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System Visualization Using Real-Time Data-Driven Models Derived from High-Resolution Sensor Profiling

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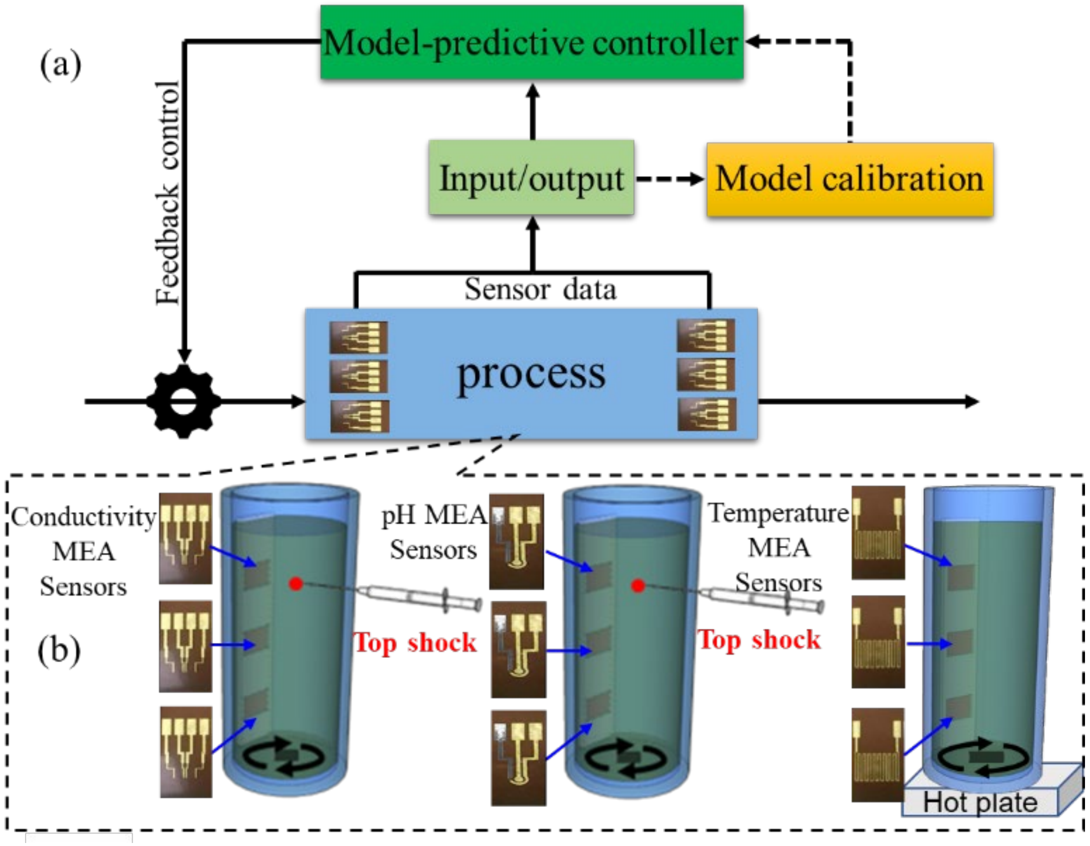
Process Systems and Operations Research Laboratory

Background

- Wastewater/water treatment plant
- Develop physics-informed data-driven model to simulate the system heterogeneity
  - Conductivity
  - pH
  - Temperature
- Three sensors are deployed along the reactor



[1] Wang, C.; Wang, T.; Xu, Z.; Cui, C.; Wang, X.; Demitrack, Z.; Dai, Z.; Bagtzoglou, A .; Stuber, M. D.; Li, B., *under review*, 2020

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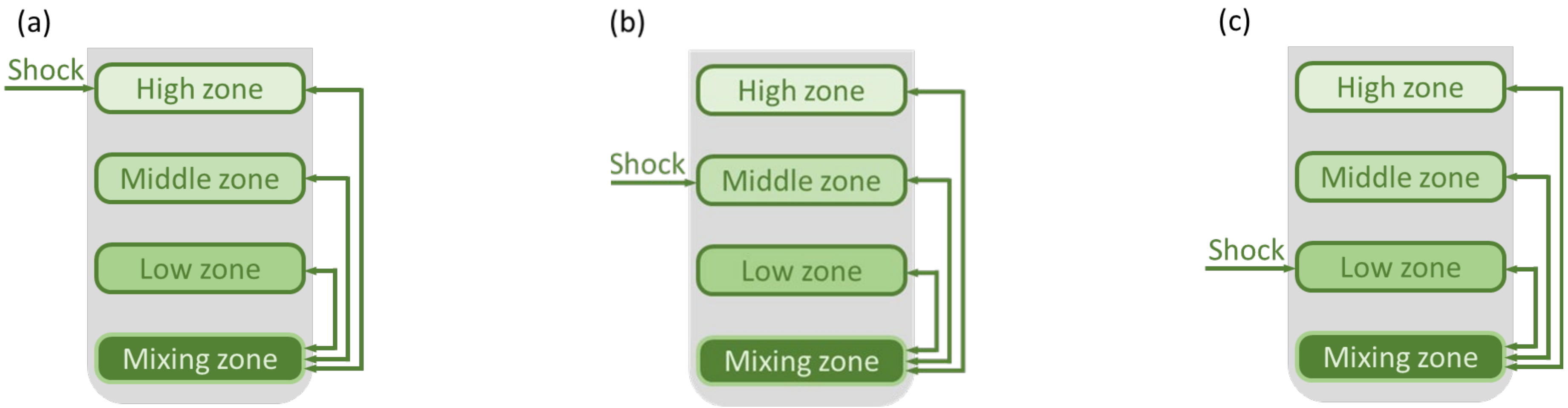
Conductivity Heterogeneity Profiling Model



