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Improving Operations of Wastewater Treatment Plants Using Economic MPC

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Process Systems and Operations Research Laboratory

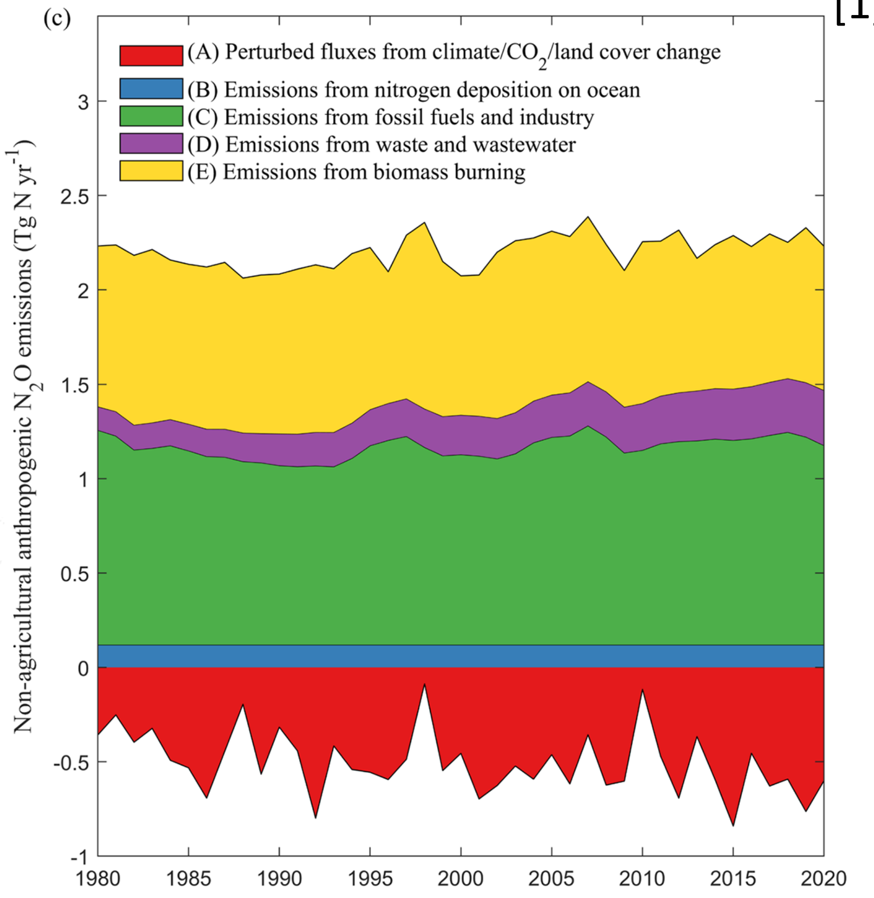
Motivation: Energy and Sustainability in WWTPs

- WWTPs emit **N_2O**, a greenhouse gas **273× stronger than CO_2**.
- **Aeration uses 50–90%** of total plant energy[2].
- Traditional (Dissolved Oxygen) DO control ignores the **energy–sustainability trade-off**.

➢ **Goal:** Operate WWTPs more efficiently — **reduce energy use while maintaining effluent quality.**

➢ **This talk:** Develops an **ASM3-based nonlinear MPC** and **eMPC** framework for **NH_4 control**, laying the groundwork for future **N_2O-integrated optimization.**

[1]



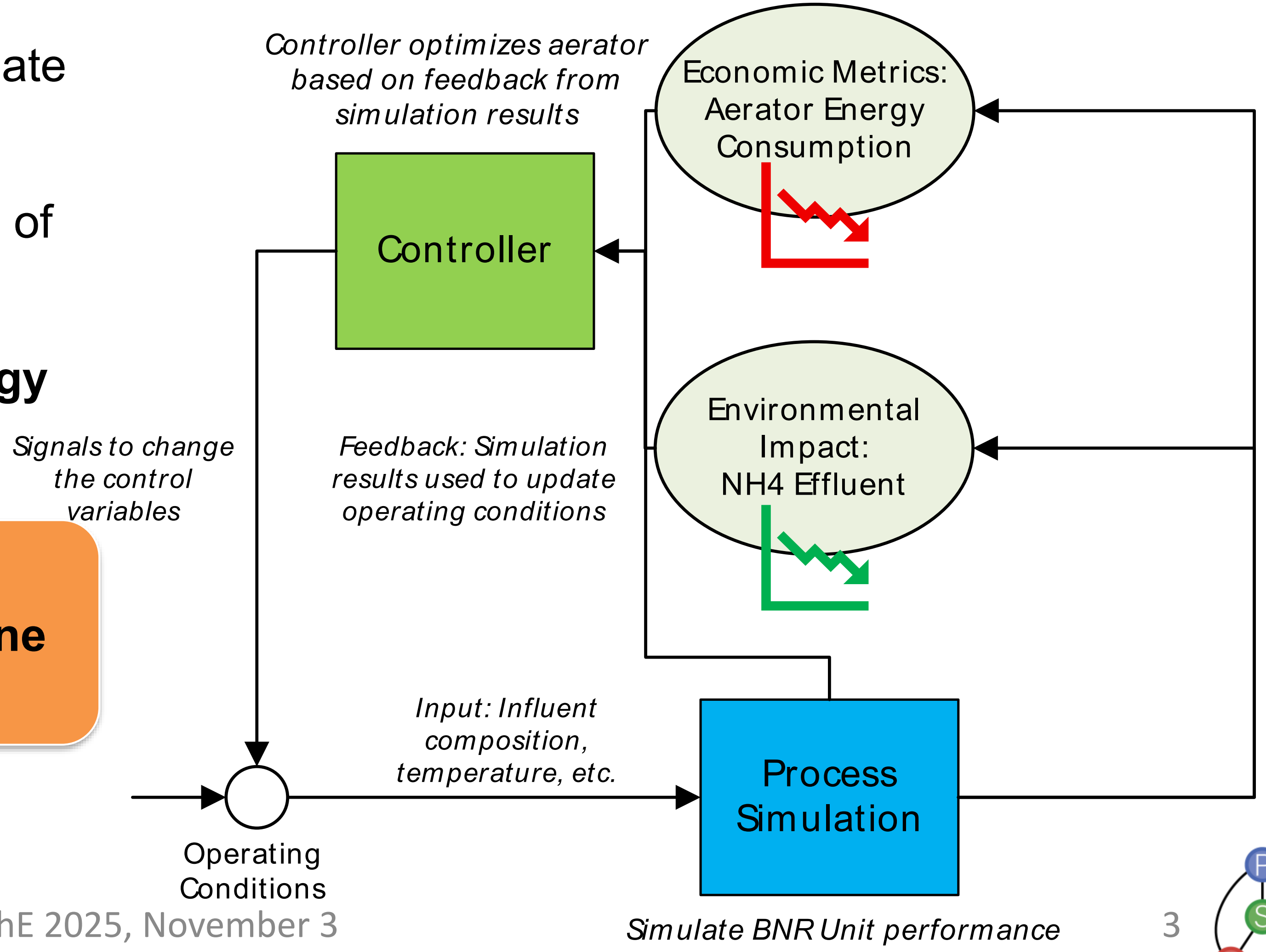
[1] Tian, H., Pan, N., Thompson, R. L., Canadell, J. G., Suntharalingam, P., Regnier, P., ... & Zhu, Q. (2024). Global nitrous oxide budget (1980–2020). *Earth System Science Data*, *16*(6), 2543-2604.

