

IDAES

Institute for the Design of
Advanced Energy Systems

Using Benchmark Simulation Models to Evaluate Biological Wastewater Treatment in WaterTAP

Adam Atia

National Energy Technology Laboratory (NETL), NETL Support Contractor

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Sandia
National
Laboratories

Carnegie Mellon

West Virginia University



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

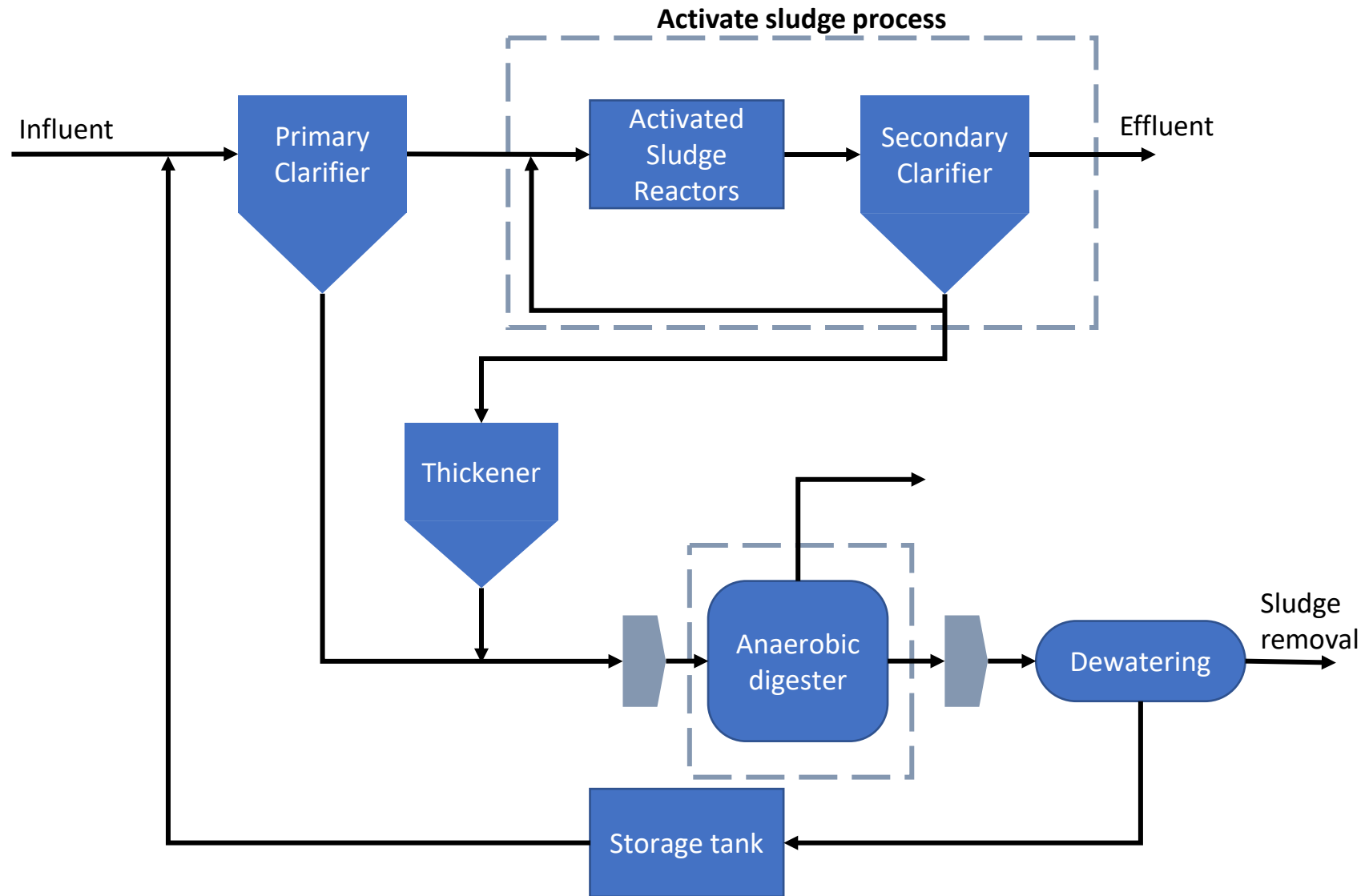


Northwestern
University

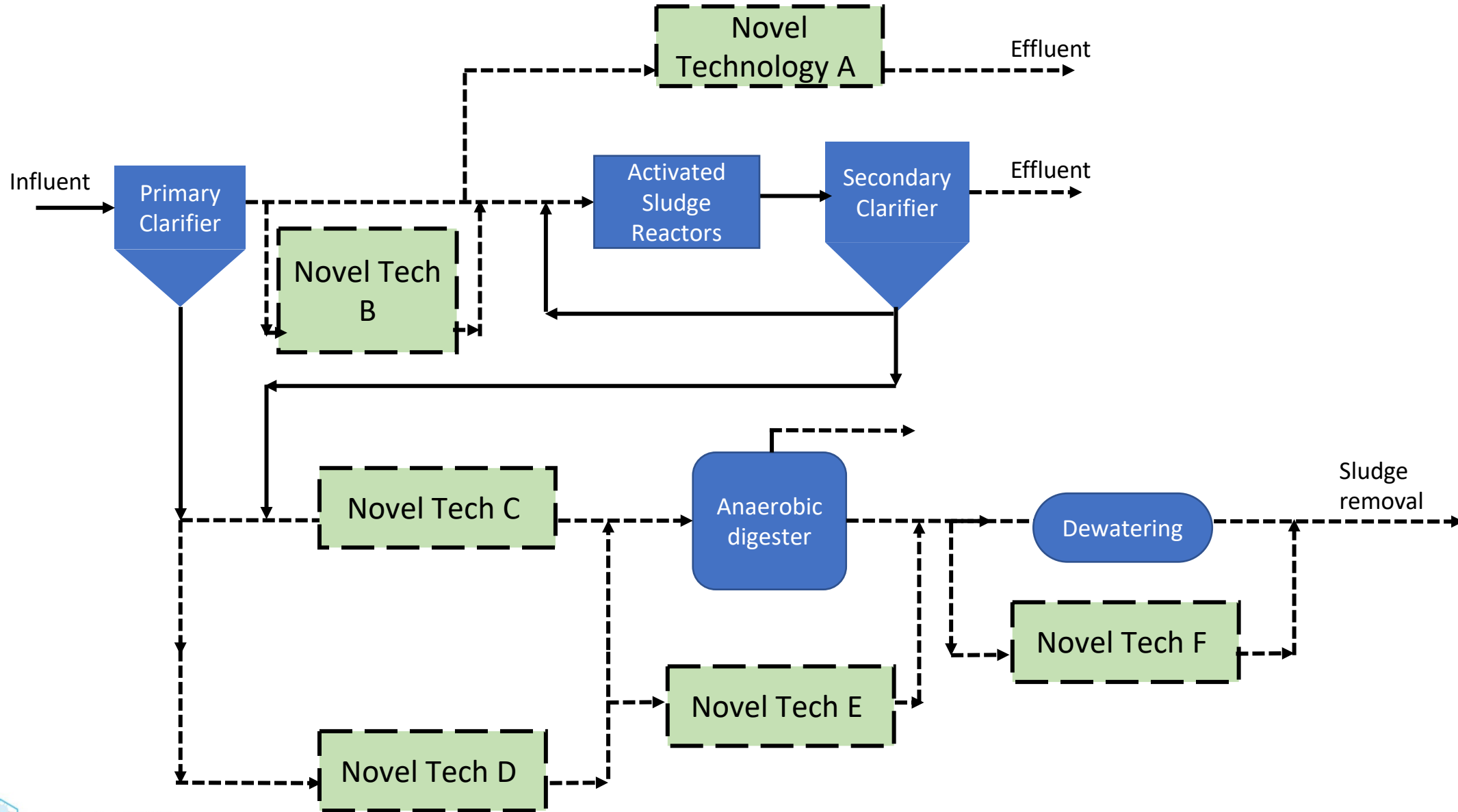
IEDO (FOA-0002336) program:

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

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



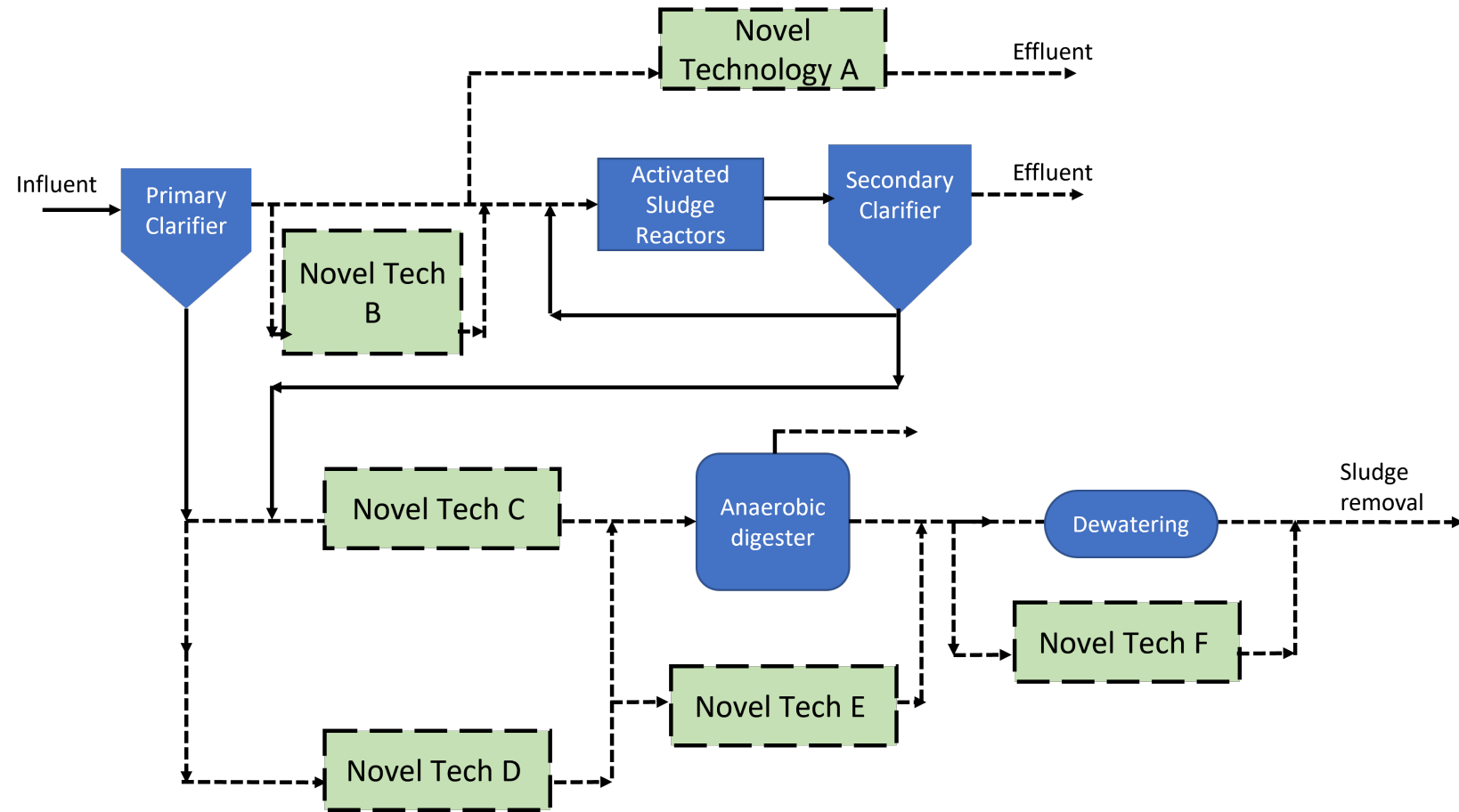
Motivation: Replace or enhance processes within conventional wastewater treatment plants to convert them into “water resource recovery facilities.”



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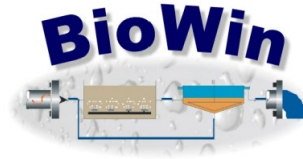
Desired outcomes:

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



Why WaterTAP?

Existing examples of commercial products for wastewater treatment modeling:



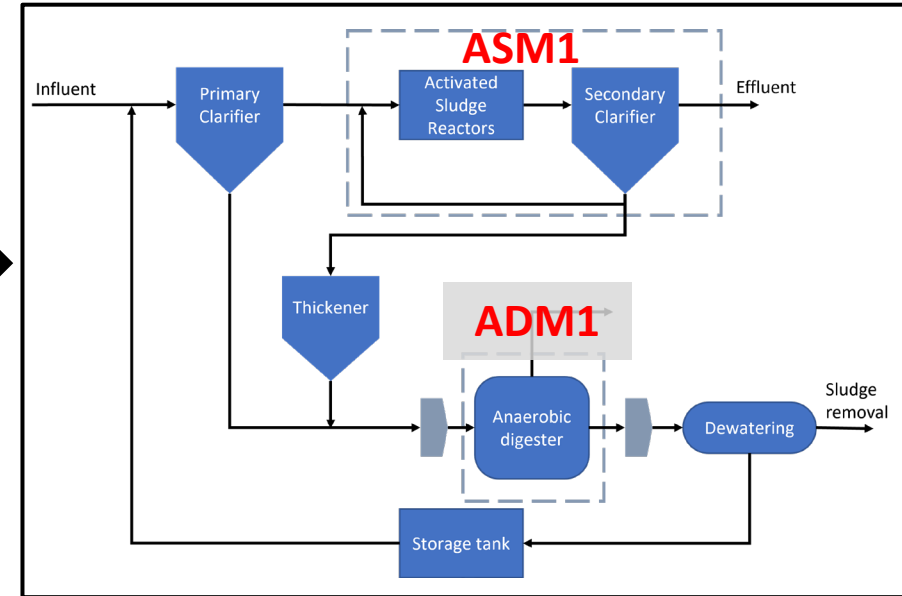
SIMBA#

- “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

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)

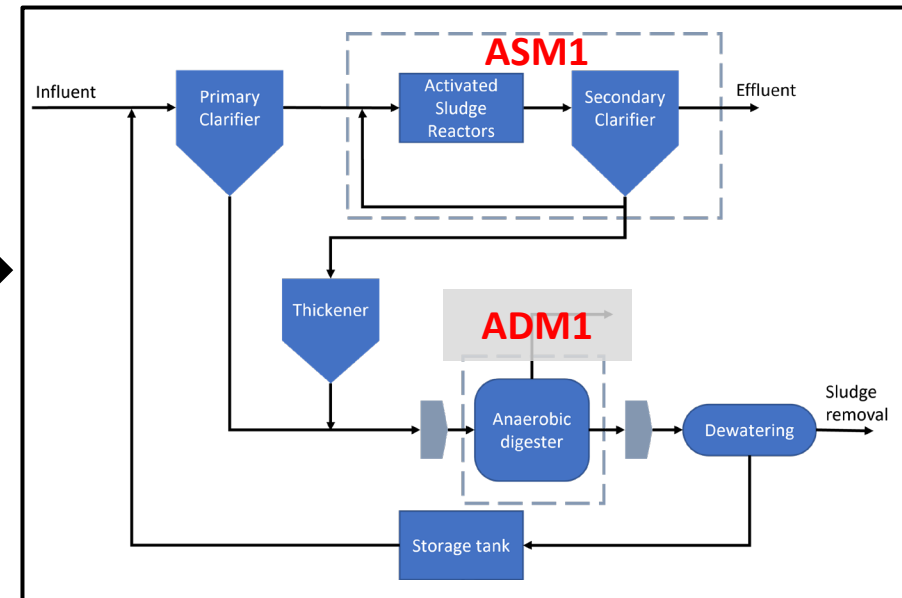


Strategy for model implementation

- Uses the **originally proposed property reaction models, i.e.,:**
 - Activated sludge model no. 1 (ASM1)
 - Anaerobic digestion model no. 1 (ADM1)
- **Excludes** tracking and biological transformation of phosphorus-related components



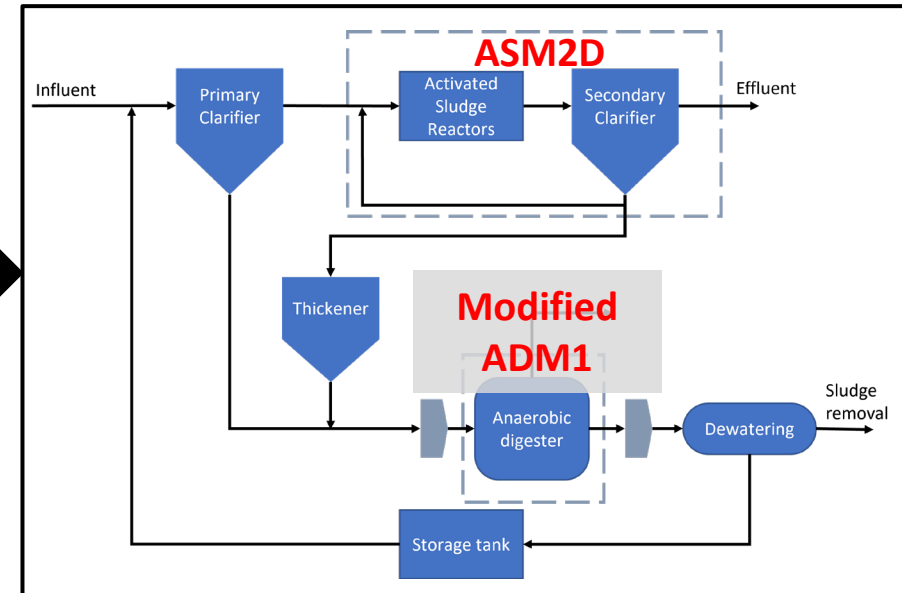
Benchmark Simulation Model No. 2 (BSM2)



