Model Predictive Control and Smart Manufacturing for Electrification of Industrial Processes such as Power-2-Ammonia

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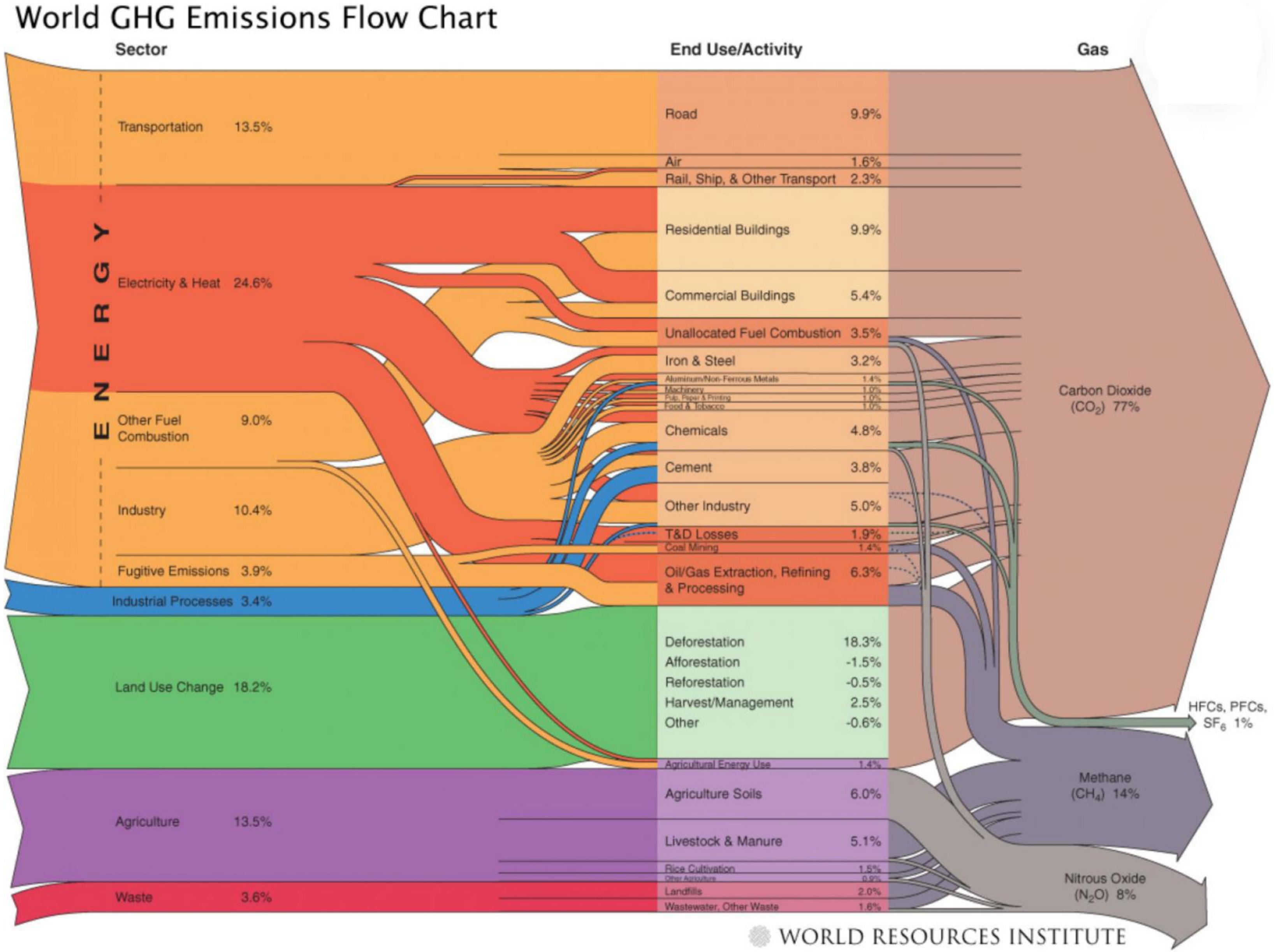
Zoom, April 26, 2023