Assumptions:

- Stirring power dominates the mass transfer
- Diffusion between adjacent zones are neglected

$$\frac{dC_i}{dt} = \frac{1}{4V} k_i (C_0 + C_4 - C_i), \qquad i = 1,2,3$$

$$\frac{dC_4}{dt} = \frac{1}{4V} k_4 (C_1 + C_2 + C_3 - 3C_4).$$

[1] Wang, C.; Wang, T.; Xu, Z.; Cui, C.; Wang, X.; Demitrack, Z.; Dai, Z.; Bagtzoglou, A .; Stuber, M. D.; Li, B., *under review*, 2020

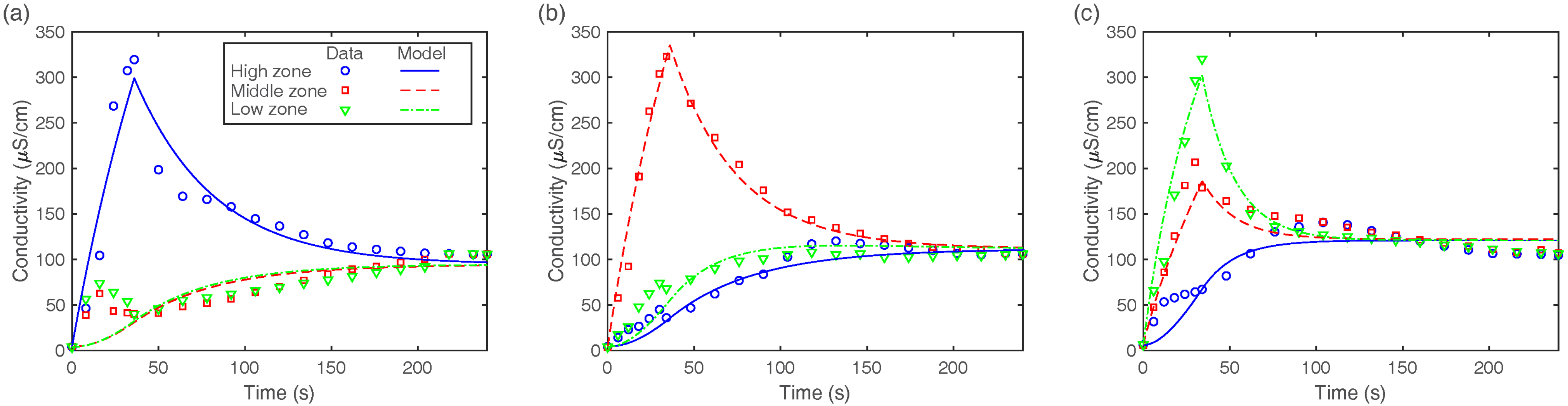
Global Optimization

$$\min_{p \in \Pi \subset \mathbb{R}^{n_p}} \phi(\mathbf{x}(\mathbf{p}, t_1), \dots, \mathbf{x}(\mathbf{p}, t_{N_t}))$$
$$\text{s.t.} \quad \dot{\mathbf{x}}(\mathbf{p}, t) = \mathbf{f}(\mathbf{x}(\mathbf{p}, t), \mathbf{p}, t), \forall t \in I = [t_0, t_f]$$
$$\mathbf{x}(\mathbf{p}, t_0) = \mathbf{x}_0(\mathbf{p}).$$

Objective function: $\phi(\mathbf{x}(\mathbf{p}, t_1), \dots, \mathbf{x}(\mathbf{p}, t_{N_t}))$

