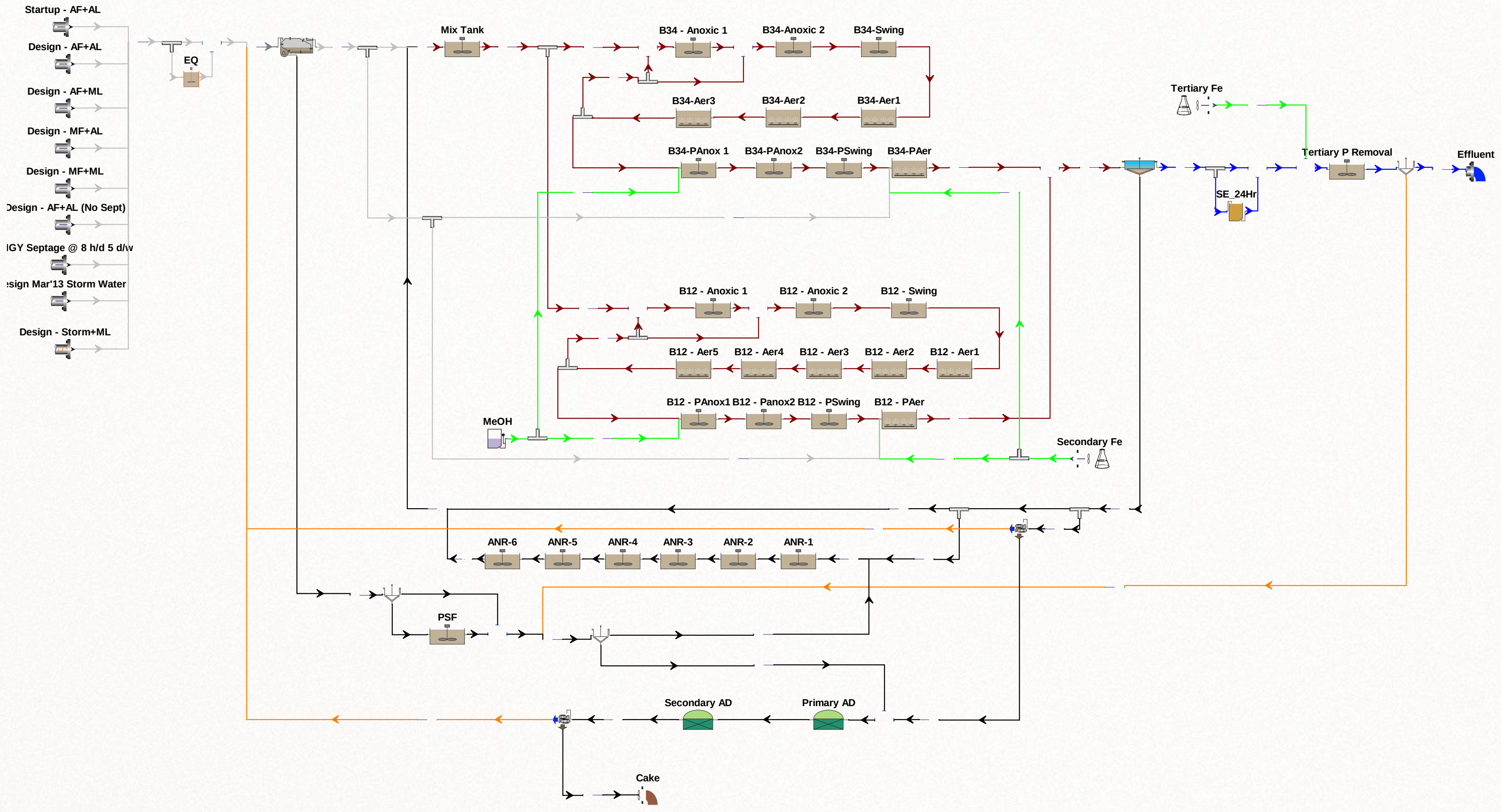
Nutrient Control Design Manual

"…modeling is the recommended approach for designing WWTP upgrades for biological nutrient removal (BNR) because of (1) its flexibility in enabling designers to quickly test many different configurations and operating scenarios and (2) its ability to simulate treatment performance under a wide range of conditions using dynamic modeling."

Simulator Options

- BioWin (Envirosim)
- GPS-X (Hatch/Hydromantis)
- SIMBA# (IFAK / InCtrl Solutions)
- SUMO (Dynamita)