- 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

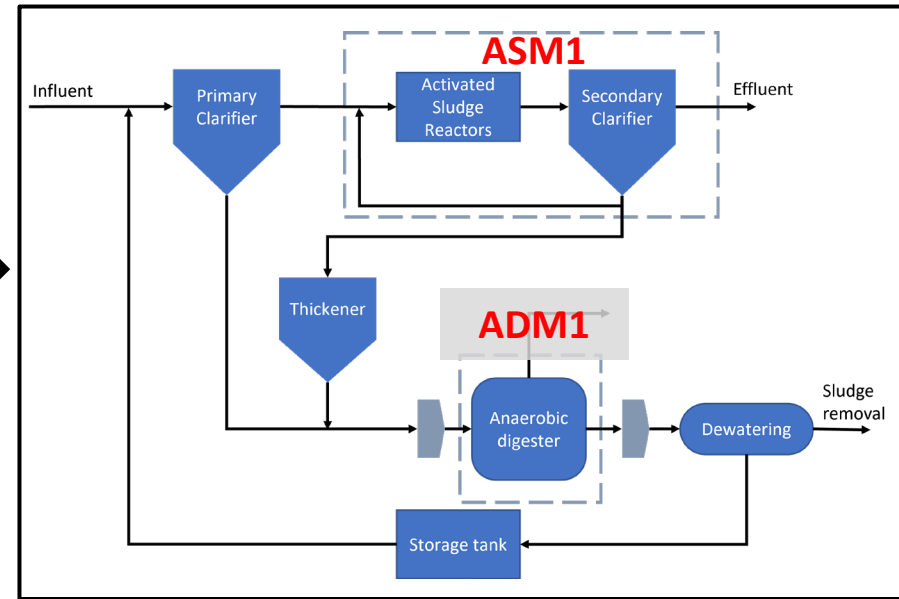


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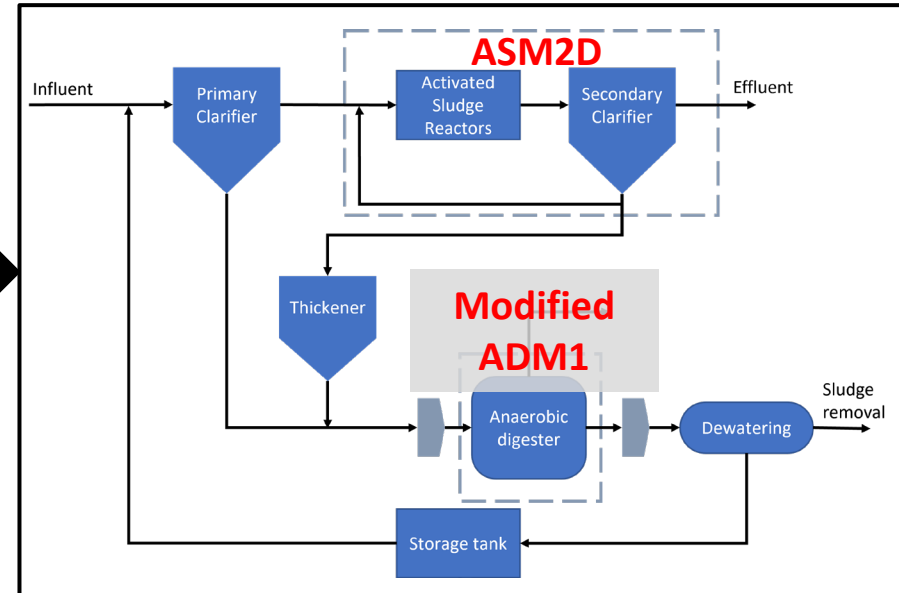
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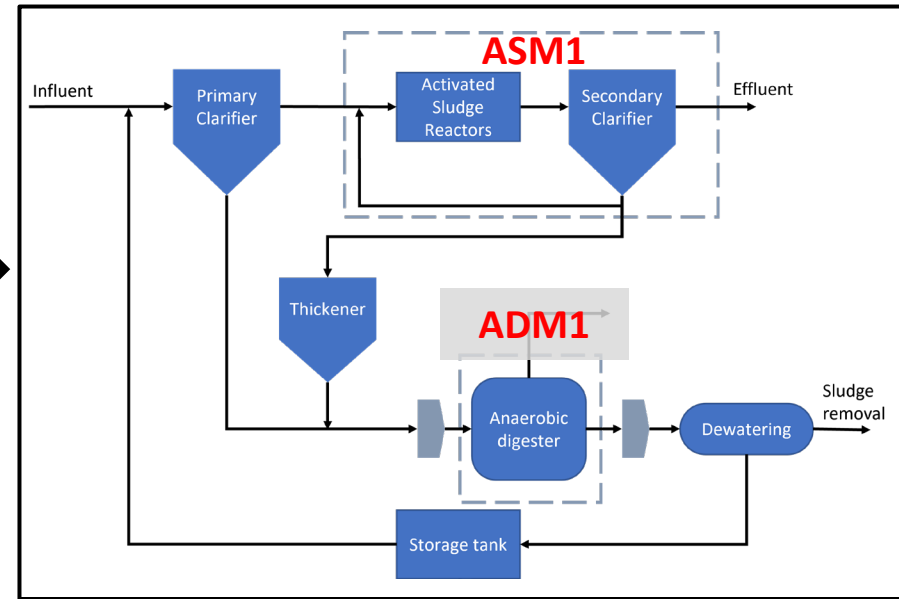


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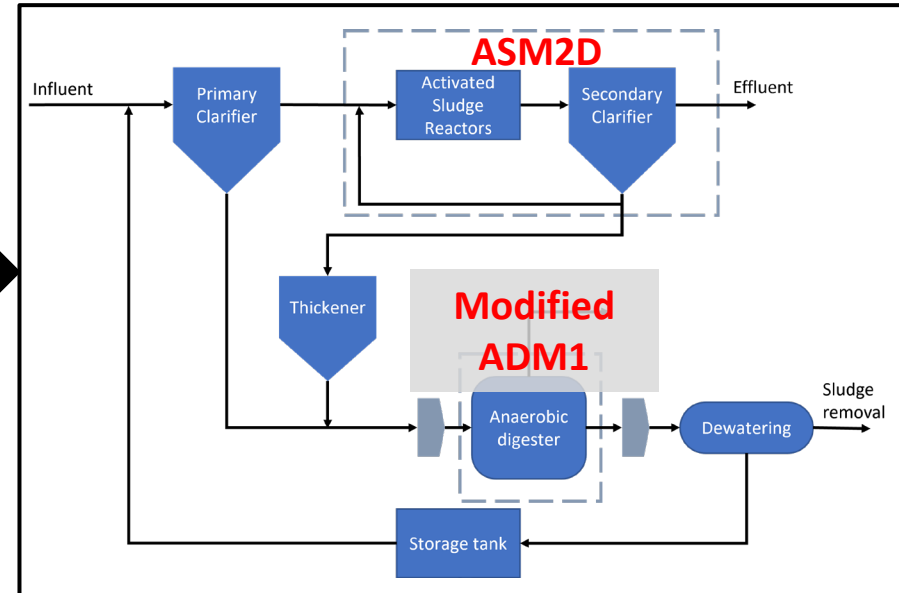
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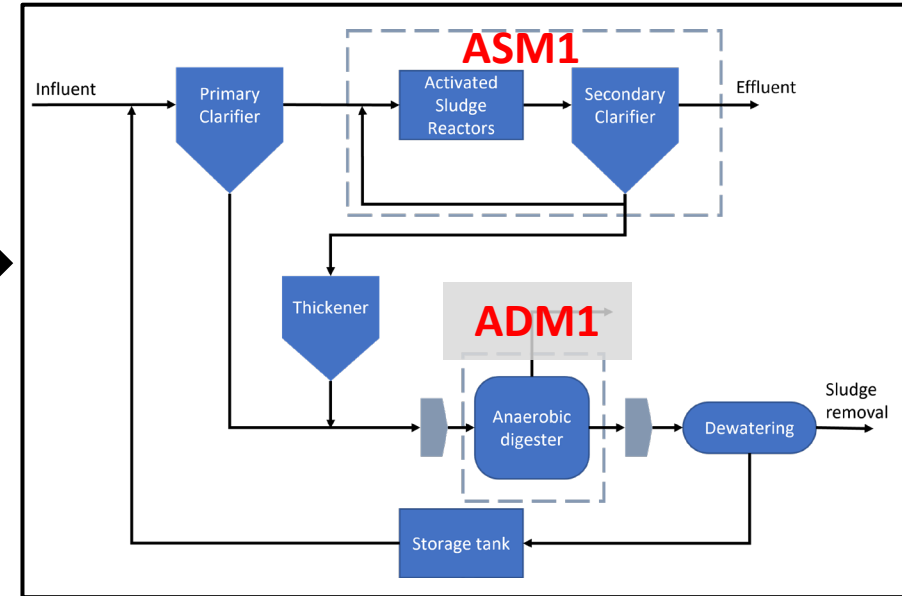
“Extended” BSM2