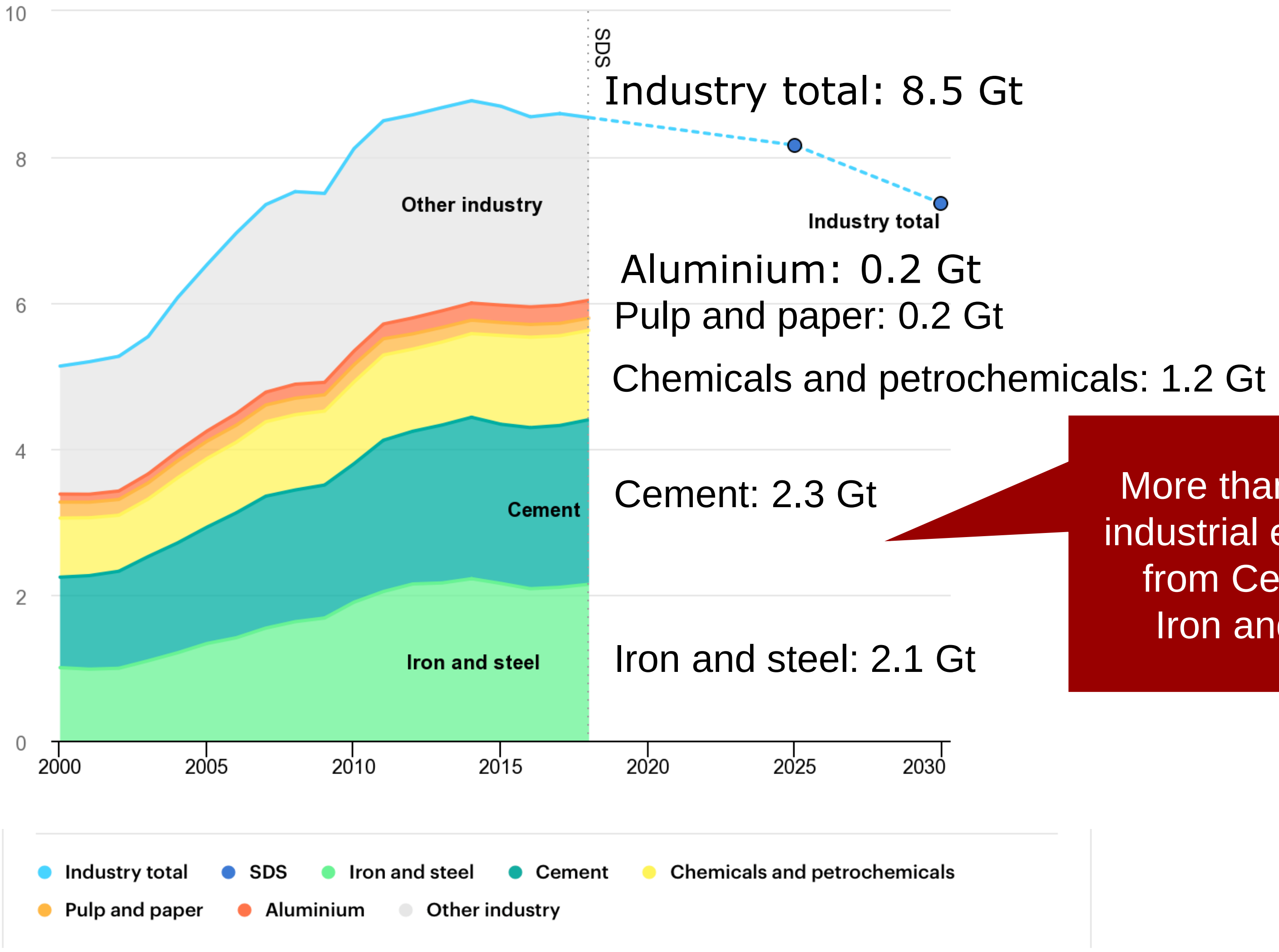
DTU Compute
Department of Applied Mathematics and Computer Science

CERE
Center for Energy Resources Engineering

Global Climate Gas Emissison by Sector – 51 Gt CO2 to zero



Industry direct CO2 emissions
- Cement & Iron and Steel more than 50%

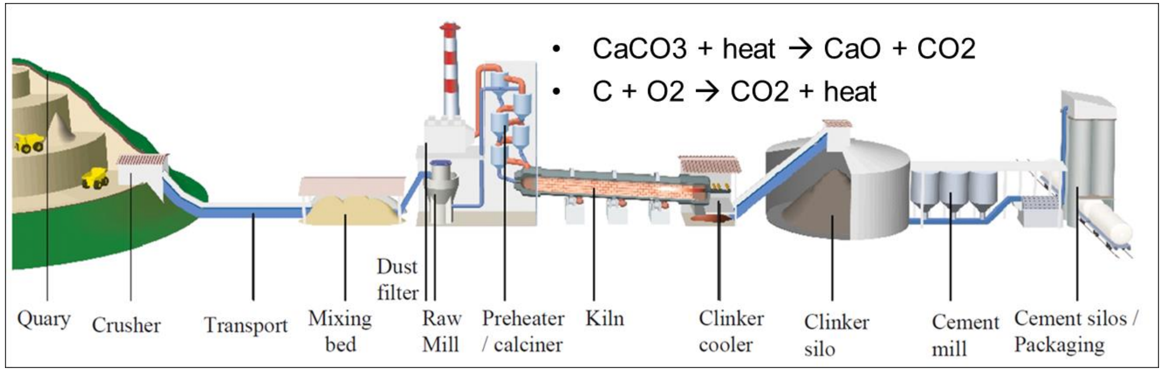


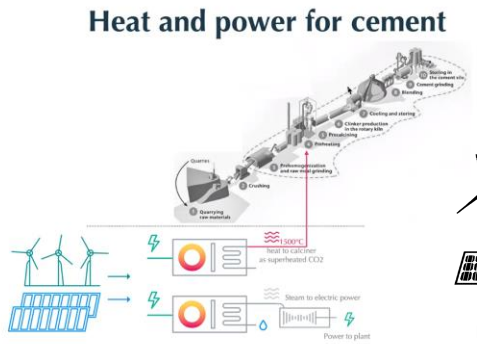
More than 50% of industrial emissions from Cement & Iron and steel

IEA, 2020

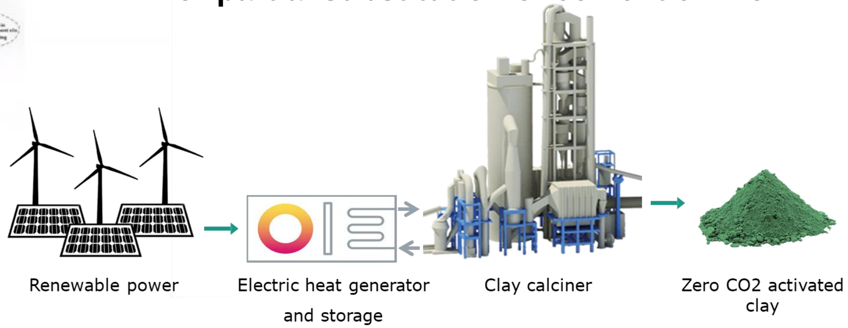
Digitalization, Control and Optimization – Model Predictive Control – for CO2 Emission Free Cement Production