BioWin

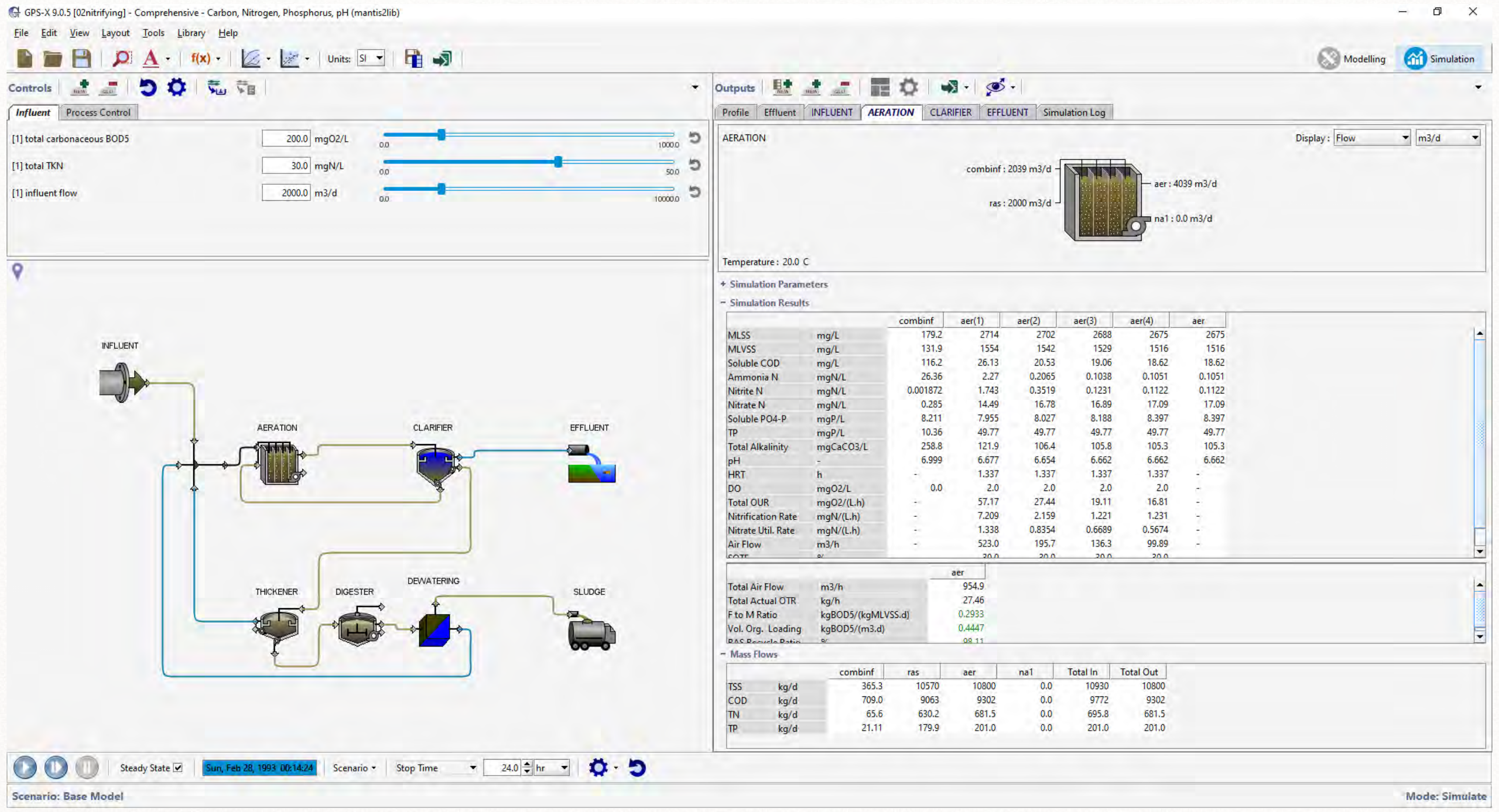


BioWin is easy to set up but offers fewer features.

Most widely adopted within industry (but maybe being usurped by Sumo?)

