Real-Time Optimization and Nonlinear Model Predictive Control for a Post-Combustion Carbon Capture Absorber

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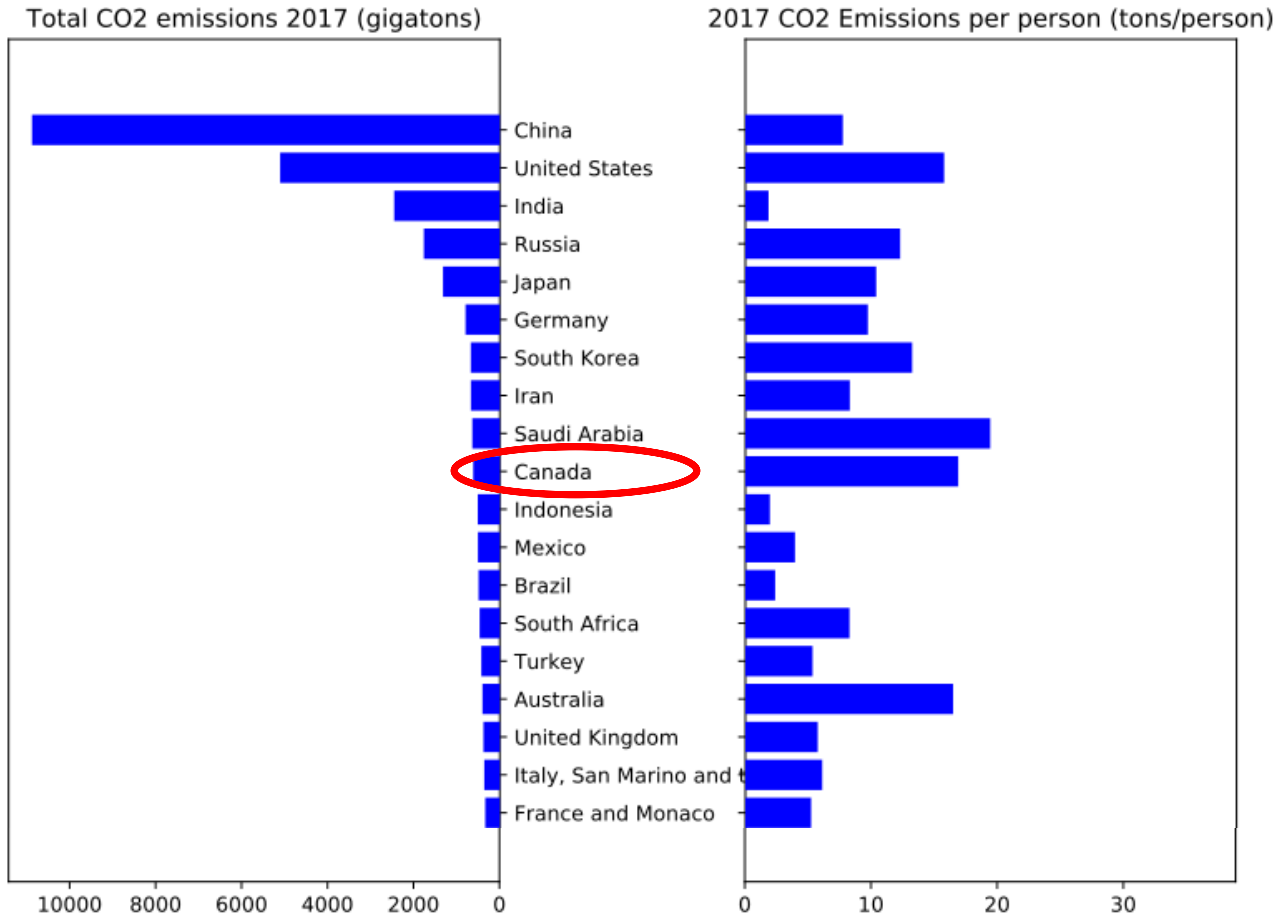
The CO_2 problem



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<u>CO2 capture methods</u>

- Pre-combustion
- Oxy-combustion
- Chemical looping combustion
- Post-combustion (PCC)*

*most mature technology

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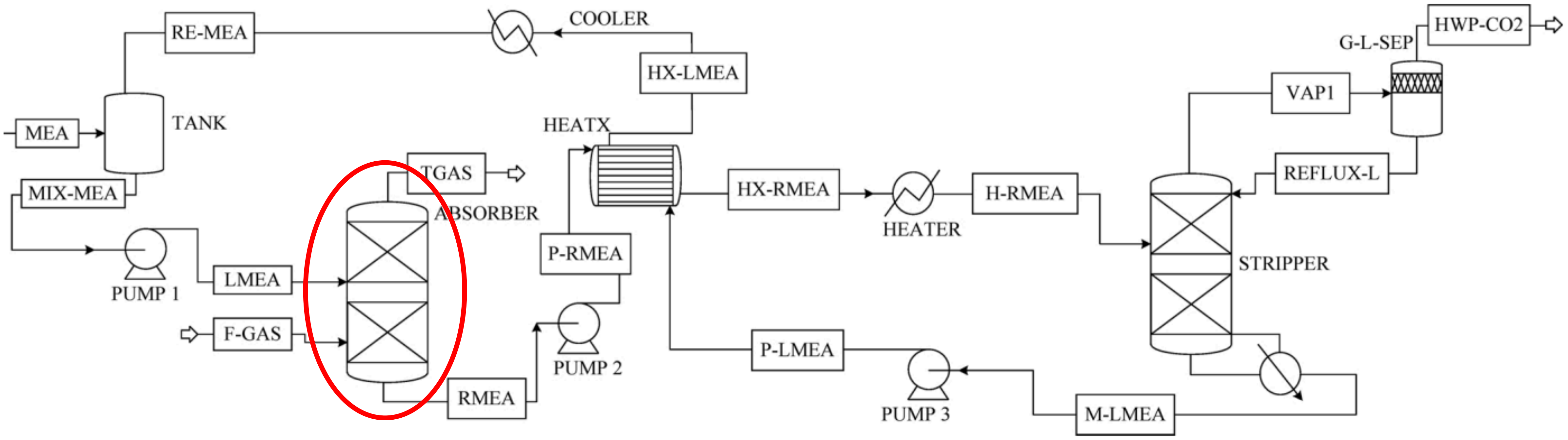
MEA Solvent Post Combustion Carbon Capture (PCC) System



