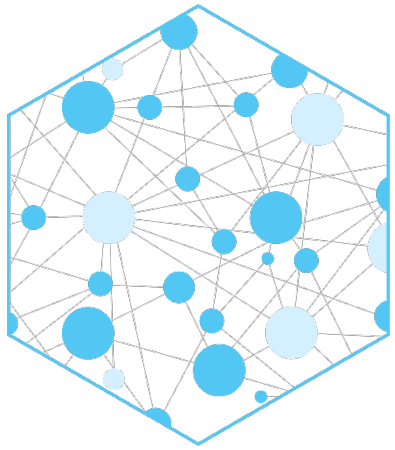

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Using Benchmark Simulation Models to Evaluate Biological Wastewater Treatment in WaterTAP

Adam Atia

National Energy Technology Laboratory (NETL), NETL Support Contractor

October 12th, 2023

NATIONAL ENERGY TECHNOLOGY LABORATORY

BERKELEY LAB

Sandia National Laboratories

Carnegie Mellon

WestVirginiaUniversity.

UNIVERSITY OF NOTRE DAME

U.S. DEPARTMENT OF ENERGY

WaterTAP development is **mainly** funded by two programs

Desalination Systems

NAWI (FOA-0001905) program:

- Advance TRL 2-4 ***desalination technologies***
- $120M over 5 years across national labs, academia, and industry

Advanced Water Resource Recovery Systems

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

NATIONAL ENERGY TECHNOLOGY LABORATORY

BERKELEY LAB

UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN

NREL NATIONAL RENEWABLE ENERGY LABORATORY

Northwestern University

IEDO (FOA-0002336) program:

- Advance TRL 4-7 ***wastewater recovery technologies***
- $27M over 3 years across 15 projects in academia and industry

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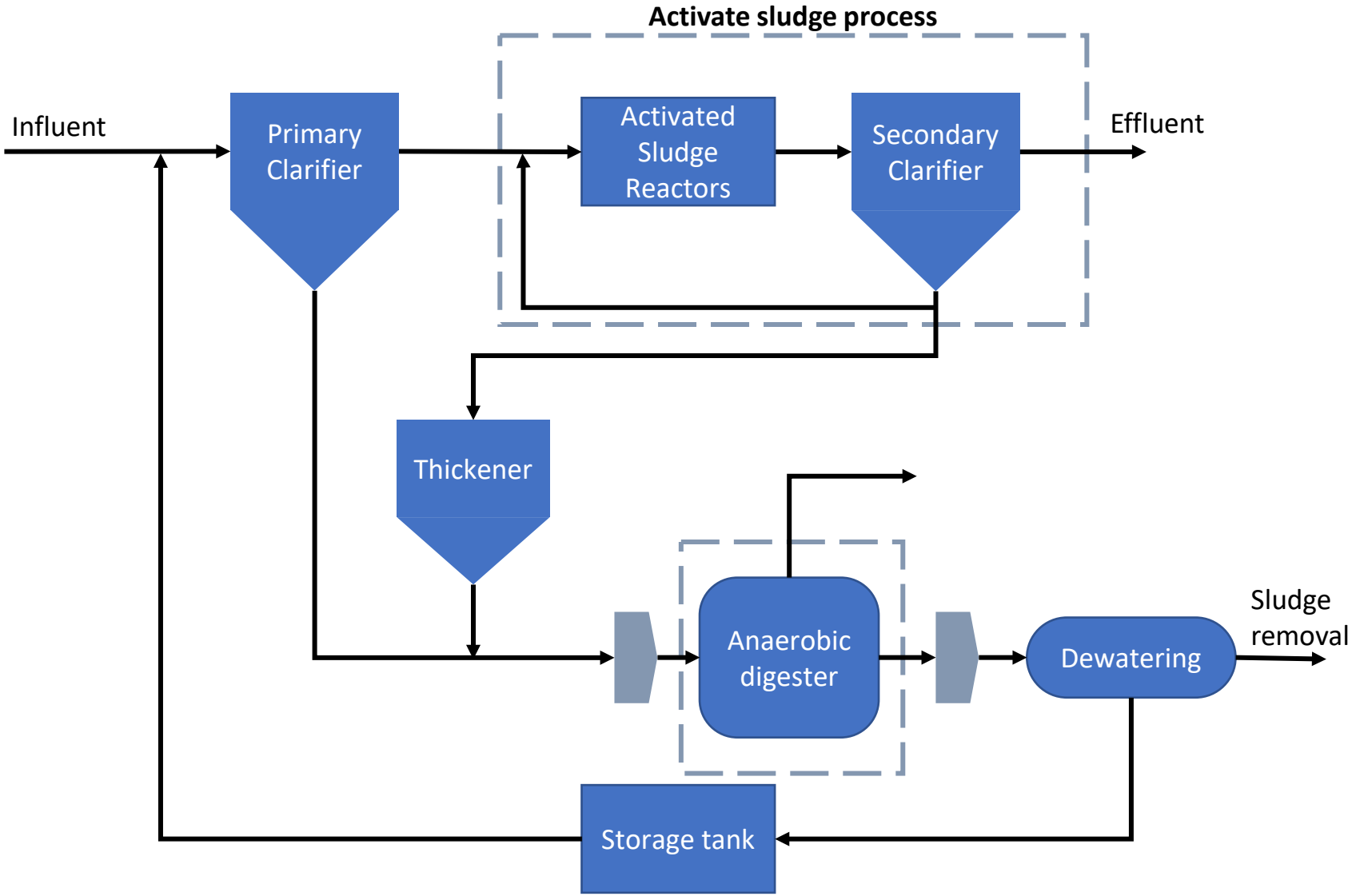
Motivation: FOA-2336 project teams are working on innovative technologies for wastewater treatment plants.



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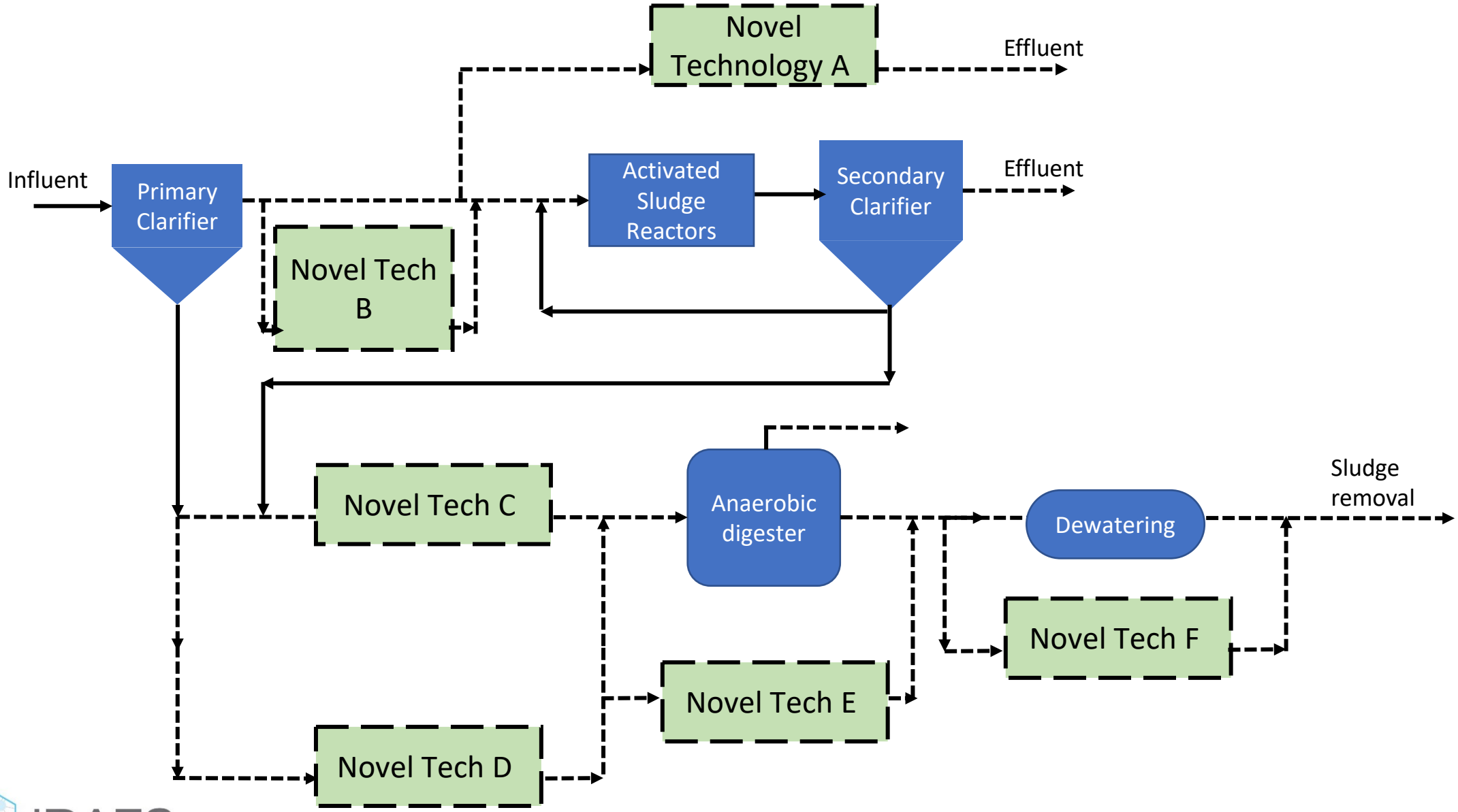
Motivation: Replace or enhance processes within conventional wastewater treatment plants to convert them into “water resource recovery facilities.”