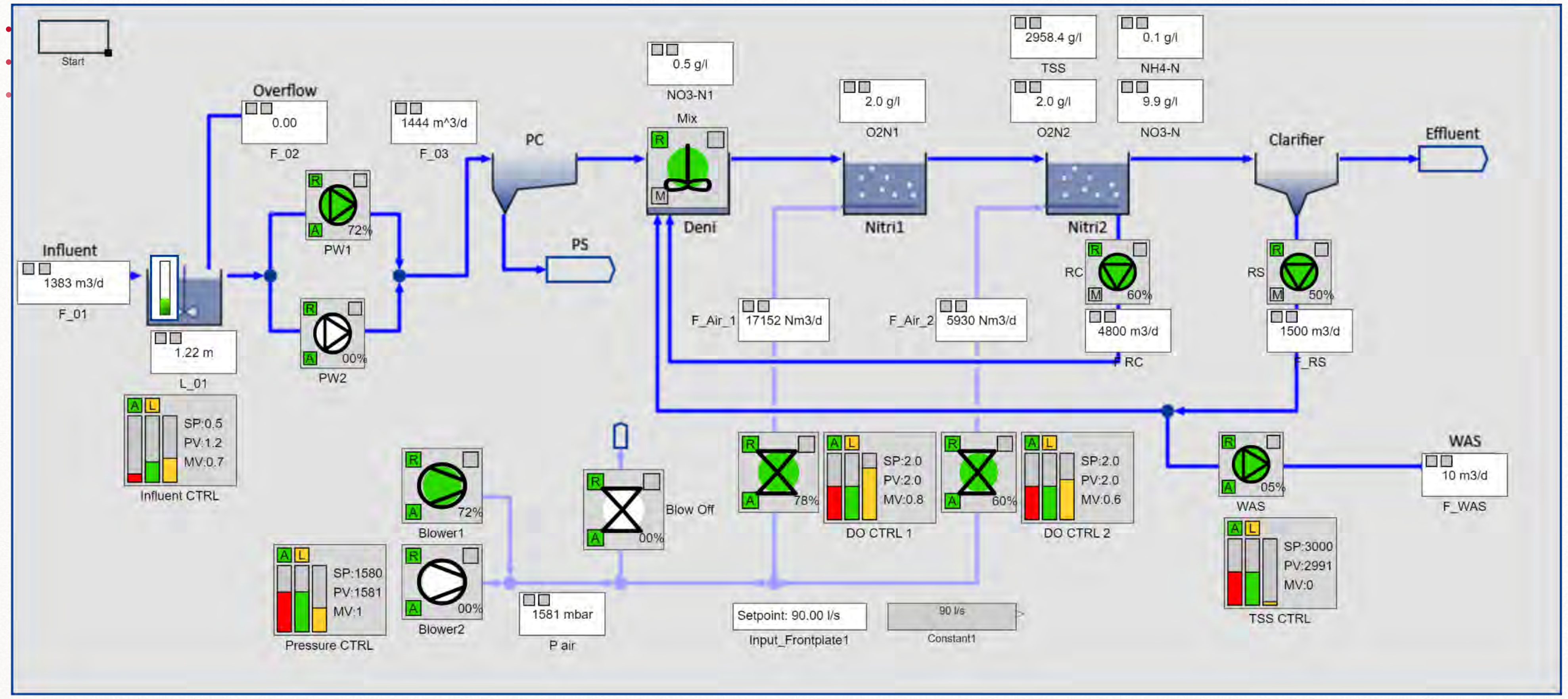
HYDROMANTIS

GPS-X

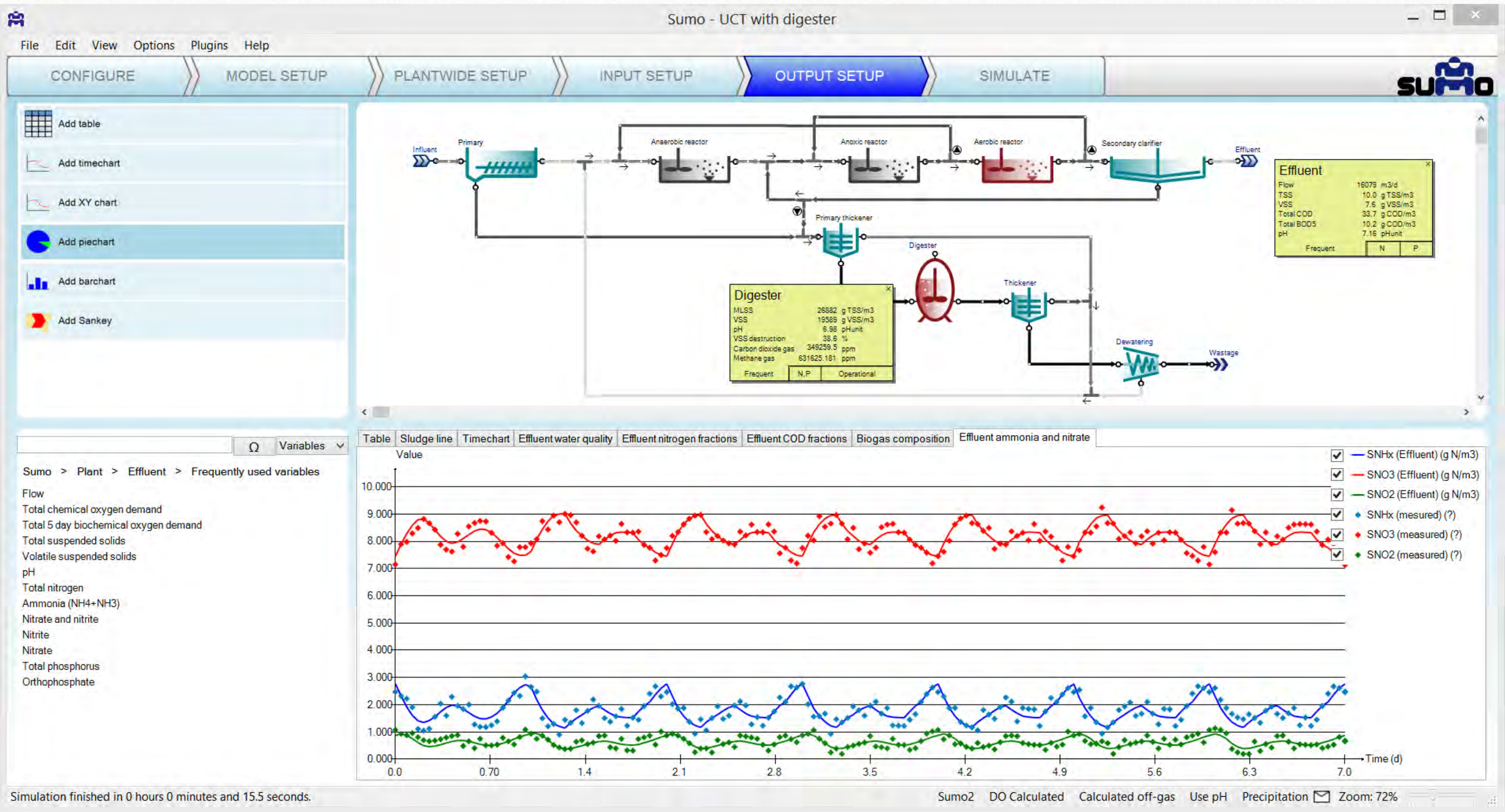


GPS-X is more challenging to build models but has more capabilities and is easier to edit inputs and run simulations after being built.

Includes industrial library.



Additional capabilities to aid in design of mechanical equipment and add value to operational modeling especially with respect to control.



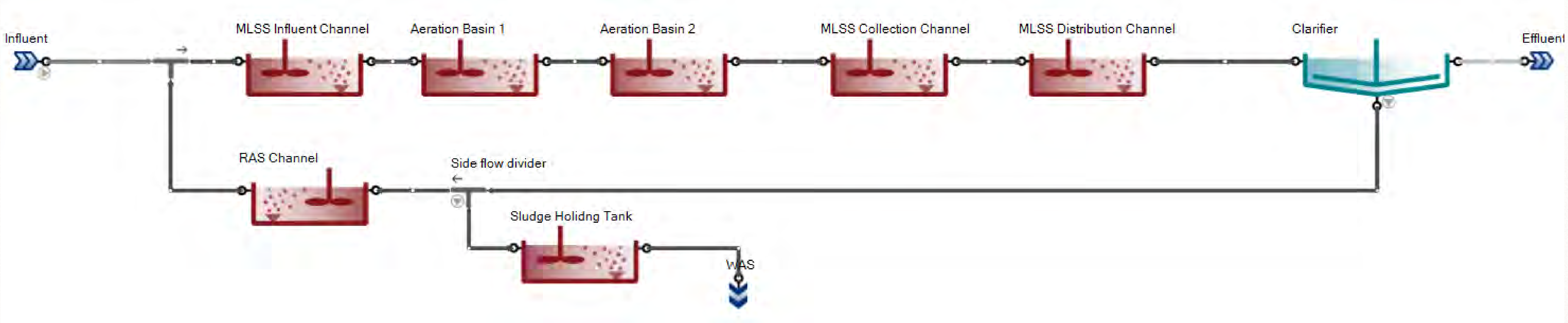
“New Kid on the Block”

Open model source code, fast and with a modern interface. Quickest to market in adding new features and easiest to modify biokinetic equations.