Optimization variable: $\mathbf{p} = (k_1, k_2, k_3, k_4, C_v)$

Generic state variable: $\mathbf{x} = (C_1, C_2, C_3, C_4)$



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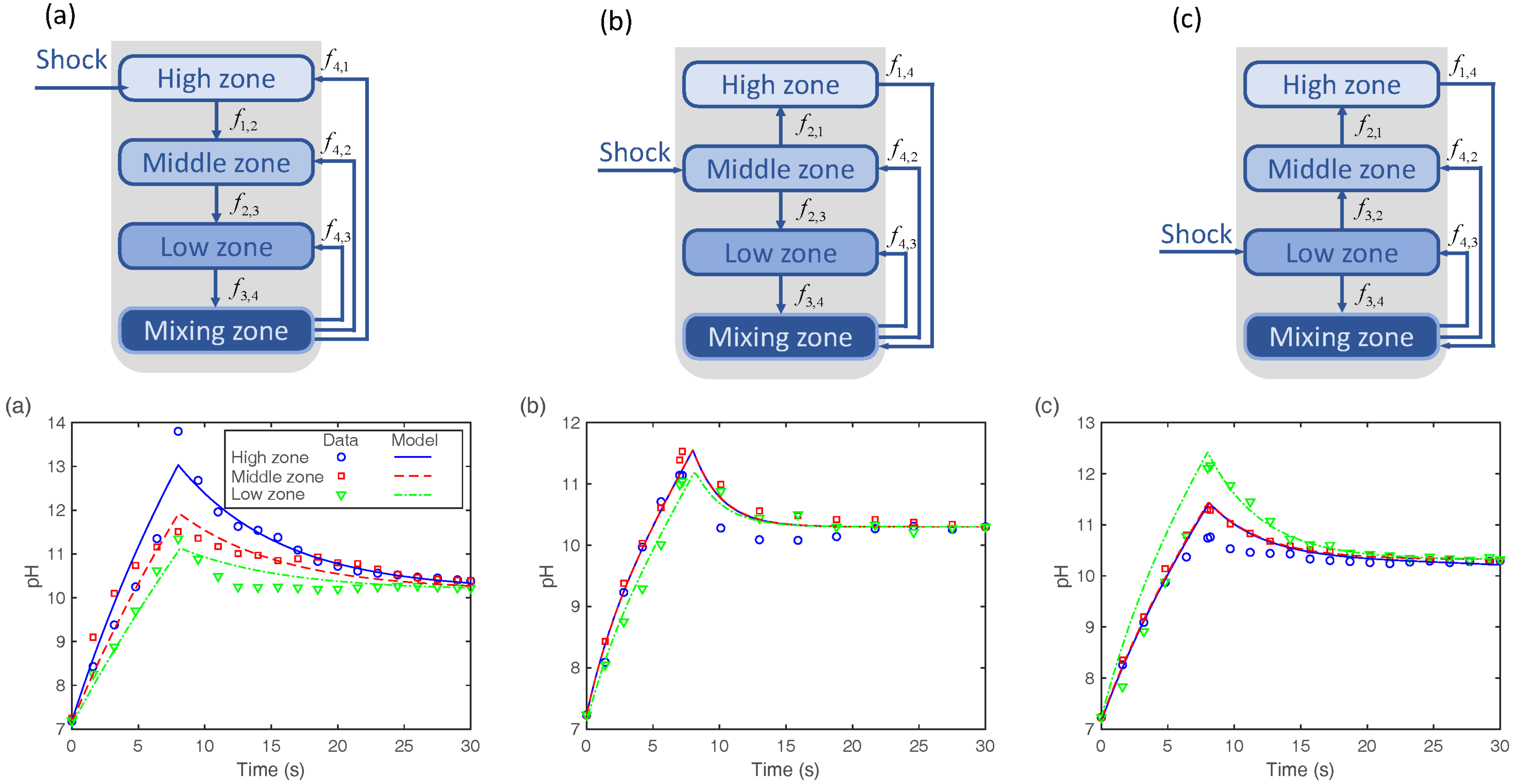
pH Heterogeneity Profiling Model



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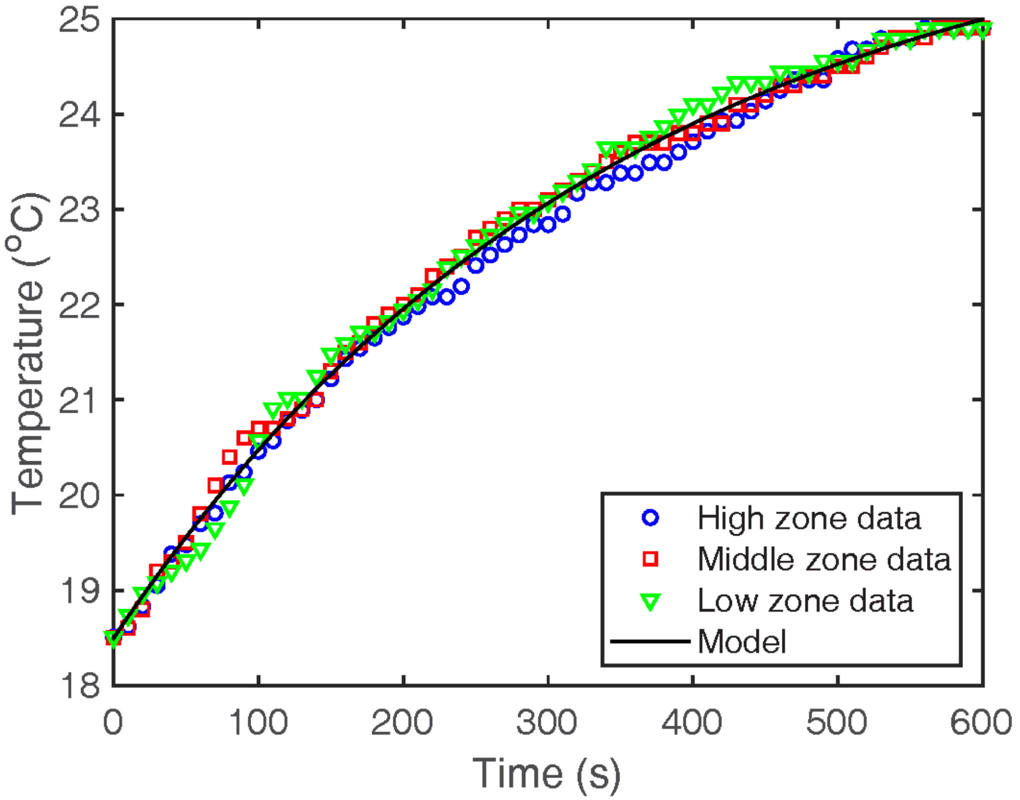
Temperature Heterogeneity Profiling Model

$$\frac{dT}{dt} = -\frac{UA_c}{V\rho C_p}(T - T_c)$$

$$T = T_c + (T_0 - T_c)\exp\left[-\frac{Ut}{L\rho C_p}\right]$$

$$\min_{T_i \in \mathcal{T} \subset \mathbb{R}, \mathbf{p} \in \Pi \subset \mathbb{R}^{n_p}} \sum_{i=1}^{N} \sum_{j=1}^{3} (T_i - T_{i,j}^{data})$$

$$\text{s.t.} \quad T_i = T_c + (T_0 - T_c)\exp\left[-\frac{Ut_i}{h\rho C_p}\right], \; i = 1, \dots, N$$