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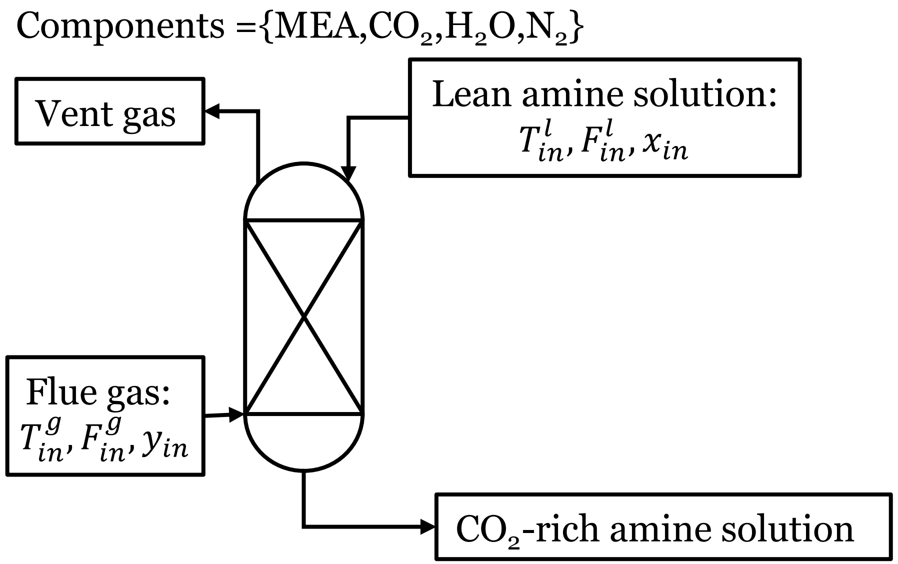
PCC economic operation and control

- Nonlinear model prediction control (NMPC)
  - Reduced order absorber model (Akeson et al.,2012)
  - Robust mechanistic absorber model (Patrón and Ricardez-Sandoval, 2020)
- Economical operation
  - Linear multivariable MPC for PCC plant (Panahi and Skogestad, 2012)
- Economic MPC
  - Chan and Chen (2018)
  - Decardi-Nelson, Liu and Liu (2018)

A two-layer RTO approach has not been tested for the PCC

Motivation, Challenges, and Objectives



Motivation

- The absorber is of economic detriment to the upstream power plant
- The power plant introduces disturbances to the absorber, creating economic suboptimality

Objectives

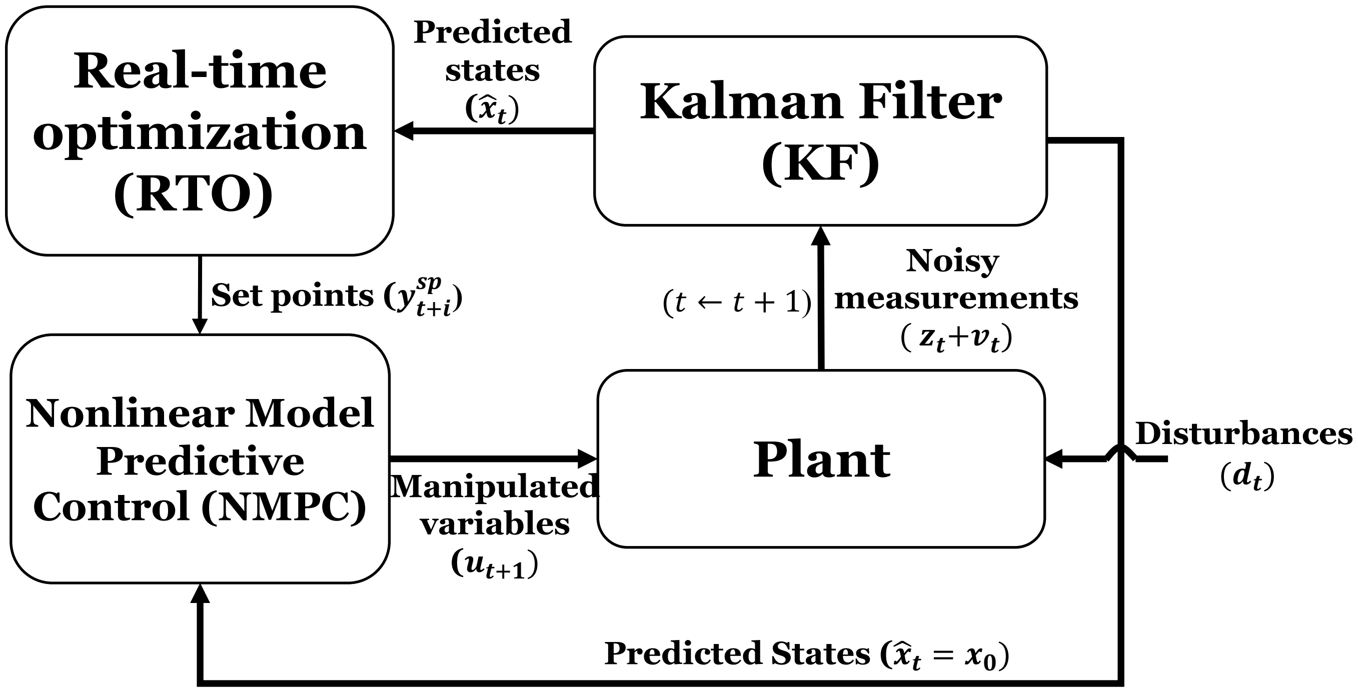
- Operate the absorber in an economically optimal way subject to upstream disturbances and changing carbon tax prices