Cement plant

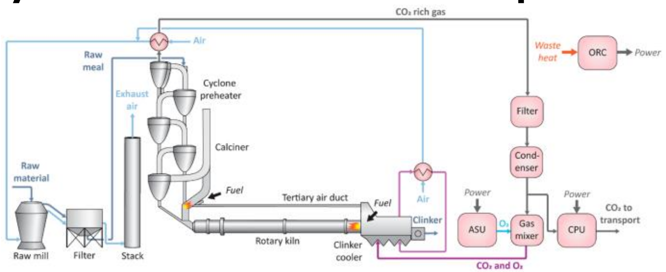




The ECOCLAY process for partial substitution of cement clinker



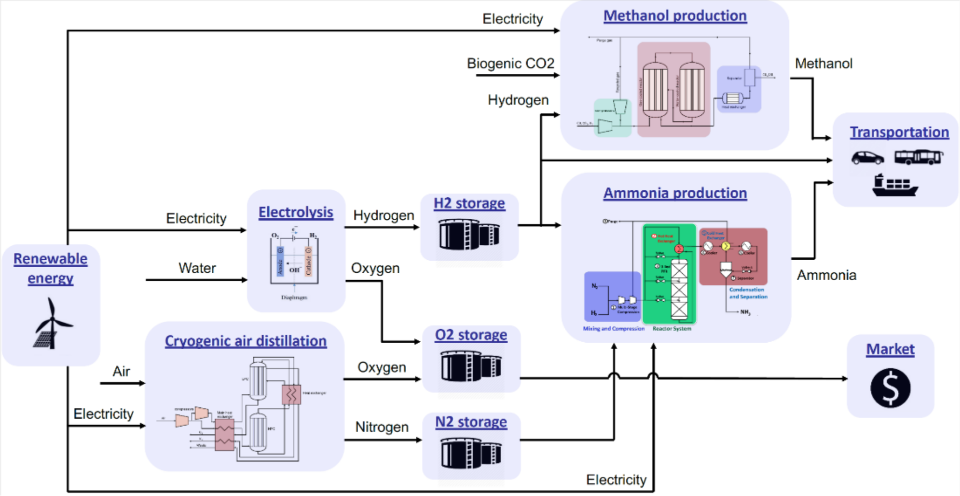
Oxyfuel combustion for CO2 capture

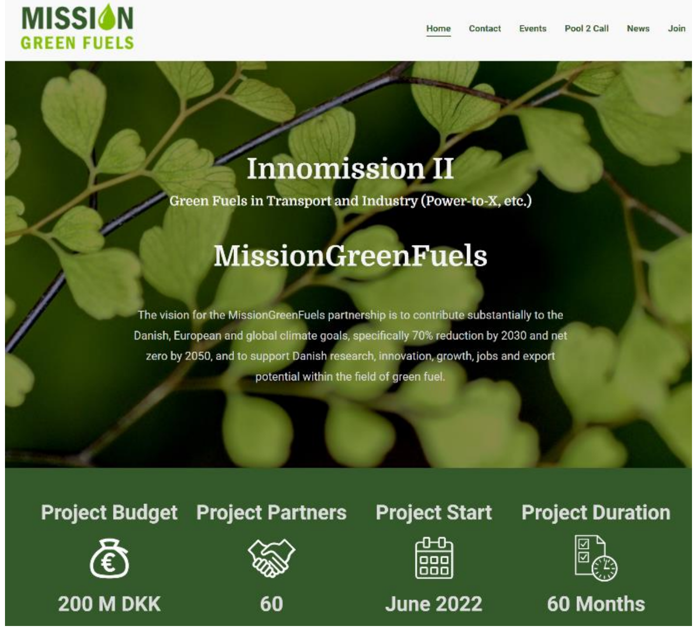


Simulation, control and optimization for CO2 emission free cement production

- Cement production is responsible for 5% of the worlds CO2 emissions
- **AI-based MPC cement production**
  - Applied to existing cement factories
  - Efficiency gains in the short term
- **ECOCLAY**
  - Electrification of cement production
  - Thermal storage of renewable energy for high-temperature industrial processes
- **NewCement**
  - CO2 capture from cement plants