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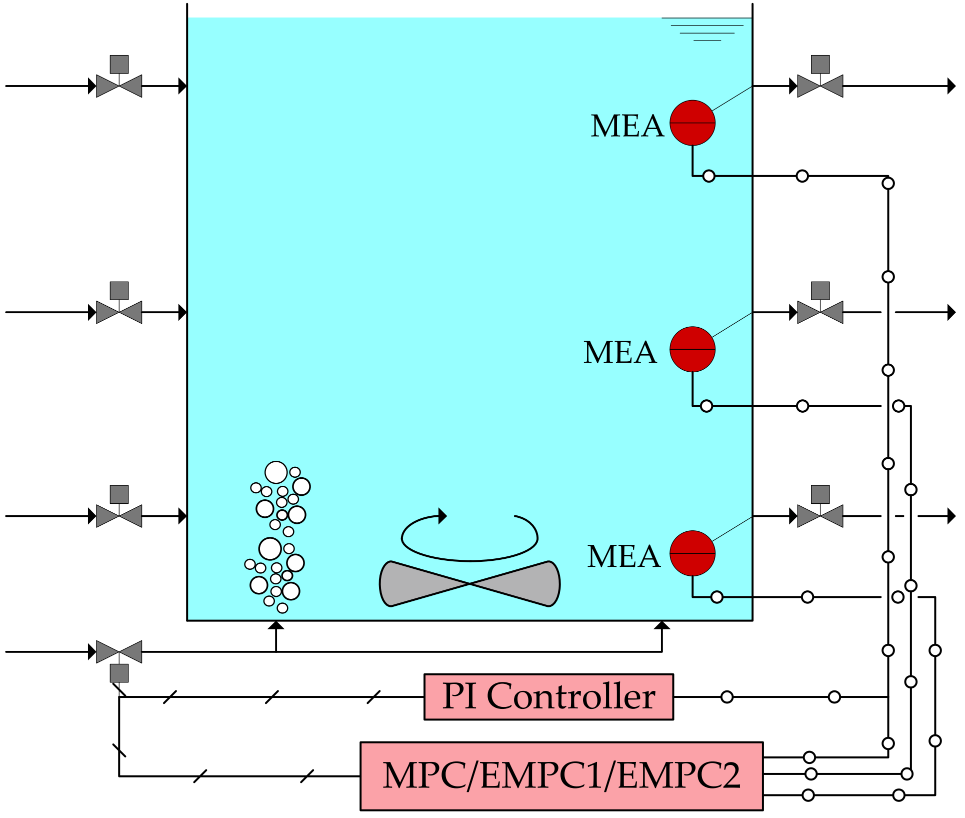
Optimal Control of Continuous Flow Nitrification Reactor

- Continuous flow nitrification reactor
- Inlet and outlet streams
  - High zone
  - Middle zone
  - Low zone
- Air diffuser
- Conductivity sensors
- Impeller
- Controller
  - PI Control
  - MPC
  - EMPC



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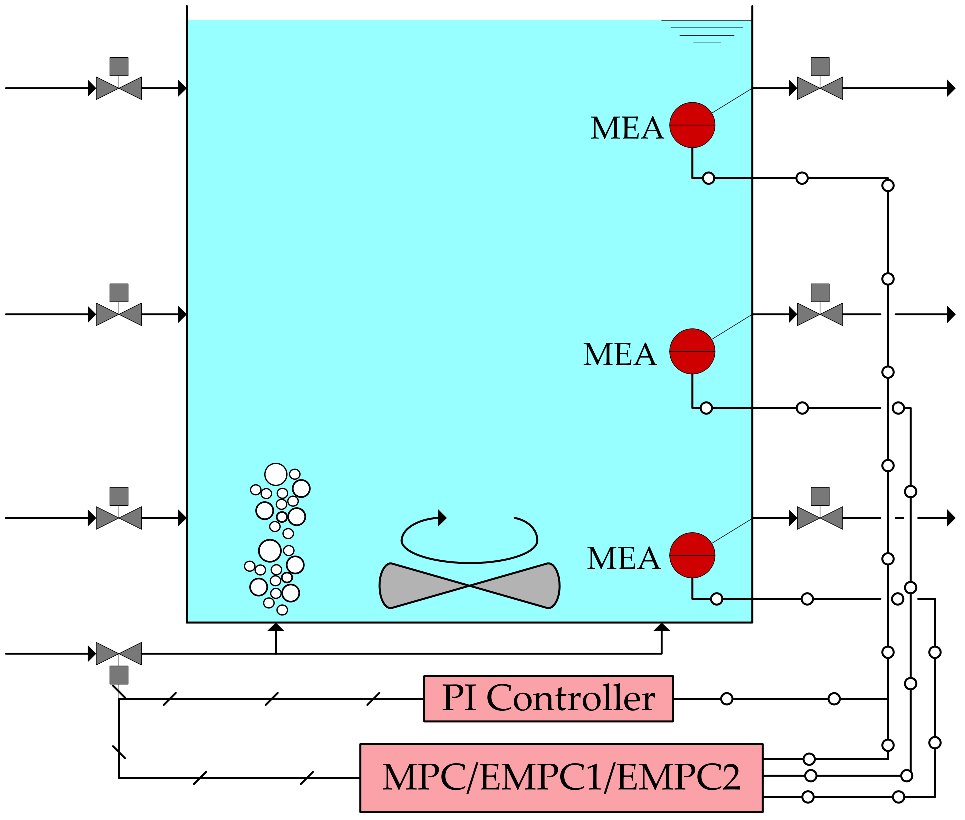
Modified Conductivity Model