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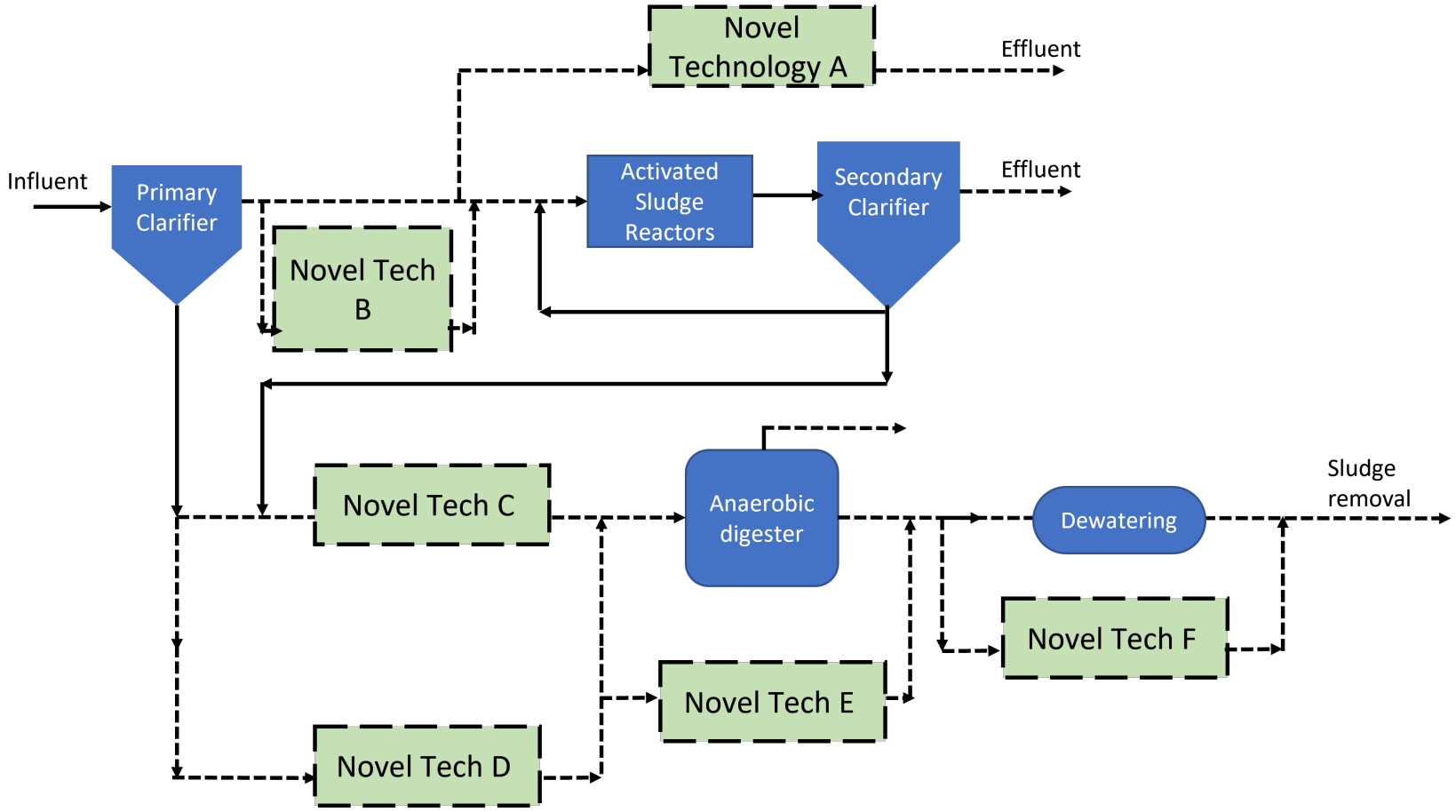
Motivation: Replace or enhance processes within conventional wastewater treatment plants to convert them into “water resource recovery facilities.”

Desired outcomes:

- Recover and valorize nutrients that otherwise would have environmental impacts, e.g.:
  - Nitrogen
  - Phosphorus
- Reduce energy & material consumption
- Reduce cost



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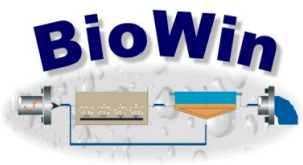
Why WaterTAP?

Existing examples of commercial products for wastewater treatment modeling:



SIMBA#

- "The data and modeling tools created by NAWI are a **central, strategic and non-biased service to NAWI members, the broader water and wastewater treatment community, and DOE to identify opportunities, assess progress, and inform RD&D.**" – FOA 2336

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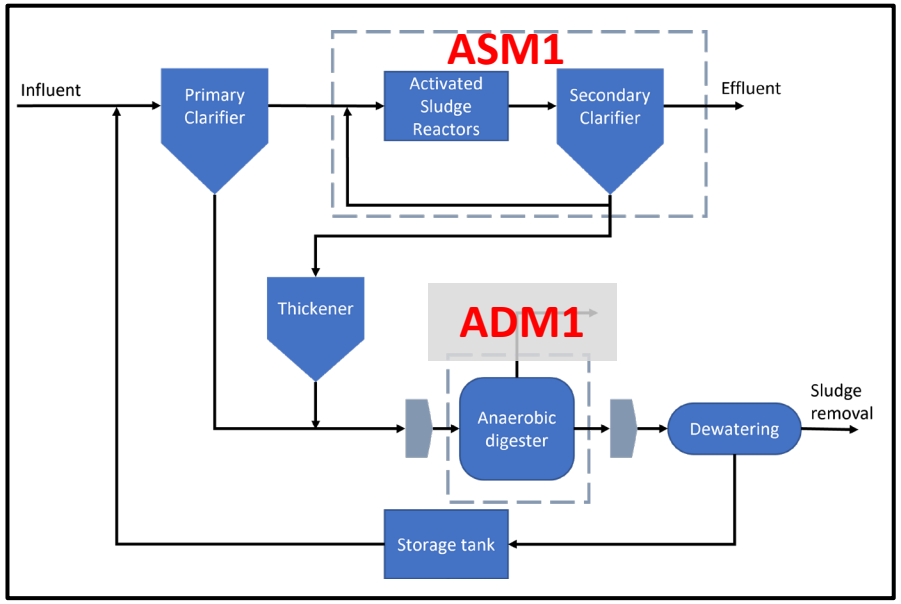
Strategy for model implementation

- Uses the **originally proposed property reaction models, i.e.,:**
  - Activated sludge model no. 1 (ASM1)
  - Anaerobic digestion model no. 1 (ADM1)

Benchmark Simulation Model No. 2 (BSM2)



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Strategy for model implementation

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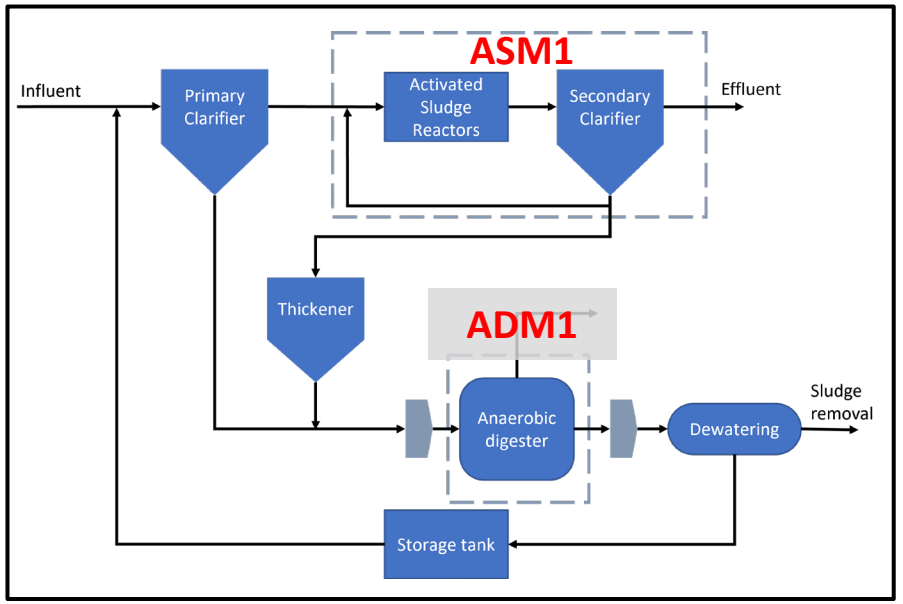
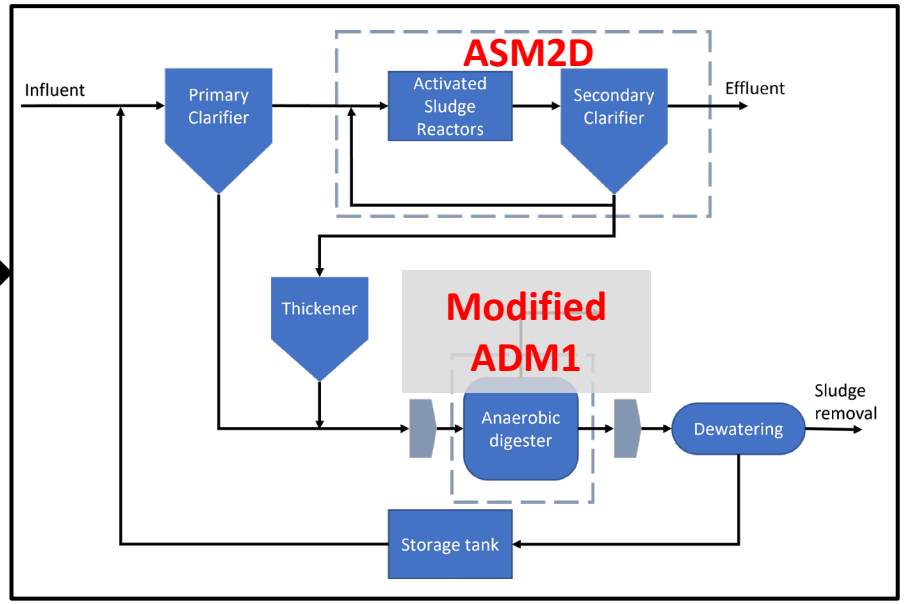


- Uses the **extended property reaction models, i.e.,:**
  - Modified activated sludge model no. 2D (ASM2D)
  - Modified anaerobic digestion model no. 1 (Modified ADM1)
- **Includes** tracking and biological transformation of phosphorus-related components

