UCONN
UNIVERSITY OF CONNECTICUT

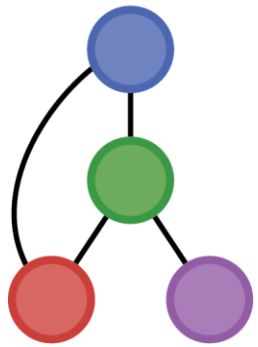
Hybrid Modeling of Wastewater Treatment Plant For Greenhouse Gas Emissions Predictions and Control

Alireza Miraliakbar, Pengfei Xu, Dimitri Alston

PI: Matthew Stuber, Pratt and Whitney Associate Professor

Nov 2, 2025

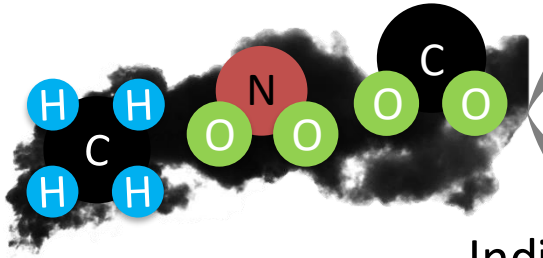
2025 AIChE ANNUAL MEETING



Process Systems and Operations Research Laboratory

When Clean Water Is Not So Clean

5% annual emission contribution



Direct

Biological Kinetic Byproduct

Indirect

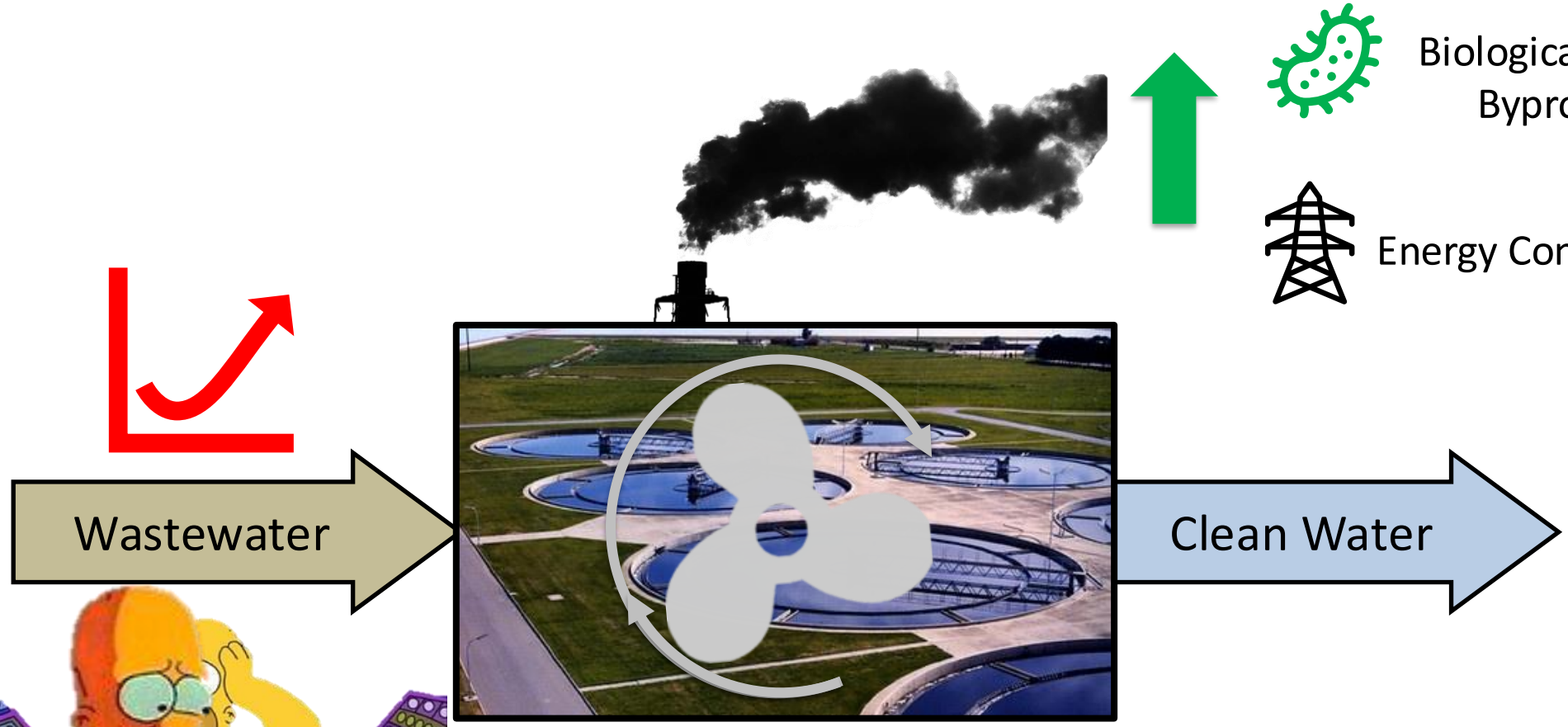
Energy Consumption

Wastewater

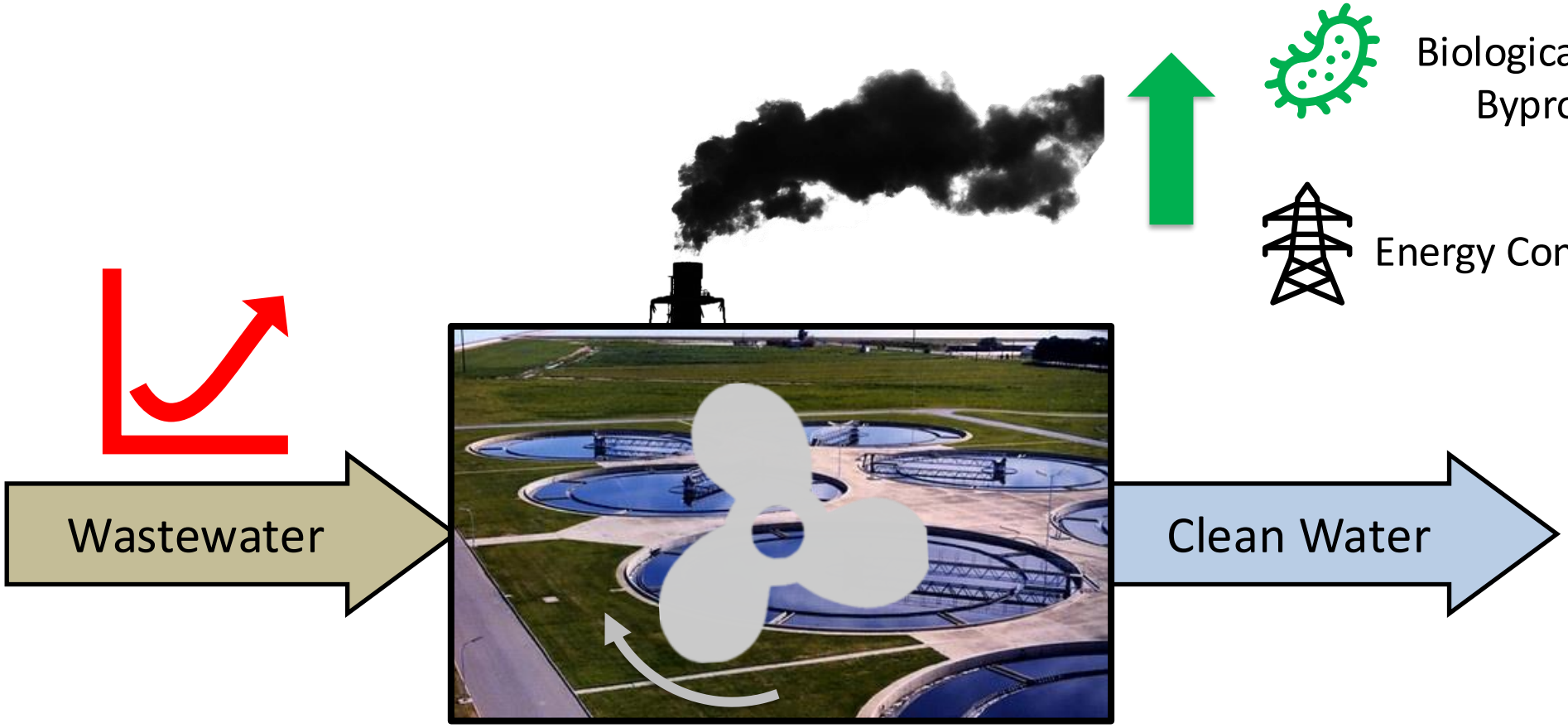
Clean Water

(Jason Ren et al. 2022)

Over-Mixing and Aeration for Shocks



Over-Mixing and Aeration for Shocks



Precise Control → Prediction Models

Wastewater Process Models

Mechanistic Models

Activated Sludge Models (ASMs)

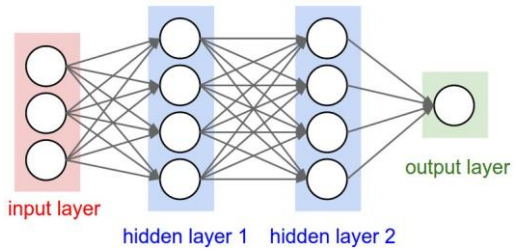
$$\frac{dX}{dt} = F_i - F_o + r_X V$$
$$\frac{dV}{dt} = \nu_i - \nu_o$$
$$\dots$$

\+ Interpretability

− Limited knowledge

Data-driven Models

Artificial Neural Networks (ANNs)