Process Modelling Application Examples

Treatment Plant Expansion (Houston Area)

- **Problem Statement-** Waste Activated Sludge Pumps and Blowers Sizing
- **Approach**
- Size the basins based on TCEQ guidelines
- Set up a calibrated model using design criteria
  - Set up the SRT tool in the model to estimate WAS
  - Extract Oxygen Uptake Rates (OURs) for the airflow calculation



Treatment Plant Expansion (Houston Area)

WAS Pump Sizing

Model Outputs

Name	WAS	Unit
Total suspended solids (TSS)	8720	lbs TSS/d
Flow rate	0.52	MGD
Total suspended solids (TSS)	2008	mg TSS/L

<u>Operational Range</u>

Concentration : 3000 to 6500 mg/L

Flow: 160 to 520 gpm

Blower Sizing

Model Outputs

Name	MLSS Influent Channel	Aeration Basin 1	Aeration Basin 2	MLSS Collection Channel	Unit
Oxygen uptake rate (OUR)	42.1	36.4	16.4	8.1	mg O2/L/h

<u>Operational Range</u>

Airflow: 8100 to 15500 scfm

<u>Model Benefit</u> - More Accurate WAS Pump and Blower Sizing.

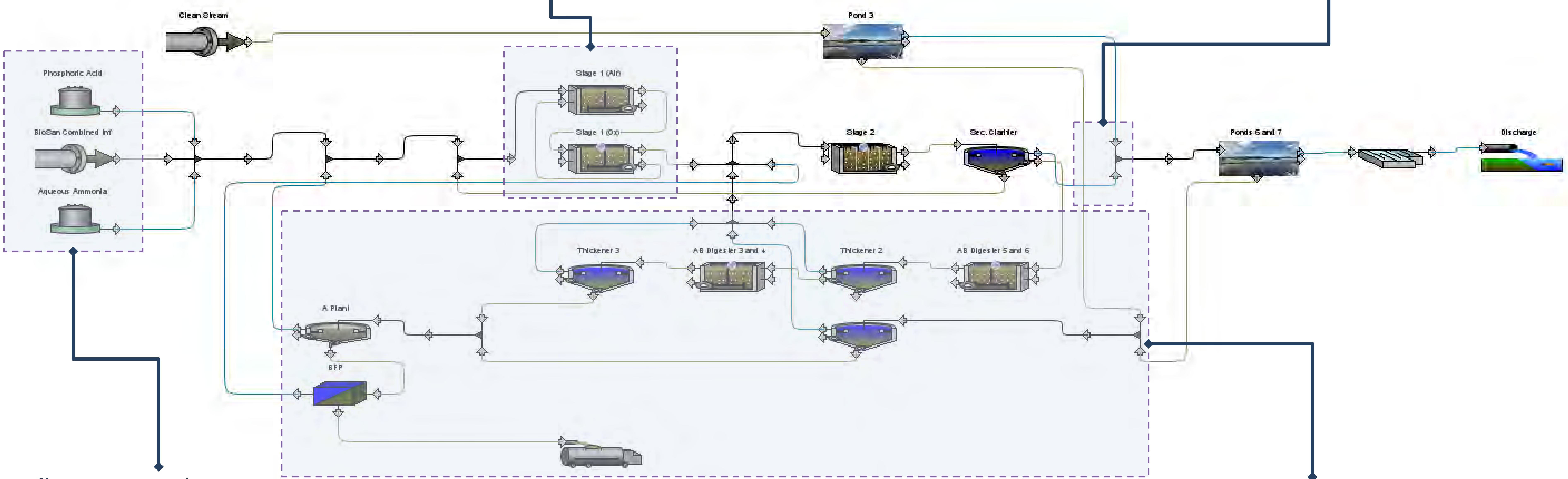
Gulf Coast Authority– Bayport Facility

- **Problem Statement**
  - Model a Pure Oxygen and Air Activated Sludge System for an Industrial Facility
  - Investigate Effluent Elevated Ammonia

Bayport Facility Process Model

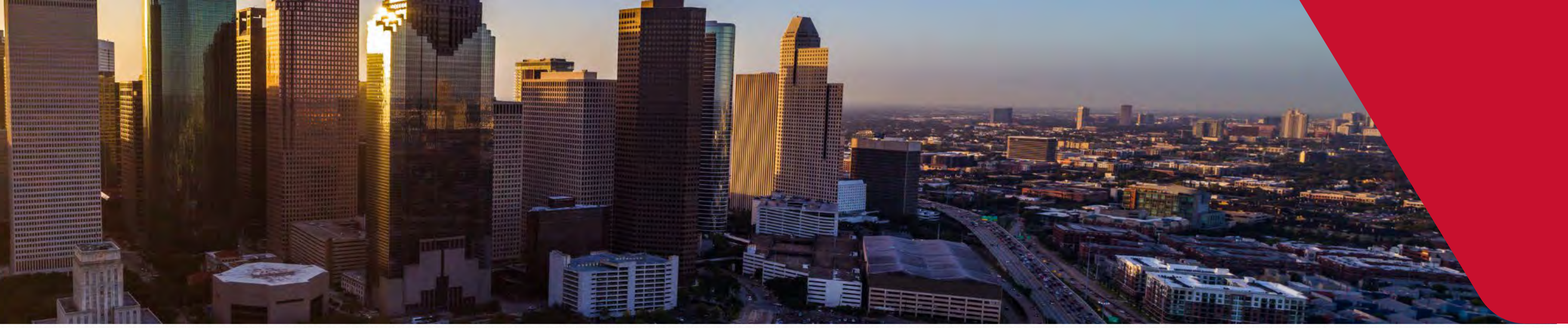
2 Modelling an Oxygen and Air System Together