Challenges

- Cost reduction and carbon capture are conflicting objectives
- State estimation is required

Research objectives

- Novel RTO formulation for absorber
- Mechanistic process model in RTO and NMPC layer
- State estimation for absorber



*all methods require models

Differential Model of CO_2 Absorber Column - $f(x)$ *

i=MEA,CO_2,H_2O, N_2

* Adapted from Harun et al. (2012)

	Mass
Liquid	$$\frac{dC_i^l}{dt} = u_l \frac{\partial C_i^l}{\partial z} + a_w N_i$$
Gas	$$\frac{dC_i^g}{dt} = -u_g \frac{\partial C_i^g}{\partial z} - a_w N_i - C_i^g \frac{\partial u_g}{\partial z}$$
	Energy
Liquid	$$\frac{dT_l}{dt} = u_l \frac{\partial T_l}{\partial z} - \frac{a_w}{\sum_{i=1}^{4} c_{p,i}^l C_i^l}\left[h_{gl}(T_l - T_g) + \Delta H_{rxn} N_{CO_2} - \Delta H_{H_2O}^{vap} N_{H_2O} + h_{out}(T_l - T_{amb})\right]$$
Gas	$$\frac{dT_g}{dt} = -u_g \frac{\partial T_g}{\partial z} + \frac{a_w}{\sum_{i=1}^{4} c_{p,i}^g C_i^g}\left[h_{gl}(T_l - T_g)\right]$$

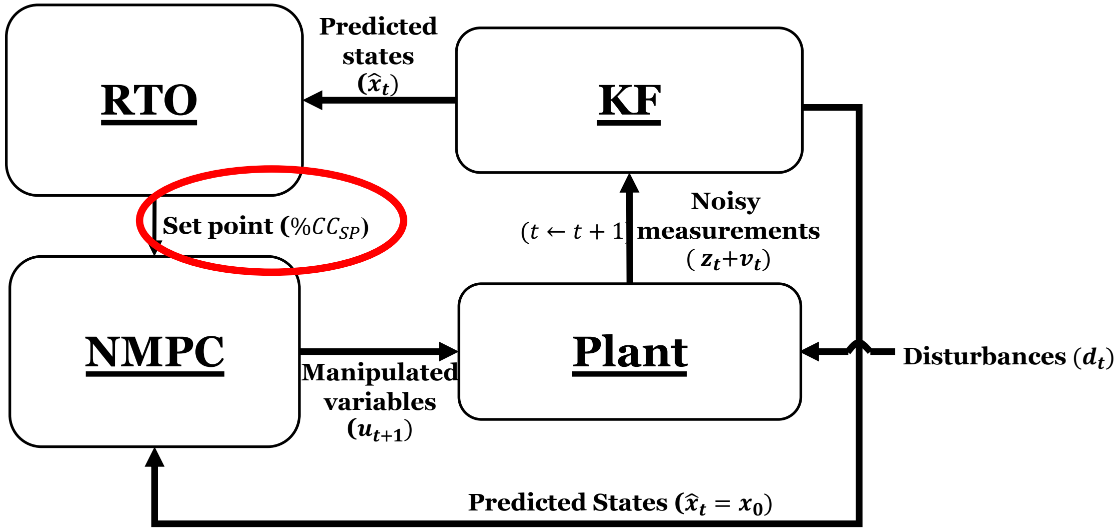
- Phenomenological and physical property equations ($\boldsymbol{h}(\boldsymbol{x})$)
- Non-discretized model has 12 PDEs and 160 AEs

Model Implementation

- PDAEs discretized by finite differences in axial domain and orthogonal collocations in time domain
- Model size (after discretization):
  - Axially (RTO) $\Rightarrow$ ~2,000 nonlinear algebraic equations
  - Axially and temporally (NMPC) $\Rightarrow$ ~64,000 nonlinear algebraic equations
- IPOPT (Wächter and Biegler, 2005)

PYOMO

RTO Formulation



- Steady-state optimization
- Three sources of cost:
  - MEA degradation (per tonne of CO_2 removed)
  - Carbon Tax (per tonne of CO_2 emitted)
  - Electricity

$$\min_{\%CC_{SP}} \mathrm{P_{MEA}}\dot{\mathrm{m}}^{\mathrm{l}}_{CO_2,out} + \mathrm{P_{CO_2}}\dot{\mathrm{m}}^{\mathrm{g}}_{CO_2,out} + \mathrm{P_e W_{pump}}$$