$$\frac{dC_i}{dt} = \frac{1}{4V}\left(k_i(C_4 - C_i) + \dot{m}_{in,i}C_{in,i} - \dot{m}_{out,i}C_i\right) + R_{\mathrm{NH}_4^+},$$

$i = 1,2,3$

$$\frac{dC_4}{dt} = \frac{1}{4V}k_4(C_1 + C_2 + C_3 - 3C_4) + R_{\mathrm{NH}_4^+},$$

$$\frac{dc_O}{dt} = r_O + \boxed{k_{la}\cdot(c_O^* - c_O)},$$



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Kinetics and Aeration

- Nitrification Process

$$2NH_4^{+} + 3O_2 \rightarrow 2NO_2^{-} + 4H^{+} + 2H_2O$$

$$2NO_2^{-} + O_2 \rightarrow 2NO_3^{-}$$

Ammonium consumption rate:

$$r_{\mathrm{NH_4^+}} = -r_{\mathrm{AOB}} X_{\mathrm{AOB}},$$

$$r_{\mathrm{AOB}} = r_{\mathrm{AOB,max}} \frac{c_{\mathrm{NH_4^+}}}{K_{\mathrm{SAOB}} + c_{\mathrm{NH_4^+}} + \frac{c_{\mathrm{NH_4^+}}^2}{K_{\mathrm{IAOB}}}} \frac{c_O}{K_{\mathrm{OAOB}} + c_O}$$

- Oxygen balance

$$\frac{dc_O}{dt} = r_O + \boxed{k_{la} \cdot (c_O^* - c_O)}$$

$$r_O = -r_{\mathrm{AOB}} \psi_{\mathrm{AOB}} X_{\mathrm{AOB}}$$

Aeration:

$$\boxed{\frac{0.2967Q \cdot \mathrm{SOTE}}{V} \left(1 - \frac{c_O}{c_O^*}\right)}$$

Air flow rate: Q

[5] Sánchez, O., Aspé, E., Martí, M.C. and Roeckel, M. (2004) The Effect of Sodium Chloride on the Two–Step Kinetics of the Nitrifying Process. Water environment research 76(1), 73-80.
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Proportional-Integral Control

$$u(t) = K_p e(t) - K_i \int_0^t e(t')dt'$$

- Control variable

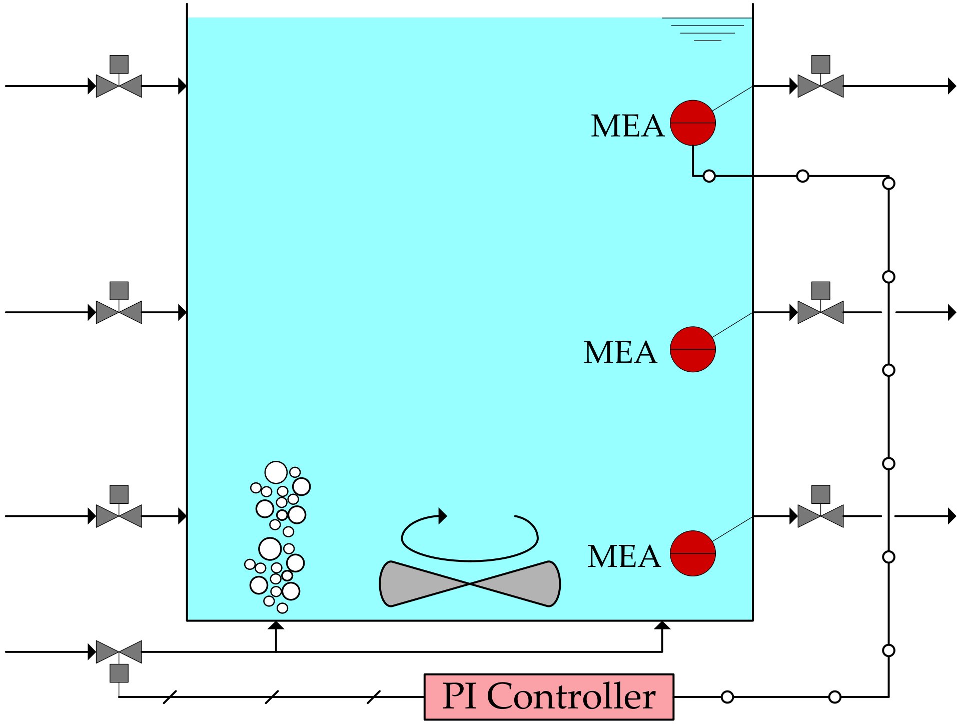
$$u(t) = Q$$

- Error

$$e(t) = \mathrm{SP} - C_1(t)$$

- Tuning coefficients

$$K_p, K_i$$



Model Predictive Control

- Primary advantage: multiple-input systems

$$\min_{u_k,\ldots,u_{k+M-1}} \sum_{i=1}^{3} \sum_{j=1}^{P} (\mathrm{SP} - \hat{C}_{i,k+j})^2$$