3 Combination of "Clean Stream" and Biologically-treated Stream



1 Influent + Track Nutrient Requirements

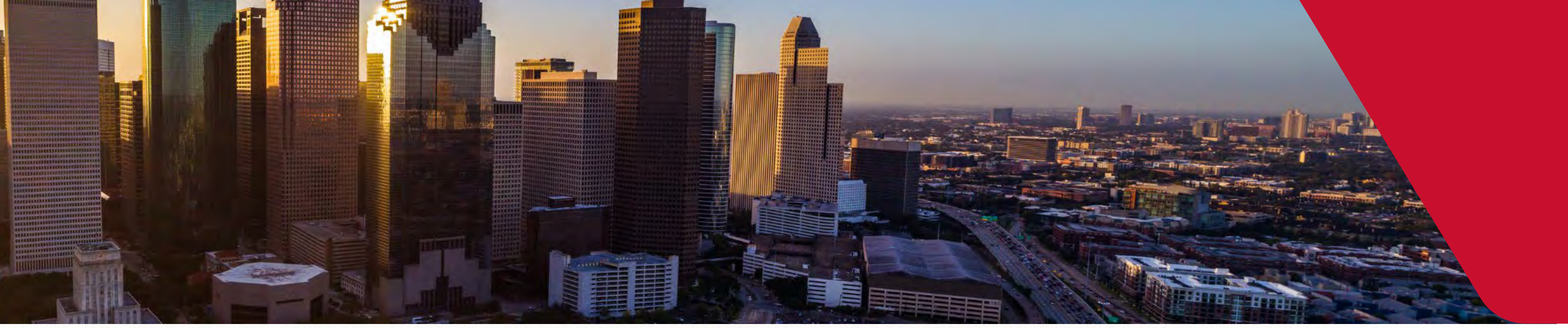
4 Repurposed Tankage for Biosolids Handling



Elevated Ammonia Investigation

Potential Cause	Approach	Model Findings	
Ammonification Rate Low	Adjusted Ammonification Rates	Increased Effluent TKN not NH_4-N	✗
Inhibition of Nitrification	Altering Half-saturation Coefficient	Increased Effluent NH_4-N	✓
Competition with Heterotrophs	Nutrient N, P Deficiency	Increased Effluent NH_4-N	✓

<u>Model Benefit- </u>Enabled to narrow the focus as the client is looking for answers



Benefits of Using Process Simulators/Modeling

- Modeling is cost-effective
- Models useful for simple calculations
  - Sludge Production and Airflow Requirements (1st case-study)
- Models for more complex applications
  - Investigation or troubleshooting (2nd case-study)

What's Next? Digital Twins!