[2] Drewnowski, J., Remiszewska-Skwarek, A., Duda, S., & Łagód, G. (2019). Aeration process in bioreactors as the main energy consumer in a wastewater treatment plant. Review of solutions and methods of process optimization. *Processes*, *7*(5), 311.

Objective: Toward Sustainable WWTP Operation

- Develop an **ASM3-based MPC** to regulate effluent **NH_4** via aeration control.
- Validate the **closed-loop performance** of the integrated model–optimizer system.
- Extend to an **eMPC** that balances **energy use** and **treatment efficiency**.

Our framework unifies modeling, optimization, and sustainability in one closed-loop system.



Toolbox: Modeling and Optimization in Julia

ModelingToolkit.jl

EOptInterface.jl

JuMP.jl

- Acausal, equation-based modeling in Julia.
- Enables symbolic formulation and simplification.
- Ideal for dynamic process simulation.

- Domain-specific optimization language in Julia.
- Supports nonlinear and mixed-integer solvers.
- Integrates with automatic differentiation tools.

[3] Ma, Y., Gowda, S., Anantharaman, R., Laughman, C., Shah, V., & Rackauckas, C. (2021). Modelingtoolkit: A composable graph transformation system for equation-based modeling. *arXiv preprint arXiv:2103.05244*.
[4] Lubin, M., Dowson, O., Garcia, J. D., Huchette, J., Legat, B., & Vielma, J. P. (2023). JuMP 1.0: Recent improvements to a modeling language for mathematical optimization. *Mathematical Programming Computation*, *15*(3), 581-589.
[5] https://github.com/PSORLab/EOptInterface.jl

EOptInterface: Connecting ModelingToolkit and JuMP

EOptInterface **automaticall**
into JuMP constraints.

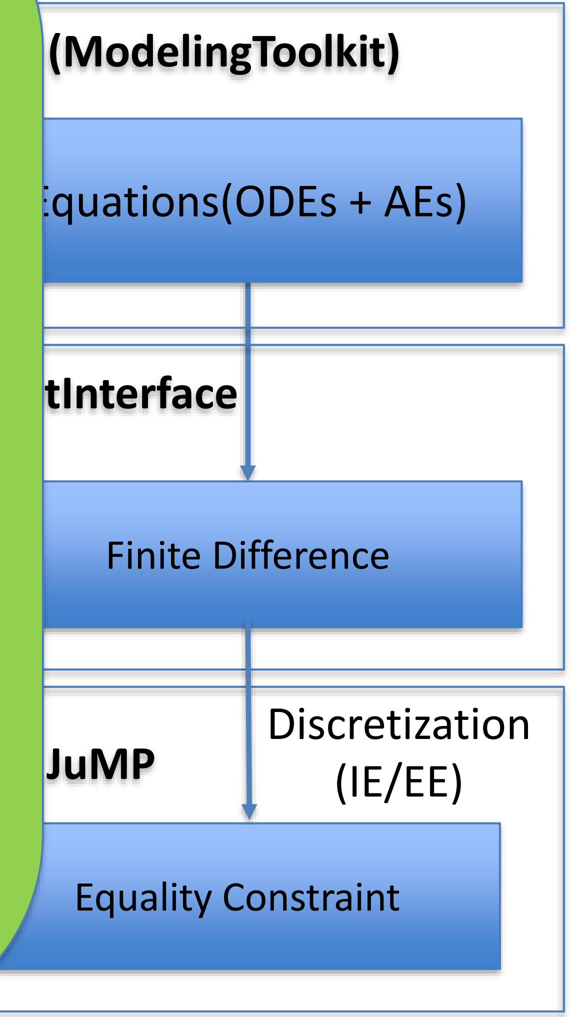
Core Functions:

- ➢ **Registers ODE systems**
  (Explicit / Implicit Euler)
- ➢ **Transforms differential**
  equality constraints.
- ➢ **Maintains consistency**
  JuMP variables.

EOptInterface.jl

Dimitri Alston (Main developer)
Optimization Abstraction Layer for
Acausal/Equation-Oriented Models in Julia
Nov 5, 2025