$$s.t.$$

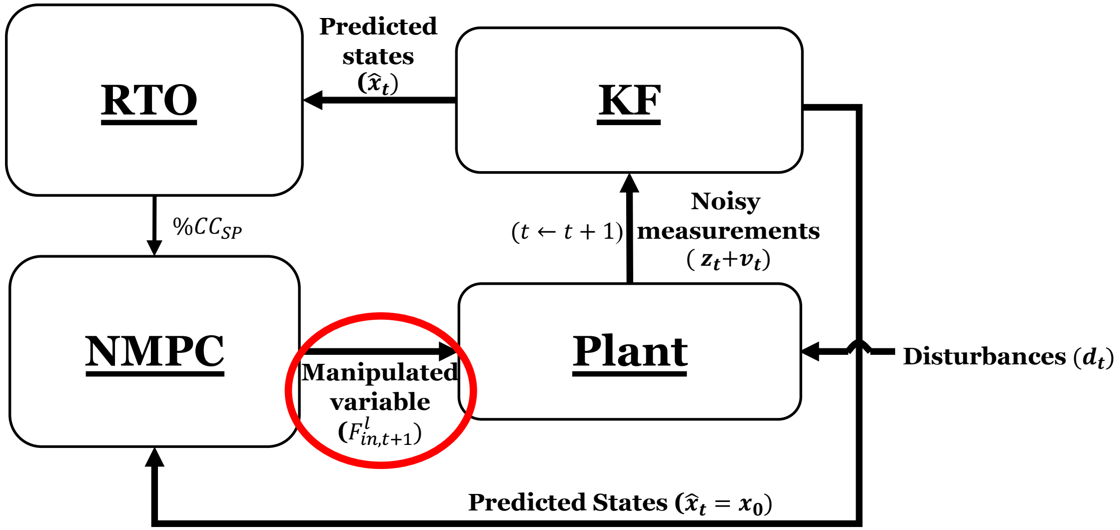
$$\boldsymbol{f(x_t, u_t) = 0}$$

$$\boldsymbol{h(x_t, u_t) = \hat{Y}_t}$$

$$\boldsymbol{u^l \le u_t \le u^h}$$

NMPC Formulation

- Dynamic optimization
- Tracking and move suppression terms
- Manipulated variable bounds



$$\min_{F^g_{in,t+j}\ \forall j \in \{1,\dots,C\}} \boldsymbol{Q} \sum_{i=1}^{P} \left(\widehat{\%CC}_{t+i} - \%CC_{SP}\right)^2 + \boldsymbol{R} \sum_{j=1}^{C} \Delta F^{l}_{in,t+j}{}^2$$

$s.t.$

$$\boldsymbol{f}(\boldsymbol{x}_t, \boldsymbol{u}_{t+j}) = \hat{\boldsymbol{x}}_{t+i}; \qquad \forall i \in \{1, \dots, P\}$$
$$\forall j \in \{1, \dots, C\}$$

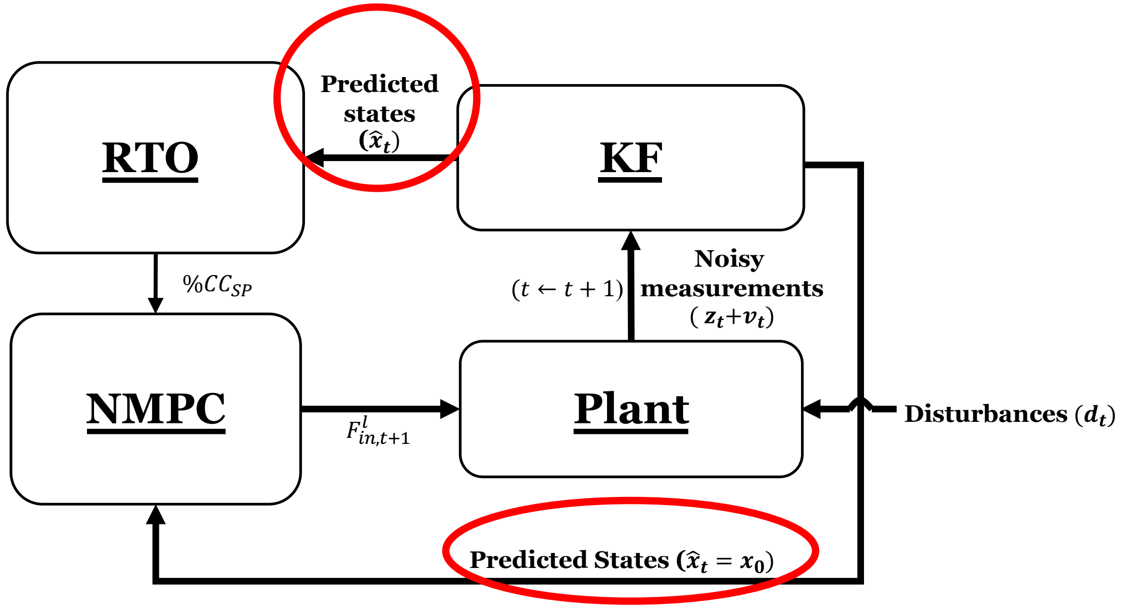
$$\boldsymbol{x}_t = \boldsymbol{x}_0$$

$$\boldsymbol{h}(\hat{\boldsymbol{x}}_{t+i}, \boldsymbol{u}_{t+j}) = \hat{\boldsymbol{Y}}_{t+i}; \qquad \forall i \in \{1, \dots, P\}$$
$$\forall j \in \{1, \dots, C\}$$

$$F^{l,l}_{in} \leq F^{l}_{in,t+j} \leq F^{l,u}_{in}; \qquad \forall j \in \{1, \dots, C\}$$