"Extended" BSM2



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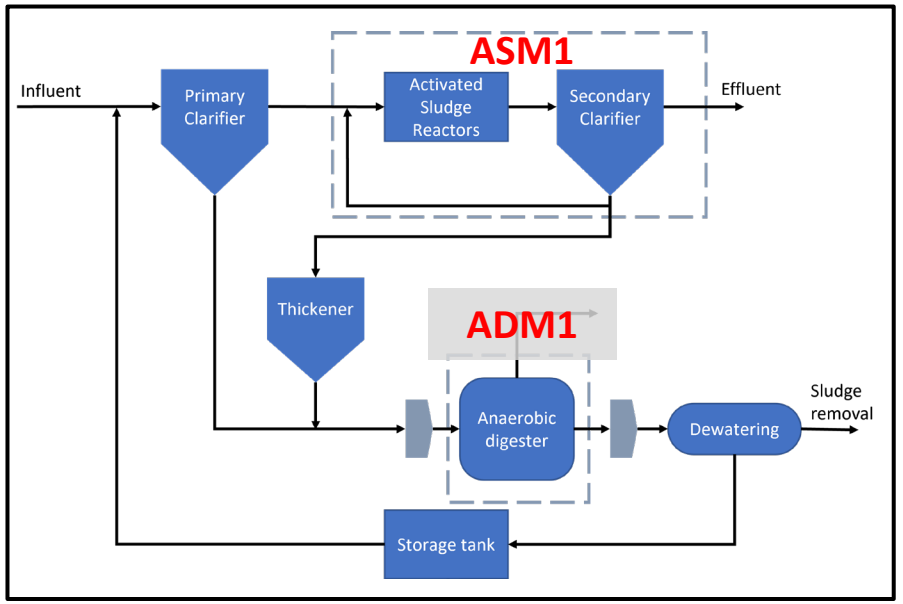

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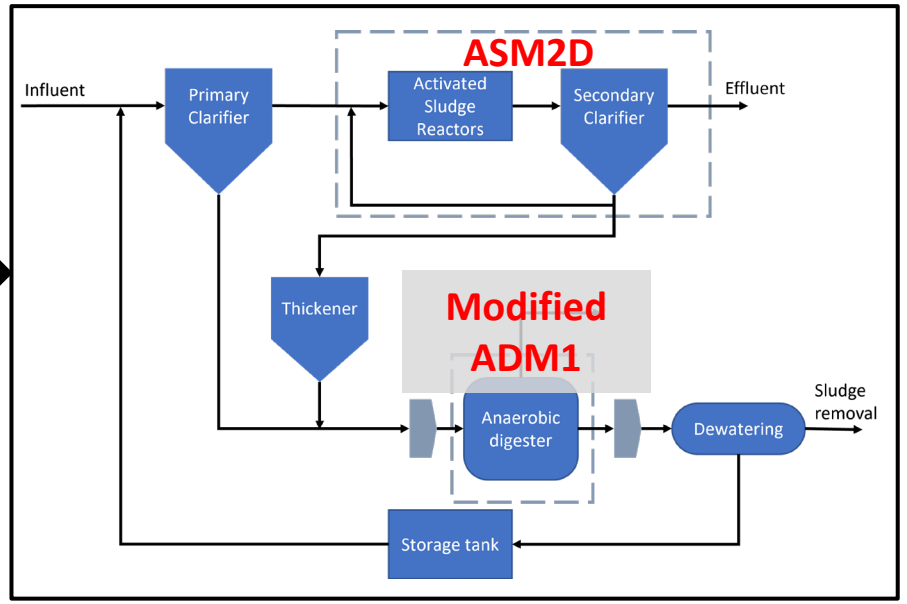

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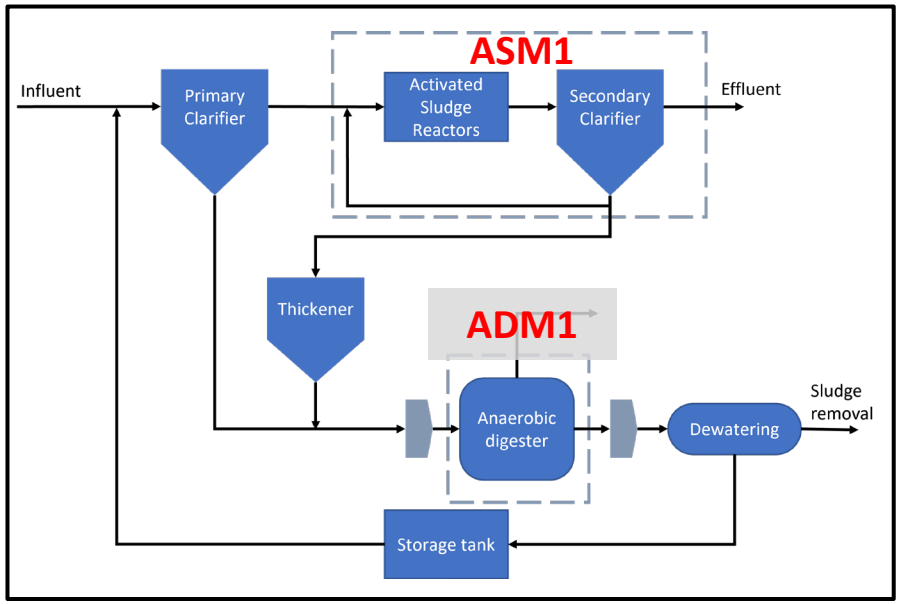

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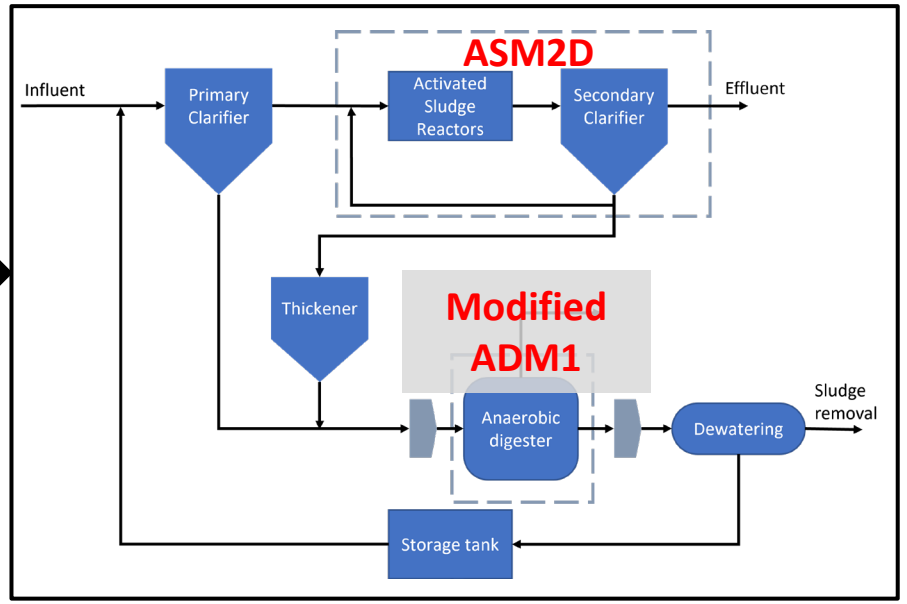

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Strategy for model implementation

- Implement the full flowsheet and get the model solving
- If successful, use this to assist completion of extended BSM2

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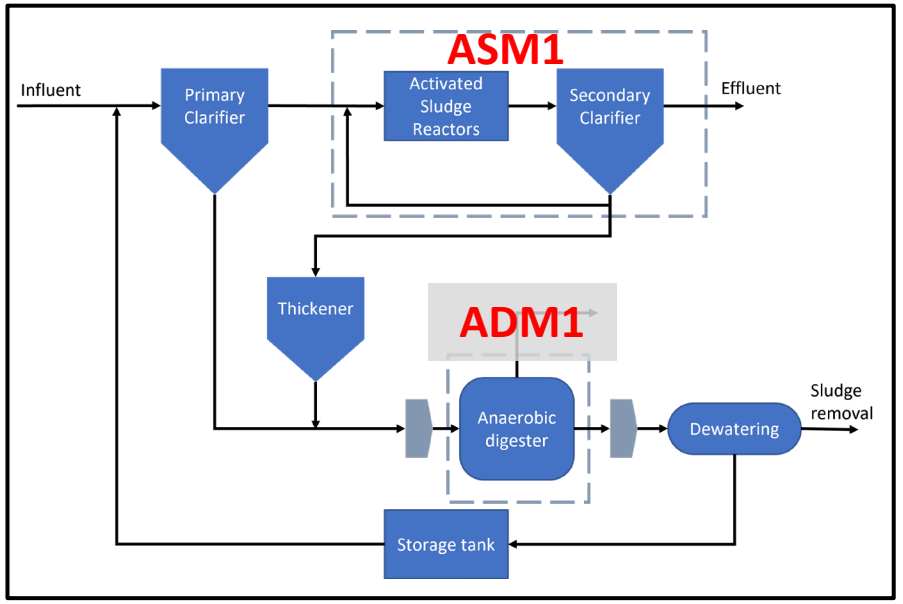