EOptInterface.jl

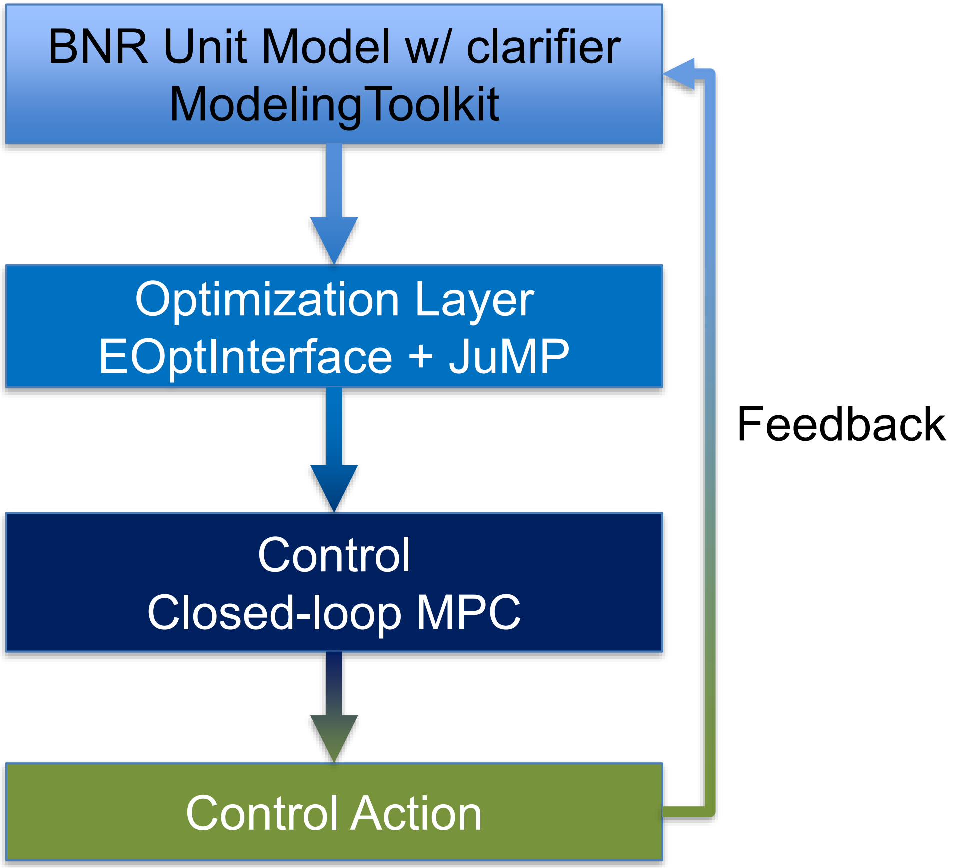


Framework Overview: From Model to Closed-loop Control

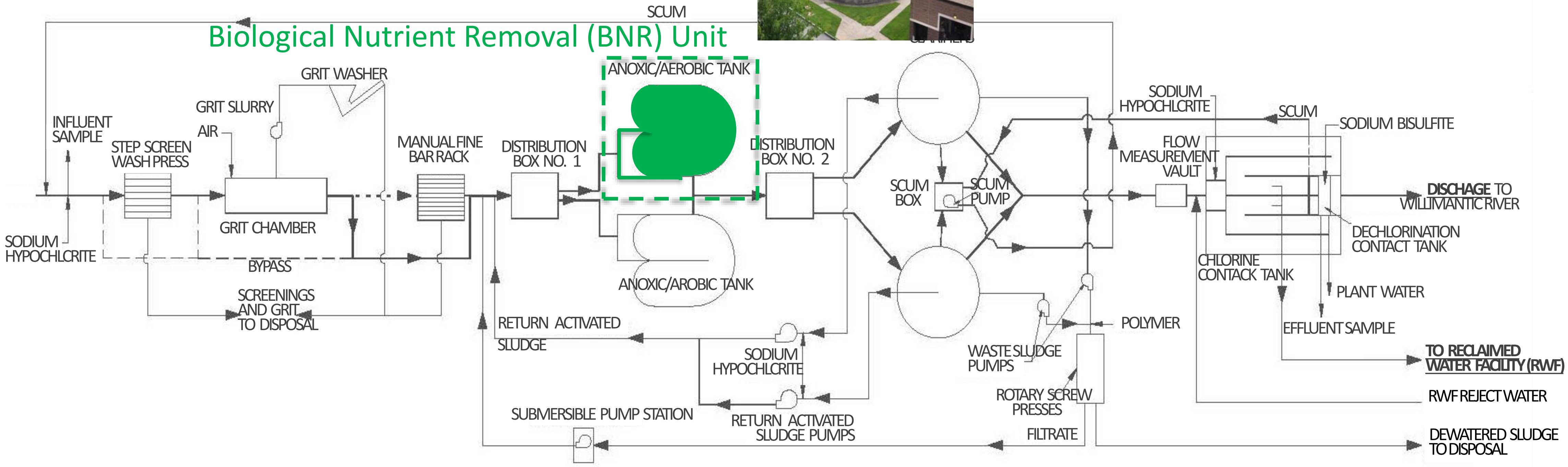
- **Mechanistic Model** (ASM3 in *ModelingToolkit*): builds the process-level ODE system.
- **Optimization Layer** (*EOptInterface* + *JuMP*): converts model equations into constraints for MPC
- **Closed-loop Control**: executes real-time MPC using updated sensor feedback.

Fully integrated feedback between simulation and optimization.

Our framework integrates modeling, optimization, and control into one unified, feedback-driven architecture.