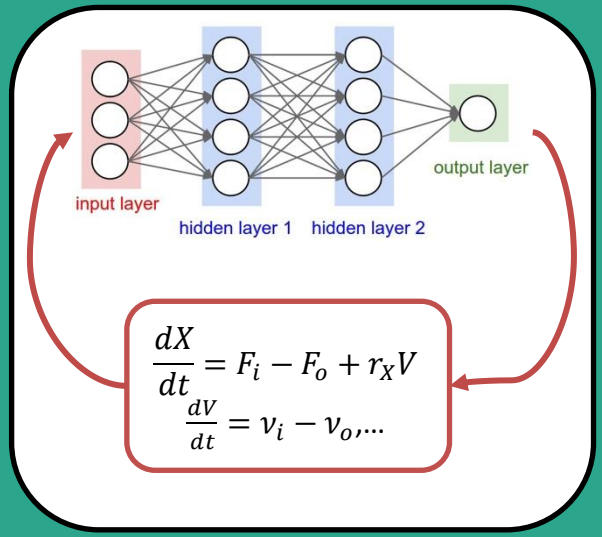


\+ No Knowledge

− Generalization

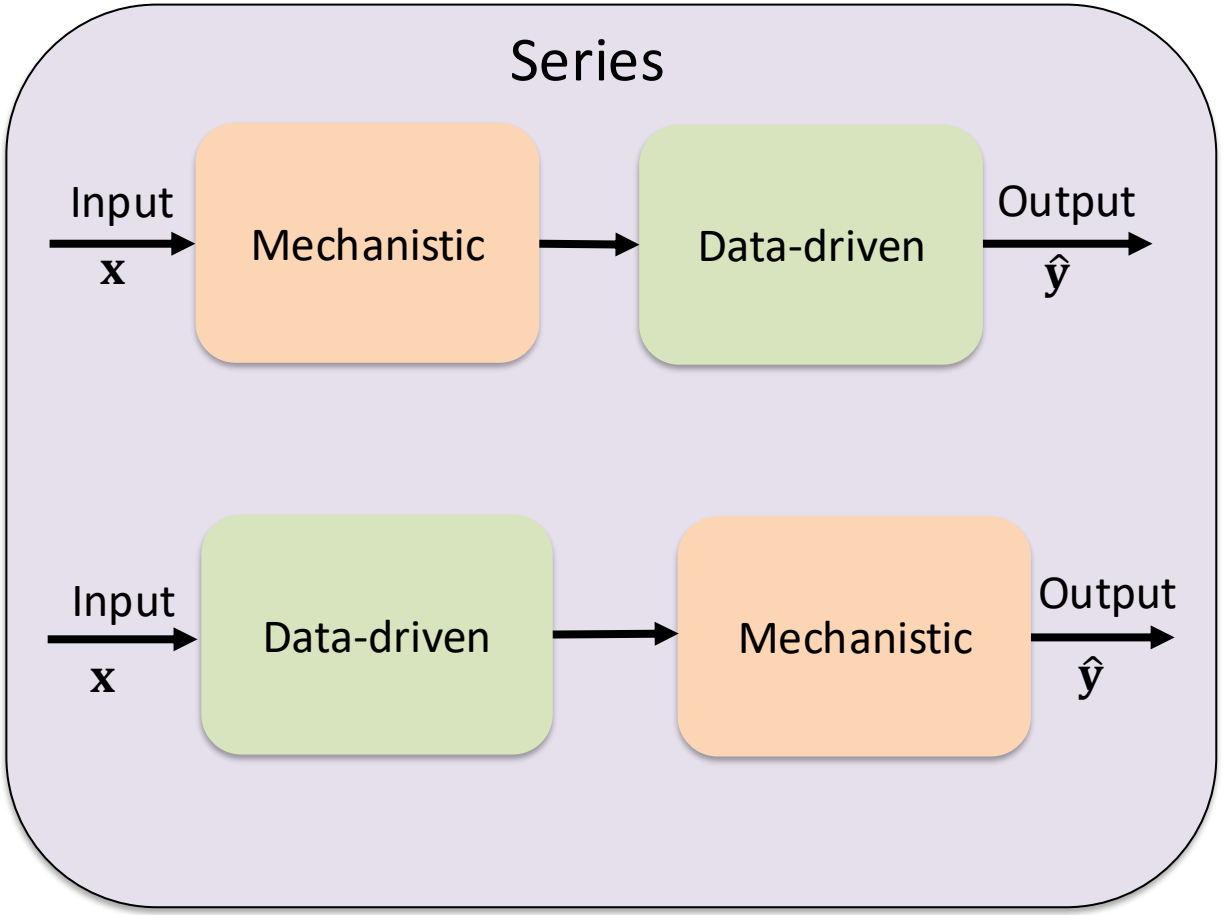
Hybrid Models

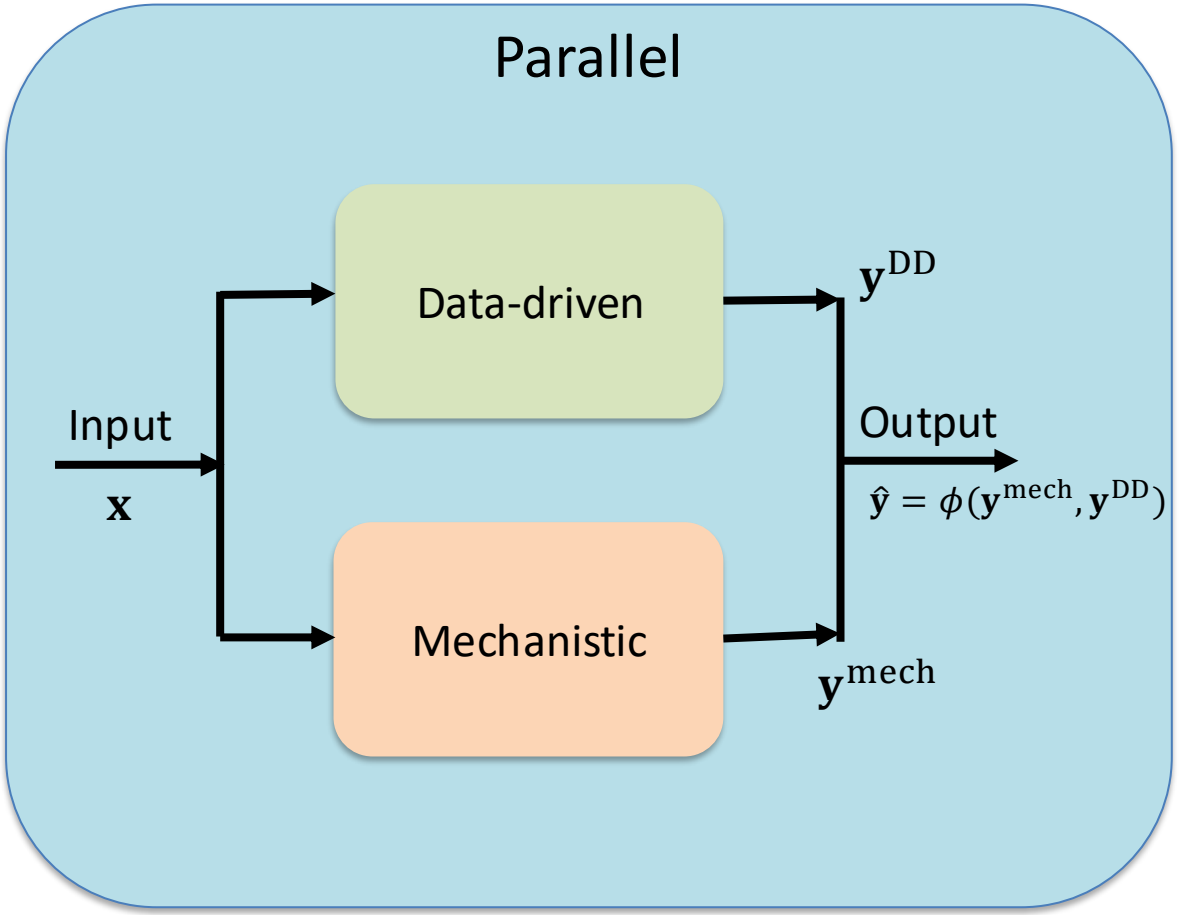
Series or Parallel



(Schneider et al. 2022)

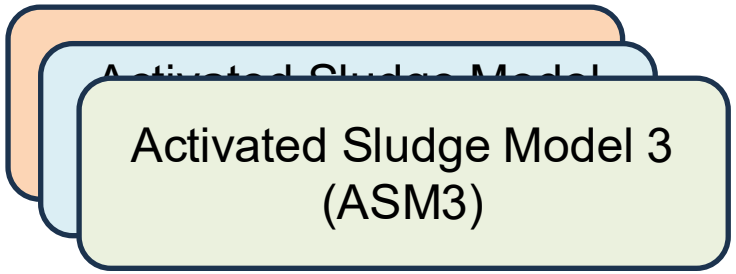
Hybrid Model Architectures





(Schneider et al. 2022)

Activated Sludge Models



- **Organic matter removal**

  Characterized by Chemical Oxygen Demand (COD)

- **Nitrogen removal by nitrification**

  Ammonium (NH_4^+) → Nitrate (NO_3^-)

- **Nitrogen removal by denitrification**

  2-step denitrification

  $$NO_3^- \rightarrow NO_2^- \rightarrow N_2$$

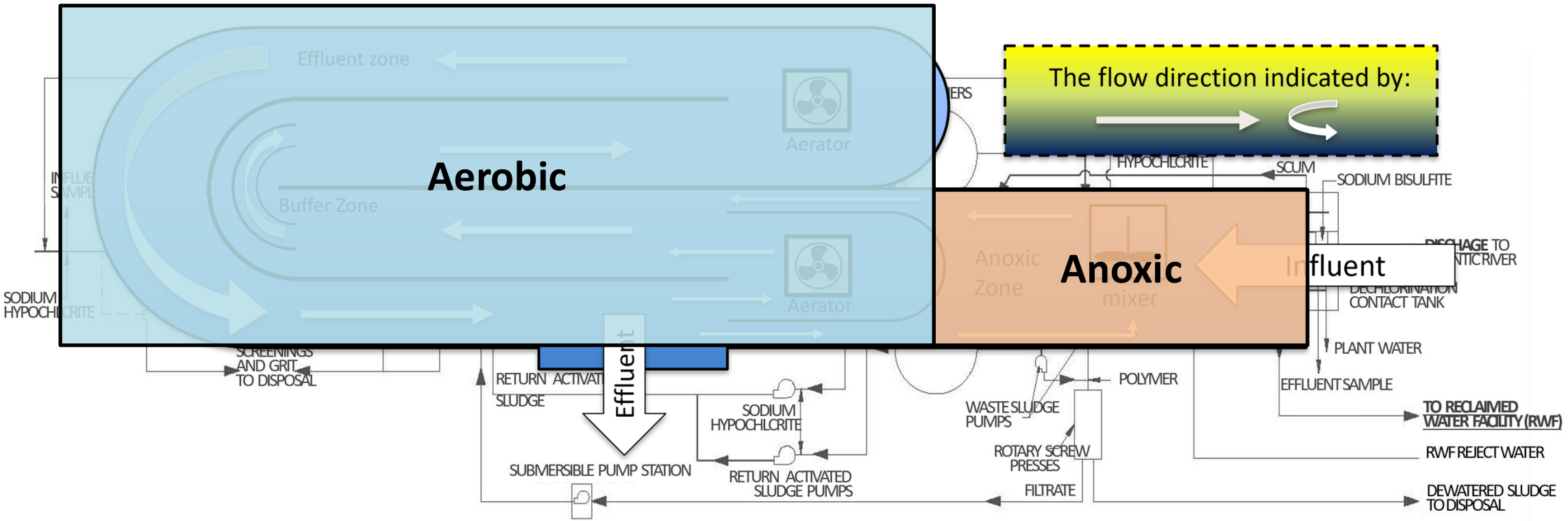
Improved nitrification and denitrification

4-step denitrification:

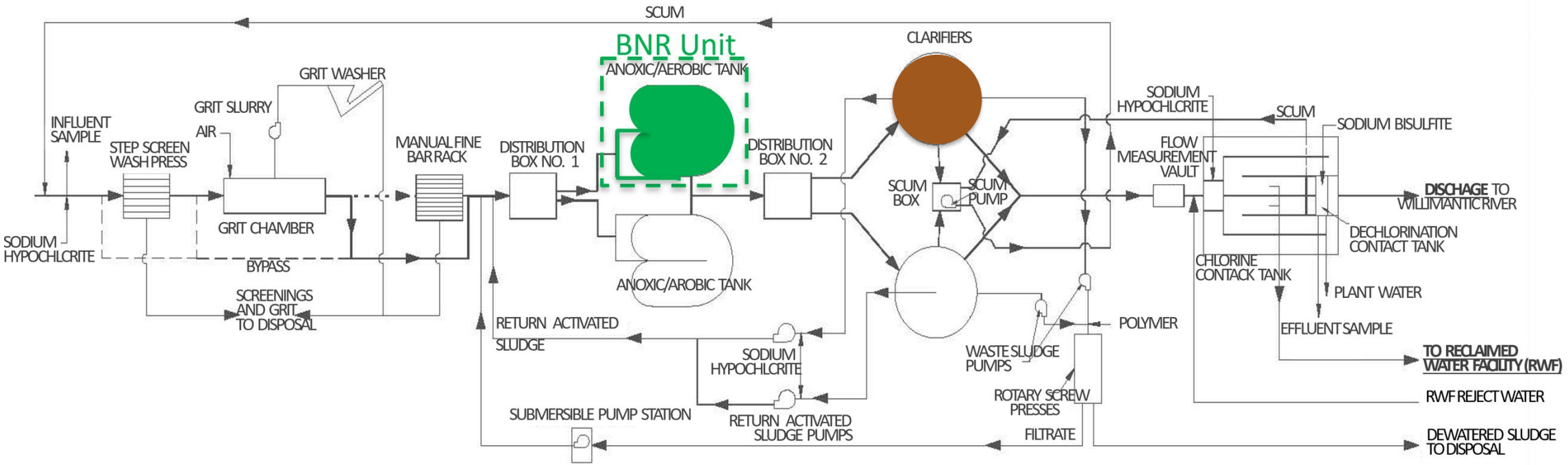
$$NO_3^- \rightarrow NO_2^- \rightarrow NO \rightarrow \mathbf{N_2O} \rightarrow N_2$$

(Henze et al. 2006) (Hiatt and Grady 2008)

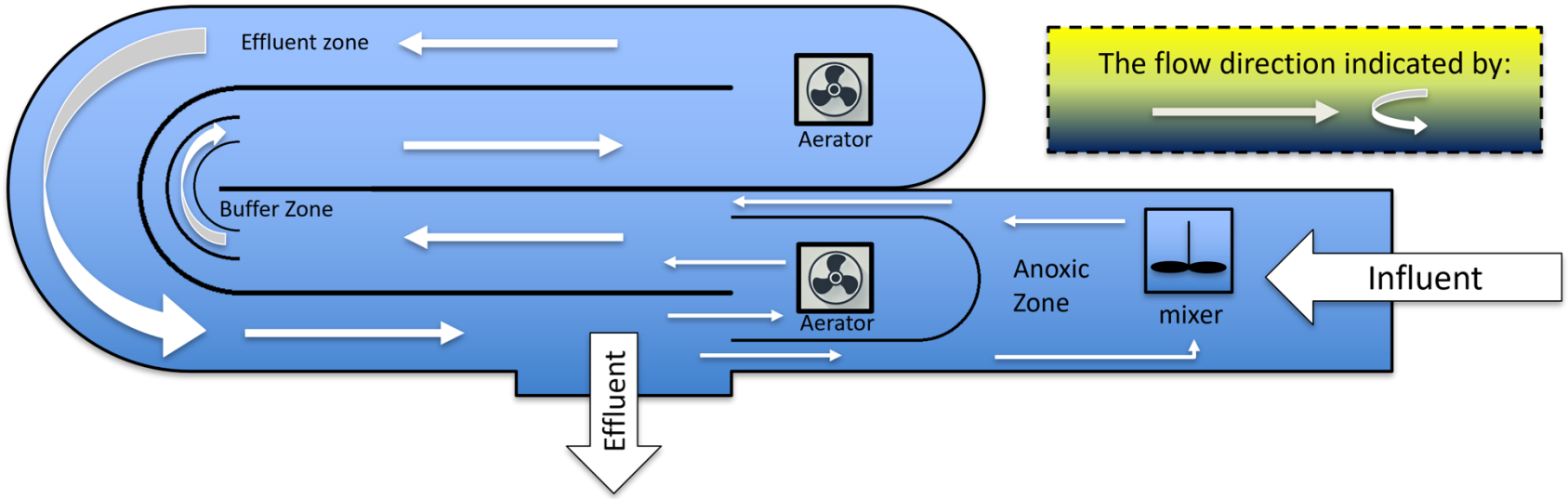
UConn Wastewater Treatment Plant

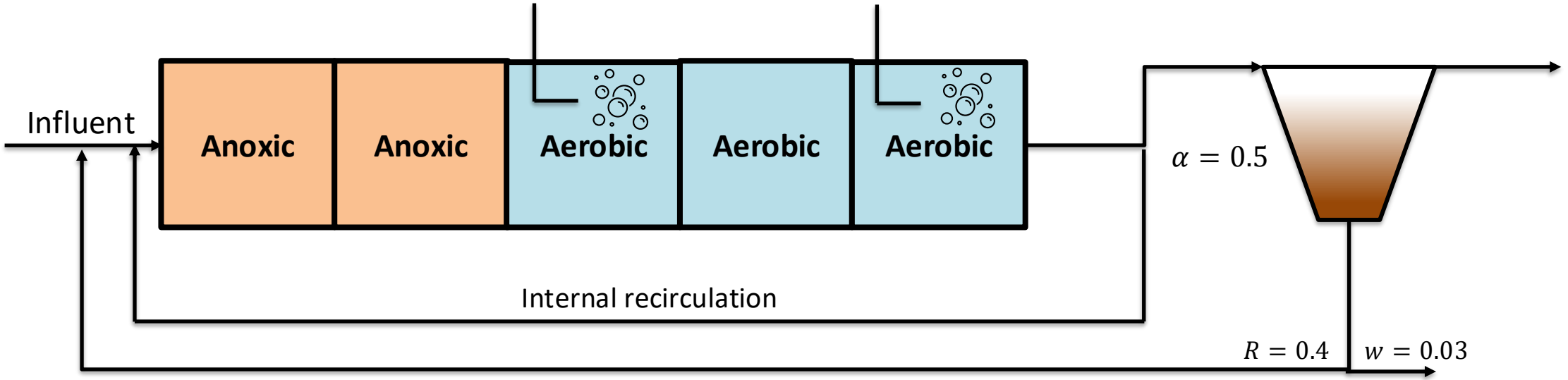


UConn Wastewater Treatment Plant



Abstracting BNR Unit with CSTRs





Entire Story

Precise control of wastewater treatment plants (WWTP) is crucial to mitigate emissions

↓

Wastewater process modeling is important to better capture the dynamic response

↓

Mechanistic models have limited knowledge and tedious calibration, Data-driven models lack interpretability → Hybrid Models

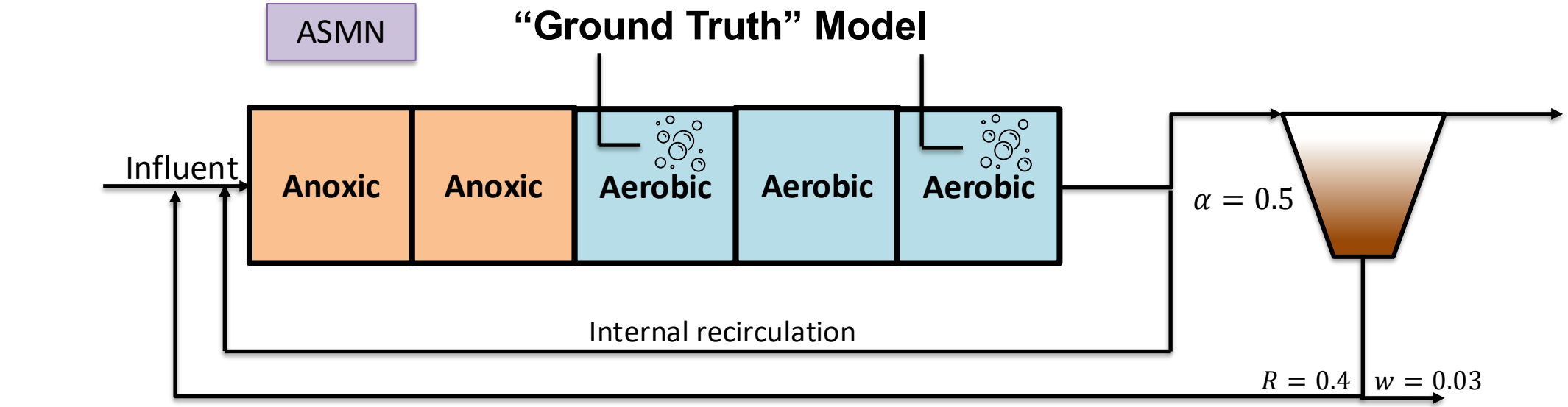
↓

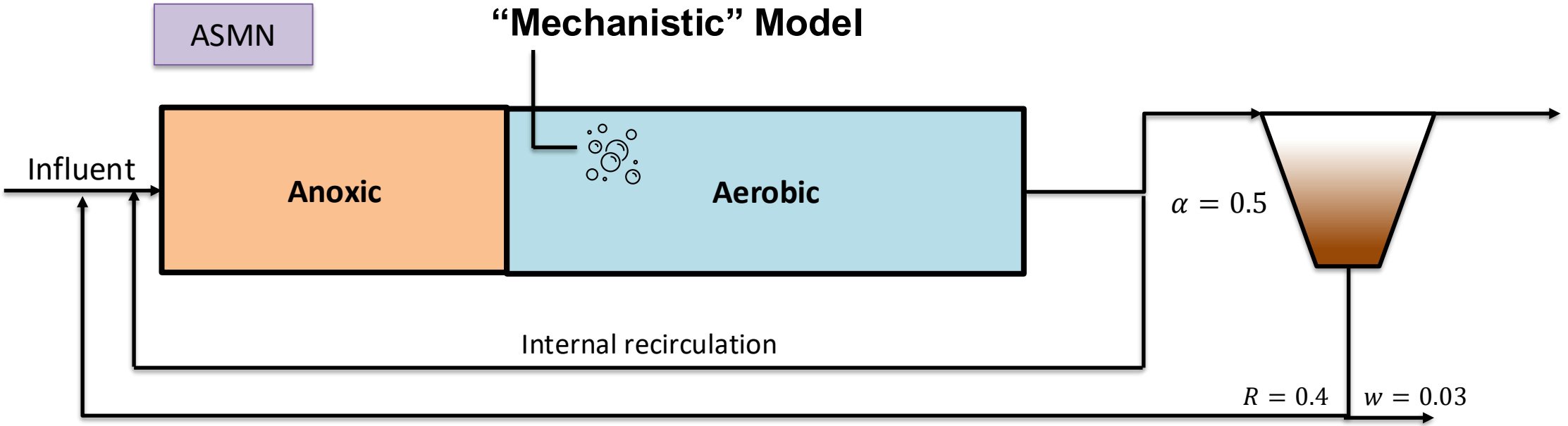
Making a hybrid model integration workflow as data is being collected from UConn plant