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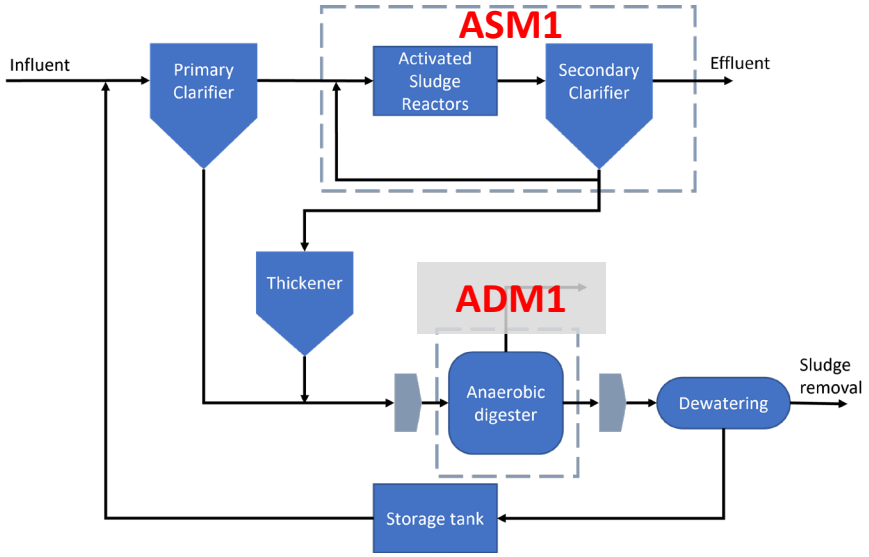
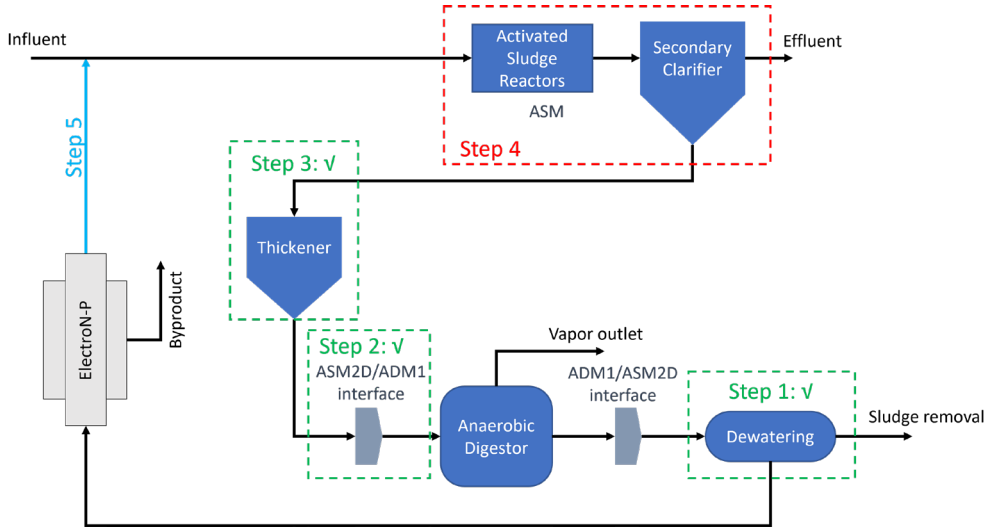


- Implement flowsheet piecewise, building out sub-flowsheets already known to be stable on BSM2 flowsheet

"Extended" BSM2



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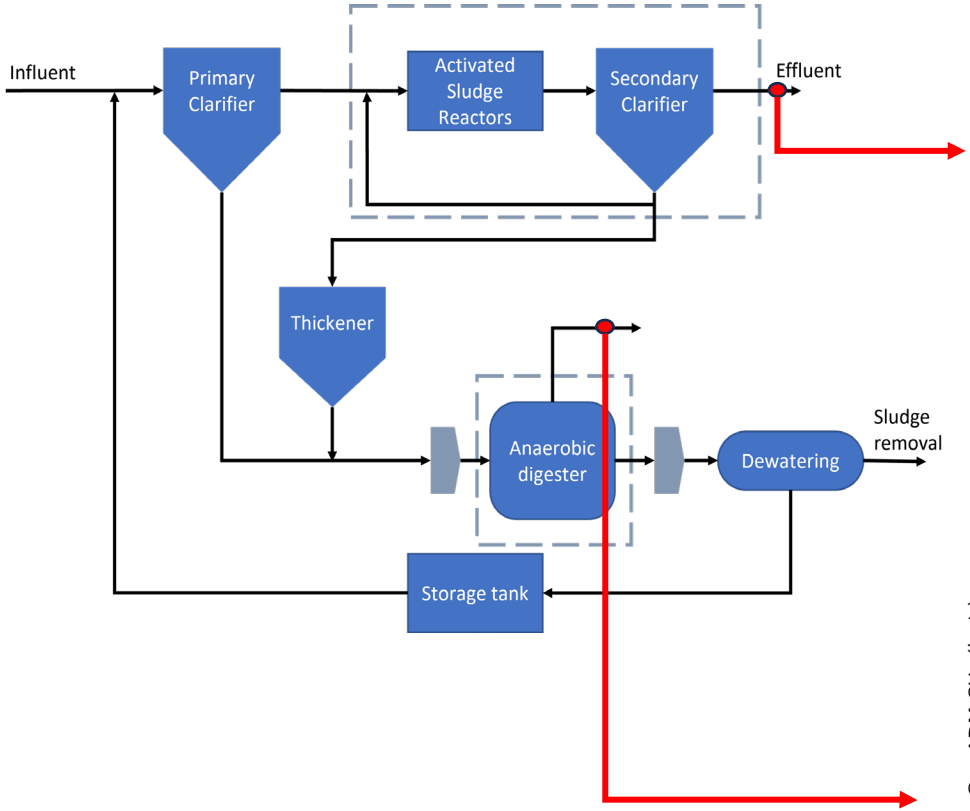
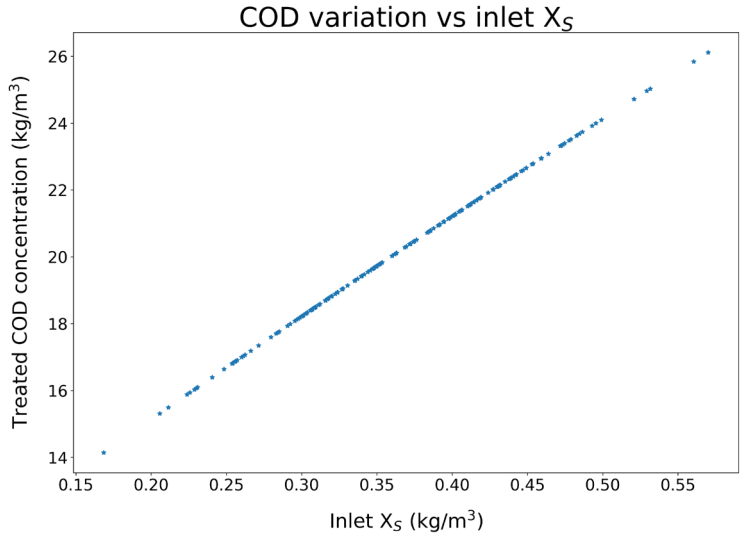
Initial simulation results demonstrating BSM2 model stability