DYNFLEX – Digitalization for Power-to-X Production





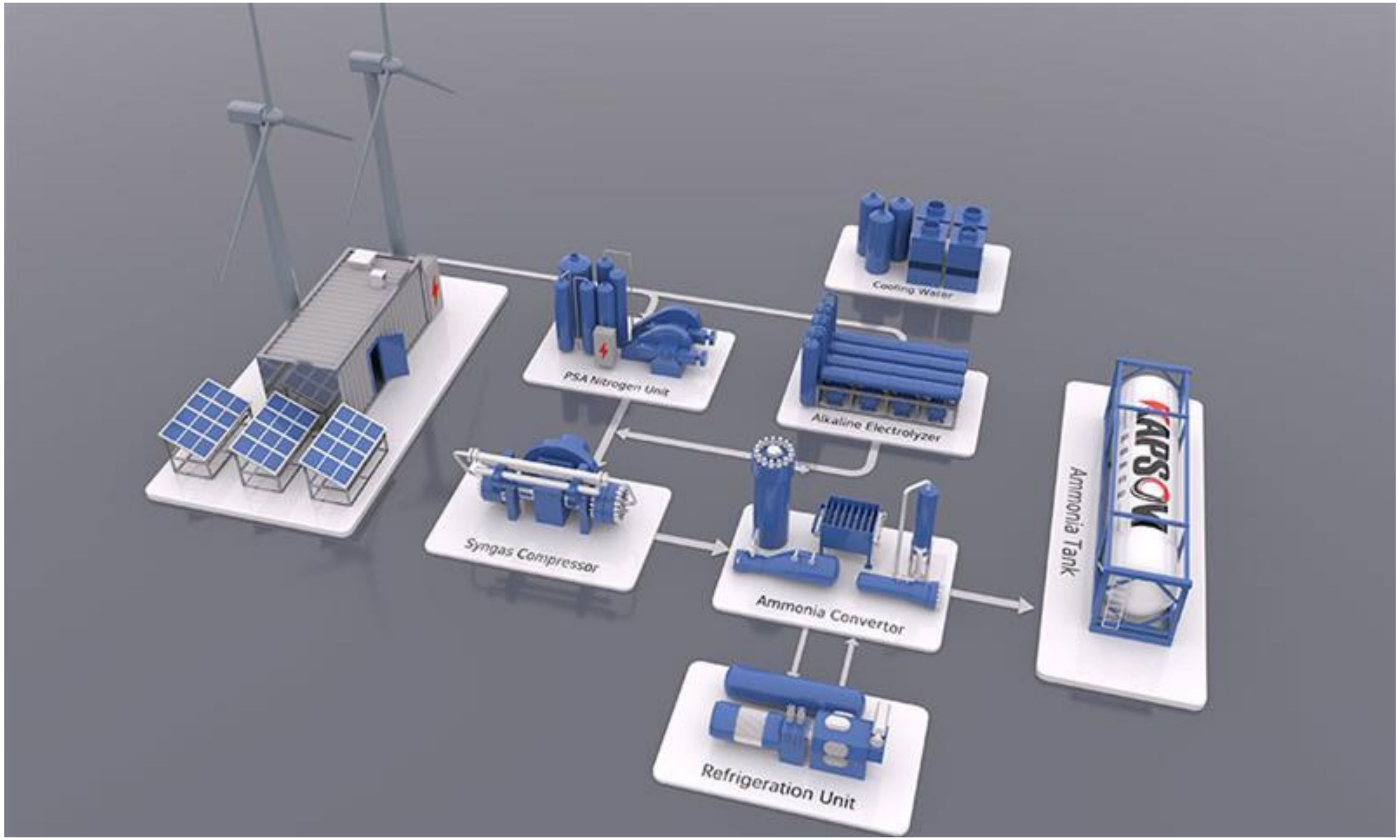
Budget	Partners	Start	Duration
33.3 M DKK	19	August 2022	3 Years

Partners

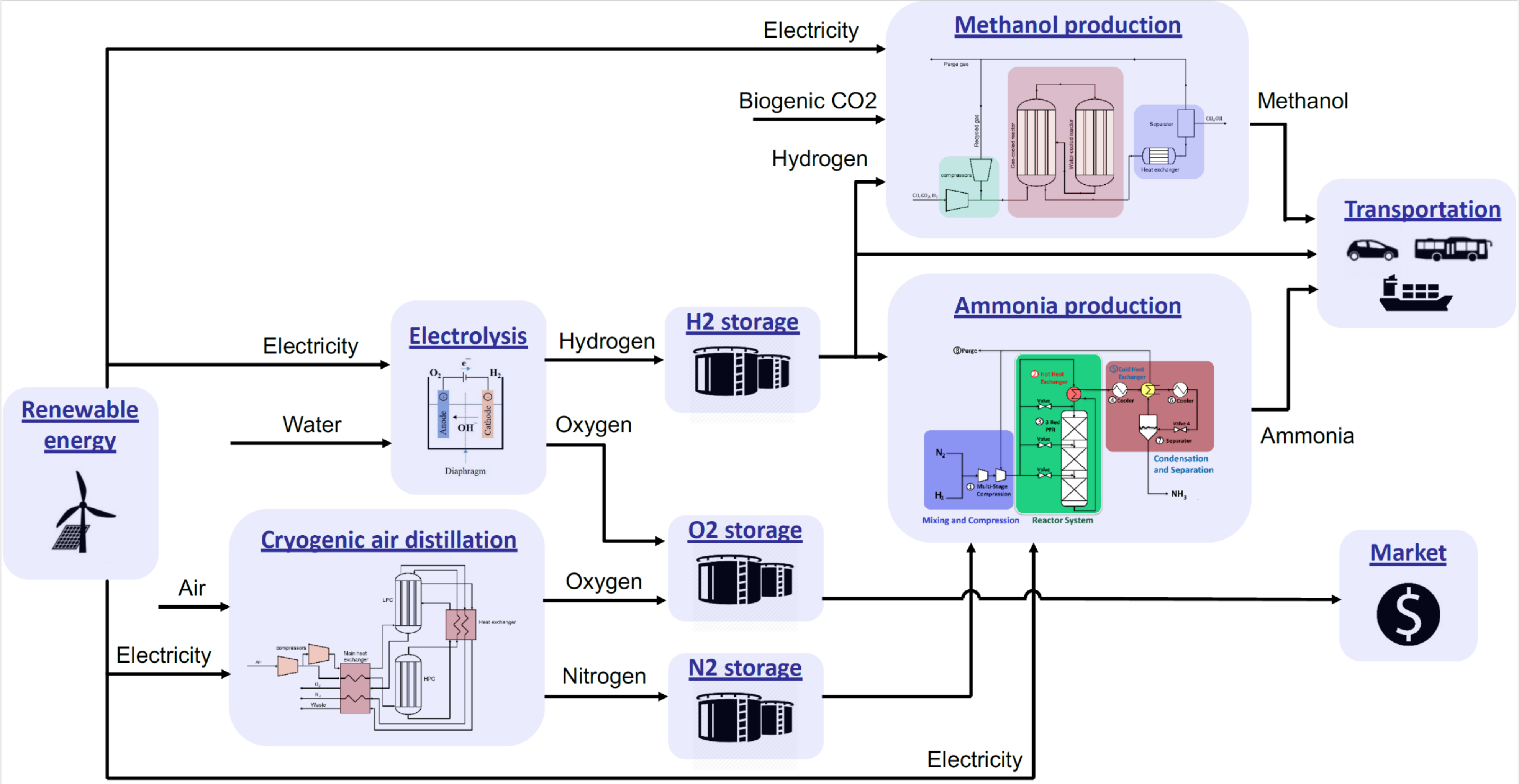
Danish Technological Institute (Coordinator), DynElectro, Aalborg University Denmark, DTU Technical University of Denmark, SDU University of Southern Denmark, Energinet, Alexandra Institutet, Aabenraa Havn, CIP Copenhagen Infrastructure Partners, EWII, European Energy, Green Hydrogen Systems, Skovgaard Invest, EMD International, Hydrogen Valley, Enfor, Energicenter Nord, 2-control