↓

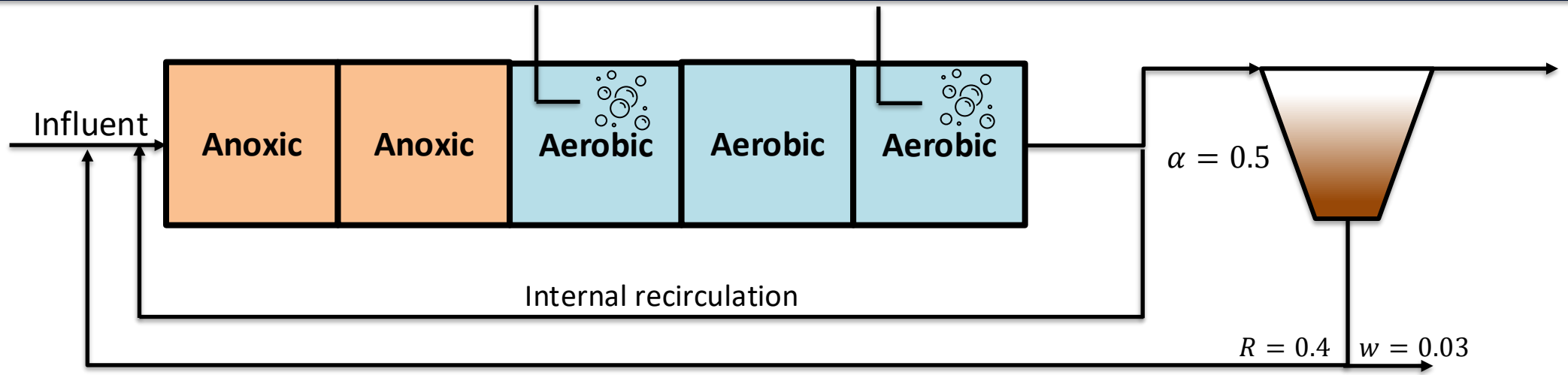
Data generation → Hybrid Model Training → Economic NMPC (eNMPC)

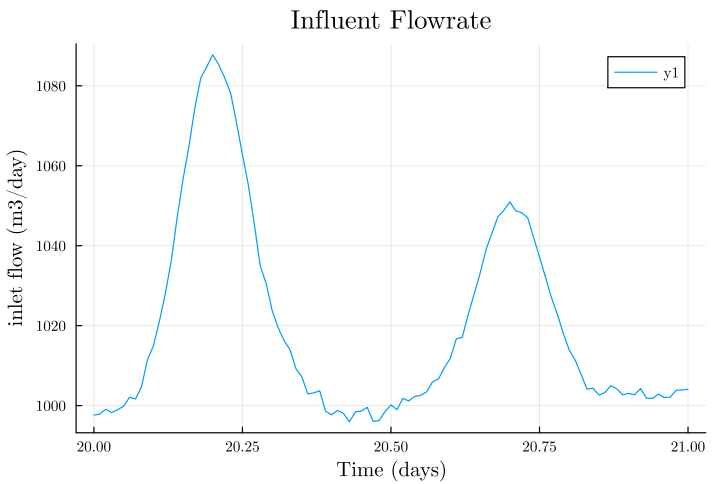
The “Ground Truth” and “Mechanistic” Models



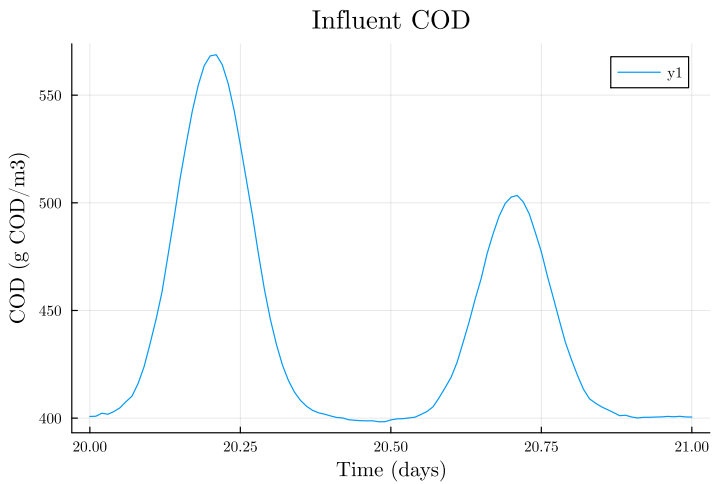


Two Peak Diurnal Influent Metrics

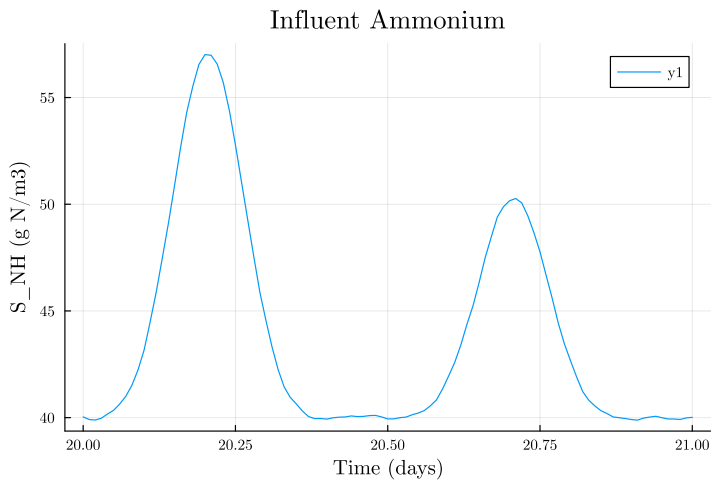




Influent Flowrate



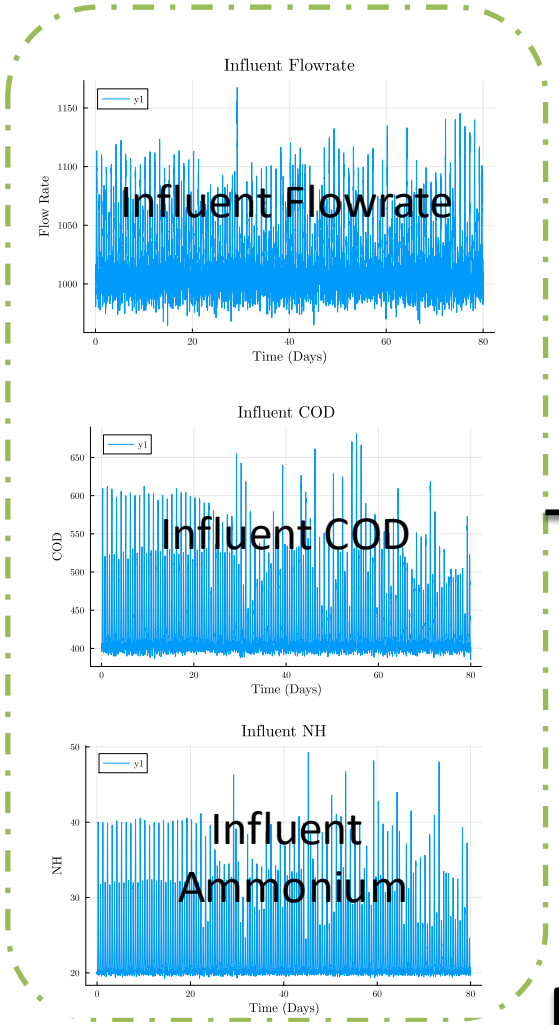
Influent COD



Influent Ammonium

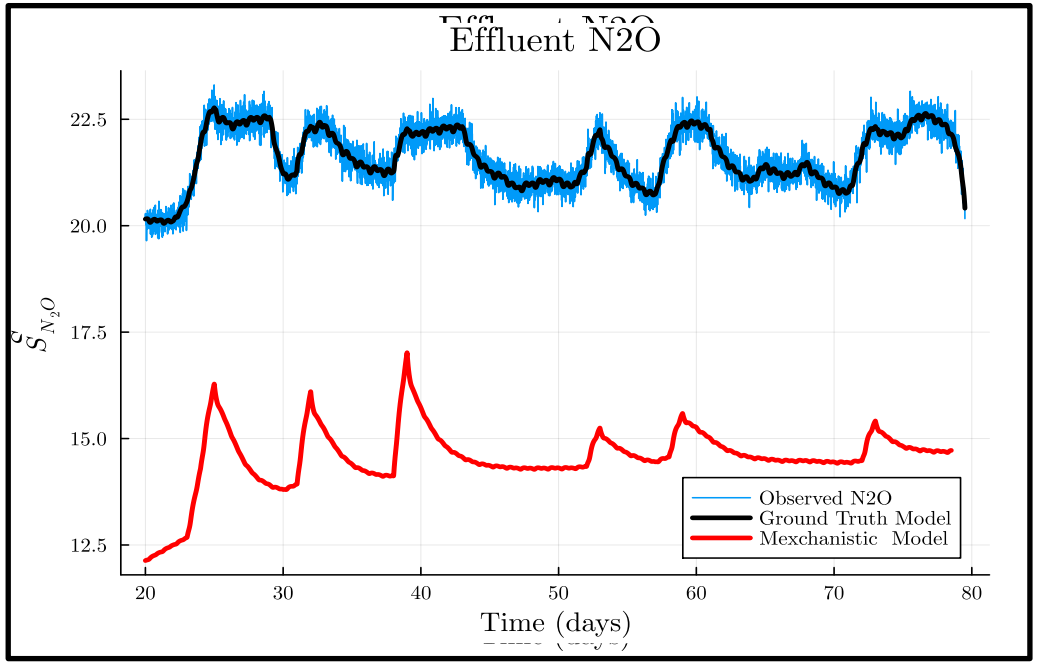
(Gernaey et al. 2011)