Strategy for model implementation

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

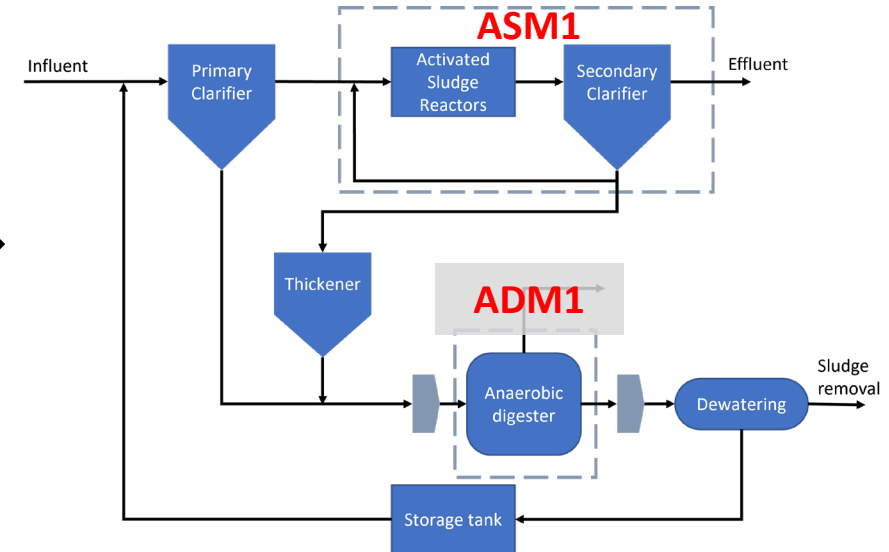
Benchmark Simulation Model No. 2 (BSM2)



Strategy for model implementation

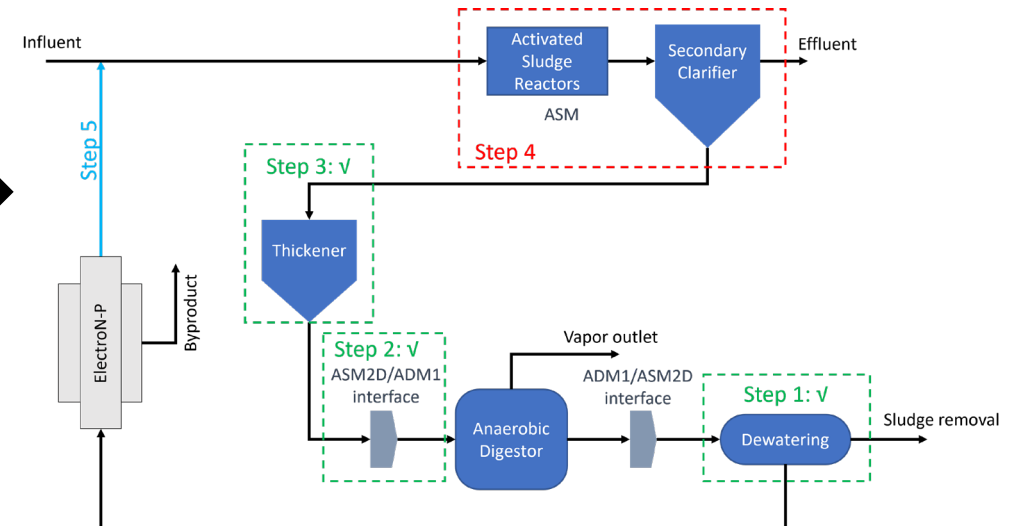
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Benchmark Simulation Model No. 2 (BSM2)



“Extended” BSM2

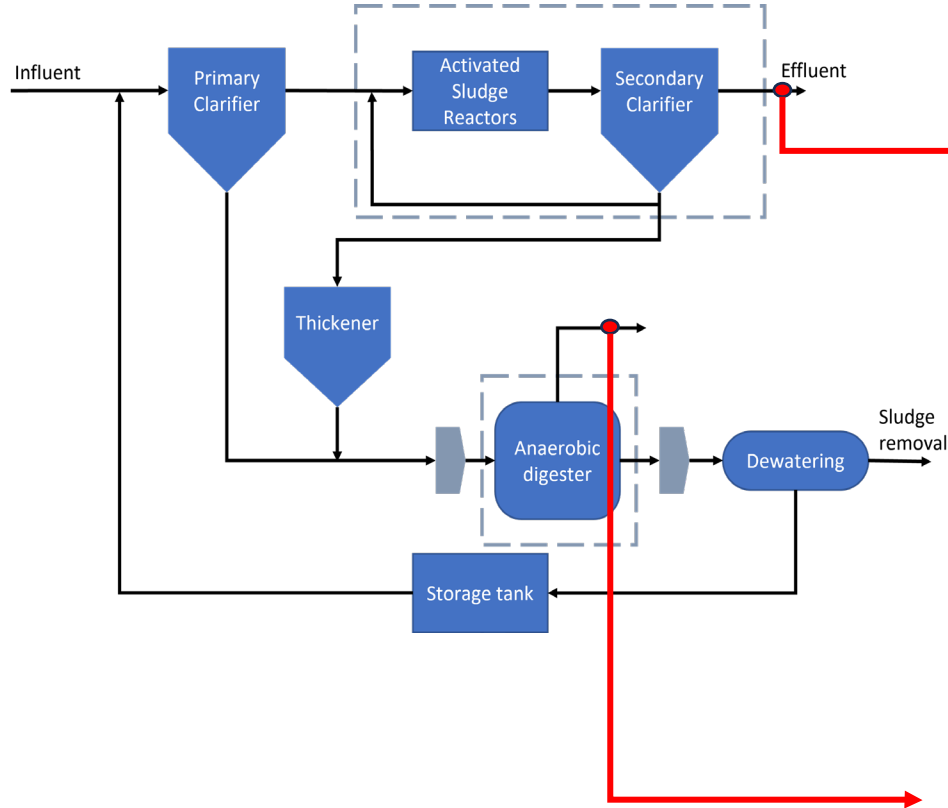
- Implement flowsheet piecewise, building out sub-flowsheets already known to be stable on BSM2 flowsheet



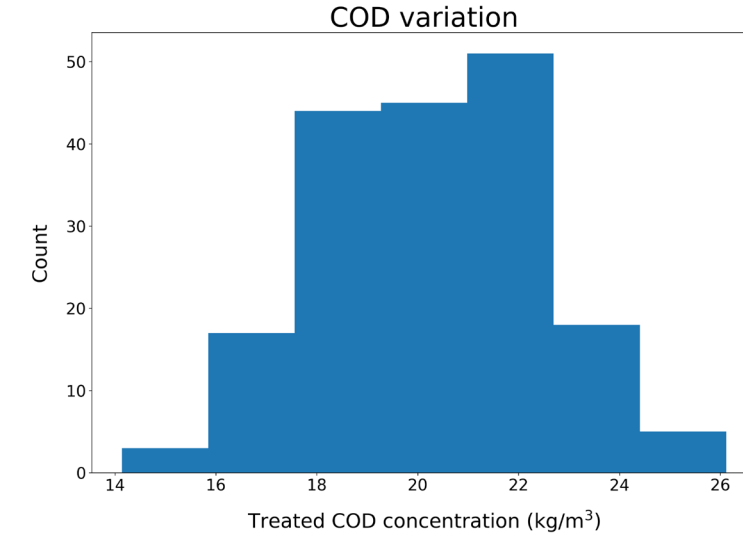
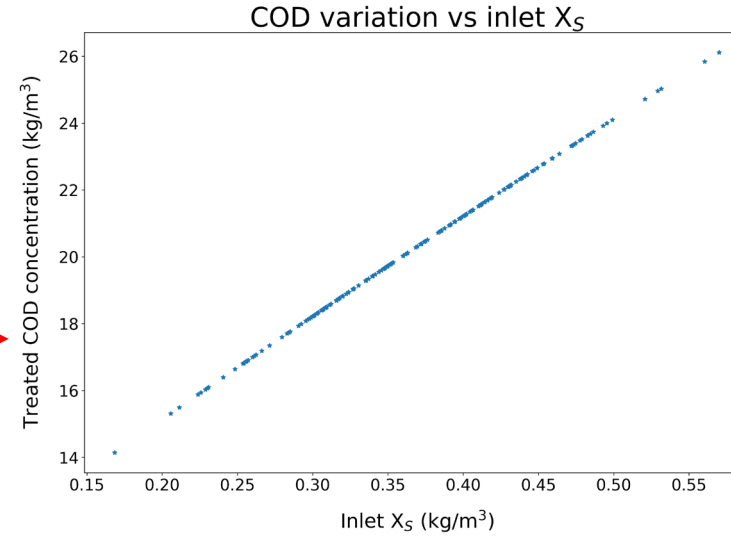
Initial simulation results demonstrating BSM2 model stability