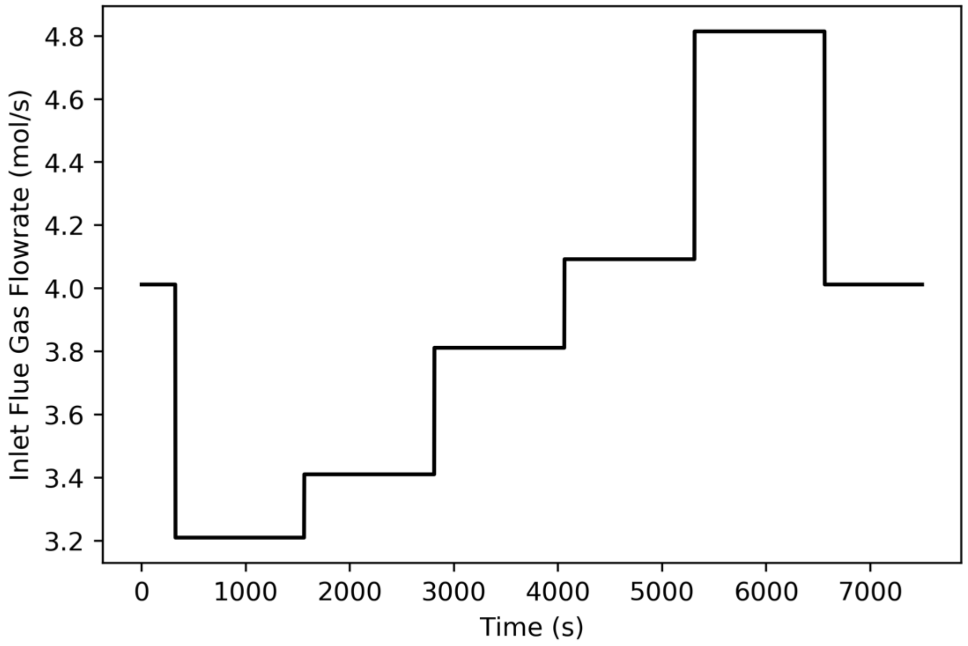
KF Formulation

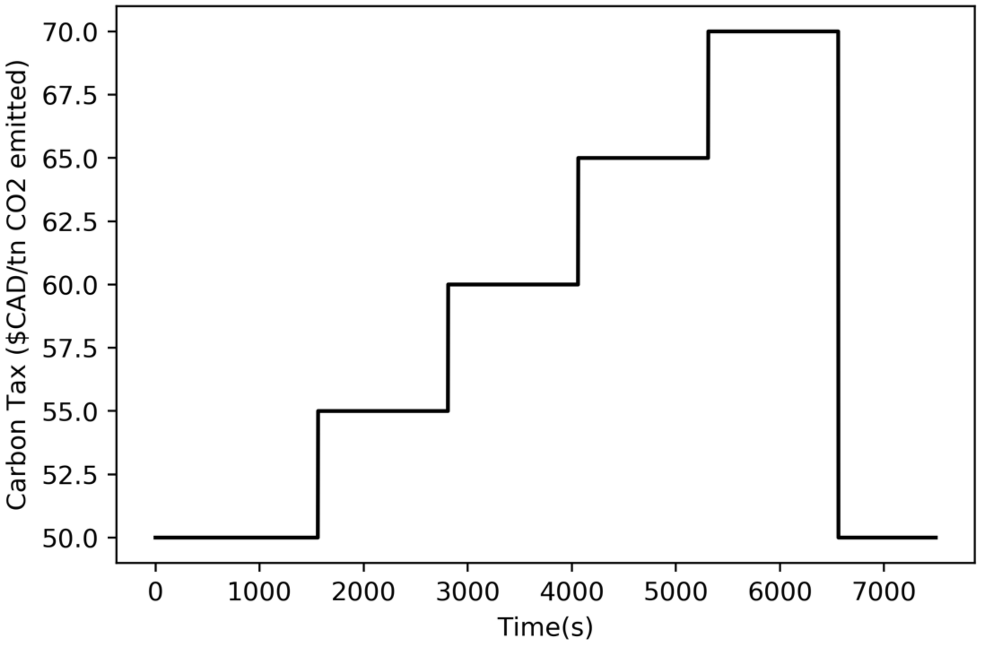
- 74/110 states measured
  - Temperatures, gas concentrations, inlet/outlet states
- *A priori* predictions generated using mechanistic model
- Jacobian matrix for generated symbolically
  - $\hat{x}_{k|k-1} = f(\hat{x}_{k-1|k-1}, u_k)$
  - $P_{k|k-1} = J_f \, P_{k-1|k-1} \, J_f^{\,T} + Q_k$
  - $K_k = P_{k|k-1} \, J_h^{\,T} (J_h P_{k|k-1} \, J_h^{\,T} + R_k)^{-1}$
  - $\hat{x}_{k|k} = \hat{x}_{k|k-1} + K_k(z_k - H_k \hat{x}_{k|k-1})$
  - $P_{k|k} = (I - K_k J_h) \, P_{k|k-1}$



Results (test scenarios)

1. NMPC only (no RTO)
2. RTO (carbon tax at fixed 50 $CAD/tn CO_2 emitted)
3. RTO (time-varying carbon tax)





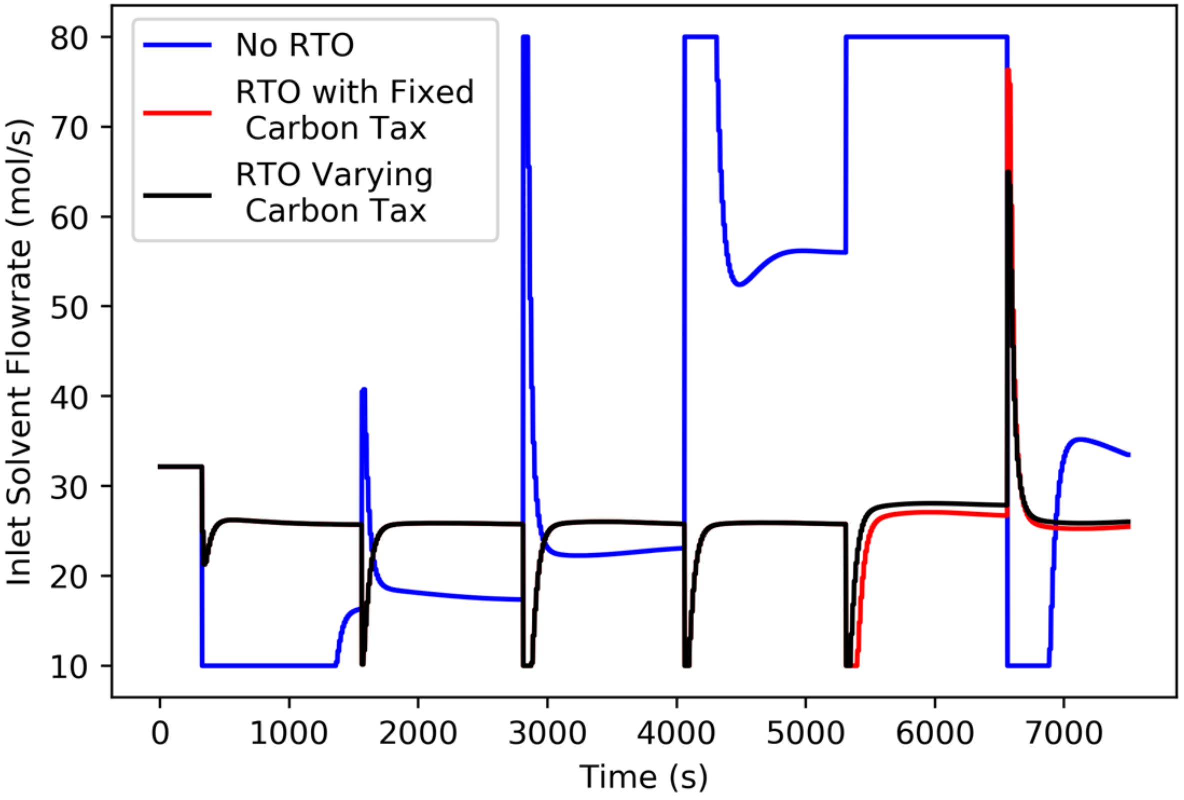
Result (process cost)