Data Generation Setup



Ground Truth Model

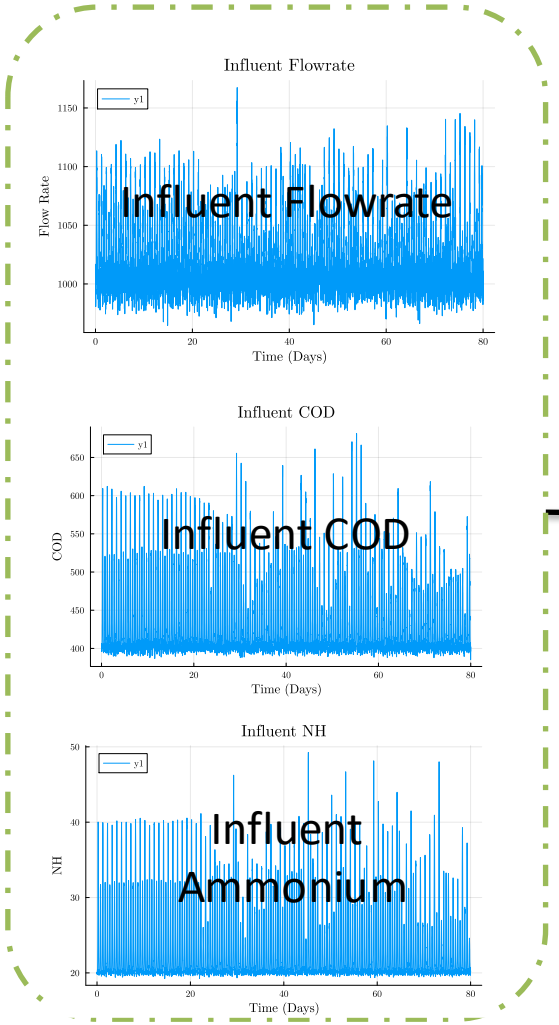
Mechanistic Model



$$\hat{x_i} = x_i + 0.01z|x_i| \quad z \in \mathcal{N}(0,1)$$

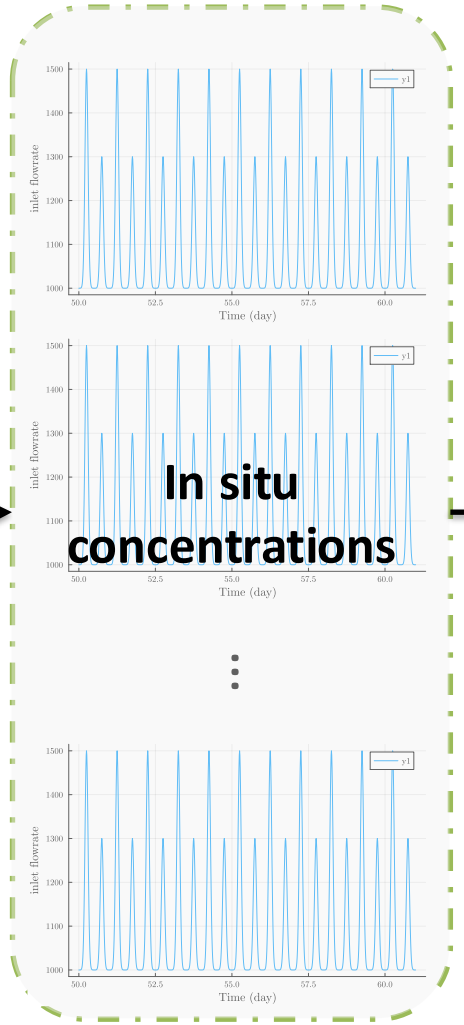
Effluent N2O as metric for greenhouse discharge of the plant

Hybrid Model Approach



ModelingToolkit.jl

Mechanistic Model

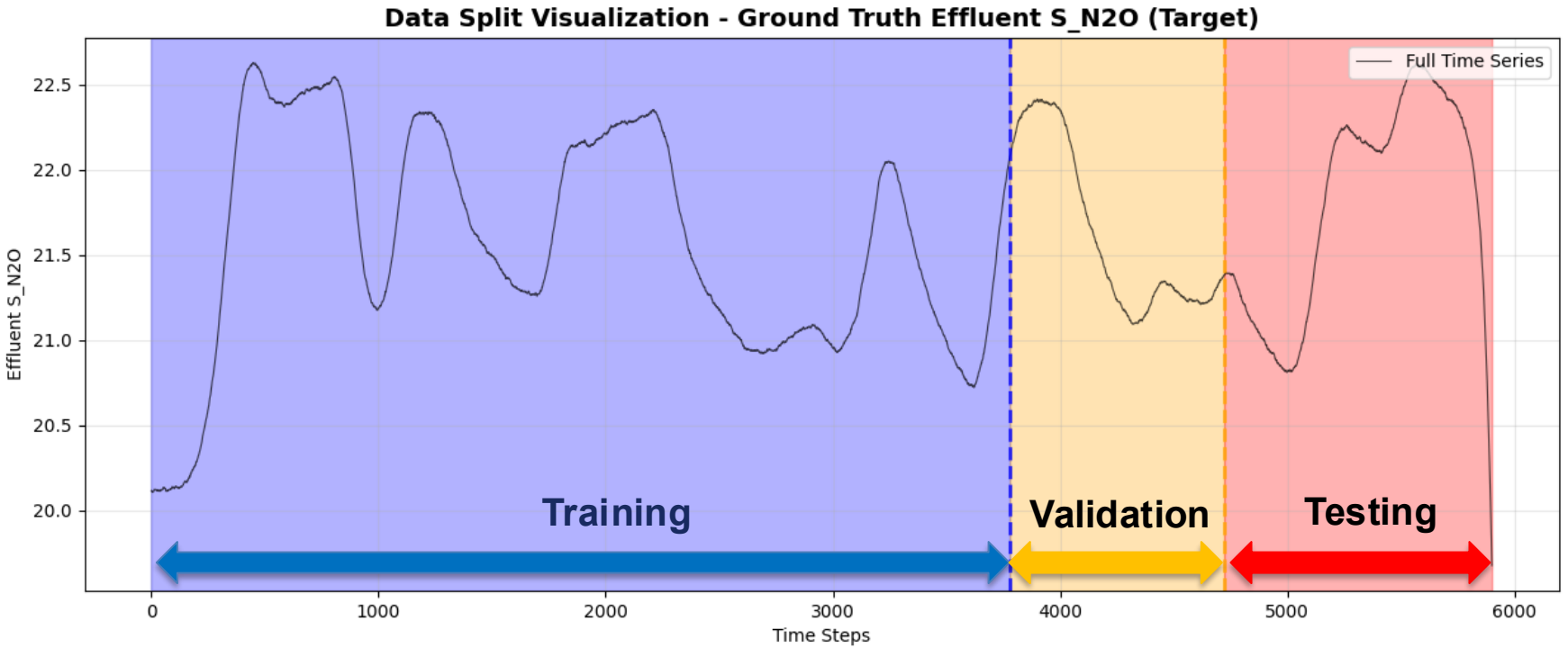


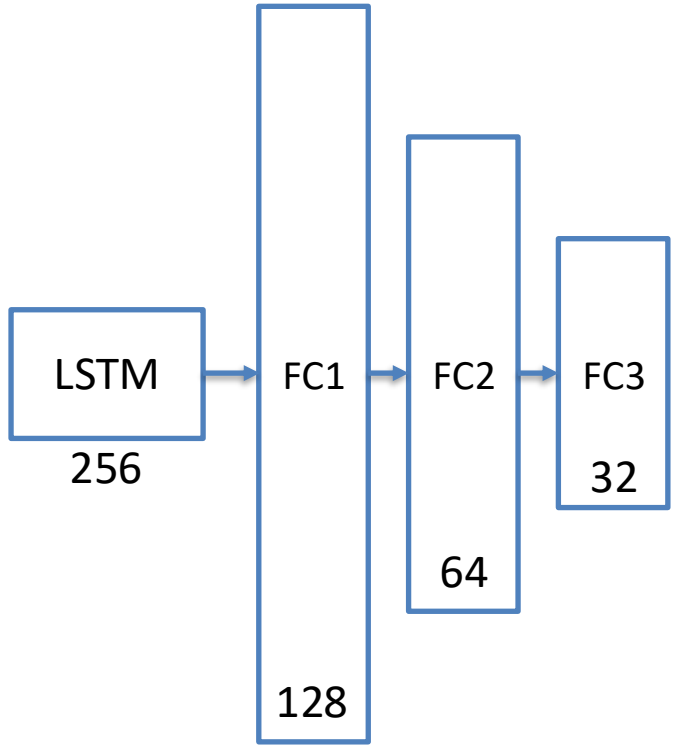
PyTorch

LSTM

Effluent N2O

Training Settings and Model Architecture





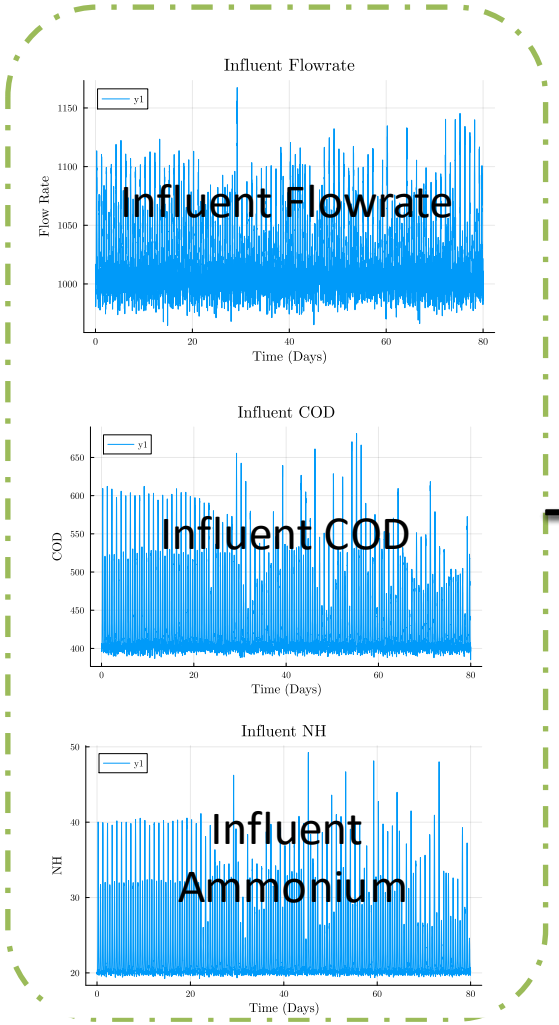
- Learning rate = 0.001
- Hidden Size LSTM= 256
- Number of LSTM Layers= 1