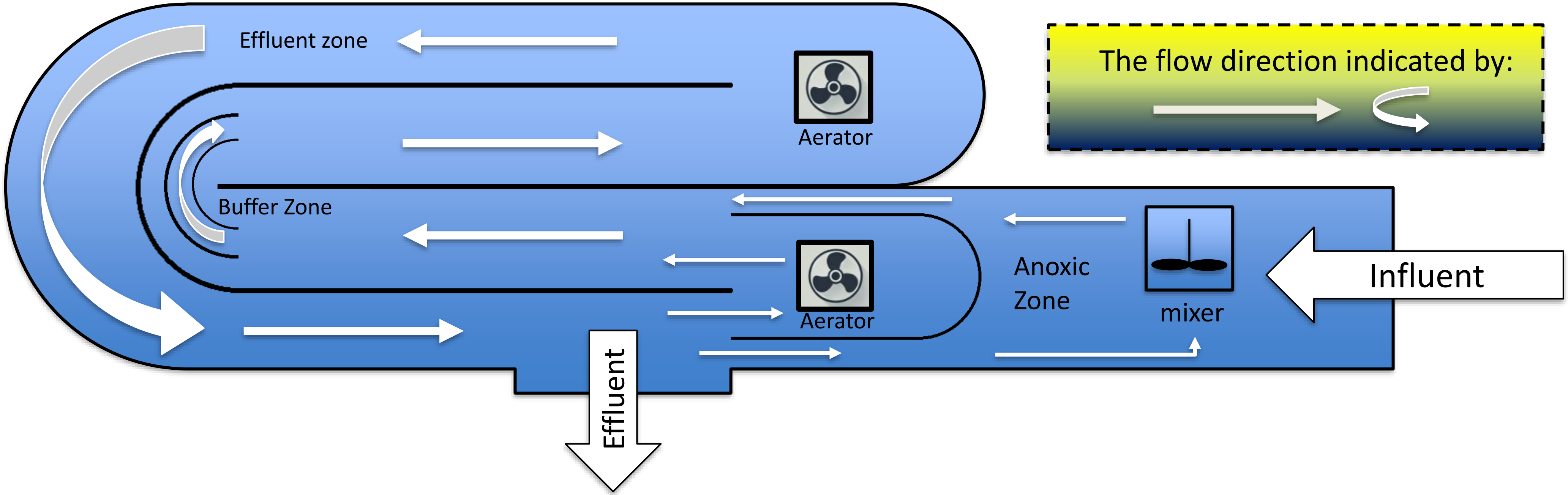


BNR System & Process Layout

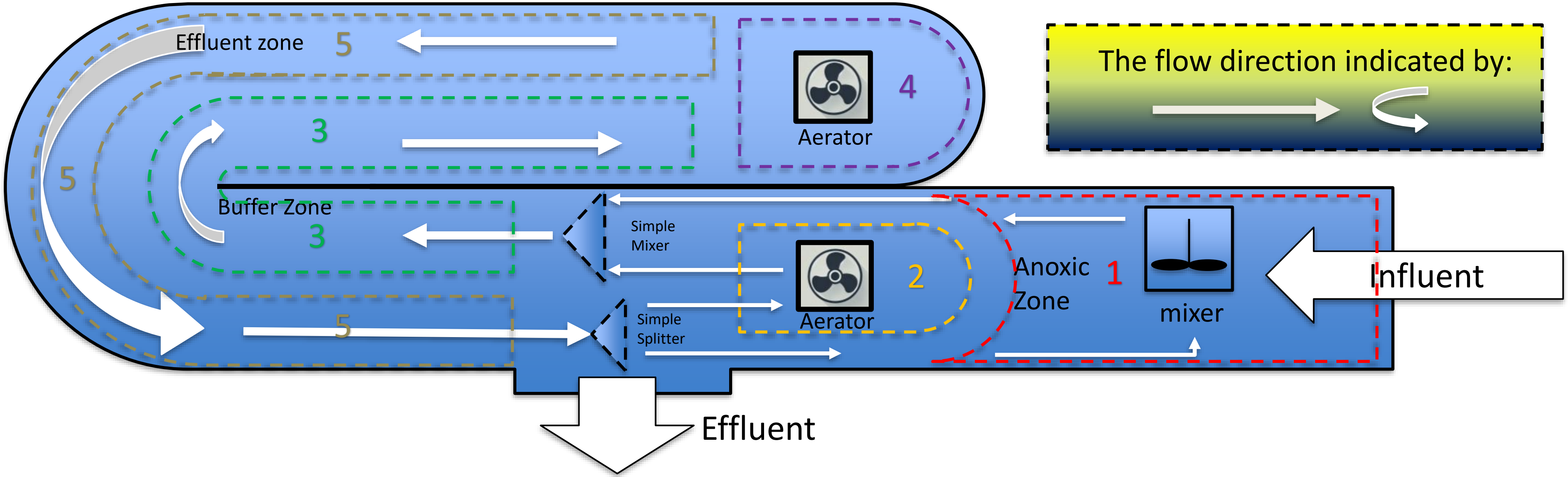


UConn Wastewater Treatment Plant (WWTP) Process Flow Diagram

Modeling of BNR Unit: Diagram



Modeling of BNR Unit: Divided Zones and ODEs



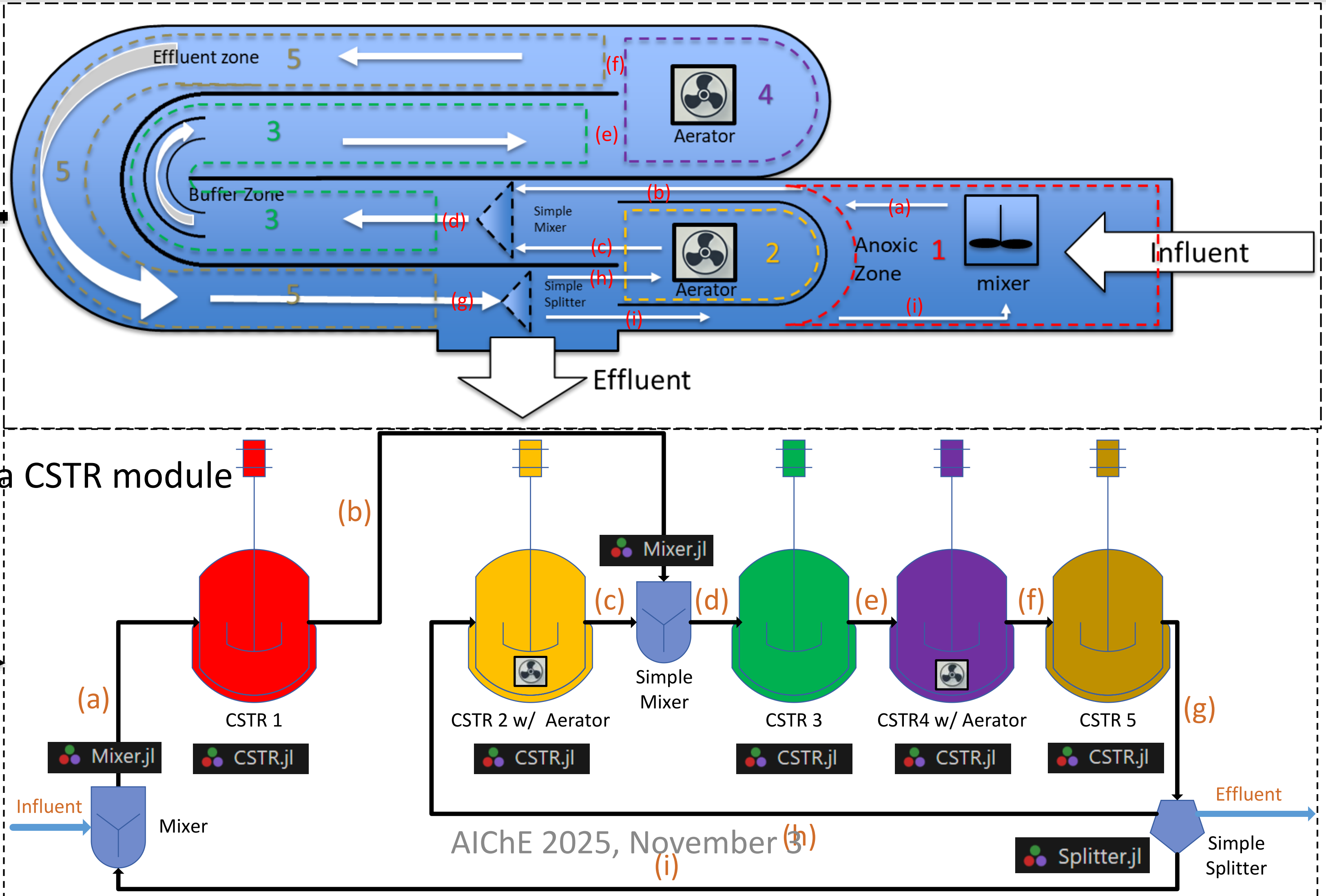
ODEs for State Variables $\mathbf{c}(t)$ in CSTRs:

$$\frac{d\mathbf{c}}{dt} = \mathbf{c}_{\text{in}}(t) - \mathbf{c}(t) + \mathbf{r}_{\text{ASM3}}(\mathbf{c}(t), t)$$