Xs: slowly biodegradable substrate

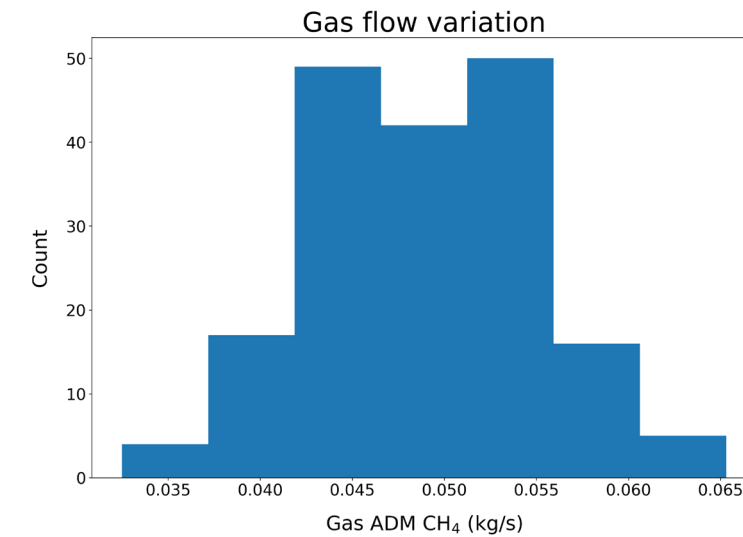
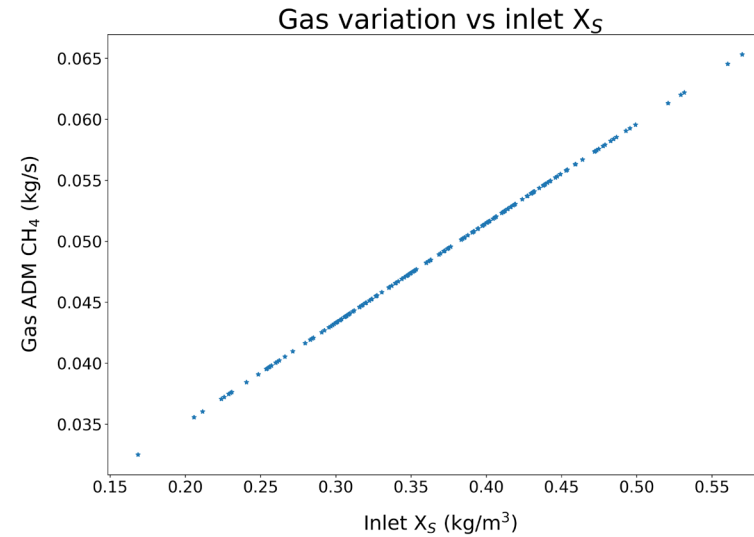
COD: chemical oxygen demand



Treated effluent COD



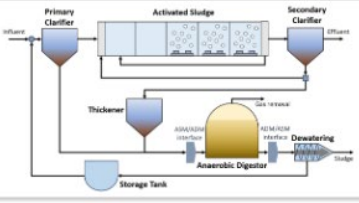
Methane Production of Anaerobic Digester



BSM2 Graphical User Interface (GUI)

INPUTS

BSM2 DEGREES OF FREEDOM: 0



SOLVE SWEEP

INPUT OUTPUT COMPARE

RESET FLOWSHEET RUN

Feed

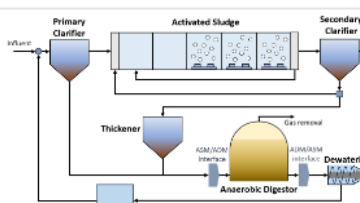
Volumetric flow rate	20648	m3/day	Fixed
S_I concentration	27	g/m3	Fixed
S_S concentration	58	g/m3	Fixed
X_I concentration	92	g/m3	Fixed
X_S concentration	363	g/m3	Fixed
X_BH concentration	50	g/m3	Fixed
X_BA concentration	0	g/m3	Fixed
X_P concentration	0	g/m3	Fixed
S_O concentration	0	g/m3	Fixed
S_NO concentration	0	g/m3	Fixed
S_NH concentration	23	g/m3	Fixed

Secondary clarifier

H2O split fraction	0.48956	fraction	Fixed
S_I split fraction	0.48956	fraction	Fixed
S_S split fraction	0.48956	fraction	Fixed
X_I split fraction	0.00187	fraction	Fixed
X_S split fraction	0.00187	fraction	Fixed
X_BH split fraction	0.00187	fraction	Fixed
X_BA split fraction	0.00187	fraction	Fixed
X_P split fraction	0.00187	fraction	Fixed
S_O split fraction	0.48956	fraction	Fixed
S_NO split fraction	0.48956	fraction	Fixed
S_NH split fraction	0.48956	fraction	Fixed

OUTPUTS

BSM2 DEGREES OF FREEDOM: 0



SOLVE SWEEP

INPUT OUTPUT COMPARE

DOWNLOAD RESULT SAVE CONFIGURATION

Feed

Volumetric flow rate **20648** m3/day
S_I concentration **27** g/m3
S_S concentration **58** g/m3
X_I concentration **92** g/m3
X_S concentration **363** g/m3
X_BH concentration **50** g/m3
X_BA concentration **0** g/m3
X_P concentration **0** g/m3
S_O concentration **0** g/m3
S_NO concentration **0** g/m3
S_NH concentration **23** g/m3
S_ALK **7** mol/m3

Secondary Clarifier Effluent

Flow rate **20640.14** m3/day
S_I concentration **61.90912** g/m3
S_S concentration **0.87127** g/m3
X_I concentration **5.44617** g/m3
X_S concentration **0.20555** g/m3
X_BH concentration **10.90312** g/m3
X_BA concentration **0.78876** g/m3
X_P concentration **2.25655** g/m3
S_O concentration **0.449** g/m3
S_NO concentration **15.4561** g/m3
S_NH concentration **0.91693** g/m3
S_ND concentration **0.64661** g/m3
X_ND concentration **0.01416** g/m3
S_ALK concentration **3.80957** mol/m3

Dewatered Sludge

Flow rate **7.83** m3/day
S_I concentration **4206.26584** g/m3
S_S concentration **233.5421** g/m3
X_I concentration **202190.22839** g/m3
X_S concentration **171143.10493** g/m3
X_BH concentration **0** g/m3
X_BA concentration **0** g/m3
X_P concentration **0** g/m3
S_O concentration **0** g/m3
S_NO concentration **0** g/m3
S_NH concentration **1515.0025** g/m3
Sludge S_ND concentration **252.92648** g/m3
X_ND concentration **9236.50219** g/m3
S_ALK concentration **52.62752** mol/m3

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

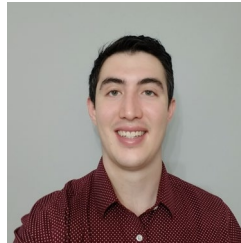
Thinking beyond 2024...

- 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



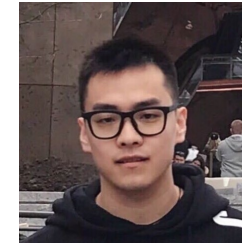
Tim Bartholomew



Adam Atia



Andrew Lee



Chenyu Wang



Travis Arnold



Marcus Holly



Alejandro Garciadiego



Elmira Shamlou



Disclaimer

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Resources and contact info



Contact information:

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BSM2 Tutorial



WaterTAP GUI

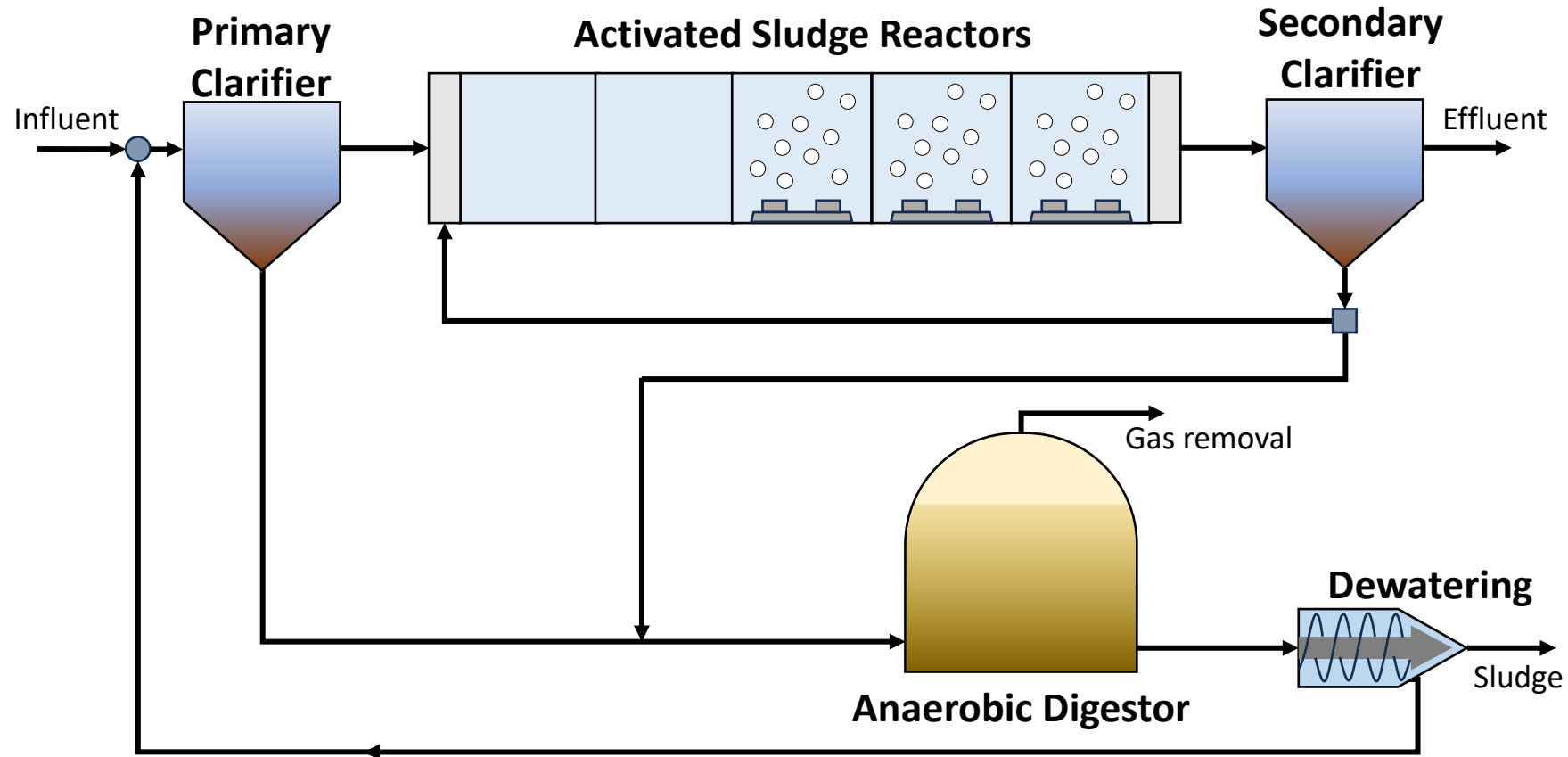


Property Model Documentation



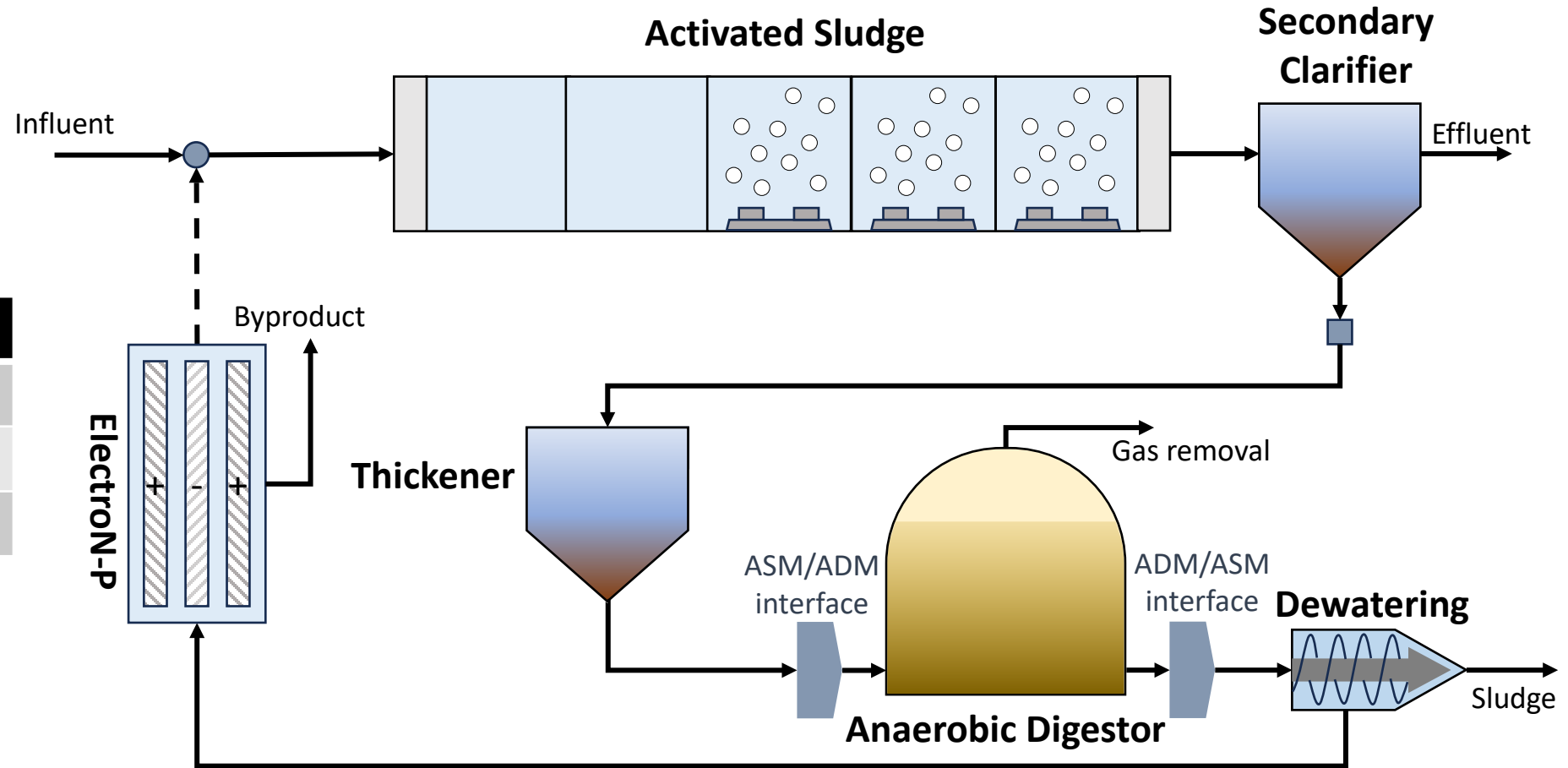
Backup Slides

Generalized figure



ElectroN-P sub-flowsheet

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



Motivation

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

ASM1

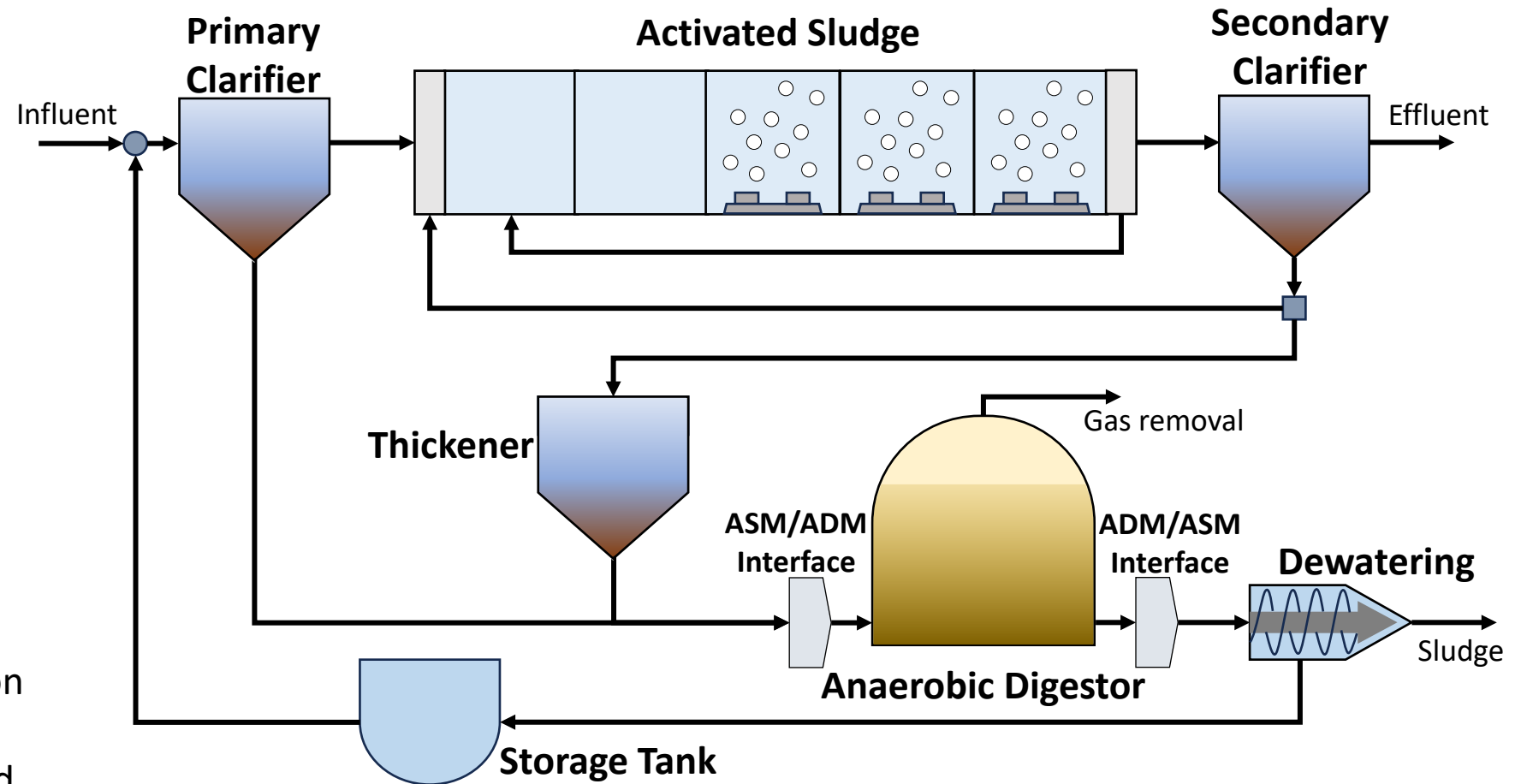
- Carbon oxidation
- Nitrification
- Denitrification