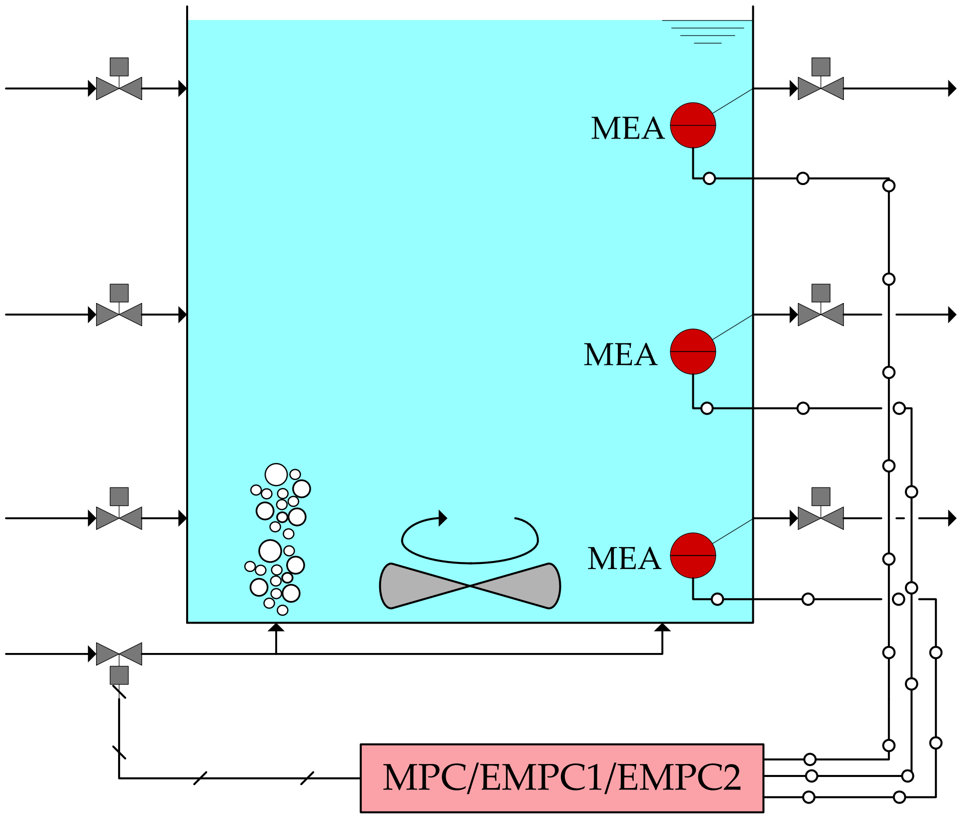
u : control variable

SP : setpoint

$\hat{C}_i$: model predicted output (DMC)

P : prediction horizon

M : control horizon



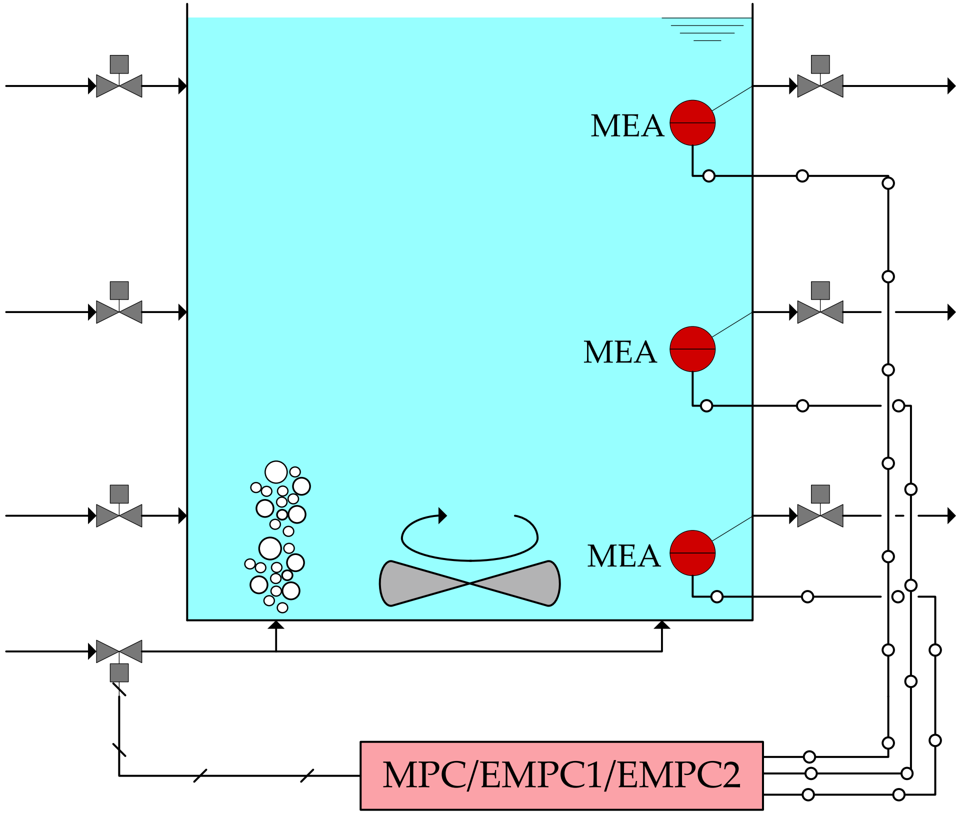
Economic Model Predictive Control

- EMPC1 - environment

$$\min_{u_k,\ldots,u_{k+M-1}} \sum_{i=3}^{3}\sum_{j=1}^{P} {D_{i,k+j}}^2 + \boxed{w\left(\sum_{i=0}^{M-1} u_{k+i} + (P-M+1)u_{k+M-1}\right)}$$