Modeling of BNR Unit – From Physical Layout to Symbolic Flowsheet

Abstraction

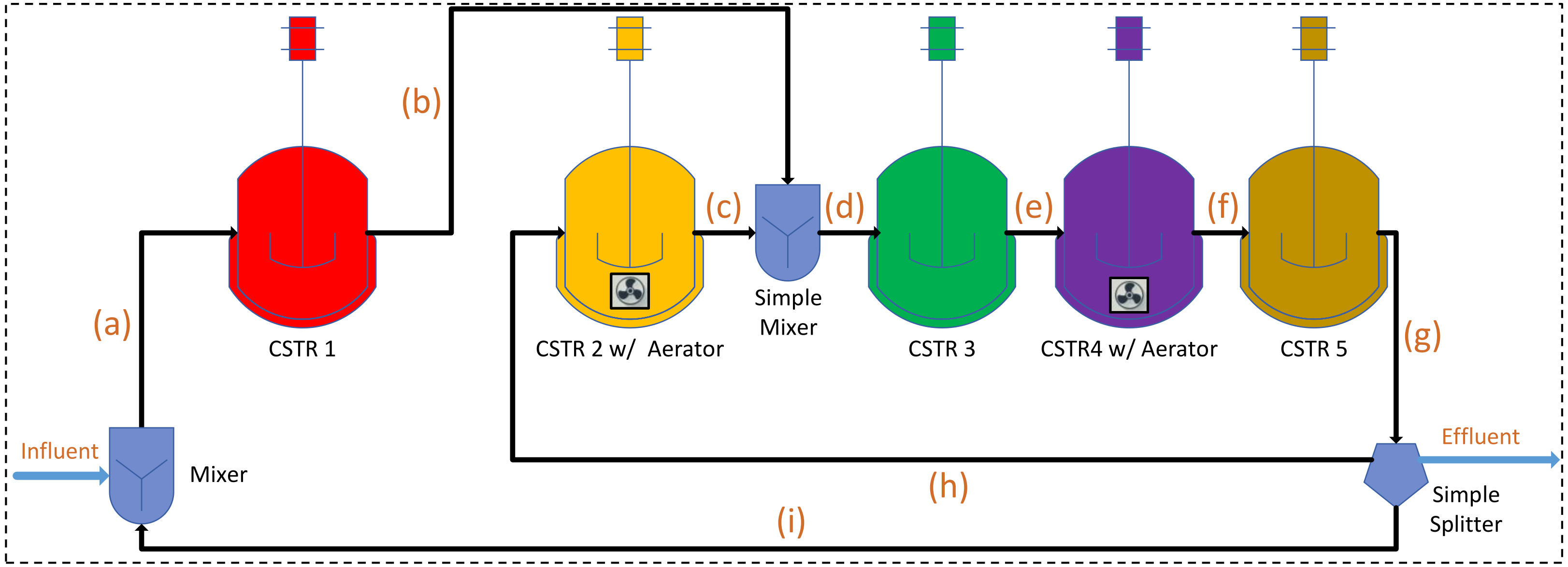
Each zone represented as a CSTR module



MaterialStream.jl

ModelingToolkit.jl

Hierarchical Modeling of the BNR Flowsheet

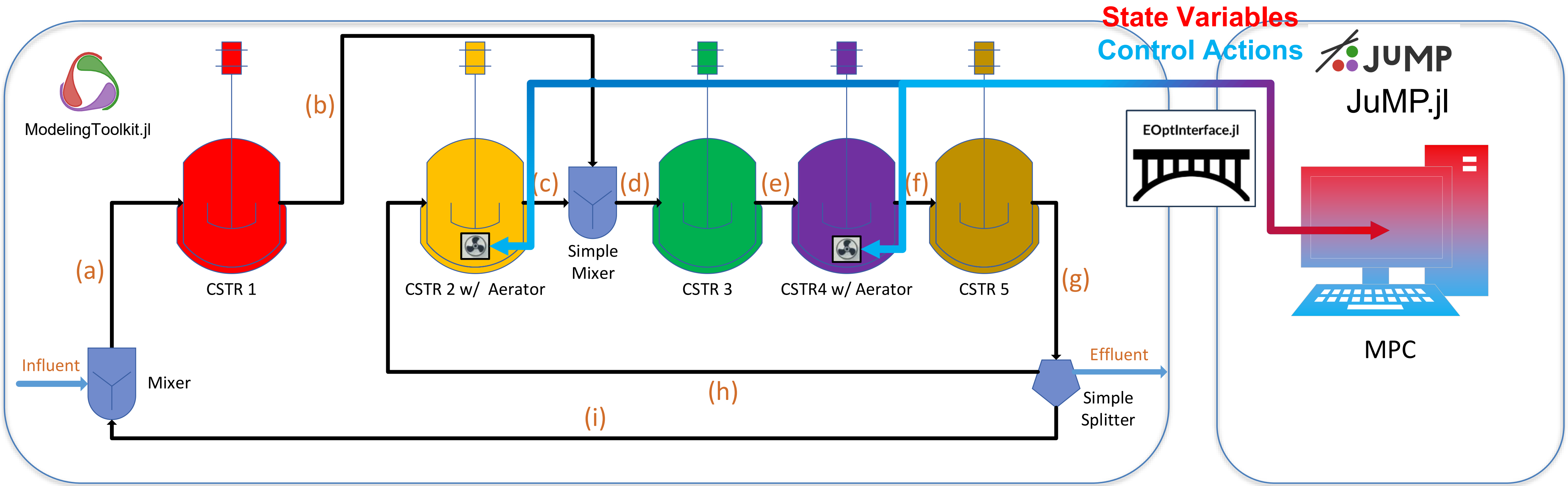



```julia
@mtkmodel WRRFPlantModel begin

    @components begin
            # Influent = DynamicInfluent()
            Influent = DynamicInfluent2()
            reactor1 = CSTR(vol=500, switch=0, Temp = inlet_temp)
            reactor2 = CSTR(vol=500, switch=0, Temp = inlet_temp)
            reactor3 = CSTR(vol=500, switch=1, Temp = inlet_temp)
            reactor4 = CSTR(vol=500, switch=0, Temp = inlet_temp)
            reactor5 = CSTR(vol=500, switch=1, Temp = inlet_temp)
            splitter1 = Splitter_1in_2out(out_factor_1 = 0.5)
            clarifier = Clarifier(R_1 = 0.4, w_1 = 0.03)
            mixer1 = Mixer_2in_1out()
            mixer3 = Mixer_2in_1out()
    end

    @equations begin
        connect(Influent.port,mixer1.In1)
        connect(splitter1.Out2,mixer1.In2)
        connect(mixer1.Out1, mixer3.In2)
        connect(clarifier.recycle_stream, mixer3.In1)
        connect(mixer3.Out1,reactor1.In)
        connect(reactor1.Out,reactor2.In)
        connect(reactor2.Out,reactor3.In)
        connect(reactor3.Out,reactor4.In)
        connect(reactor4.Out,reactor5.In)
        connect(reactor5.Out,splitter1.In)
        connect(splitter1.Out1, clarifier.inlet_stream)
    end
end

@mtkcompile sys = WRRFPlantModel()
```

ModelingToolkit.jl

- Each reactor, mixer, and splitter is a reusable ModelingToolkit component.
- All units are connected symbolically using simple syntax to form the BNR flowsheet.
- Mass and energy balances are enforced automatically.
- The full model runs directly for steady-state and dynamic simulation.

Adding MPC to the Flowsheet



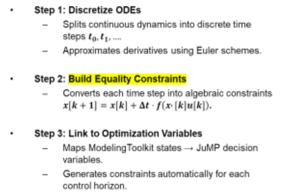
- The assembled model communicates directly with the MPC optimizer.
- **Control actions (Aerator)** are updated at each step using system feedback.
- This integration enables closed-loop dynamic control under the ASM3 framework.

MPC: Automating Discretization and Constraint Generation

- **Step 1: Discretize ODEs**
  - Splits continuous dynamics into discrete time steps $\boldsymbol{t_0}, \boldsymbol{t_1}, ...$
  - Approximates derivatives using Euler schemes.

- **Step 2: Build Equality Constraints**
  - Converts each time step into algebraic constraints $\boldsymbol{x}[\boldsymbol{k}+\mathbf{1}] = \boldsymbol{x}[\boldsymbol{k}] + \boldsymbol{\Delta t} \cdot \boldsymbol{f}(\boldsymbol{x}, [\boldsymbol{k}]\boldsymbol{u}[\boldsymbol{k}])$.

- **Step 3: Link to Optimization Variables**
  - Maps ModelingToolkit states → JuMP decision variables.
  - Generates constraints automatically for each control horizon.