- Mathematical modeling, simulation, control and optimization for Power-to-X production
- Forecasting and optimization-based control
- Production of green fuels (H2, NH3, MeOH) from renewable energy source (solar and wind)
- DYNFLEX is the largest project in InnoMission II and conceived by DTU Compute
- Demonstration of controllers on real plants: Power-to-Ammonia and Power-to-Methanol

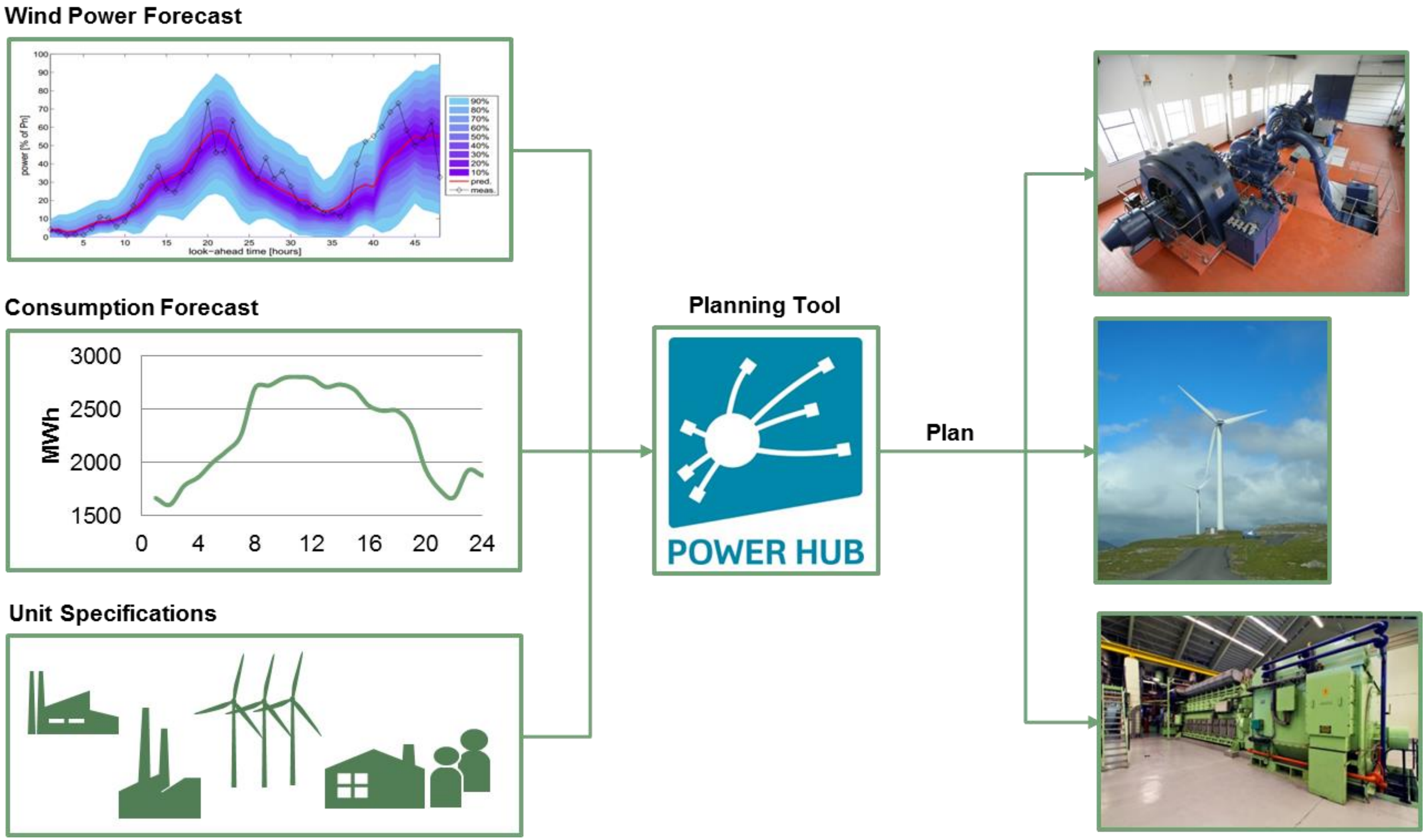
Power-2-Ammonia



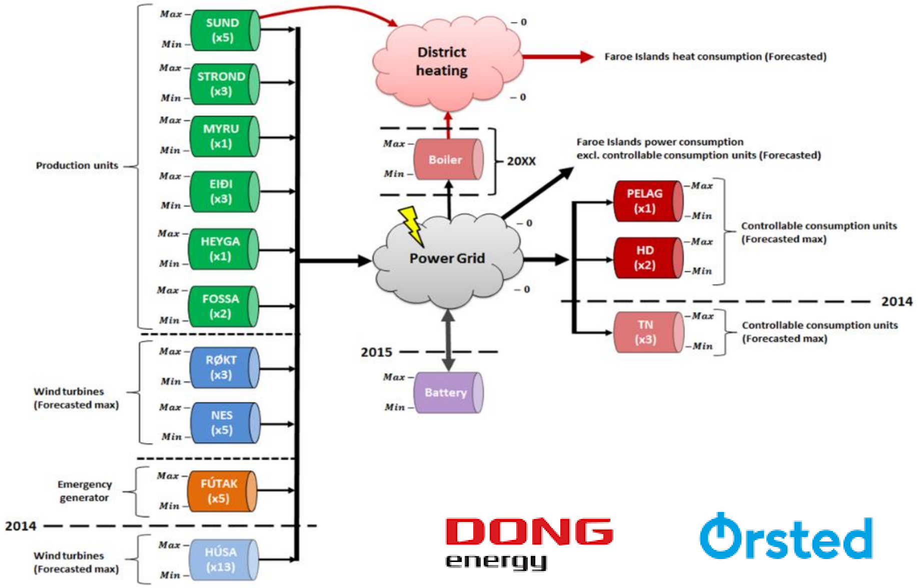
Power-2-X for Green Fuels (H2, NH3, CH3OH)

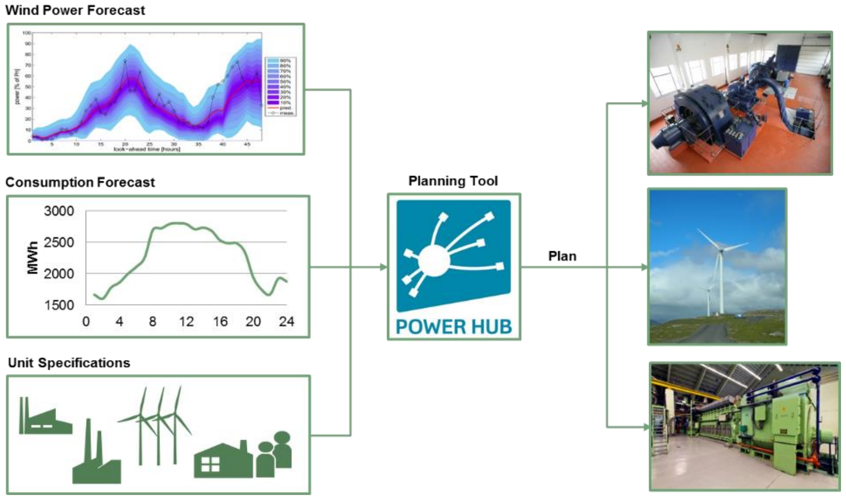


Control of Energy-Smart Systems
= Economic Model Predictive Control

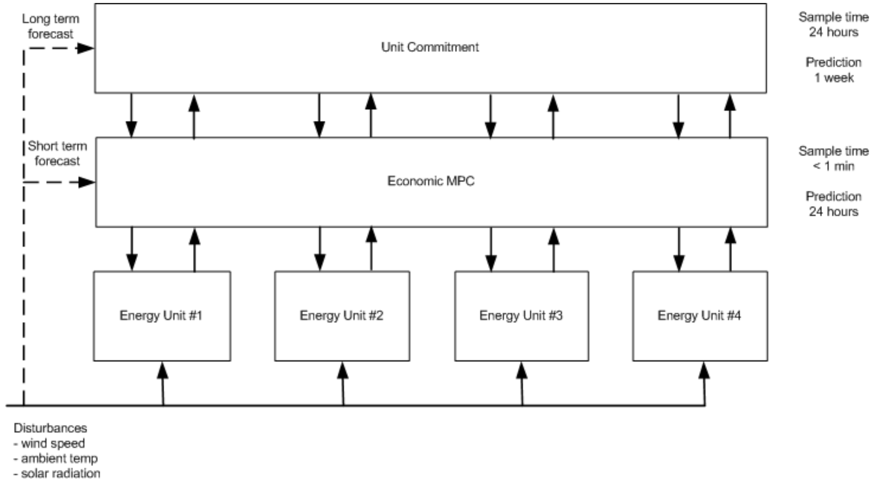


The Faroe Island Power System





- Controlled the entire Faroe power system for 3 months