Penalty function

$$D_{i,k+j} = \begin{cases} \hat{C}_{i,k+j} - \mathrm{SP} & \text{if } (\hat{C}_{i,k+j} - r) > 0 \\ 0 & \text{if } (\hat{C}_{i,k+j} - r) \le 0. \end{cases}$$



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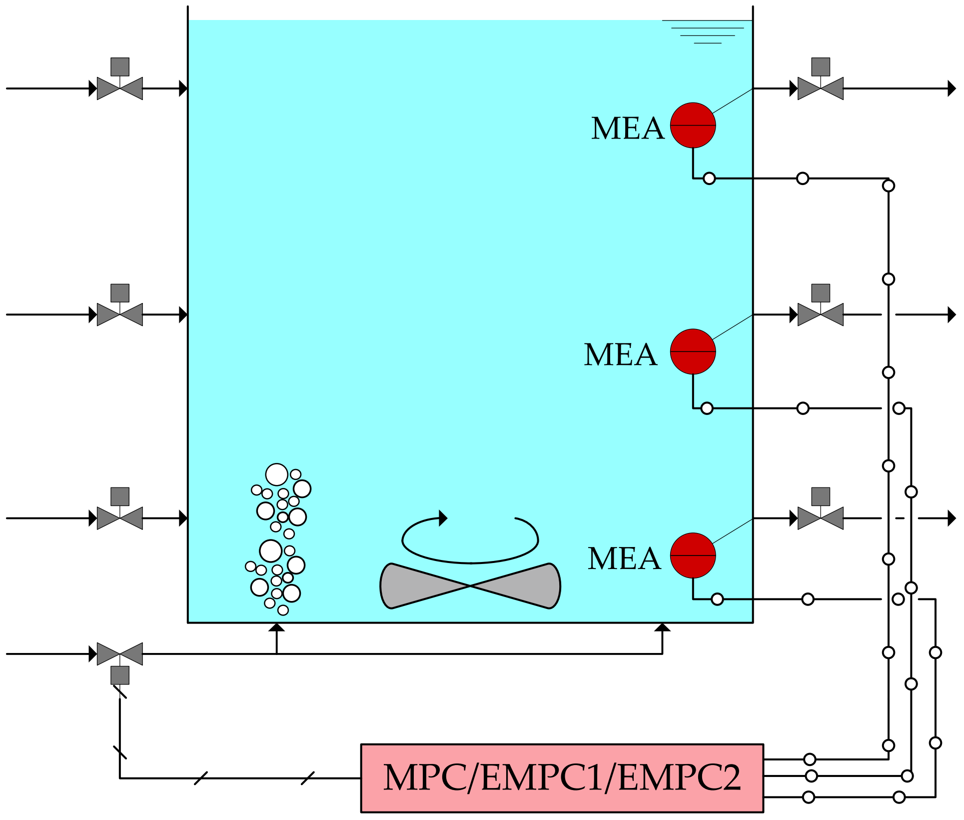
Economic Model Predictive Control

- EMPC2 - energy

$$\min_{u_k,\ldots,u_{k+M-1}} \delta\left(\sum_{i=0}^{M-1} u_{k+i} + (P-M+1)u_{k+M-1}\right)$$

s.t. $\hat{C}_{i,k+j} - \mathrm{SP} \le 0$

$\forall i = 1,2,3, \quad j = 1,\ldots,M,P$



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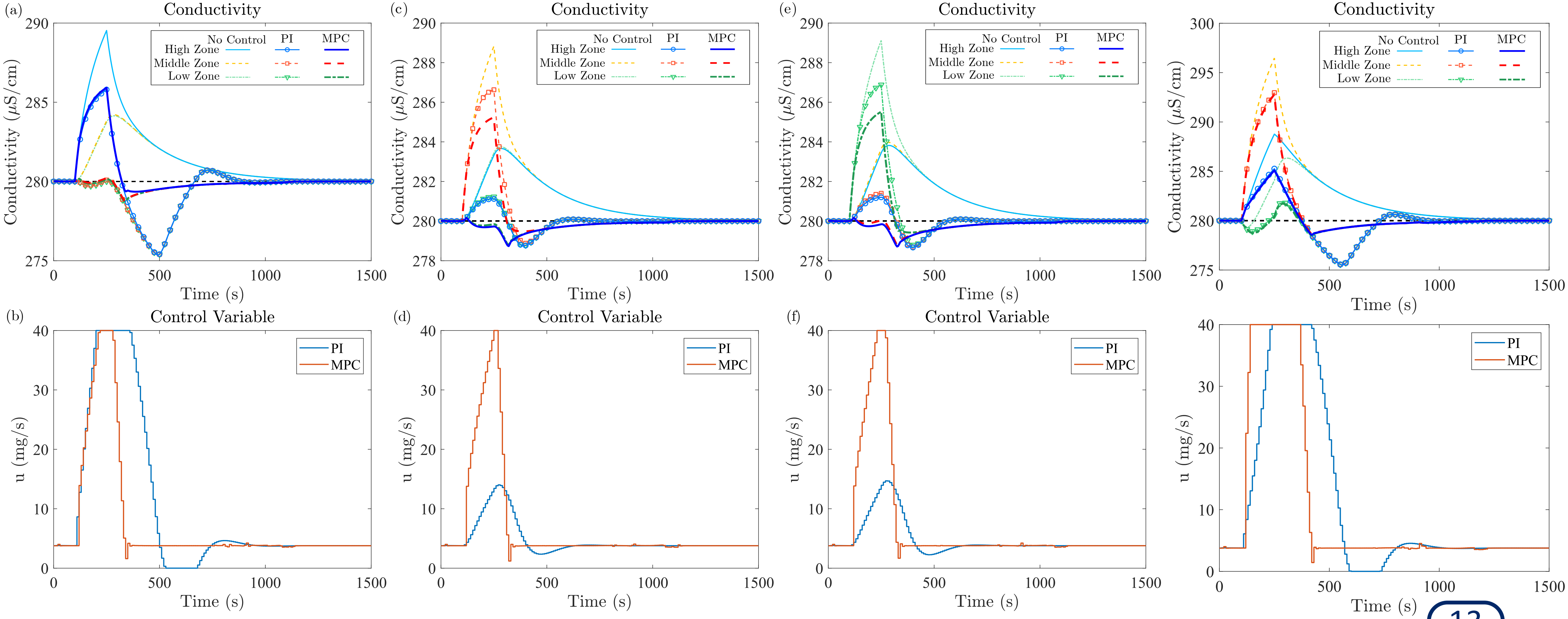
Results