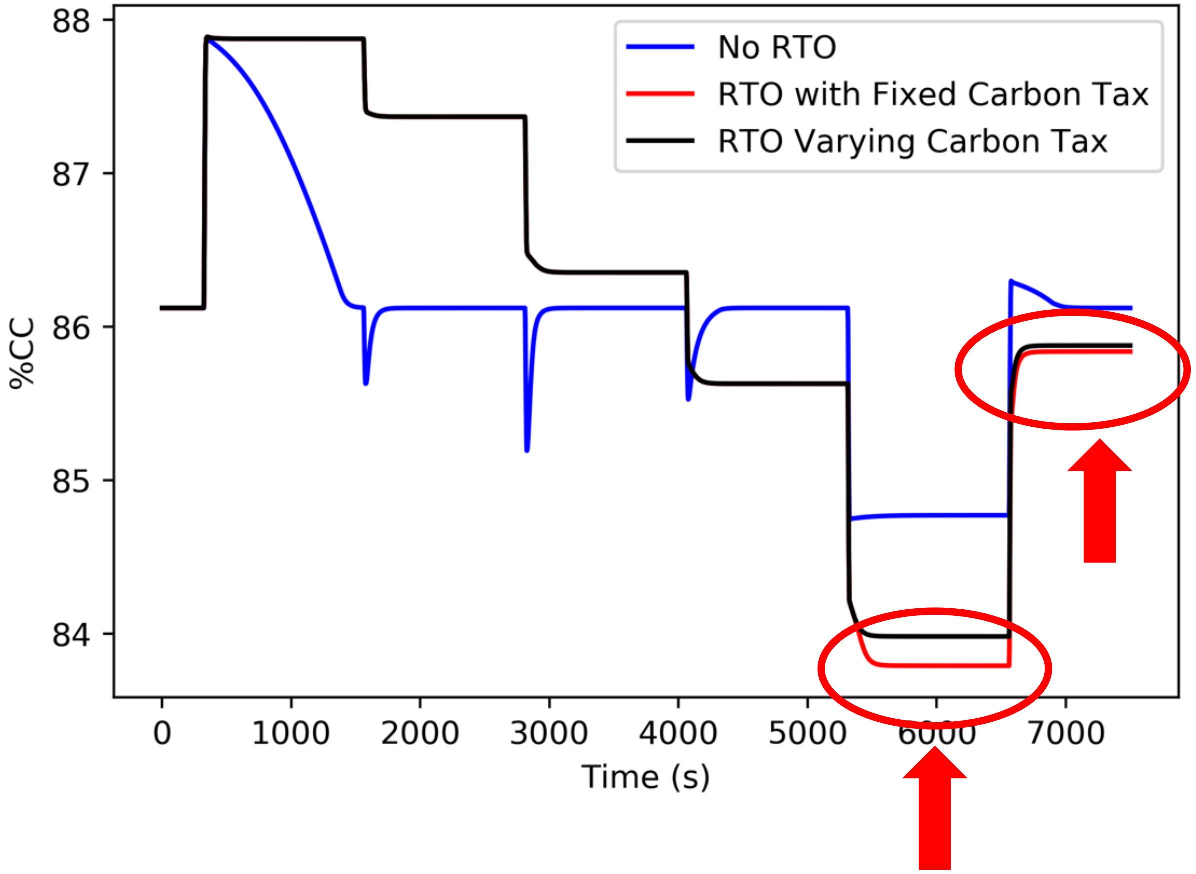
*costs in $CAD

Scenario	Total Cost	Tax Cost	MEA Cost	Electrical Cost
No RTO (fixed tax)	13.46	6.31	7.13	0.01
No RTO (varying tax)	14.64	7.50	7.13	0.01
RTO (fixed tax)	11.98	6.31	5.67	0.01
RTO (varying tax)	13.23	7.51	5.70	0.01