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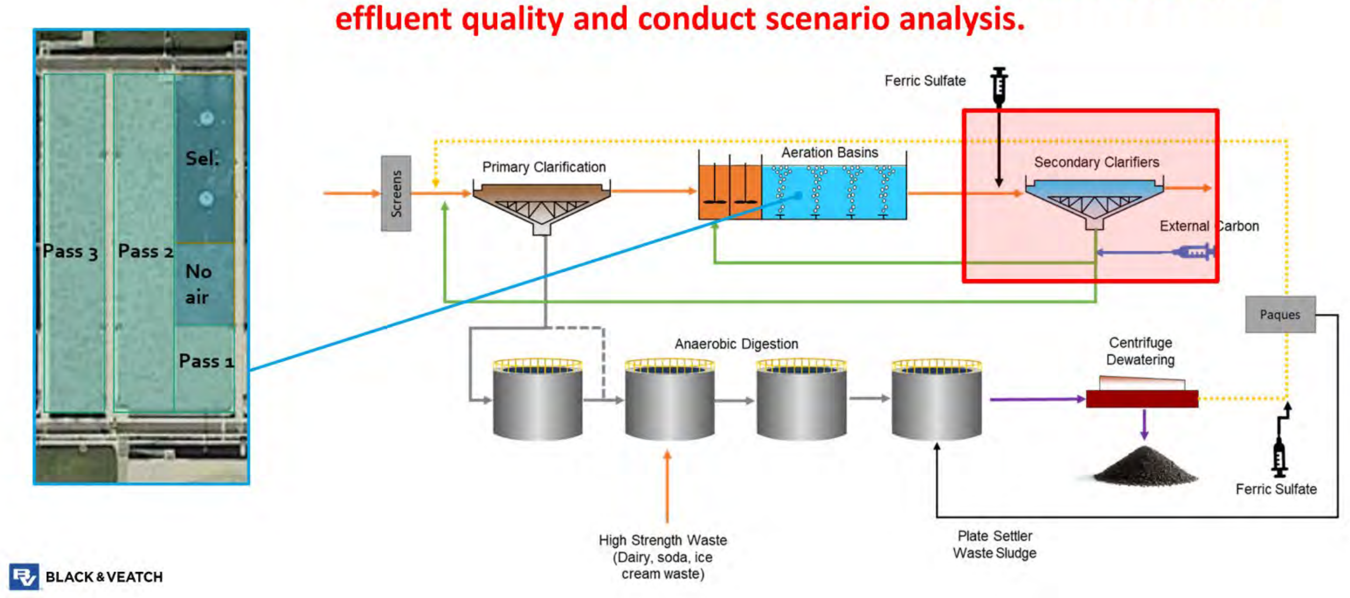
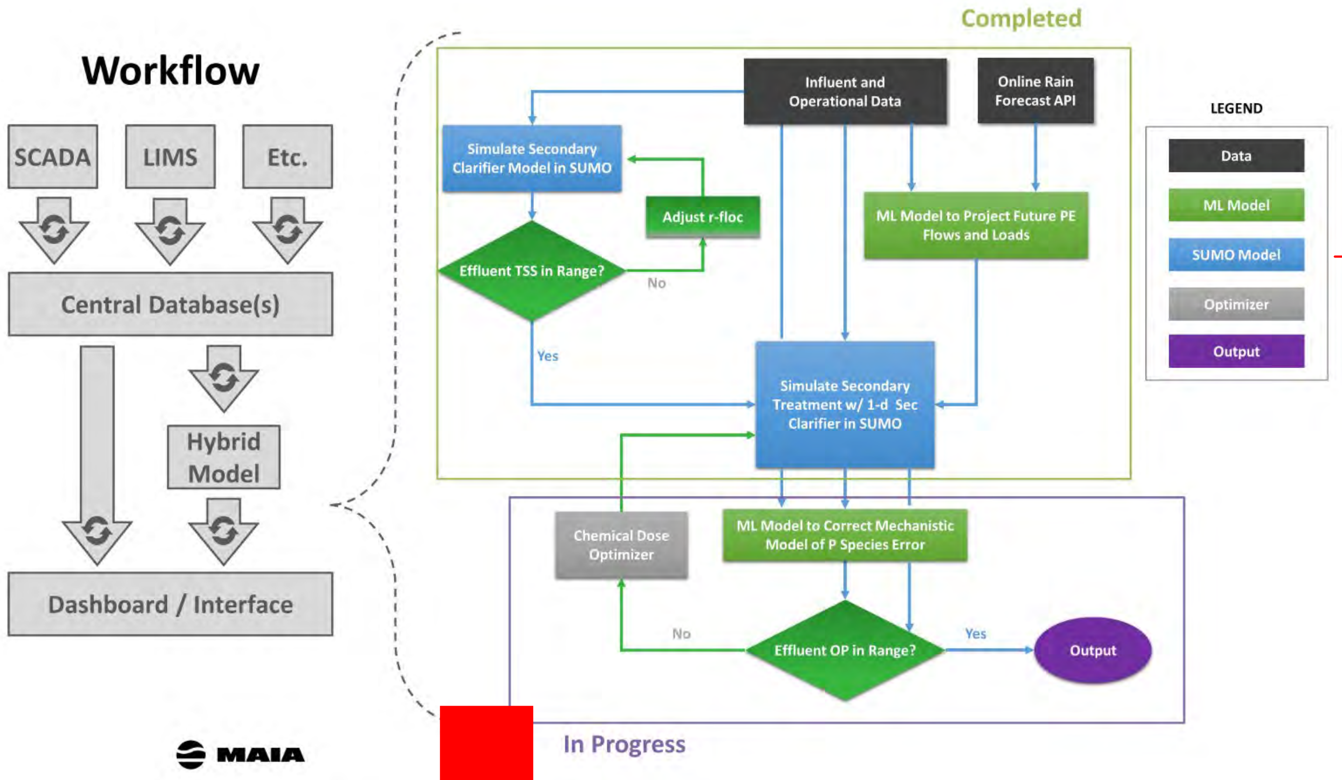
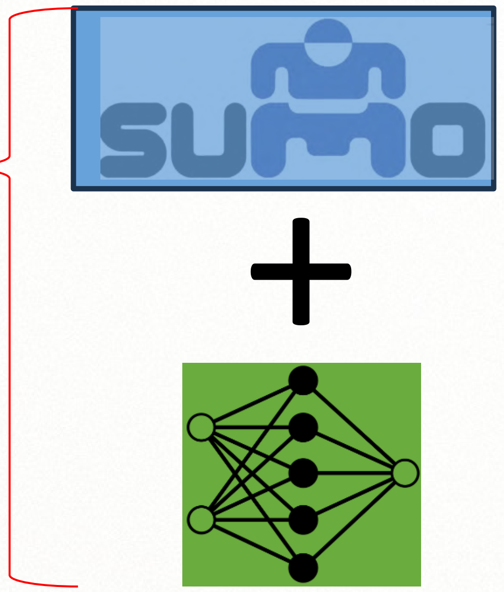
Fond du Lac Hybrid Model

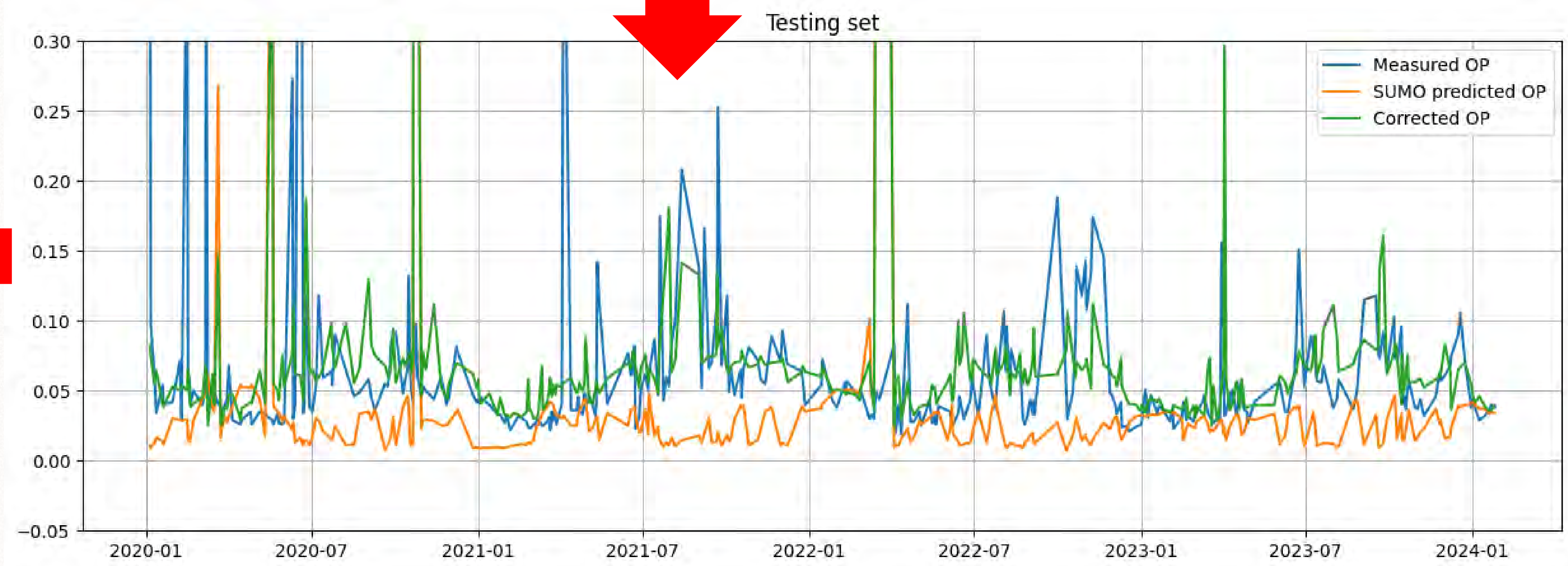
Overview of the Fond du Lac Treatment Process