(i) $C_{in,1}$ = 320 µS/cm (ii) $C_{in,2}$ = 320 µS/cm (iii) $C_{in,3}$ = 320 µS/cm (iv) Multiple shocks



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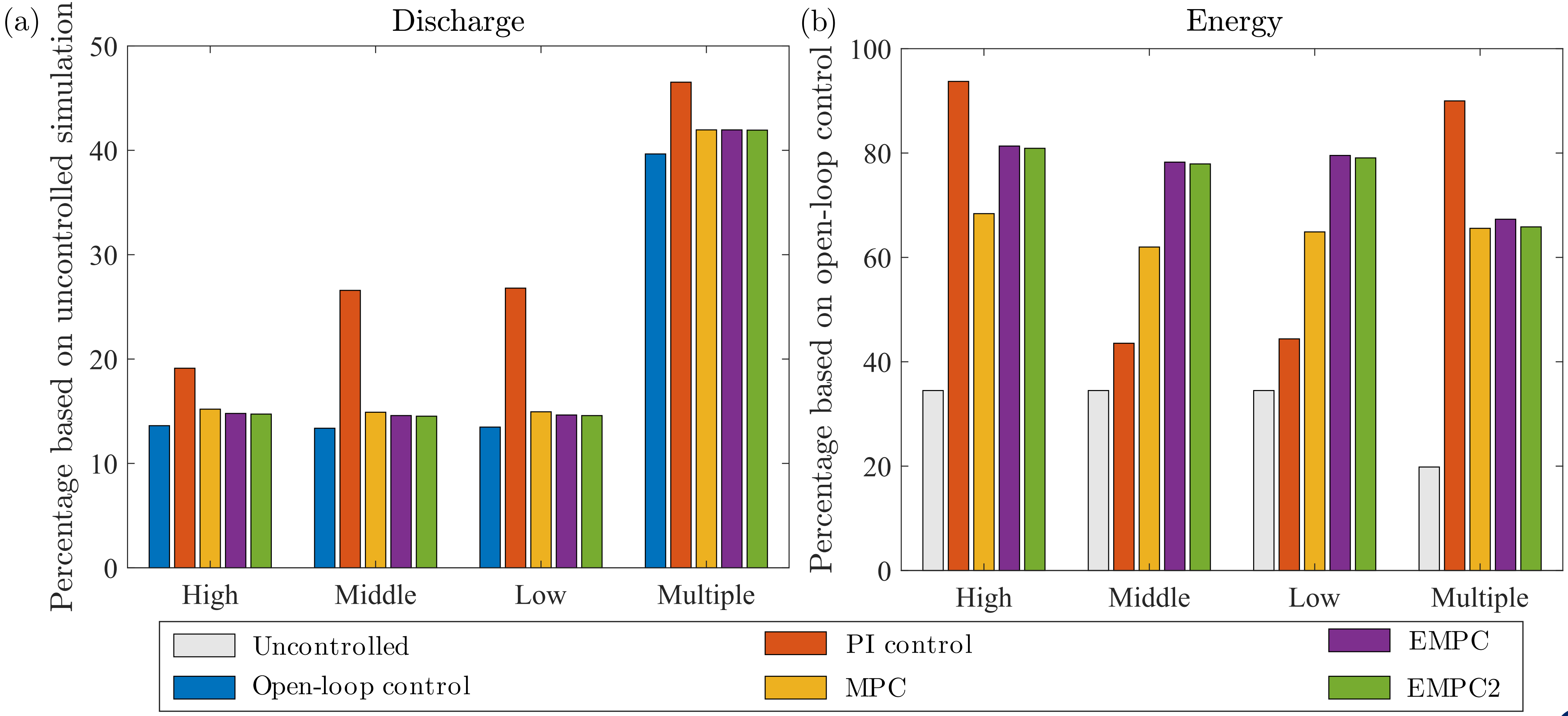
Discharge & Energy



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Any questions?

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