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



Benchmark Simulation Model 2 (BSM2)

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

ASM1

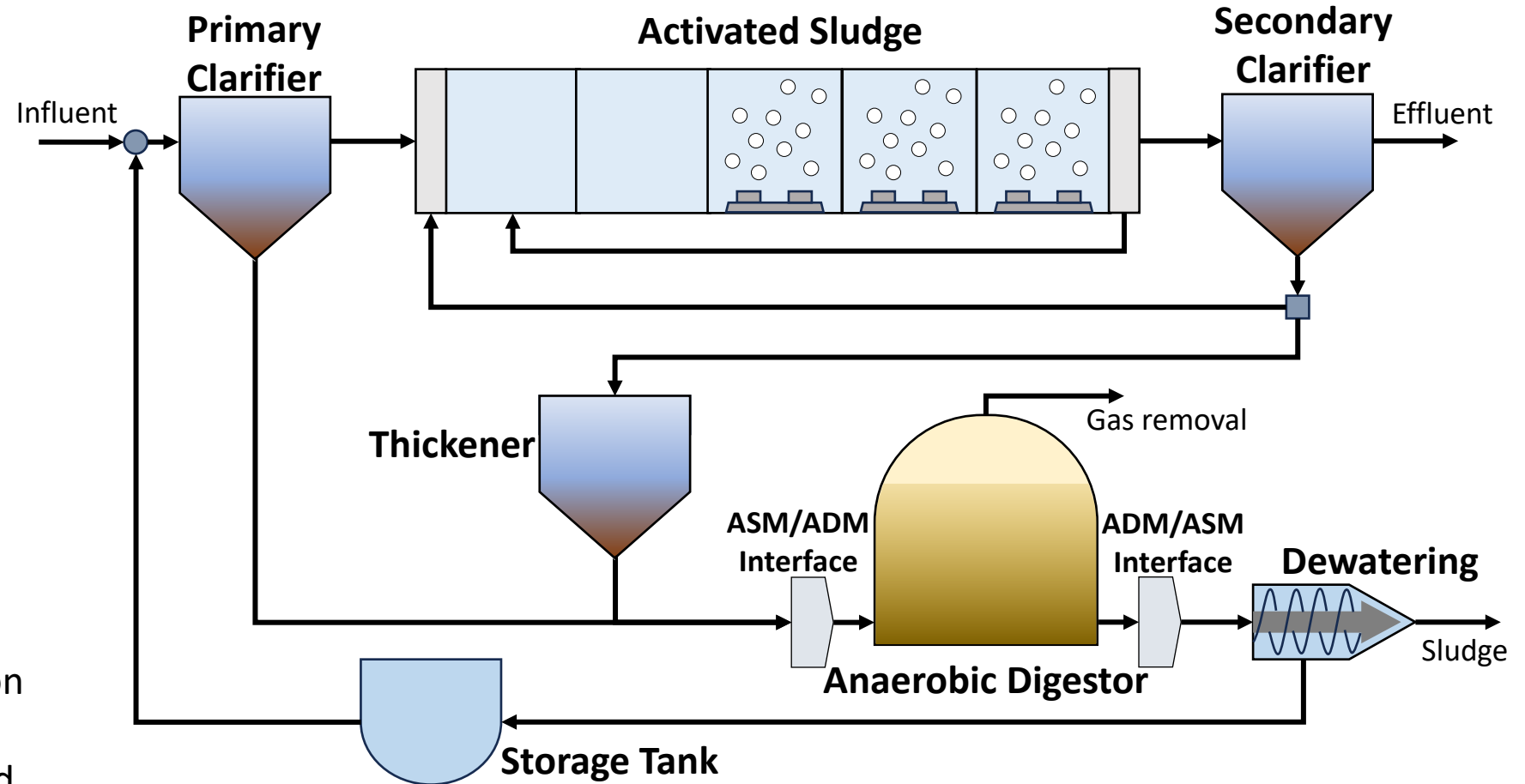
- Carbon oxidation
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ASM2d

- Additional biological process
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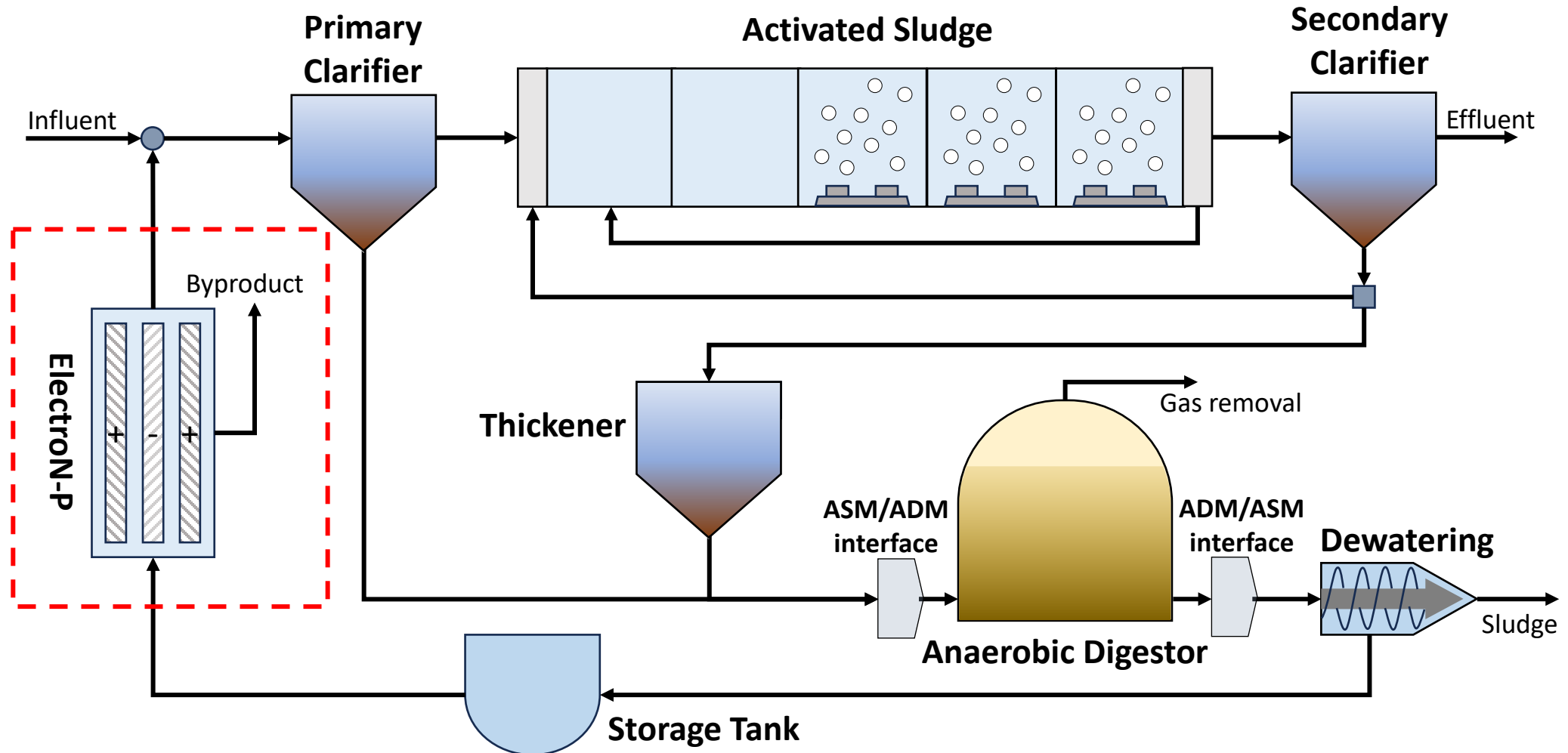
ADM1