Step 1: Discretize ODEs
Splits continuous dynamics into discrete time steps $t_0, t_1, ...$
Approximates derivatives using Euler schemes.
Step 2: Build Equality Constraints
Converts each time step into algebraic constraints $x[k+1] = x[k] + \Delta t \cdot f(x\cdot[k]u[k])$.
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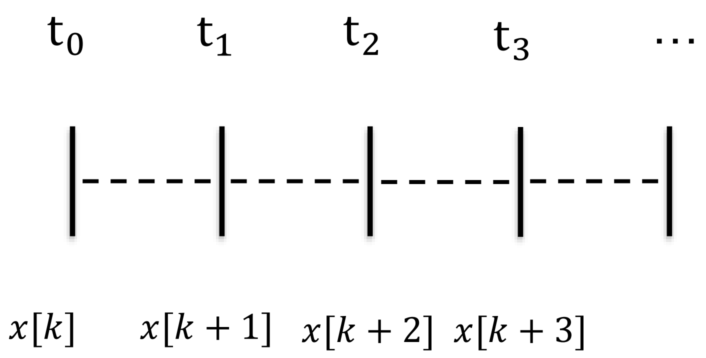


$$x[k+1] = x[k] + \mathrm{D}t \times f(x[k], u[k])$$

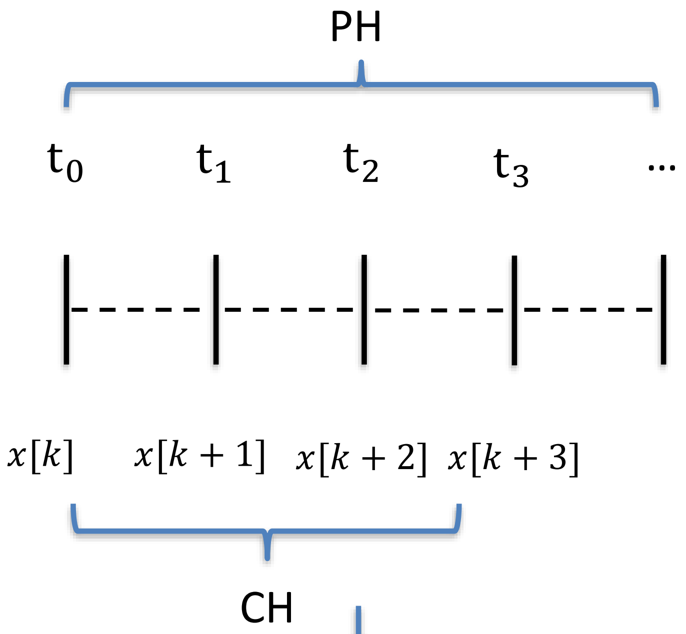
Time discretization with IE/EE to build equality constraints

MPC: Architecture

- **Prediction horizon (PH):** future simulation window based on ASM3 dynamics.
- **Decision variables:** oxygen transfer coefficients (kLa_2, kLa_4)
- **Control horizon (CH):** number of steps where aeration (kLa_2, kLa_4)
- **Objective function:**

$$J = w_1 \sum_{i=1}^{PH} \left| y_{NH_4}(kLa_{2,i}, kLa_{4,i}, X_i) - y_{\text{target}, NH_4, i} \right|^2 + w_2 \sum_{j=1}^{CH-1} \left(|\Delta kLa_{2,j}|^2 + |\Delta kLa_{4,j}|^2 \right)$$

- The optimization runs recursively at each step using new sensor feedback.



Measurement Update → Optimization → Apply first move (Kla)

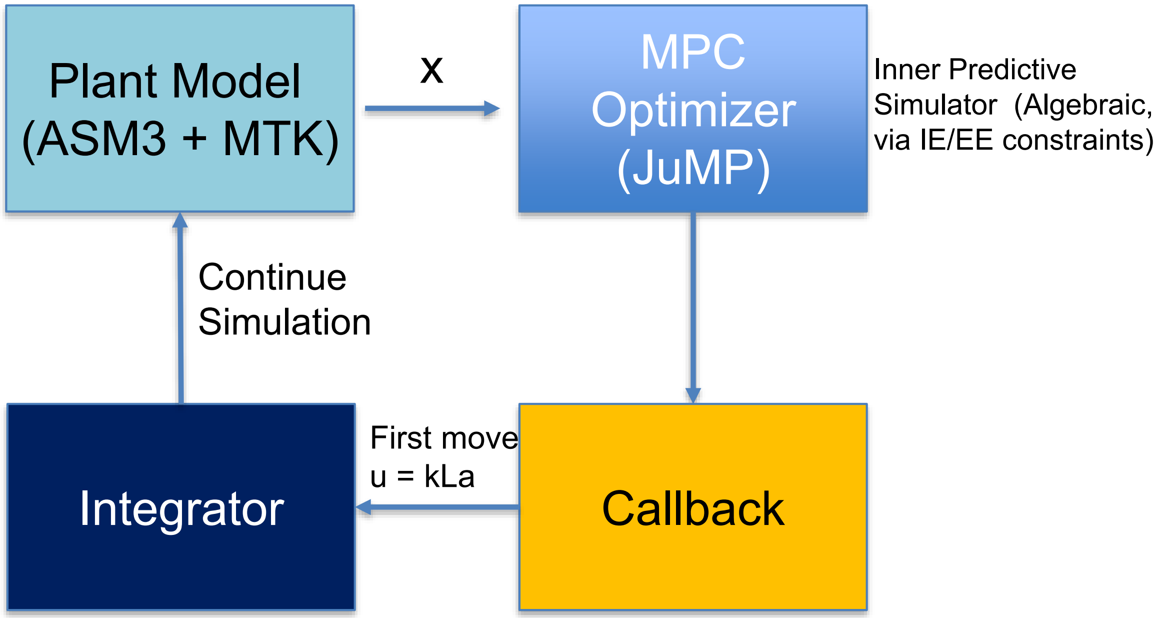
Objective: Track NH_4 while smoothing control.

Closed-loop MPC Execution in Real Time

Algorithm 1 Closed-loop MPC: Code-level Cycle

Initialize:
Build ASM3 model in `ModelingToolkit`
Create outer ODE integrator (continuous simulation)
Register ODE system with `EOptInterface` (IE/EE discretization)
Define optimization model and objective J
while simulation time $t < T_{\text{end}}$ **do**
Read current state x_k from outer integrator
Pin initial condition in JuMP: $x_{\text{pred}}[1] \leftarrow x_k$
Discretize and predict over horizon P_H
Solve MPC optimization problem
Apply first control move $u_k = (KLa_2, KLa_4)$
Advance outer integrator by Δt to obtain x_{k+1}
Feed back x_{k+1} and repeat
end while
Output: effluent NH_4 trajectory, control profiles, energy indicators

Real-time coupling of dynamic simulation and optimization.



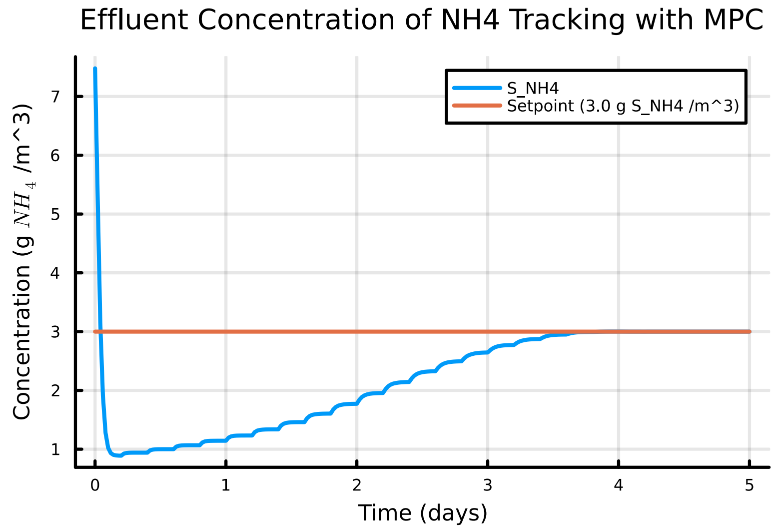
Real-time MPC coupling achieves dynamic consistency between model prediction and plant response.