- Hidden Size FC1= 128
- Hidden Size FC2= 64
- Hidden Size FC2= 32

- Adam Optimizer

PyTorch

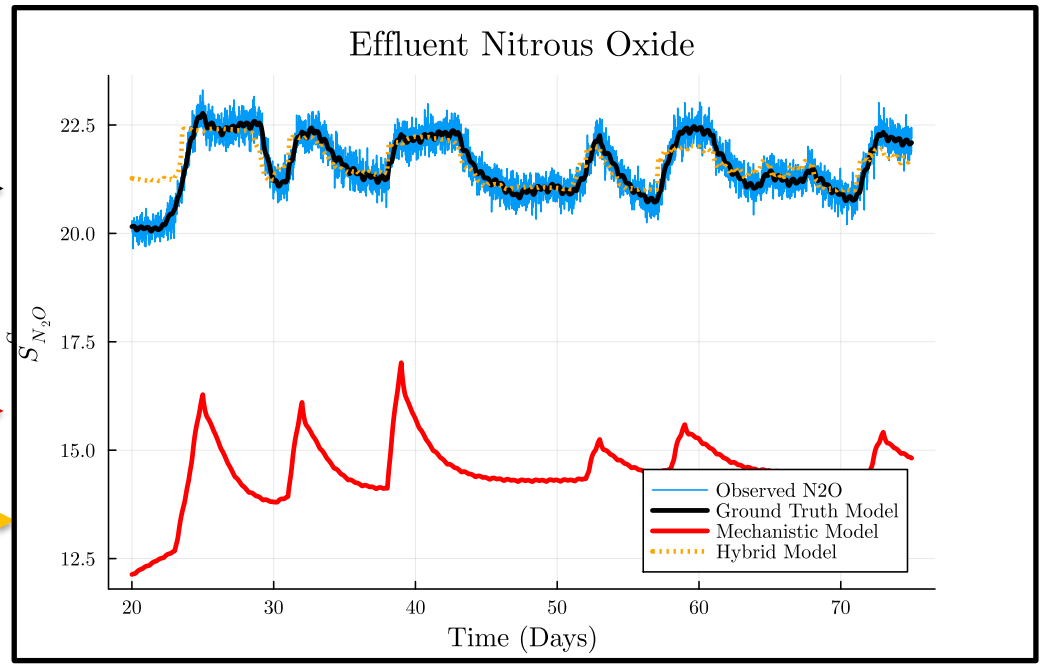
Hybrid Model Prediction Results



Ground Truth Model

Mechanistic Model

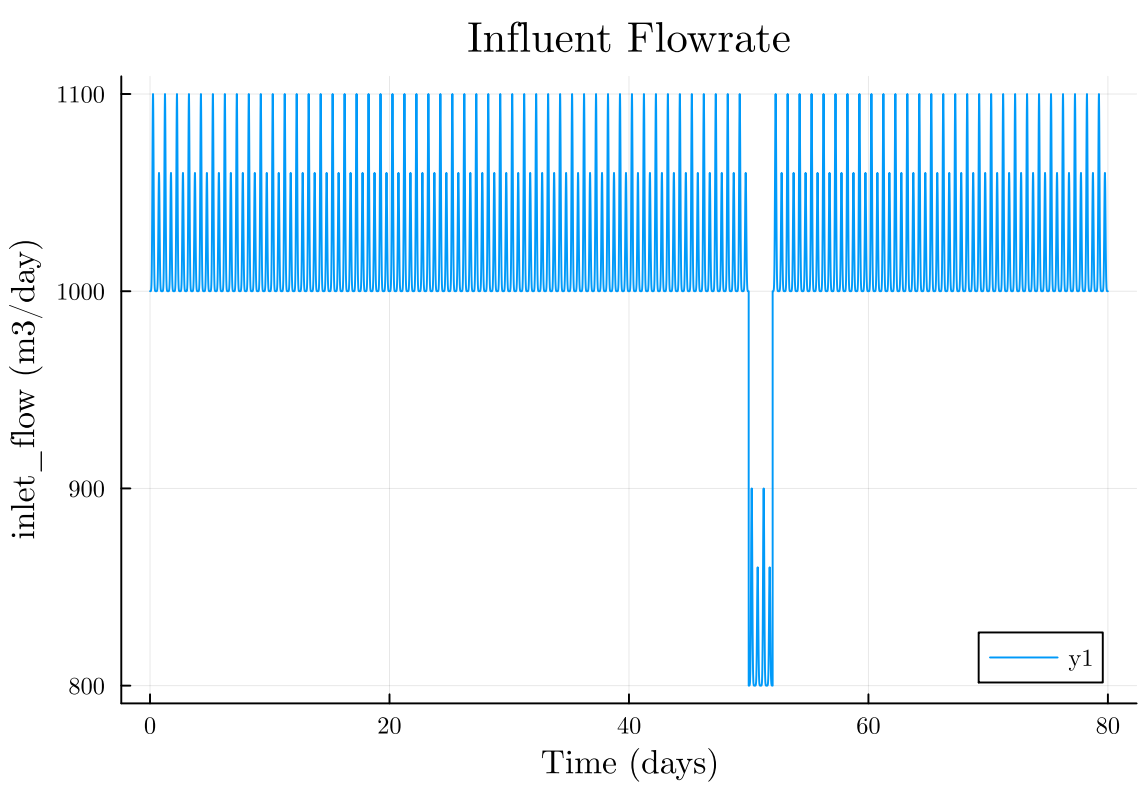
Hybrid Model

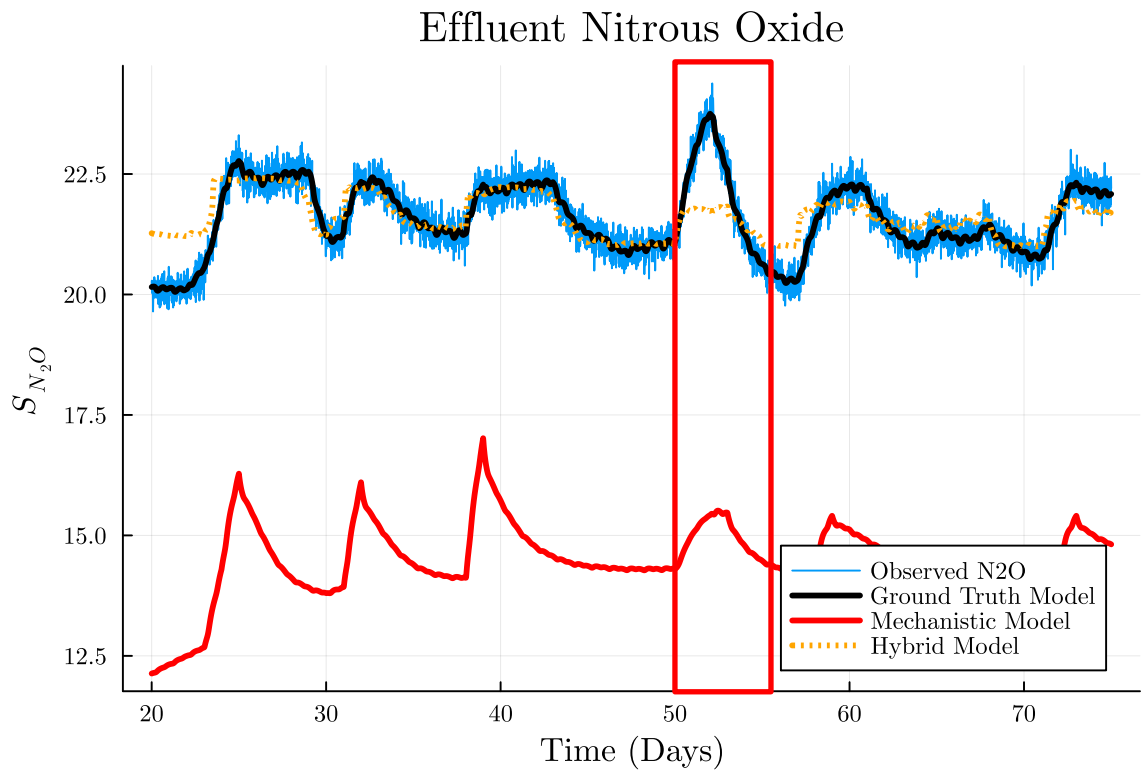


Mean Squared Error of Mechanistic = 49.54

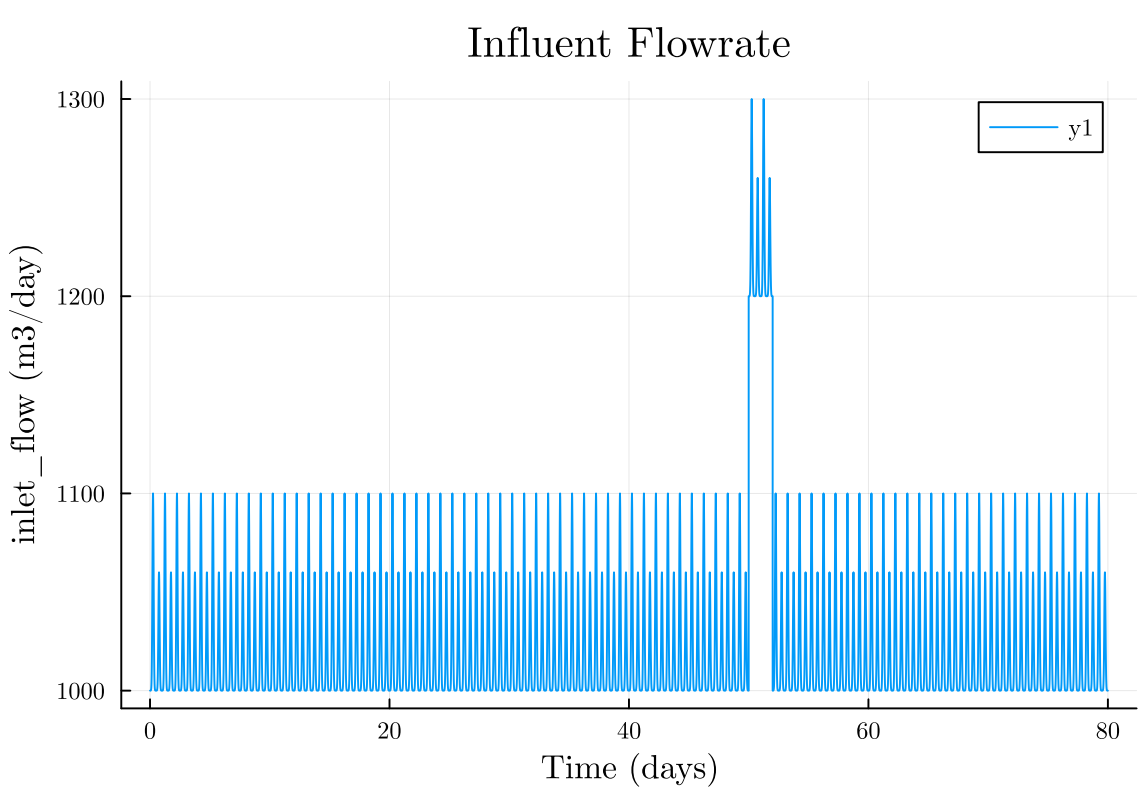
Mean Squared Error of Hybrid = 0.18

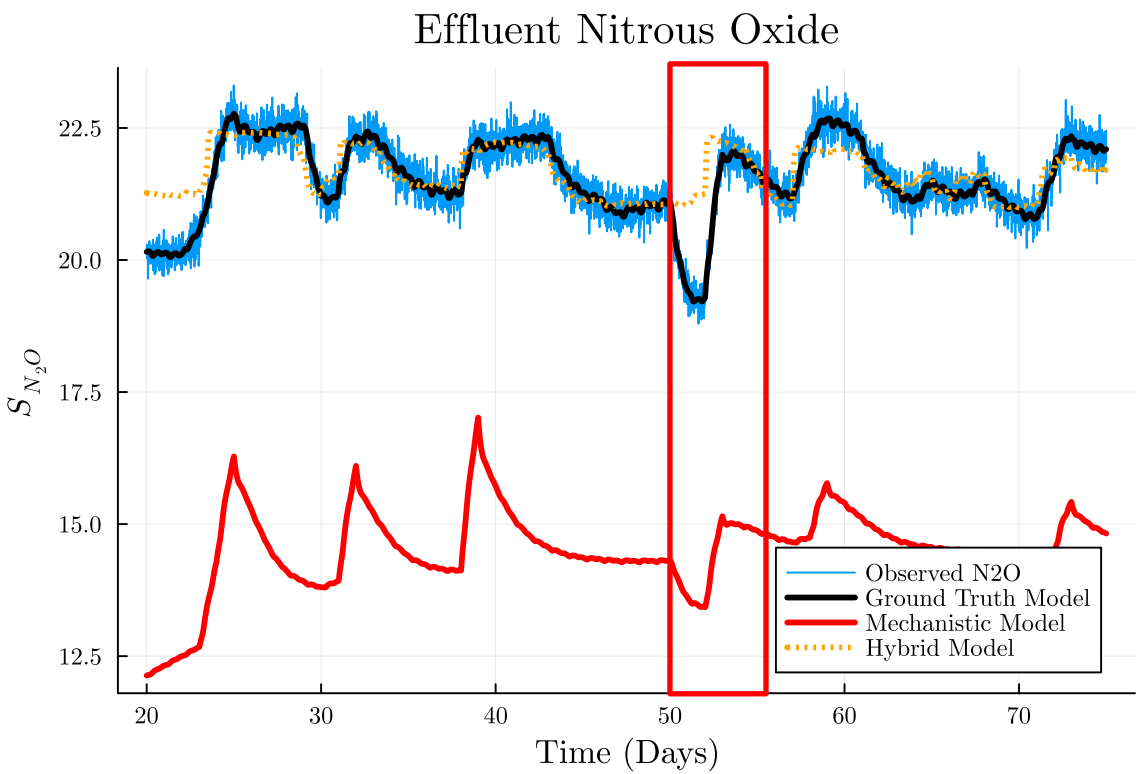
Hybrid Model Performance under Influent Shocks