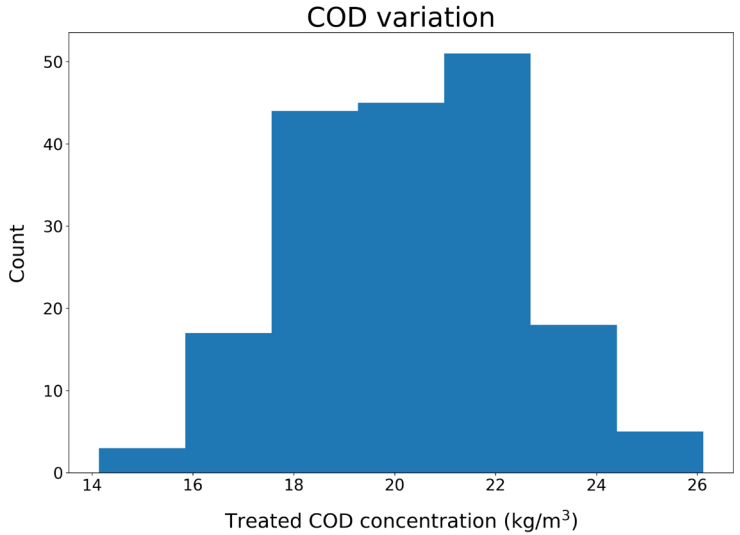
Xs: slowly biodegradable substrate

COD: chemical oxygen demand

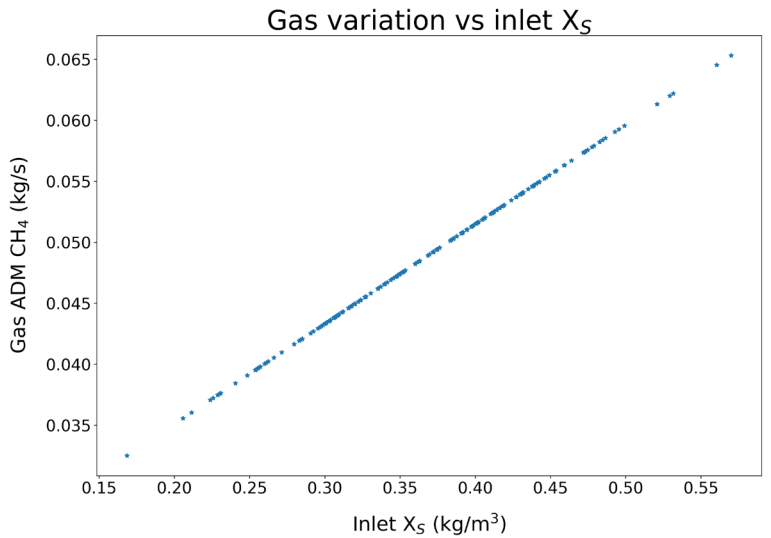


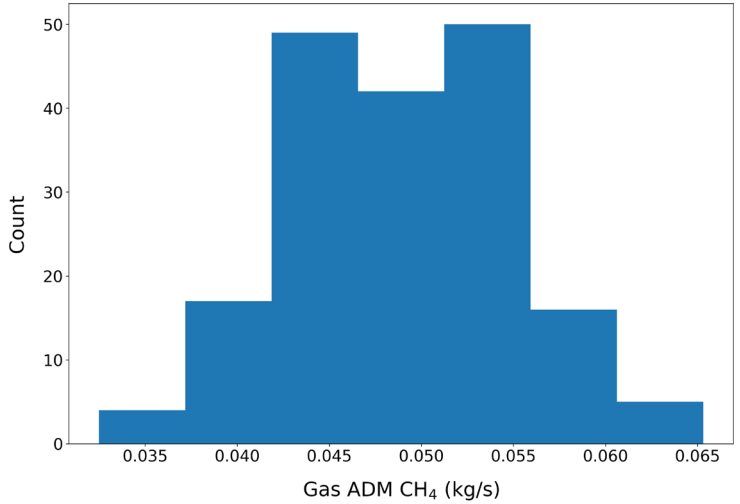
Treated effluent COD





Methane Production of Anaerobic Digestor





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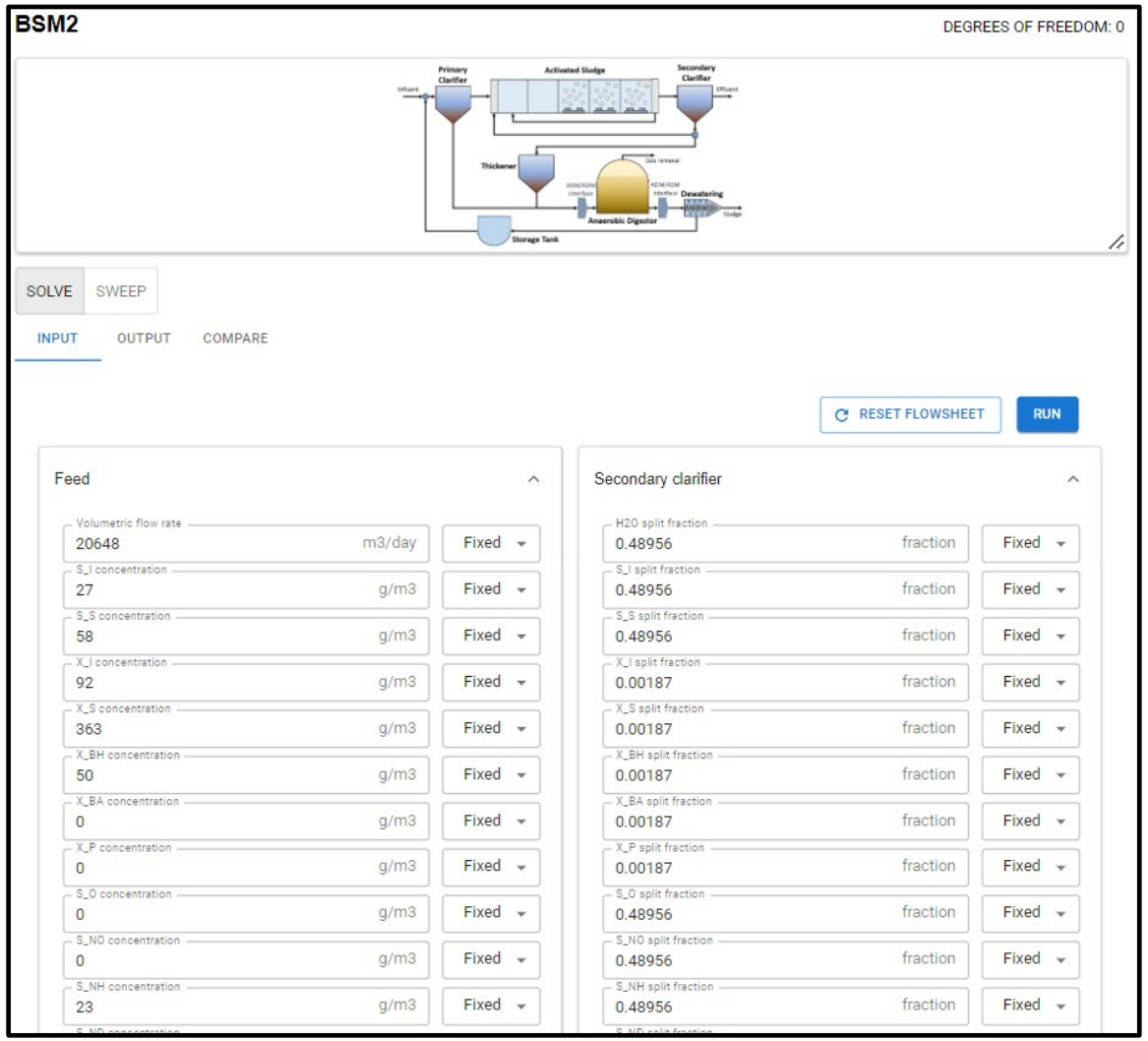
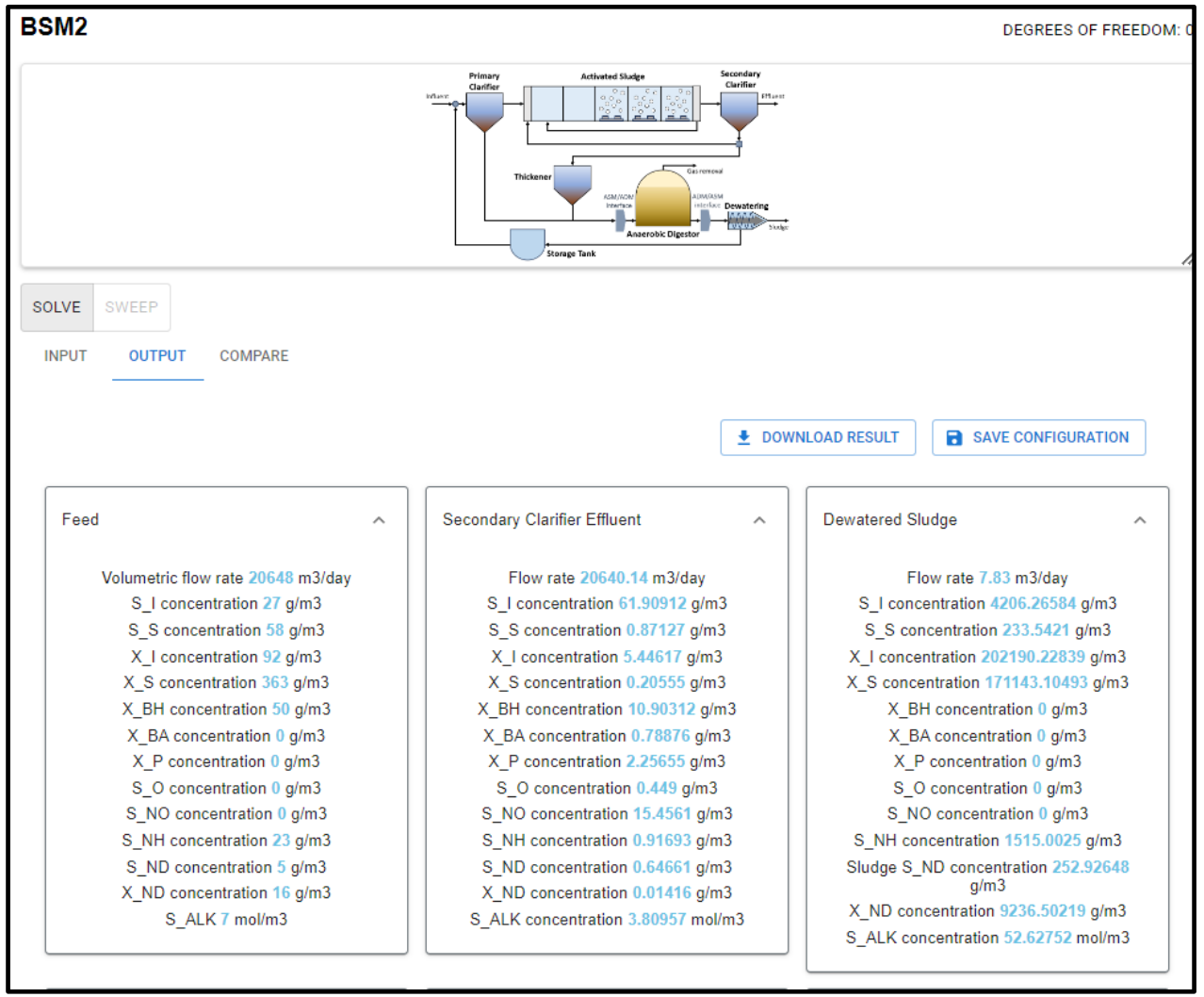
BSM2 Graphical User Interface (GUI)

INPUTS



OUTPUTS



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Future Work: short-term

- Stabilize the extended BSM2 flowsheet to enable plant-wide modeling with phosphorus tracking
- Add unit- and flowsheet-level costing and performance metrics
- Plug in models of novel technologies to conduct comparative, detailed techno-economic analyses for select 2336 awardees
- Model extensions, e.g.:
  - Ion speciation
  - Precipitation reactions
  - pH prediction

Future Work: long term

Thinking beyond 2024…

- Supporting WRRF-related projects funded by DOE?
- WaterTAP + WNTR ➔ WRRF plant modeling with network-scale resilience modeling?

- NAWI 2.0 → Regional-scale modeling? Building-scale reuse modeling?
- Dynamic modeling or quasi-steady-state using multiperiod modeling from the DISPATCHES workflow

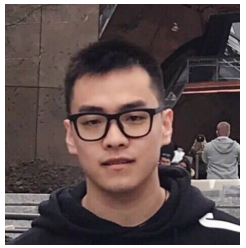
Acknowledgments

NATIONAL ENERGY TECHNOLOGY LABORATORY


Tim Bartholomew


Adam Atia


Andrew Lee


Chenyu Wang


Travis Arnold


Marcus Holly


Alejandro Garciadiego


Elmira Shamlou

NREL
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Lawrence Berkeley National Laboratory