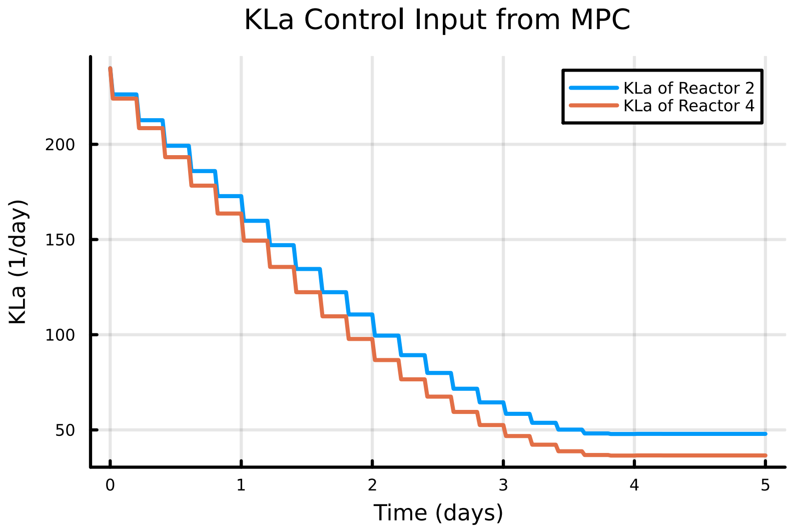
NMPC: Setpoint Tracking Performance

Goal: Regulate effluent NH_4 by adjusting aeration rates (kLa_2, kLa_4).

Result: Smooth convergence to 3.0 g NH_4/m^3 within 4 days, with no overshoot.

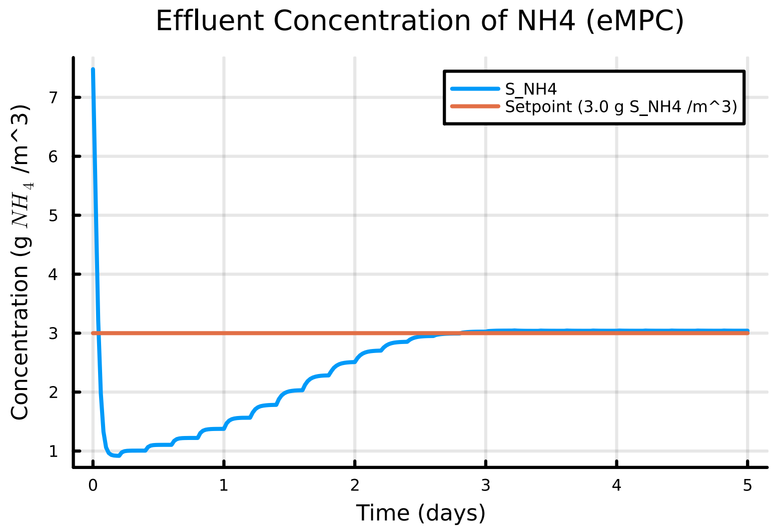
Insight: Stable, realistic control actions confirm robust MPC–simulation coupling.