- Economic MPC system developed by
  - Orsted (Dong Energy)
  - DTU Compute



NMPC based on SDEs

Introduction to NMPC based on SDEs
– Model Predictive Control for Closed-Loop Performance

- Advanced Process Control / Model Predictive Control
  - Estimation
  - Experimental design (input design)
  - System identification
  - Control and optimization

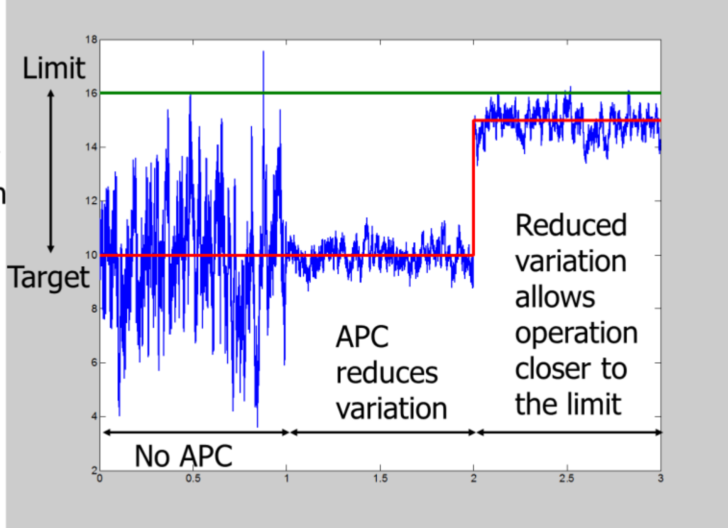
- Model predictive control technology
  = Mathematical / statistical models for
  - **Monitoring** of key process variables (fault detection)
  - **Forecasting** of key process variables.
  - **Control** of key process variables by adjustment of process inputs
  - **Computer science** for
    - real-time systems
    - Monte-Carlo simulation