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Disclaimer

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Resources and contact info

Contact information:
Adam A. Atia
adam.atia@netl.doe.gov

BSM2 Tutorial

WaterTAP GUI

Property Model Documentation

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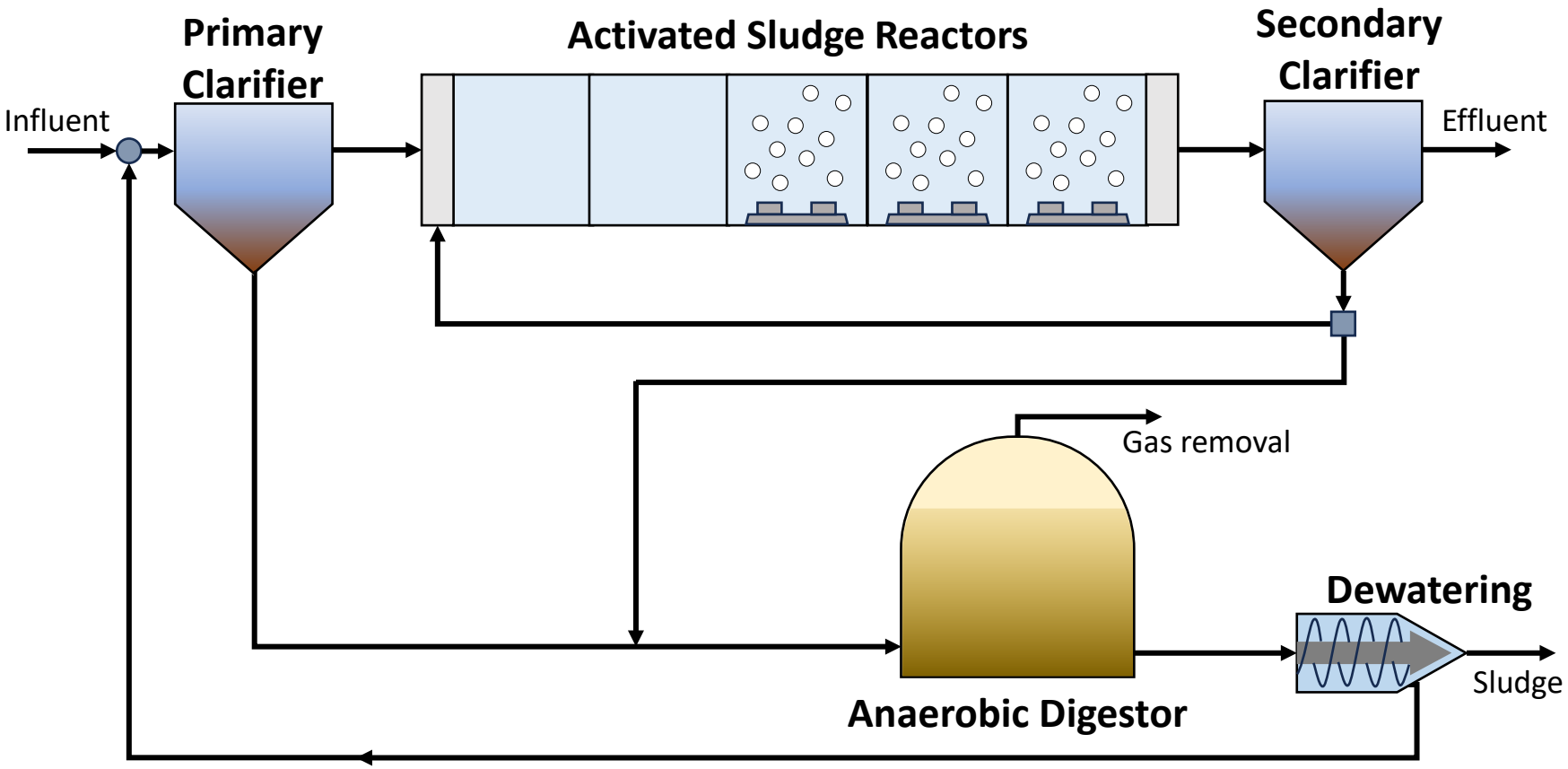
Backup Slides

Generalized figure



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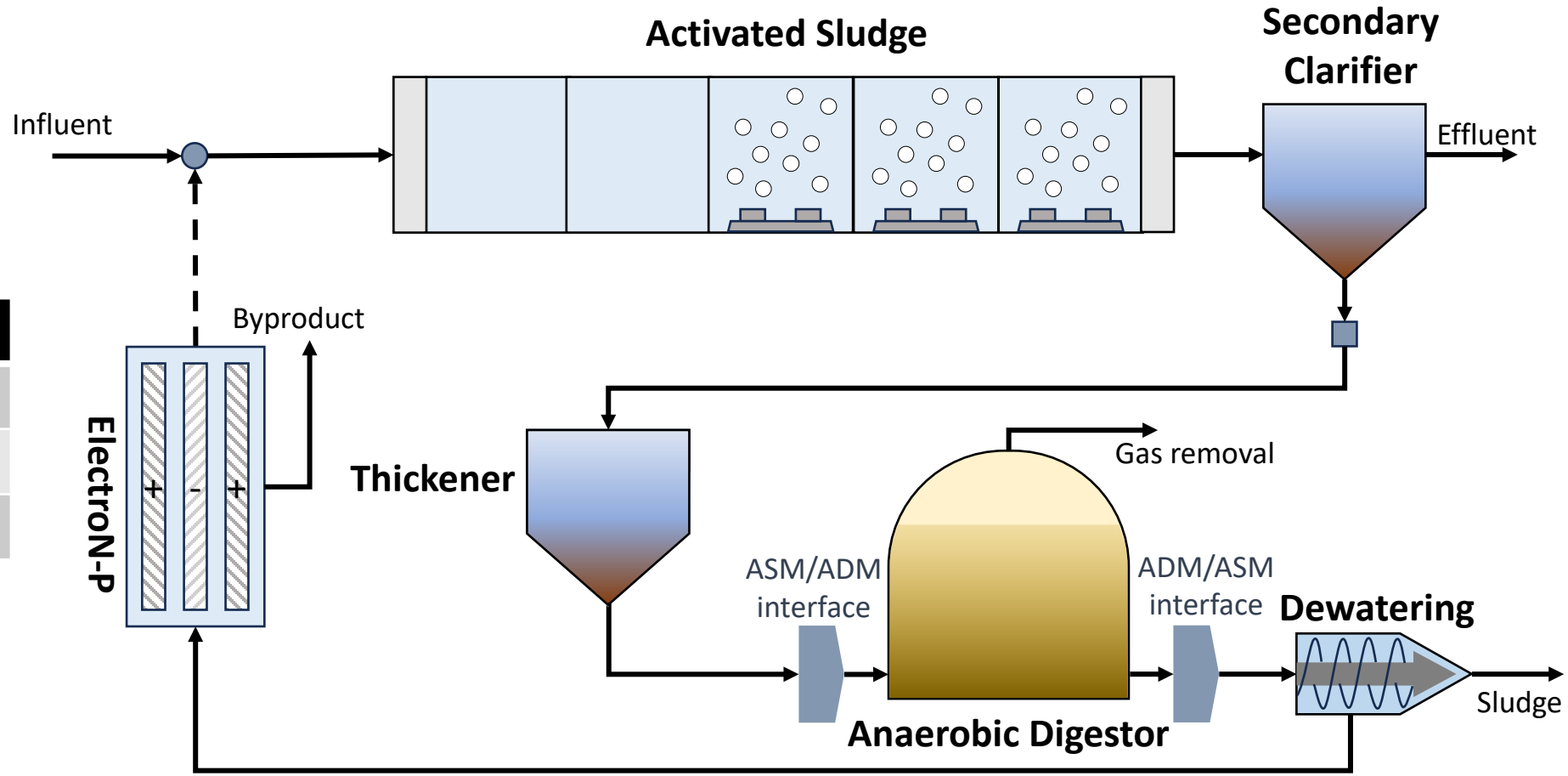
ElectroN-P sub-flowsheet

Name	Value
Flow rate (m3/d)	20648
Temperature (K)	298.15
Pressure (Pa)	101325



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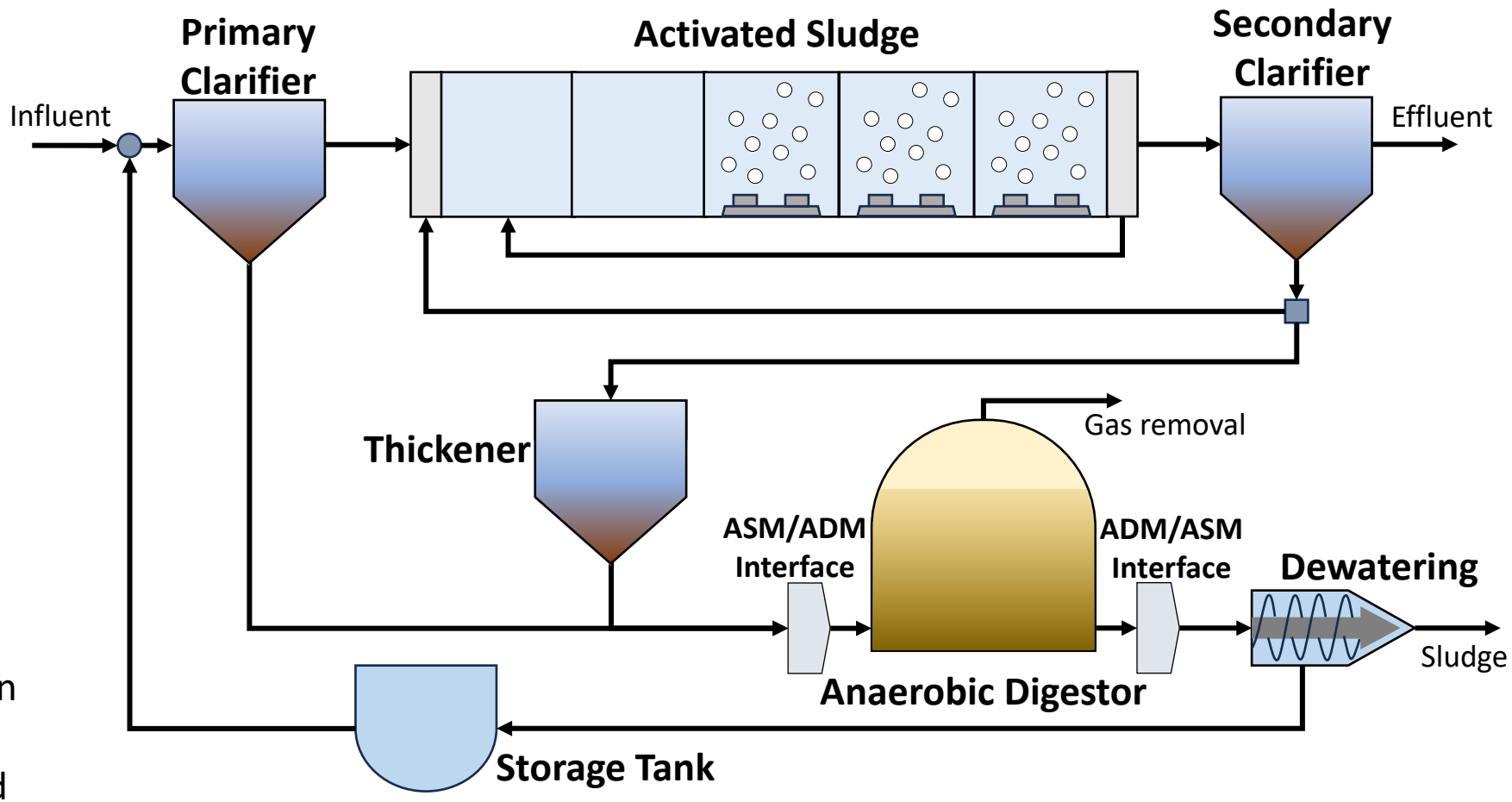
Motivation