RTO sensitive to MEA cost

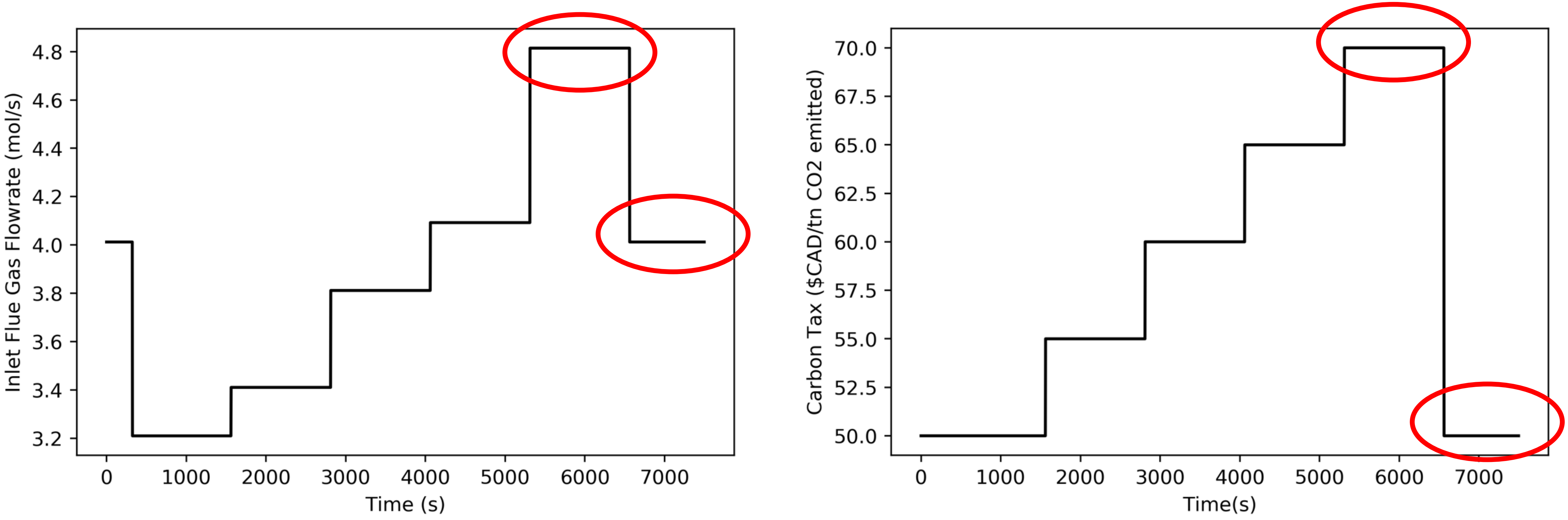
Results (profiles)





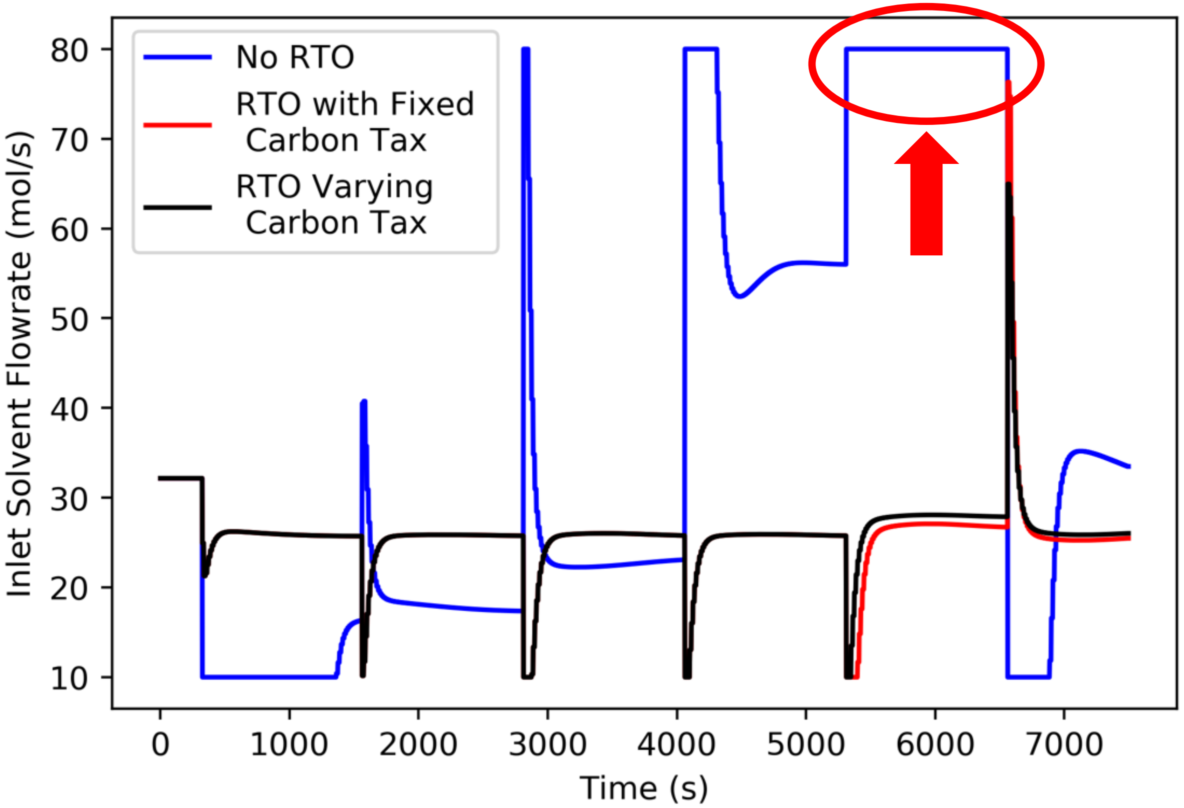
- Fixed and varying tax case are only substantially different in final two RTO periods