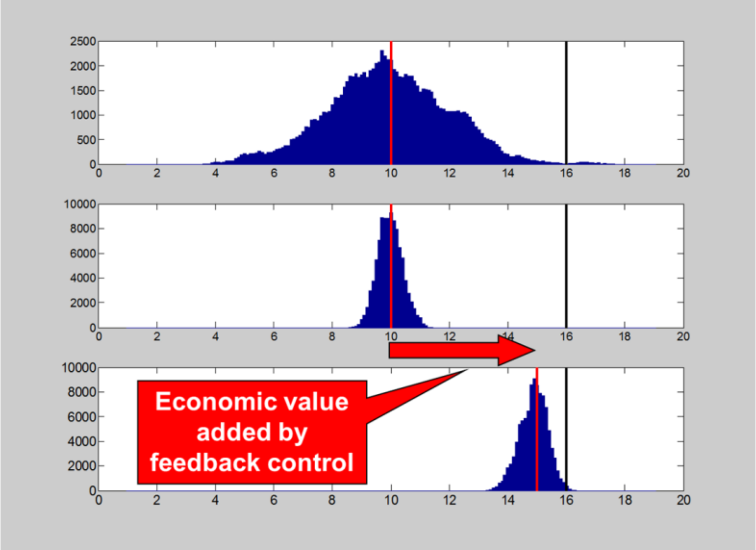
- **Continuous-discrete model – stochastic differential equations**

$$\boldsymbol{x}(t_0) = \hat{\boldsymbol{x}}_0 \qquad \hat{\boldsymbol{x}}_0 \sim N(\hat{x}_0, \hat{P}_0)$$

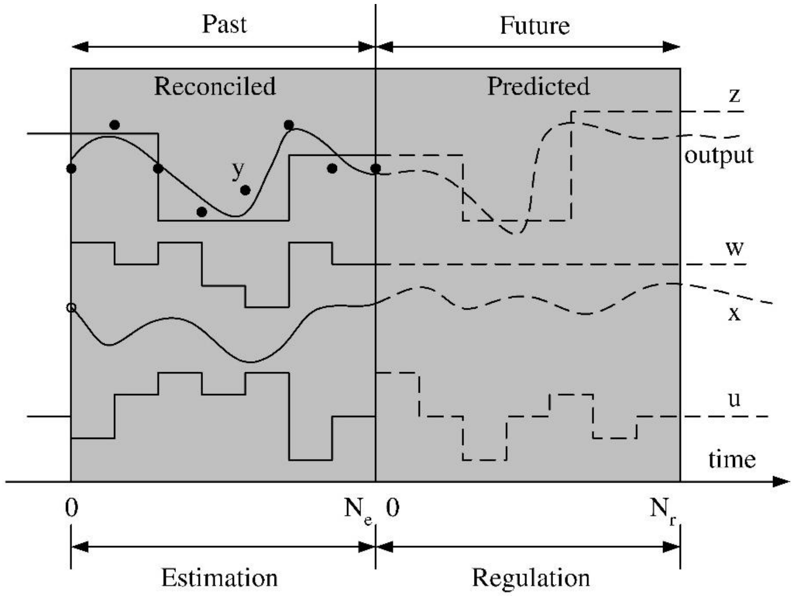
$$d\boldsymbol{x}(t) = \overbrace{f(\boldsymbol{x}(t), u(t), d(t), \theta)dt}^{=\text{drift}} + \overbrace{\sigma(\boldsymbol{x}(t), u(t), d(t), \theta)d\boldsymbol{\omega}(t)}^{=\text{diffusion}} \qquad d\boldsymbol{\omega}(t) \sim N_{iid}(0, Idt)$$

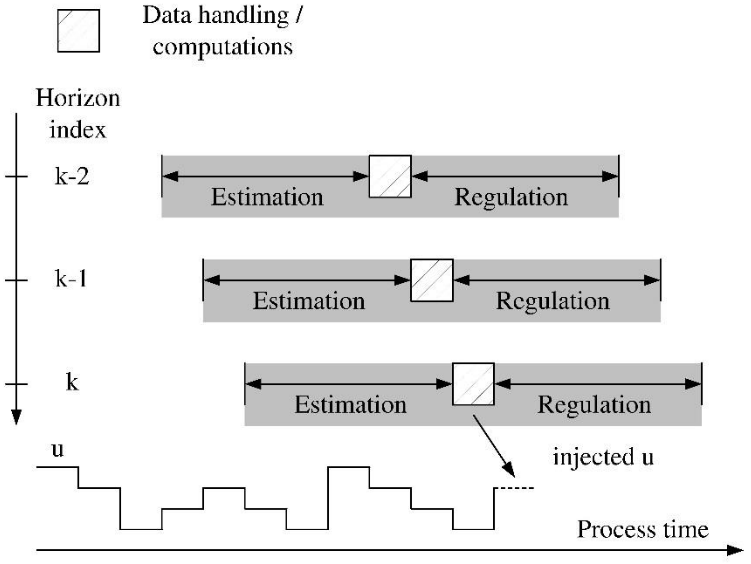
$$\boldsymbol{y}(t_k) = g(\boldsymbol{x}(t_k), \theta) + \boldsymbol{v}(t_k) \qquad \boldsymbol{v}(t_k) \sim N_{iid}(0, R(\theta))$$