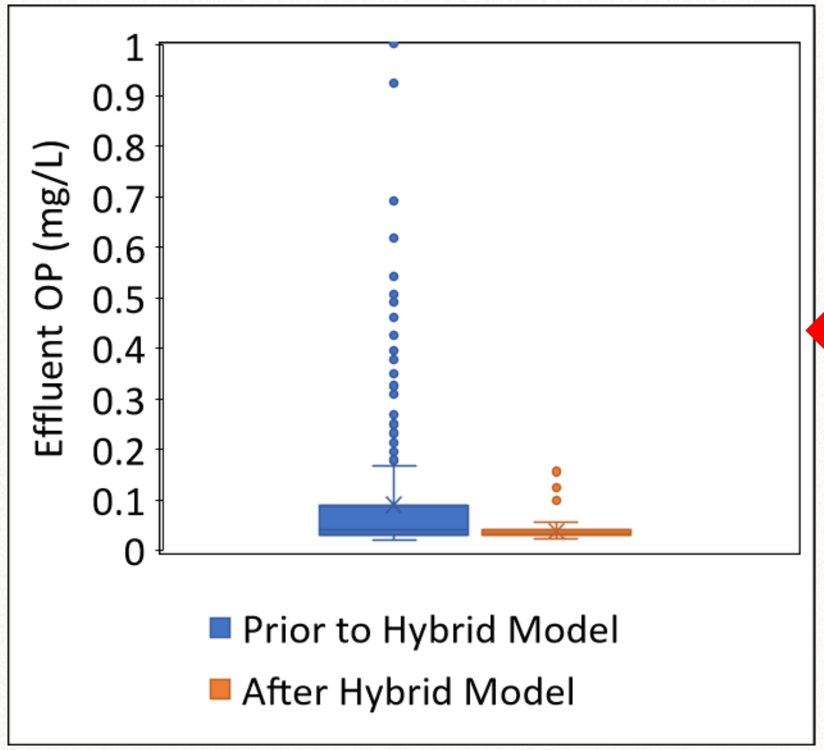
- **Use a fully calibrated plant-wide mechanistic model to predict effluent quality and conduct scenario analysis.**