BSM2 is an industry standard model for modeling a conventional wastewater treatment plant

ASM1
- Carbon oxidation
- Nitrification
- Denitrification

ASM2d
- Additional biological process
- Phosphorus removal
- Cell internal structure

ADM1
- Biochemical:
  - Extracellular process
  - Intracellular process
- Physico-chemical:
  - Ion association/dissociation
  - Gas-liquid transfer
  - Precipitation – to be added



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Benchmark Simulation Model 2 (BSM2)

BSM2 is an industry standard model for modeling a conventional wastewater treatment plant

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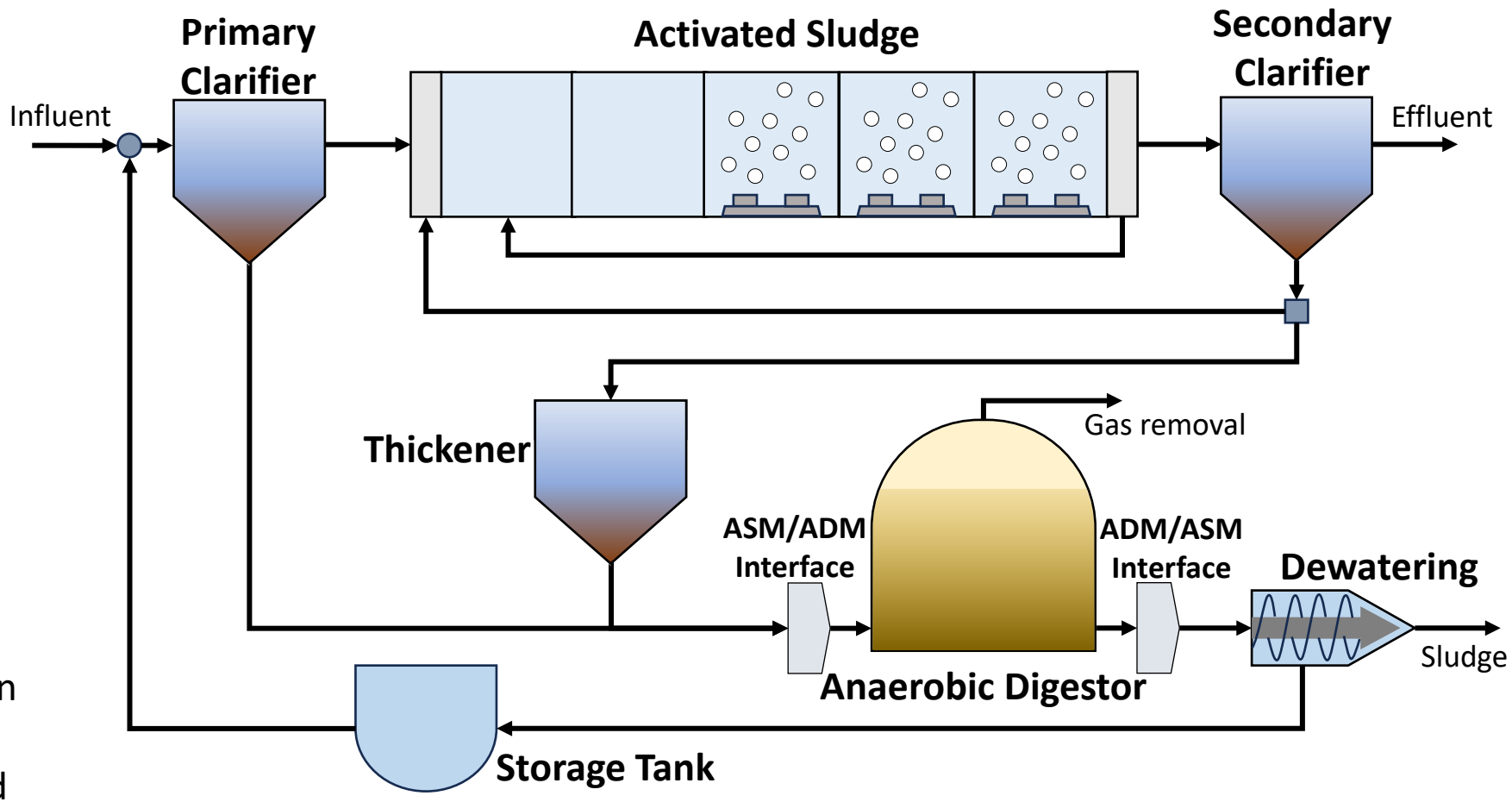

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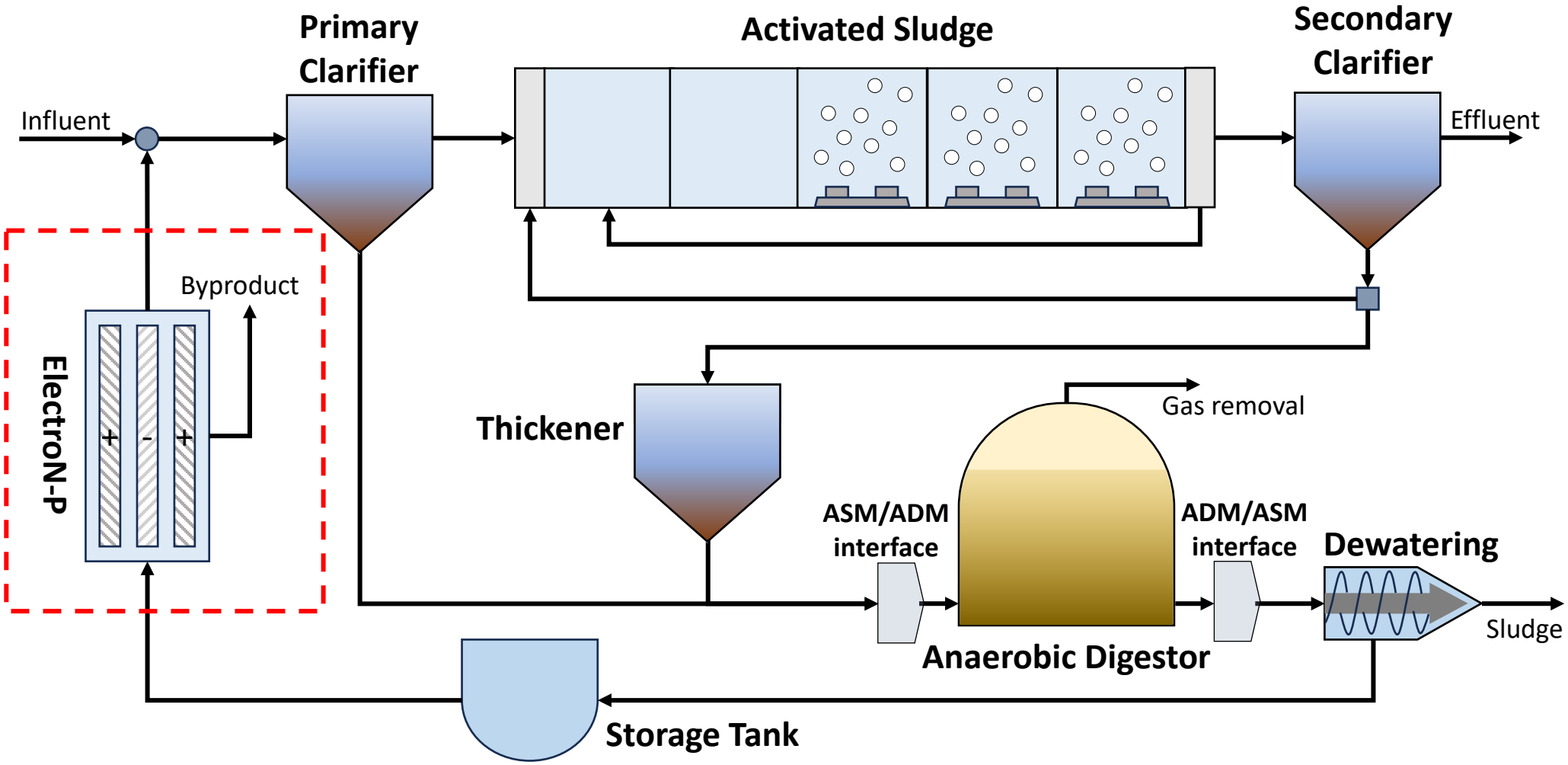
ElectroN-P

ElectroN-P: extract nitrogen and phosphorous from municipal wastewater



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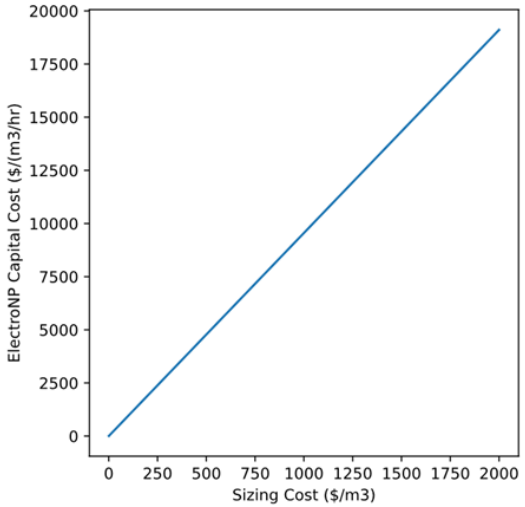
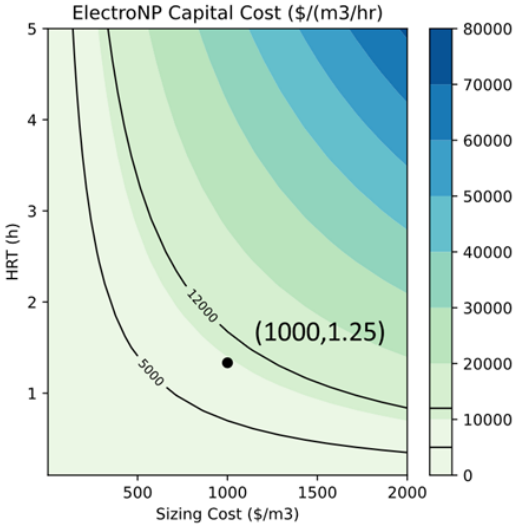
Results