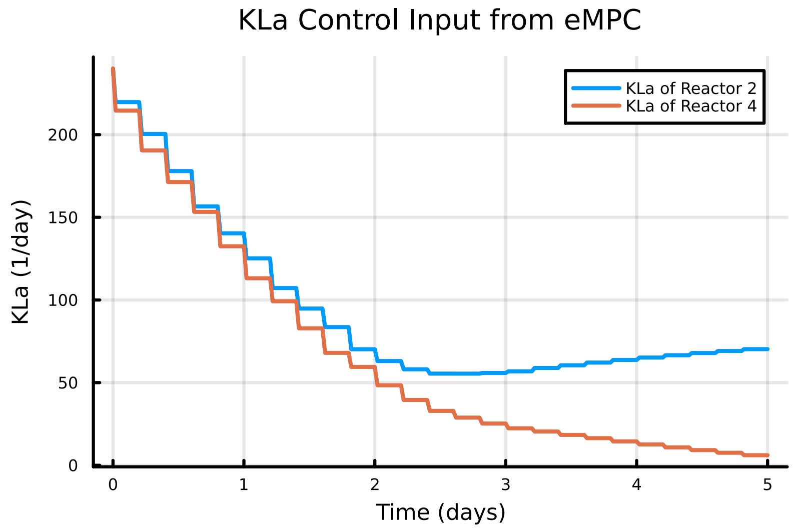




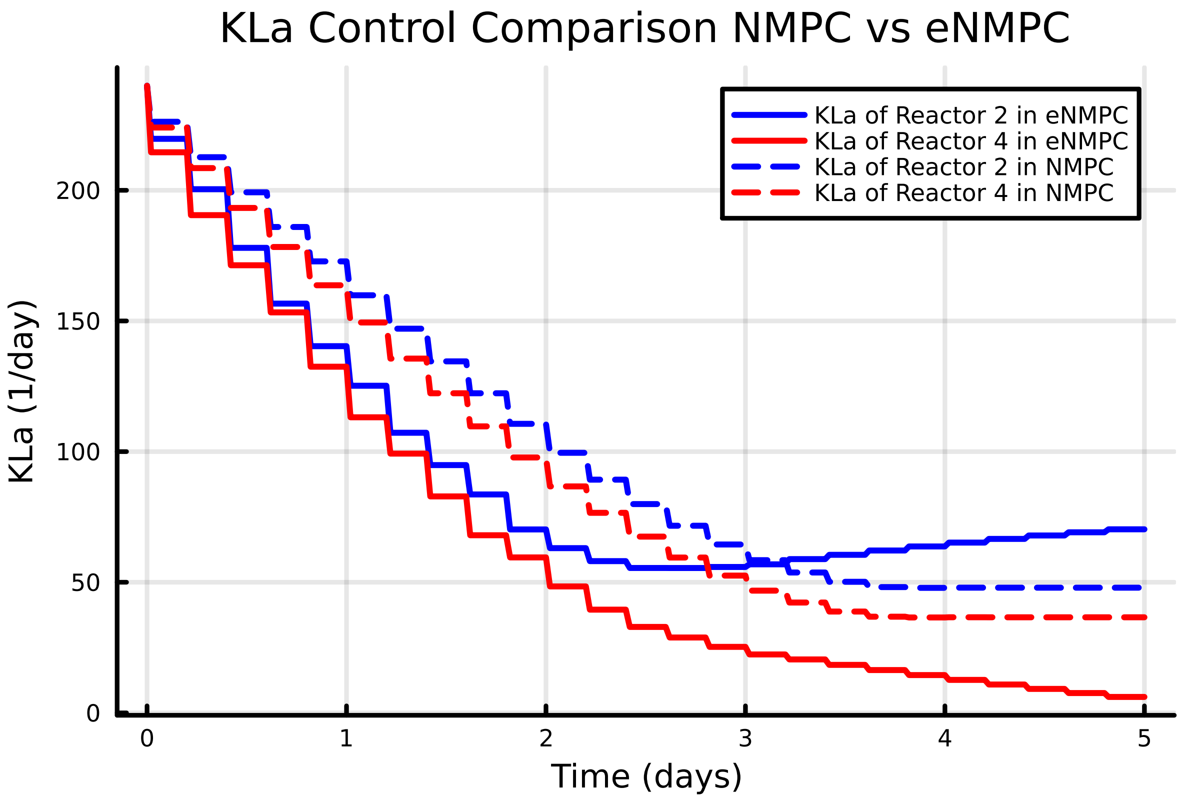
eNMPC Performance

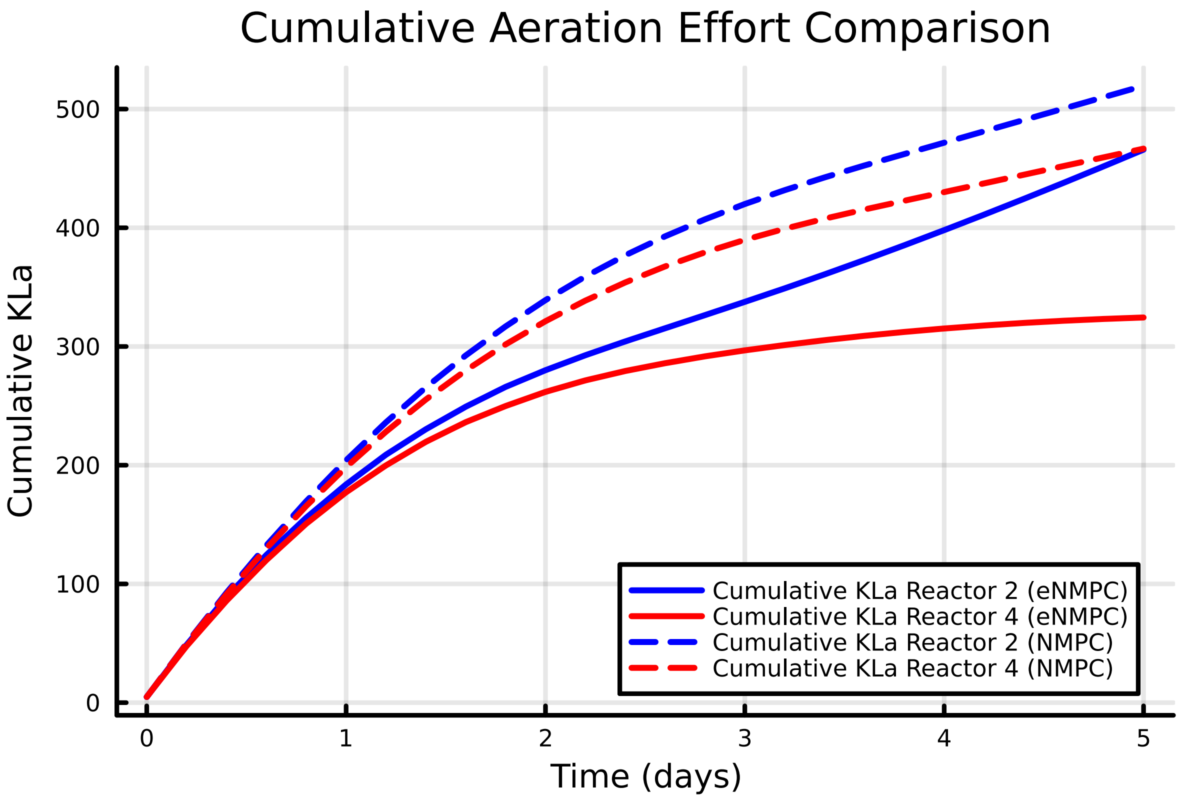
- **Goal:** Add an economic layer balancing energy use and sustainability.
- **Effect:** Slightly higher aeration improves NH_4 stability and reduces GHG impact.
- **Insight:** Establishes the energy–environment trade-off frontier for future N_2O integration.





Energy Efficiency: eNMPC vs NMPC

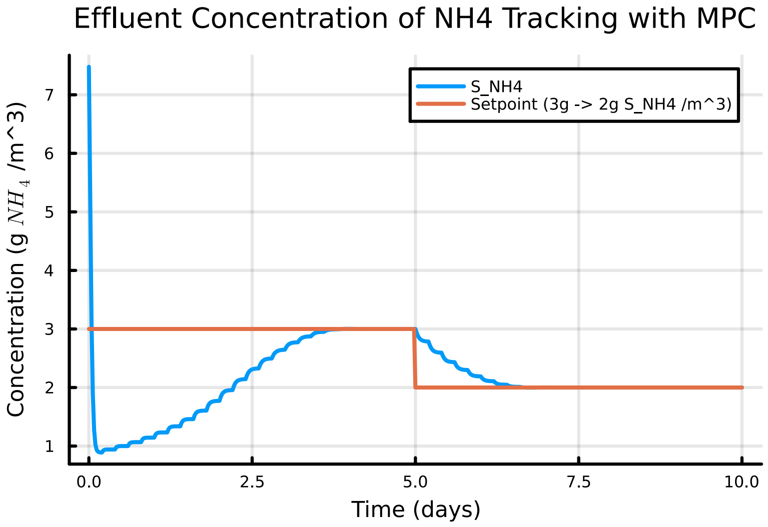


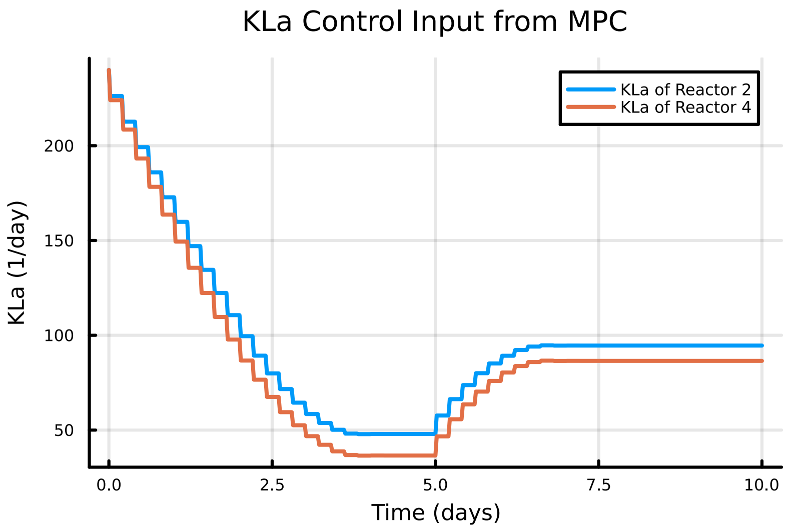


Cumulative KLa serves as a proxy for aeration energy use.

Controller Robustness and Practical Feasibility: NMPC

- **Test:** Step change (NH_4: 3 → 2 mg/L) shows smooth and stable transition.
- **Control:** kLa_2, kLa_4 adjust gradually within feasible limits.
- **Result:** Stable and energy-efficient response under realistic disturbances.





The NMPC framework stays feasible, stable, and efficient under varying setpoints and loads

Conclusions

- The ASM3-based eMPC framework successfully integrates mechanistic modeling, optimization, and control in a unified Julia environment.
- EOptInterface automates ODE discretization and constraint generation, enabling real-time closed-loop simulation.
- The controller achieves regulation of effluent NH_4 concentration.
- The framework remains feasible and robust under realistic operating variations, including setpoint changing.

Outlook

- Incorporate GHG emission objectives (N_2O-inclusive optimization).
- Introduce time-varying influent and recycle conditions for real-plant scenarios.

Acknowledgements

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