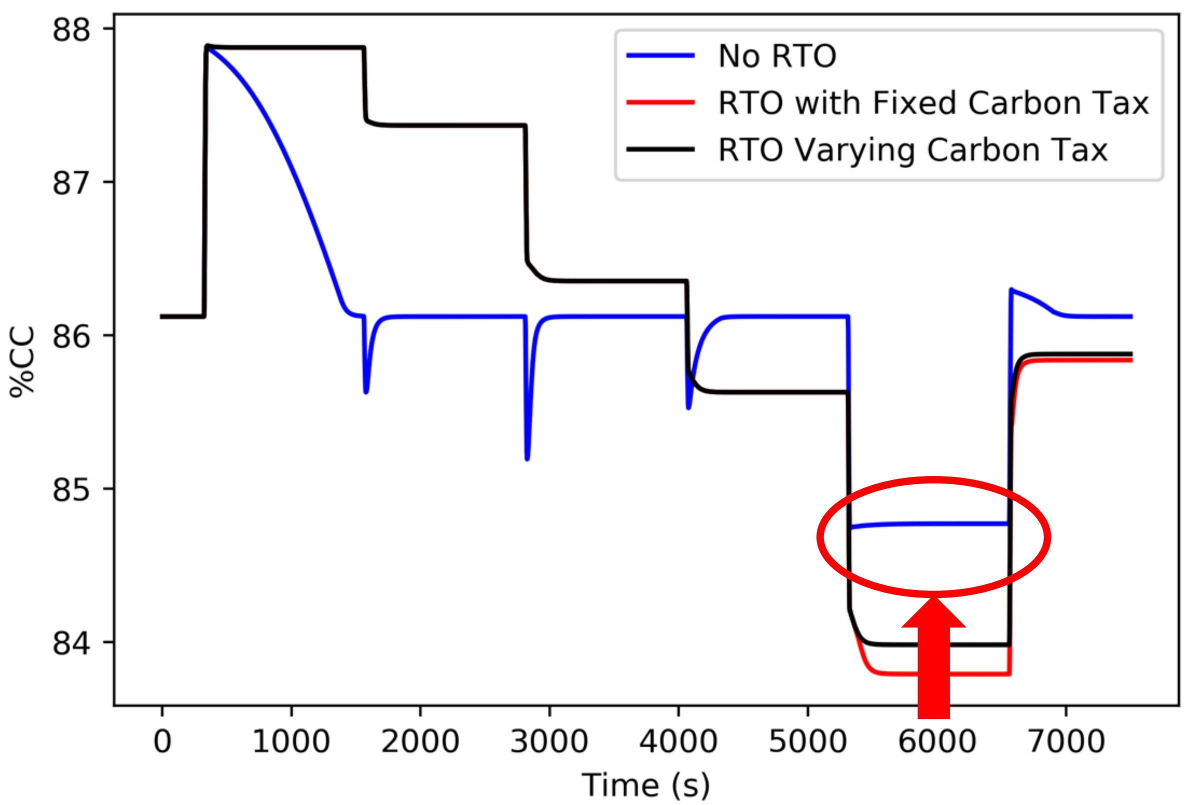
Results (profiles)



- RTO only sensitive to tax rate when it coincides with large disturbances

Results (profiles)

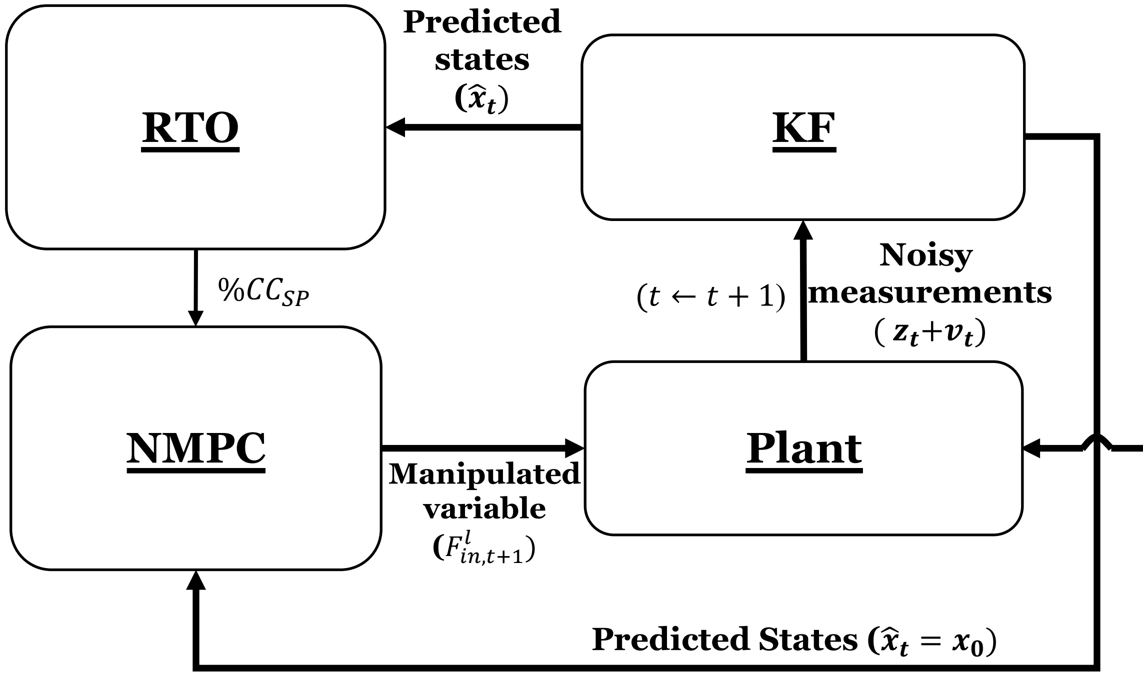




- Large disturbances cause unreachable set points in no RTO scenario
- These are avoided by the executing the RTO

Results (computational times)

	CPU time [s]	Number of equations	Key outputs
RTO	~15 s	1,861	1 ($\%CC_{SP}$)
NMPC	~60 s	64,480	9 ($F^{l}_{in,t+1}$)
KF (a priori)	~4 s	1,861	110 ($\hat{x}_t$)
KF (a posteriori)	<1 s	110	



Conclusions

- RTO provides substantial economic benefit and avoids unreachable setpoints
- Carbon tax rate only impacts economics when under large disturbances
- KF is able to compute states at a computational cost

Future Work

- Investigate more advanced estimation schemes (i.e. moving horizon estimation)
- Account for plant—model mismatch via parameter or modifier adaptation
- Merge RTO and NMPC layers by formulating an economic NMPC
- Consider entire post-combustion CO2 plant (i.e. stripper, heat exchange units, tanks)

Thank you

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https://uwaterloo.ca/chemical-process-optimization-multiscale-modelling-process-systems/

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