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



ElectroN-P

ElectroN-P: extract nitrogen and phosphorous from municipal wastewater

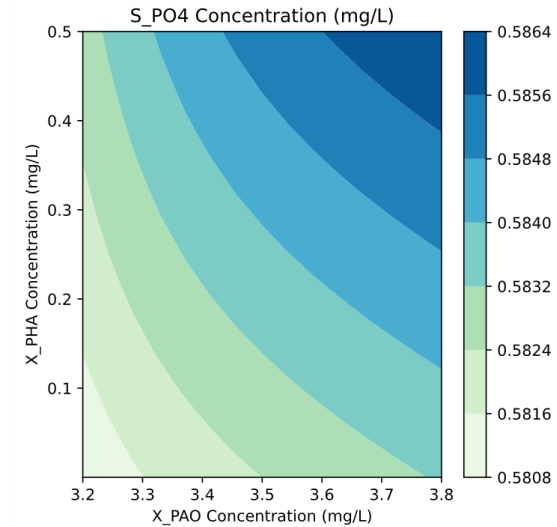
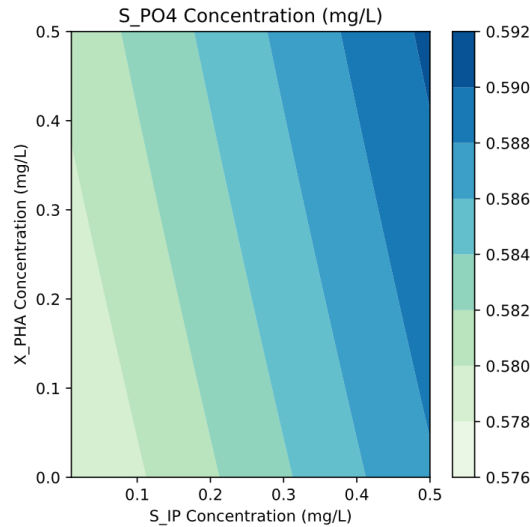
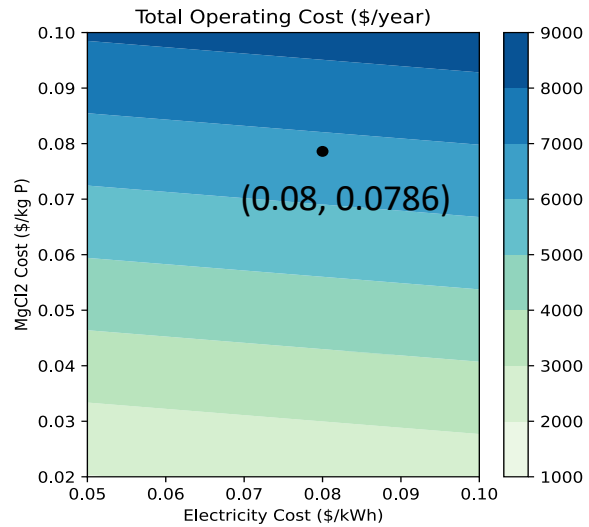
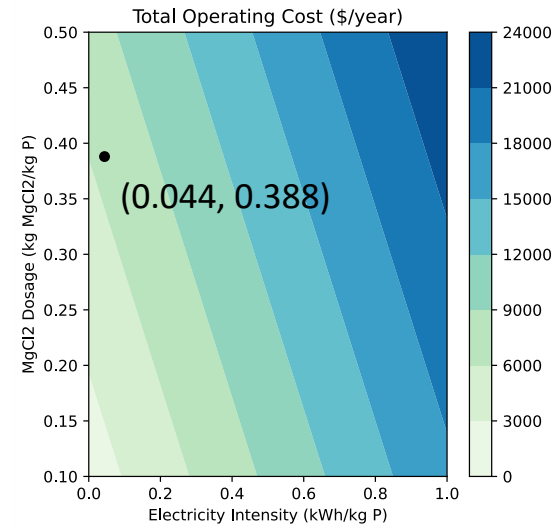
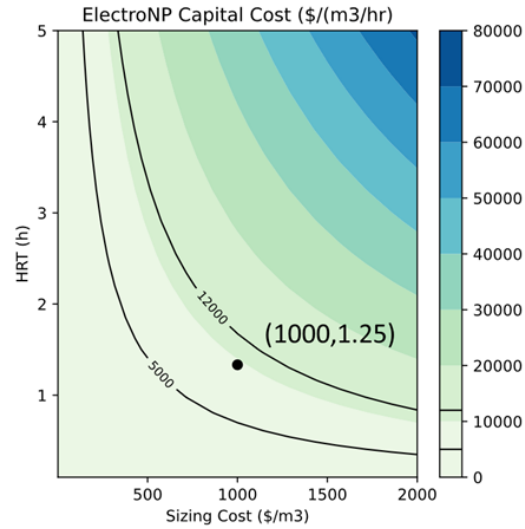
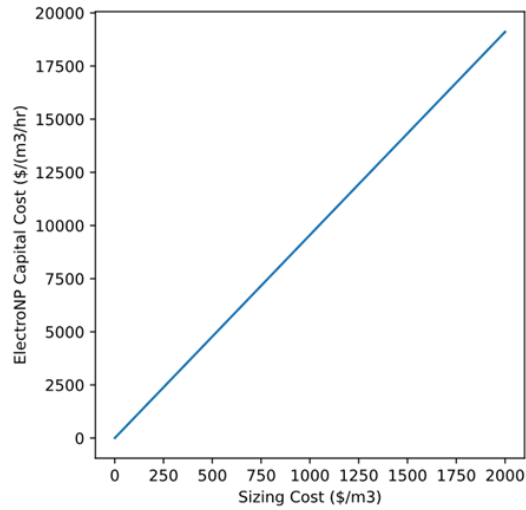


Results

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



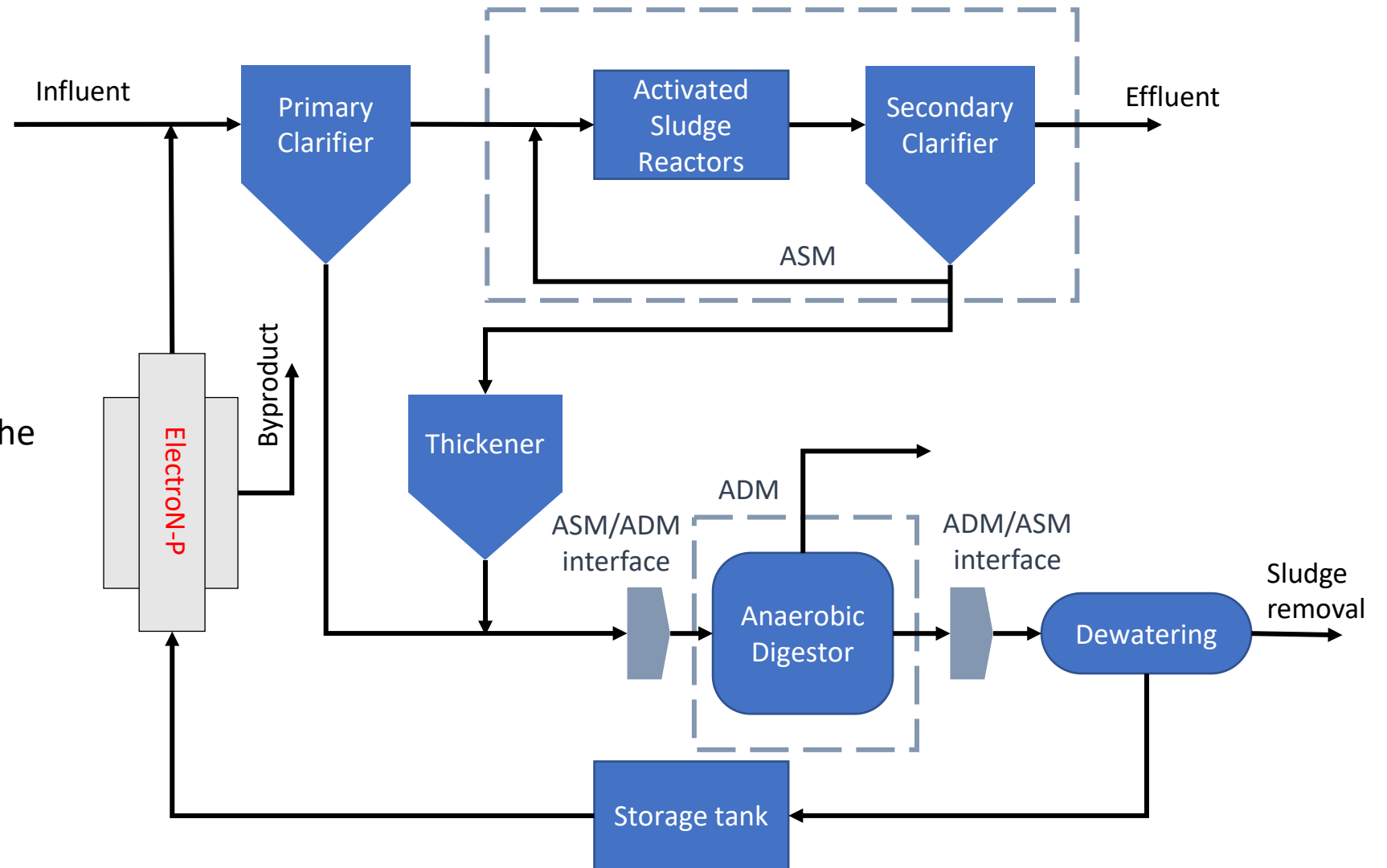
Progress updates and future plan

Progress updates:

- Full BSM2 flowsheet (ASM1) v: PR under review
- ASM2D; ADM1 reformulated for resolving scaling issue
- ElectroN-P OD 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



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 digester 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