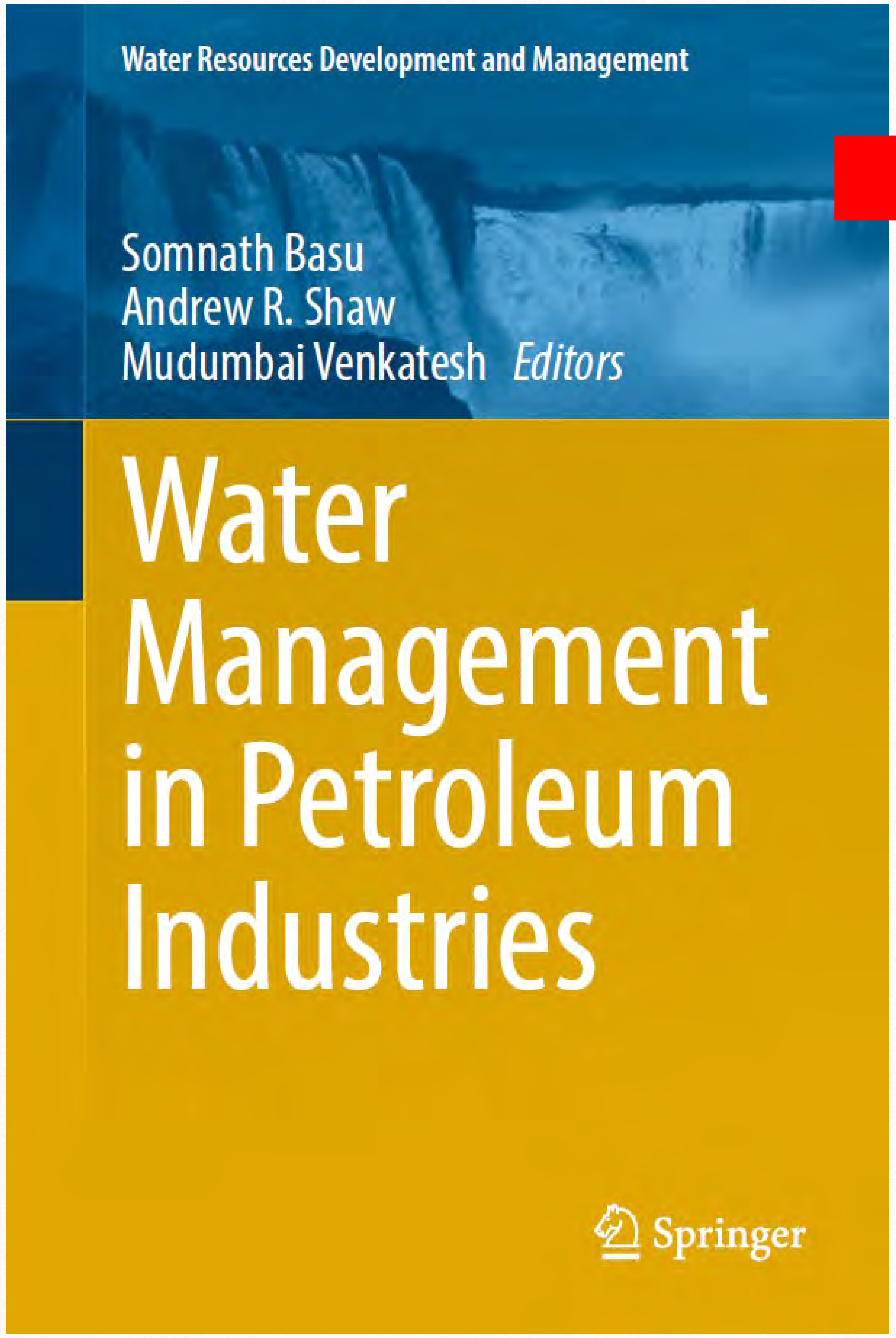


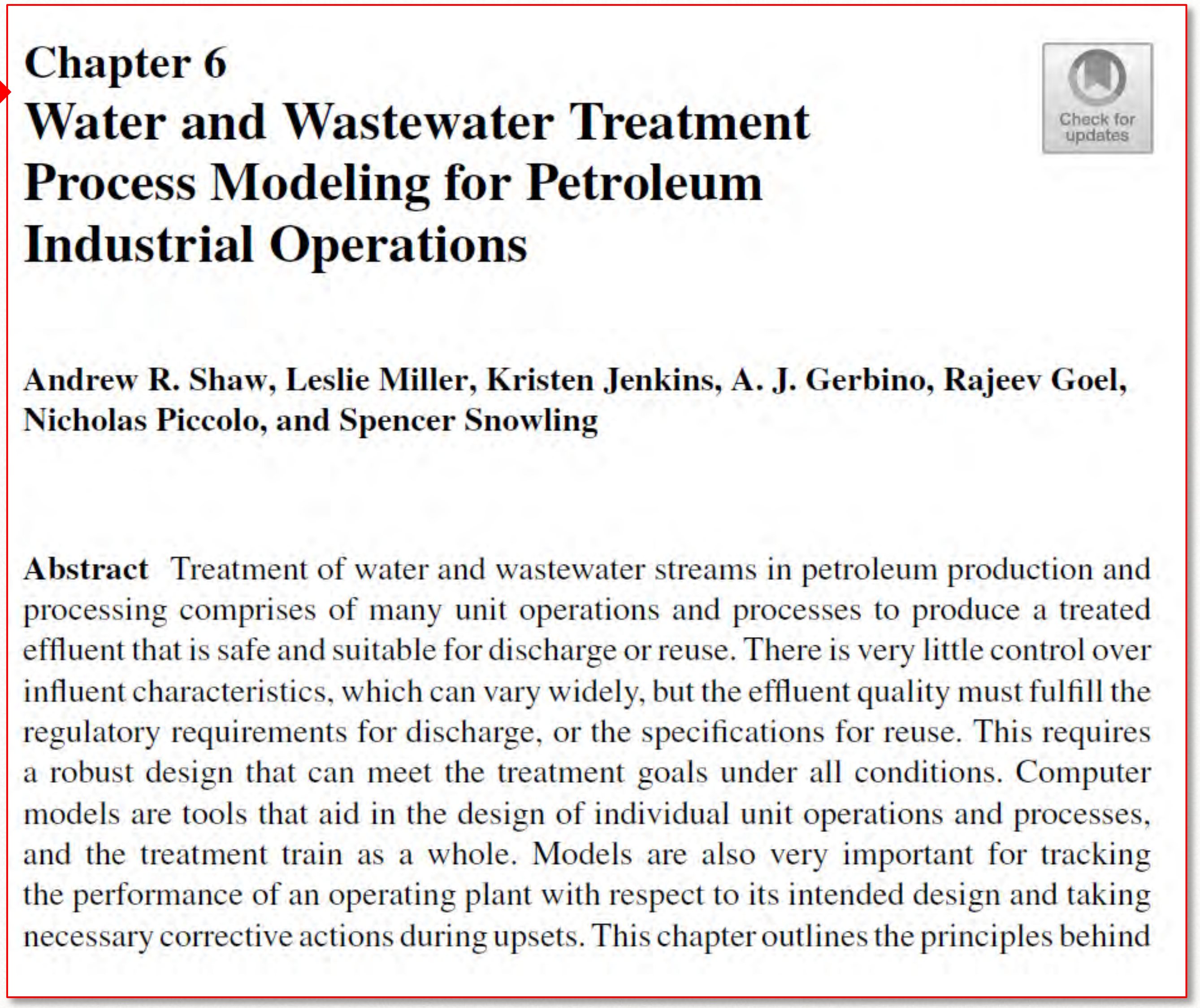






Learn More





Chapter 6
Water and Wastewater Treatment Process Modeling for Petroleum Industrial Operations

Andrew R. Shaw, Leslie Miller, Kristen Jenkins, A. J. Gerbino, Rajeev Goel, Nicholas Piccolo, and Spencer Snowling

Abstract Treatment of water and wastewater streams in petroleum production and processing comprises of many unit operations and processes to produce a treated effluent that is safe and suitable for discharge or reuse. There is very little control over influent characteristics, which can vary widely, but the effluent quality must fulfill the regulatory requirements for discharge, or the specifications for reuse. This requires a robust design that can meet the treatment goals under all conditions. Computer models are tools that aid in the design of individual unit operations and processes, and the treatment train as a whole. Models are also very important for tracking the performance of an operating plant with respect to its intended design and taking necessary corrective actions during upsets. This chapter outlines the principles behind

https://link.springer.com/book/10.1007/978-981-19-3159-8

BLACK & VEATCH

THANK YOU!

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