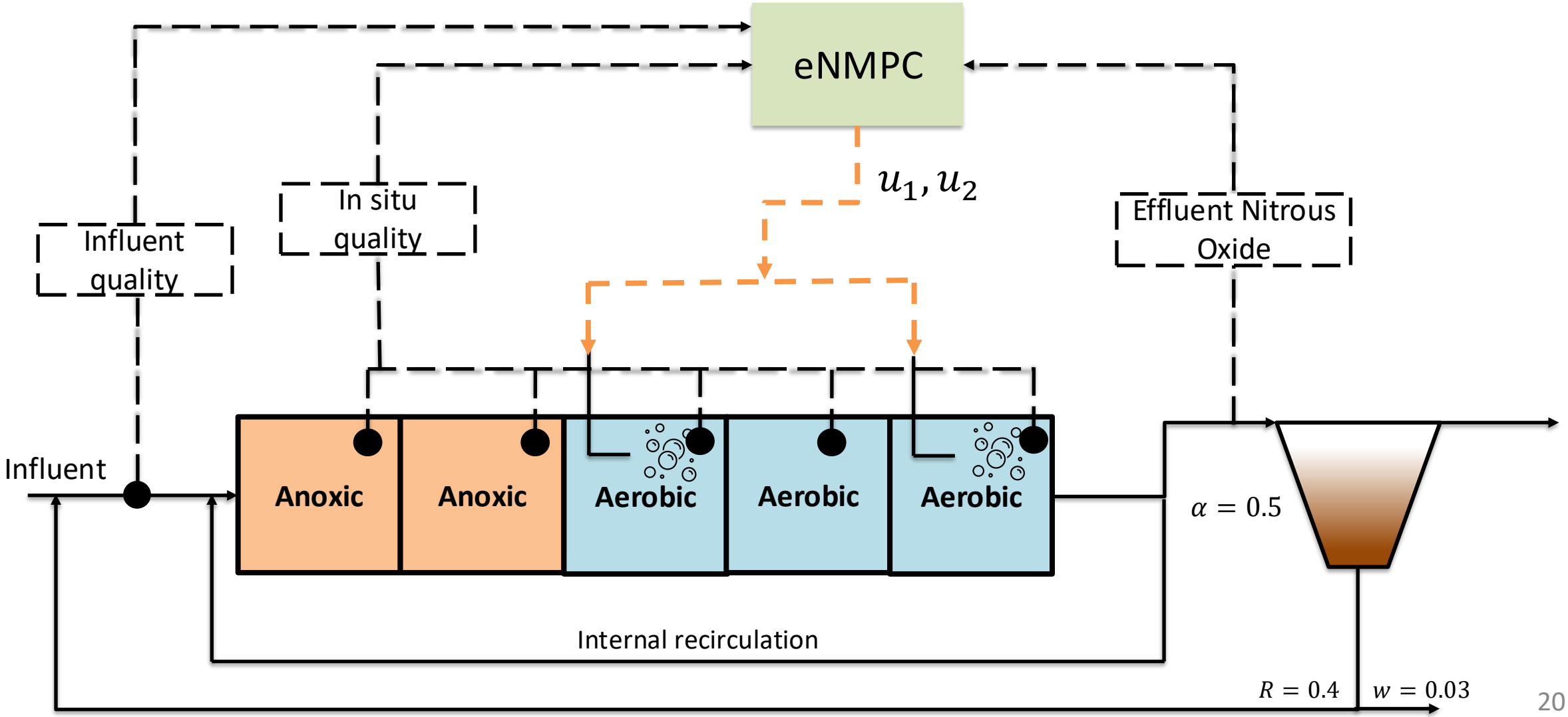


Hybrid Model Performance under Influent Shocks

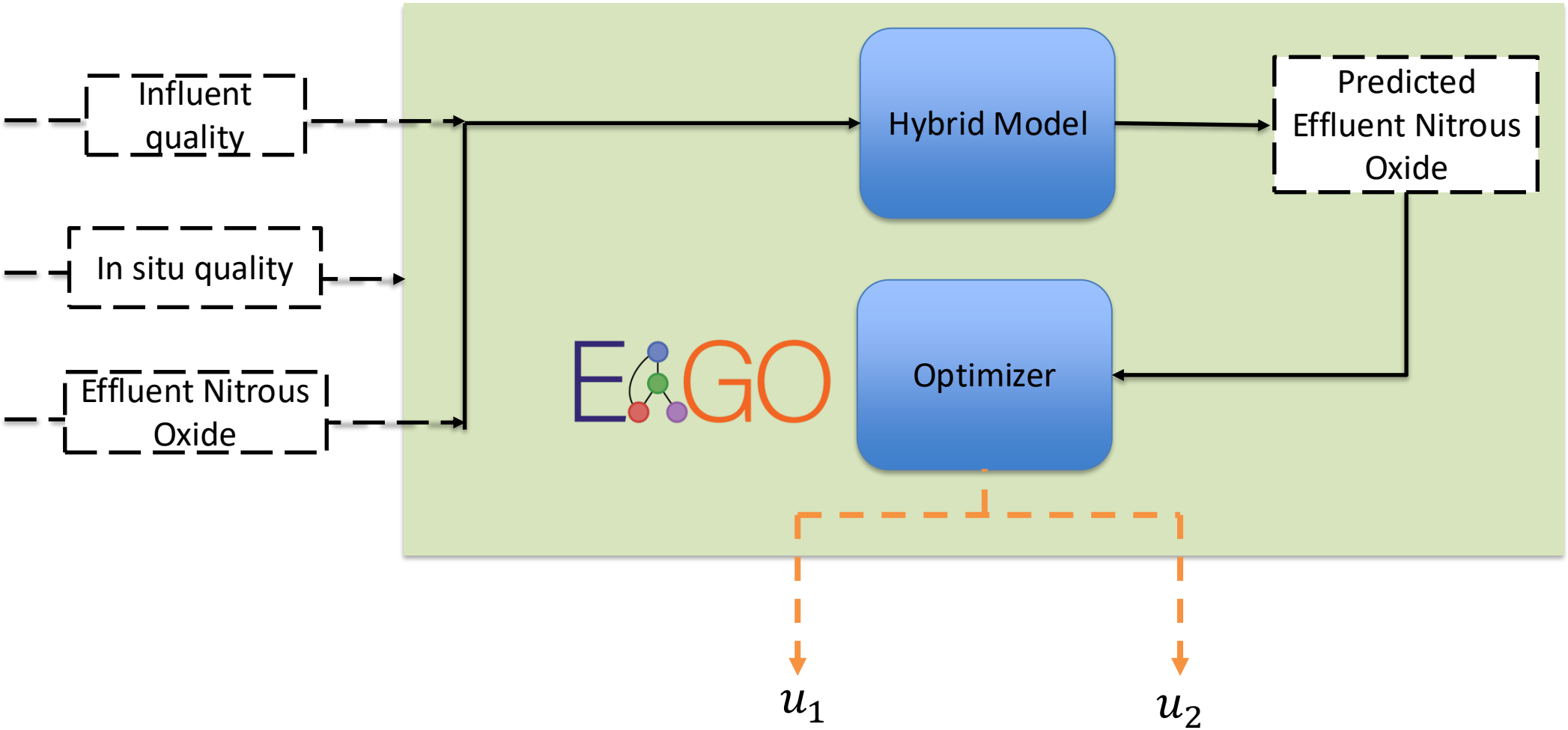




Economic Model Predictive Control

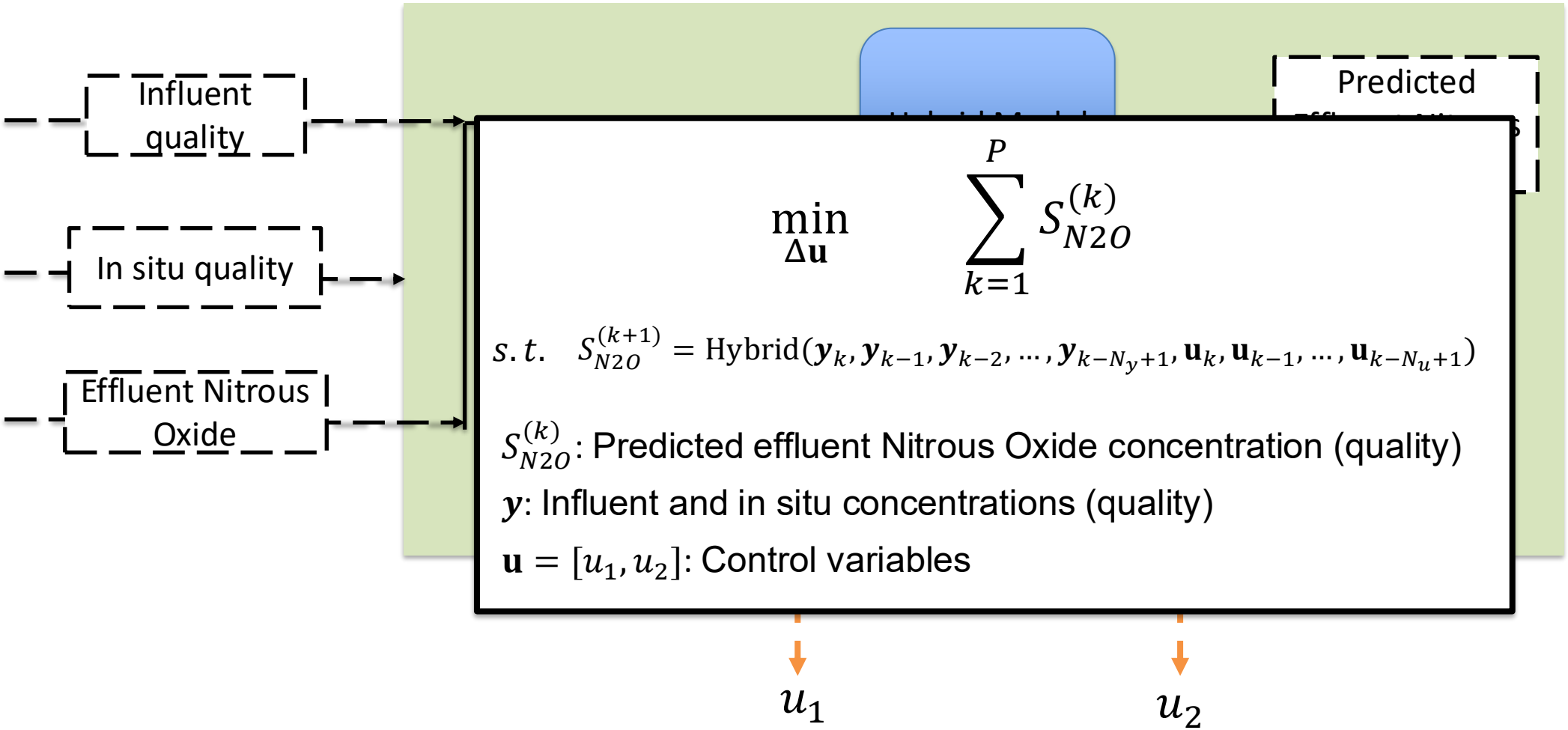


EMPC Controller Setup



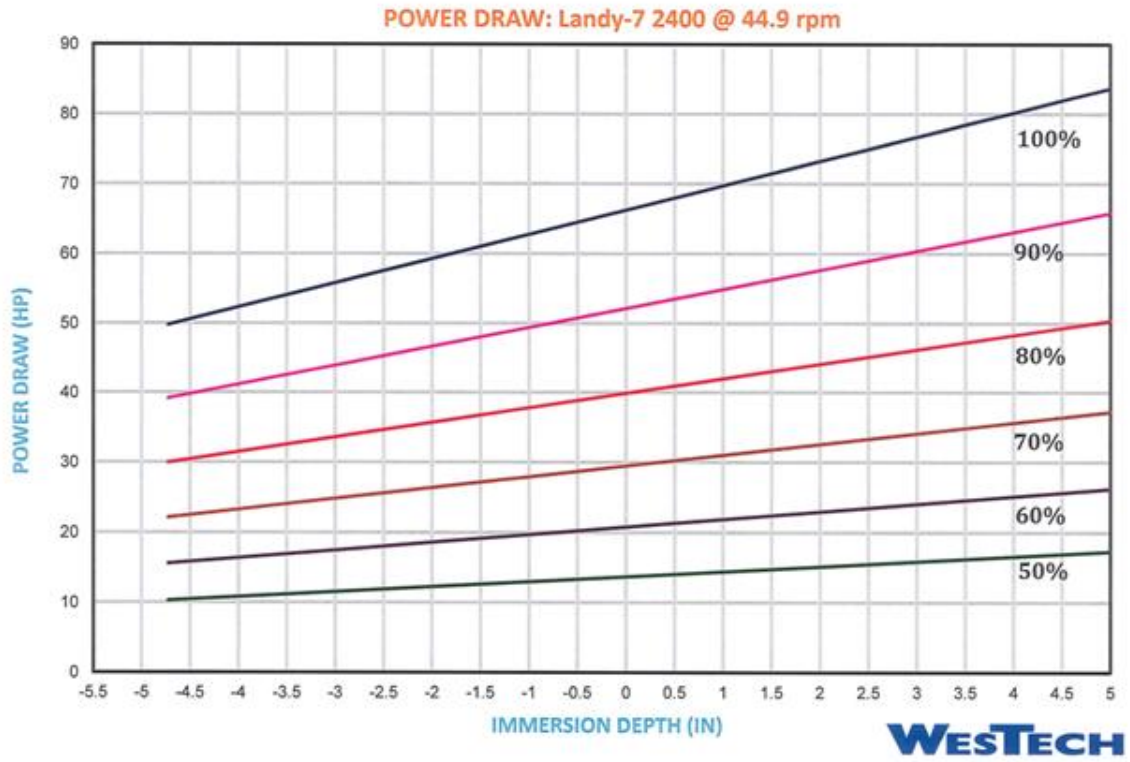
(Doncevic et al. 2020) (Schweidtmann and Mitsos 2019) (Wilhelm and Stuber 2022)

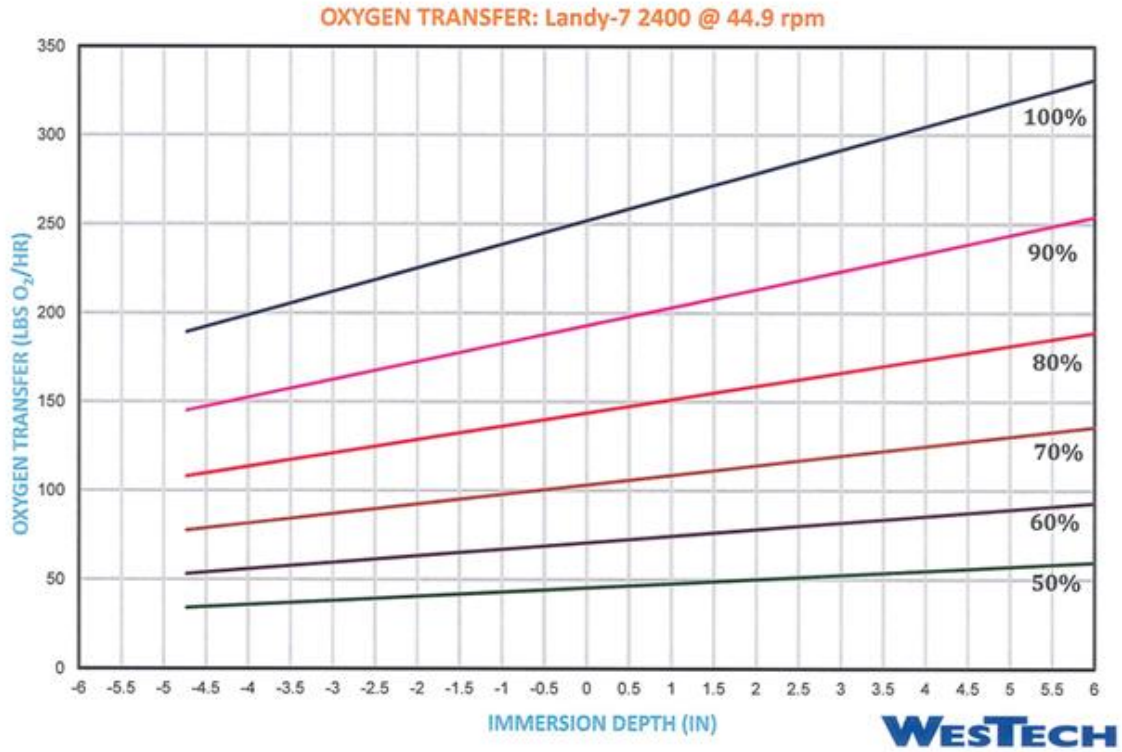
EMPC Controller Setup



(Doncevic et al. 2020) (Schweidtmann and Mitsos 2019) (Wilhelm and Stuber 2022)

Control Variable Surrogates



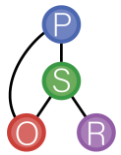


u_1:Immersion Depth

u_2: Operational Capacity

Conclusion

- Wastewater treatment plants (WWTPs) directly and indirectly contribute to greenhouse gas emissions – especially nitrous oxide
- Over-aeration and mixing are common response to influent shocks, increasing both direct and indirect emissions
- Precise control of WWTPs is crucial, therefore process modeling is important
- Sequential hybrid modeling can improve the predication accuracy of mechanistic modeling significantly
- Hybrid models can further be embedded in an economic nonlinear model predictive control (eNMPC) framework to mitigate the emissions



Acknowledgement

Members of the Process Systems and Operations Research Laboratory at the University of Connecticut (https://www.psor.uconn.edu)

UCONN COLLEGE OF ENGINEERING

Pratt & Whitney Engineering Endowed Professorship

Institute for Advanced Systems Engineering
UNIVERSITY OF CONNECTICUT

Process Systems and Operations Research Laboratory

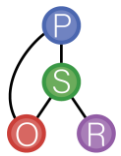
https://www.psor.uconn.edu

Funding:

National Science Foundation, Award No.: **2029428**
Pratt and Whitney Institute of Advanced Systems Fellowship
Pratt and Whitney Engineering Endowed Professorship

Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation or IASE institute or the United States Government.

Thank you!



Other talks from our lab

Robert Gottlieb
468e - GPU-Enhanced Deterministic Global Optimization
Nov 5, 9:24 AM, Hynes Convention Center Room 111

Dimitri Alston
593g - Optimization Abstraction Layer for Acausal/Equation-Oriented Models in Julia
Nov 5, 5:18 PM, Hynes Convention Center Room 108

Pengfei Xu
124e - Improving Operations of Wastewater Treatment Plants Using Economic MPC
Nov 5, 5:18 PM, Hynes Convention Center Room 108