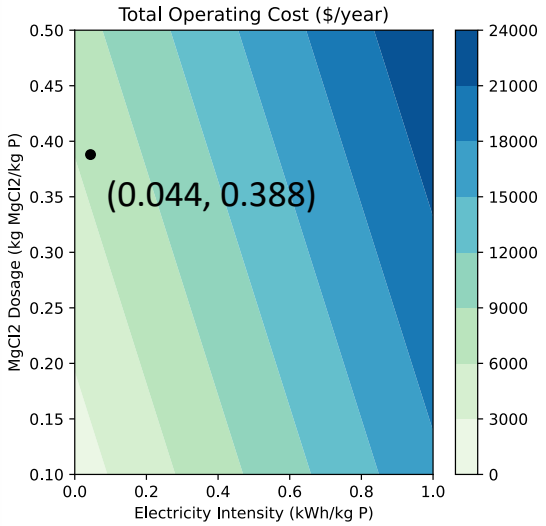
Activated Sludge Process

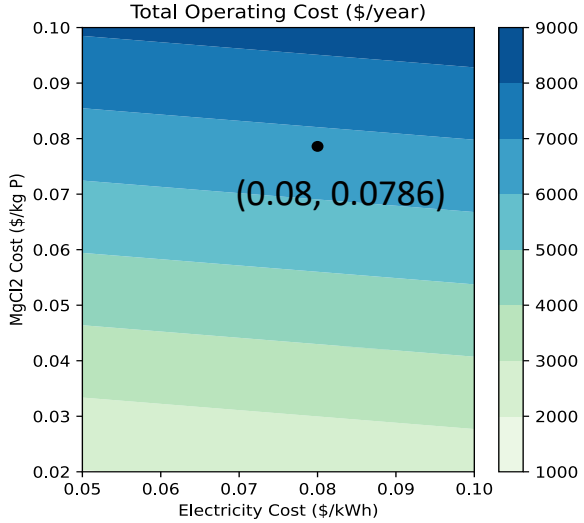
Components	Description	Influent concentration (g/L)	ASM outlet concentration (g/L)	ElectroN-P inlet concentration (g/L)	ElectroN-P outlet concentration (g/L)
S_IC	Inorganic Carbon	0.079	0.083	2.918	2.918
S_I	Soluble Inerts	0.030	0.030	0.030	0.030
S_A	Acetate	0.020	0.012	0.084	0.084
S_F	Fermentable	0.030	0.019	19.495	19.495
S_N2	Dinitrogen	0.015	0.015	0	0
S_NH4	Ammonium plus ammonia nitrogen	0.016	0.014	4.142	2.899
S_NO3	Nitrate plus nitrite nitrogen	0	0	0	0
S_O2	Dissolved oxygen	0	0	0	0
S_PO4	Inorganic soluble phosphorus	0.0036	0.0033	0.905	0.018
S_K	Potassium	0	0	0	0
S_Mg	Magnesium	0	0	0	0
X_I	Particulate Inerts	0.025	0.025	0.349	0.349
X_PHA	Polyhydroxyalkanoates	0	0	0	0
X_PP	Polyphosphates	0	0	0	0
X_PAO	Phosphorus Accumulating Organisms	0	0	0	0
X_AUT	Autotrophic nitrifying organisms	0	0	0	0
X_H	Heterotrophic organisms	0.030	0.053	0	0
X_S	Slowly biodegradable substrates	0.125	0.105	0.0006	0.0006

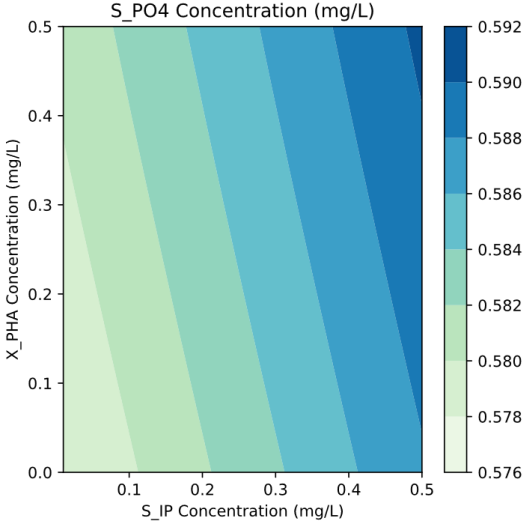
Sensitivity Analysis

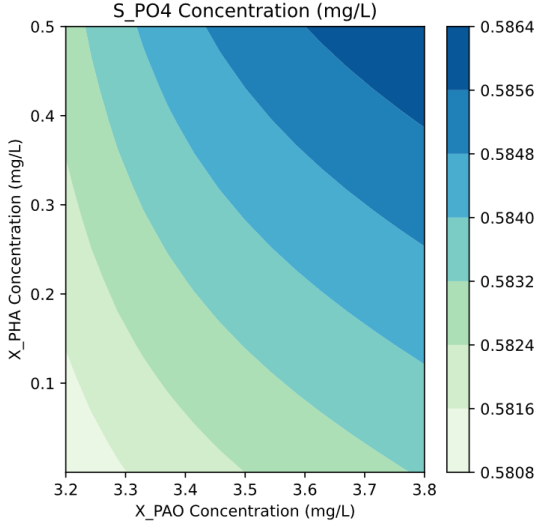












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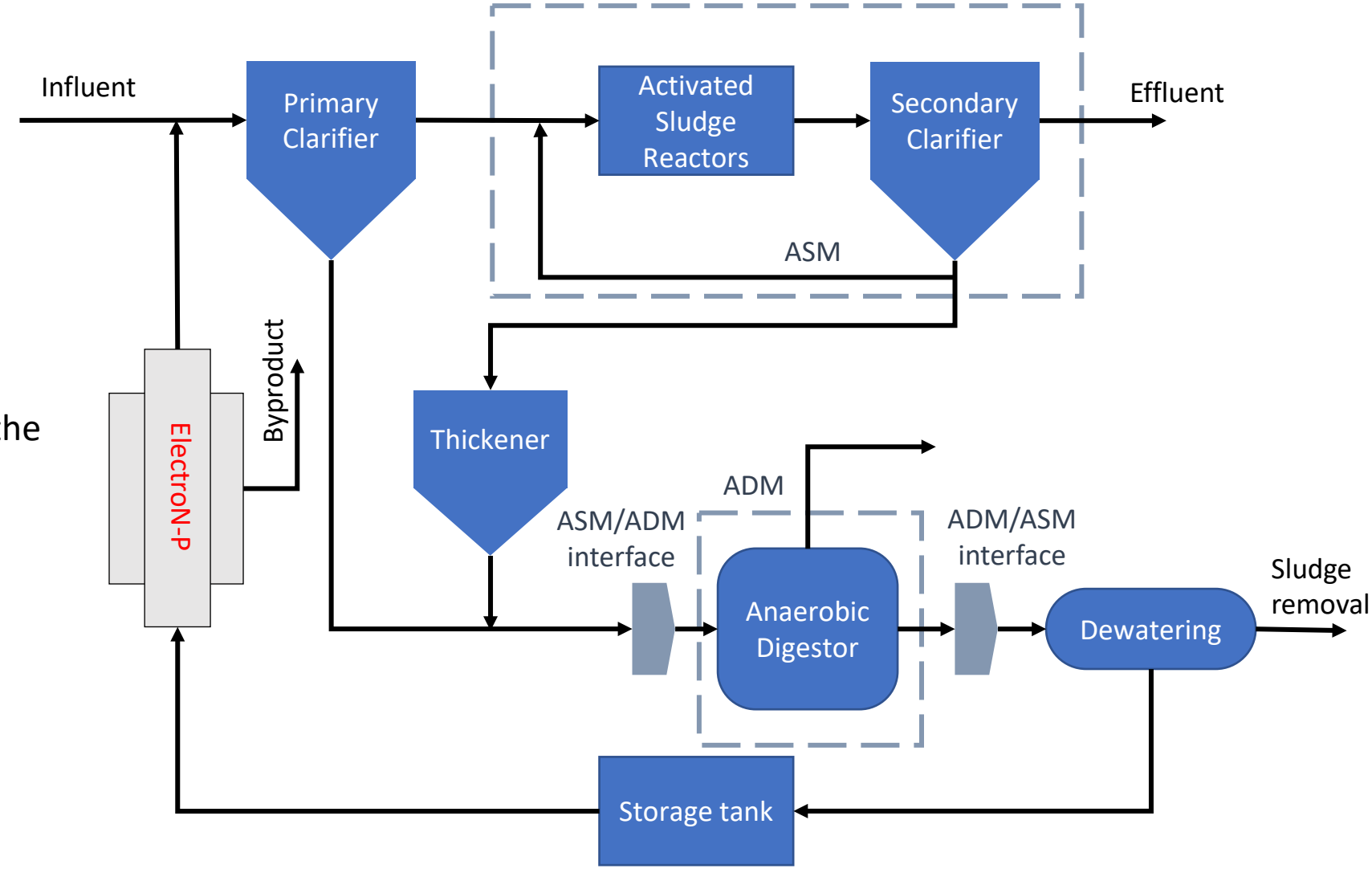
Progress updates and future plan

Progress updates:

- Full BSM2 flowsheet (ASM1) √: PR under review
- ASM2D; ADM1 reformulated for resolving scaling issue
- ElectroN-P 0D model reformulated

Future plan:

- Integrate these modifications into the electroN-P sub-flowsheet
- Finish Step 4
- Revise costing method of AD
- Add costing for thickener, activated sludge reactor and clarifiers
- Finish Step 5



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Results

Description	Units	Value
Levelized Costs (without revenue from products)		
Levelized cost of feed water	$/m^3 of feed water	14.827
Capital costs		
Investment costs (including direct capital, indirect capital, installation, siting, etc.)	$/(m^3/hr)	897949
Total capital costs	k$	433.857
Anaerobic digestor capital cost	k$	216.301
ElectroN-P capital cost	k$	0.627
Operating costs		
Electricity cost	$/m^3 of feed water	0.005
Magnesium chloride cost	$/m^3 of feed water	0.026
Energy Consumption		
Total specific electricity consumption	kWh/m^3 of feed water	0.0666

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