Model Predictive Control Principle





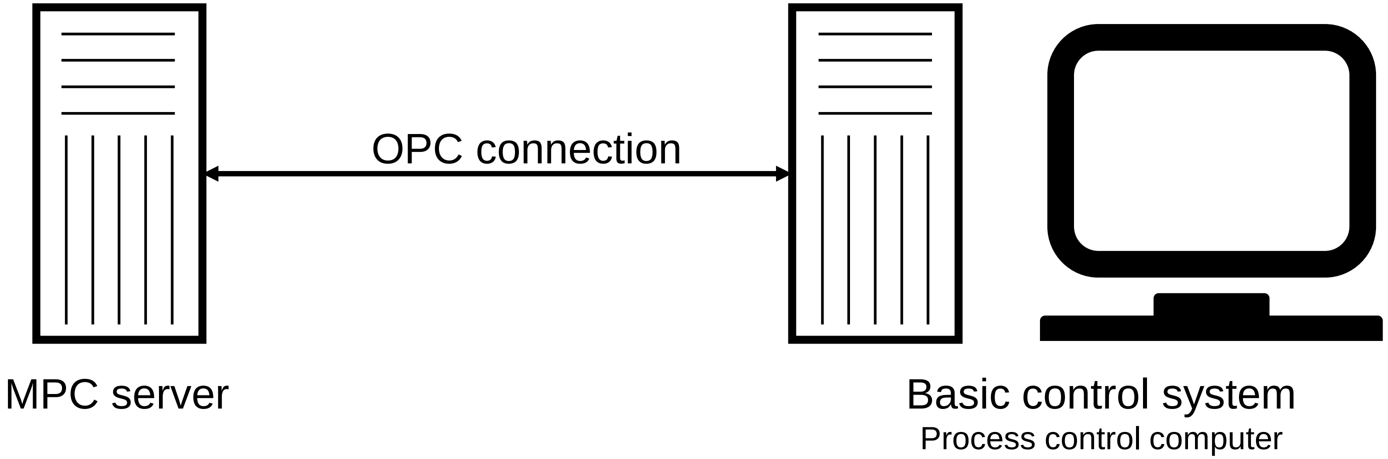
Estimation

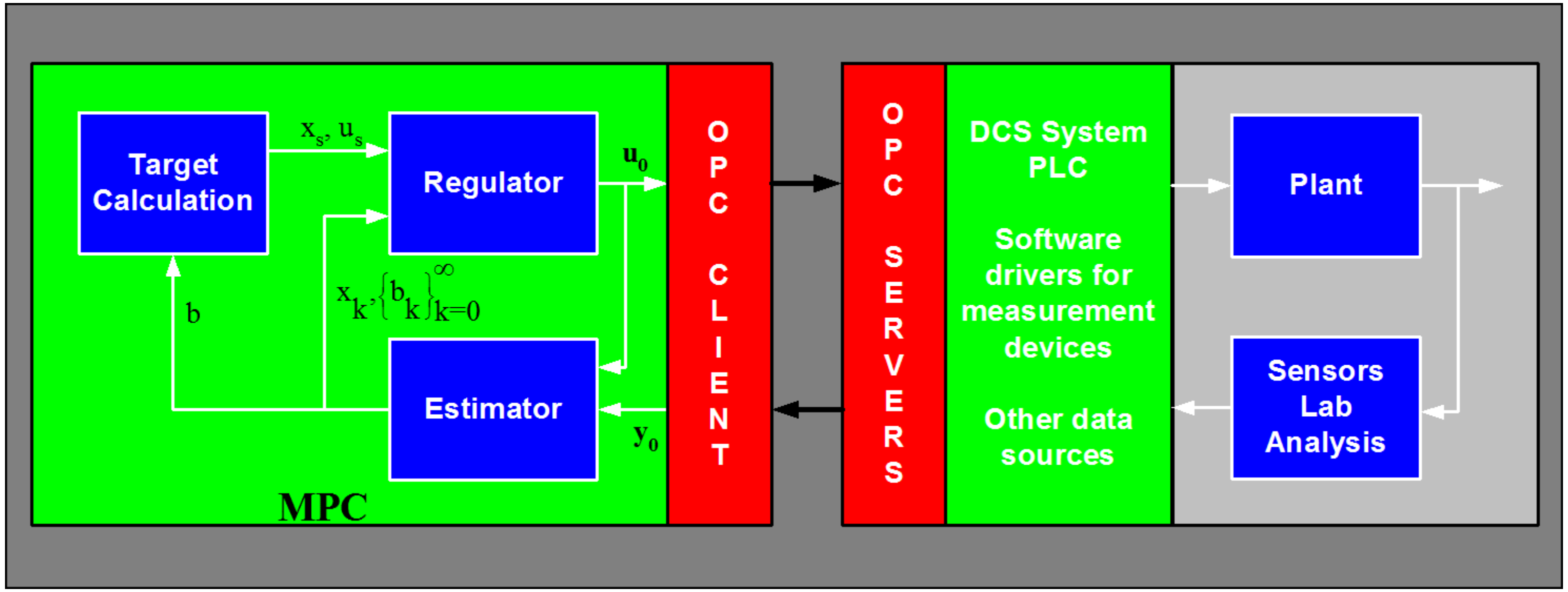
Use historical measurements and the model to compute the most likely historical process trajectory and process disturbances.

Regulation (control)

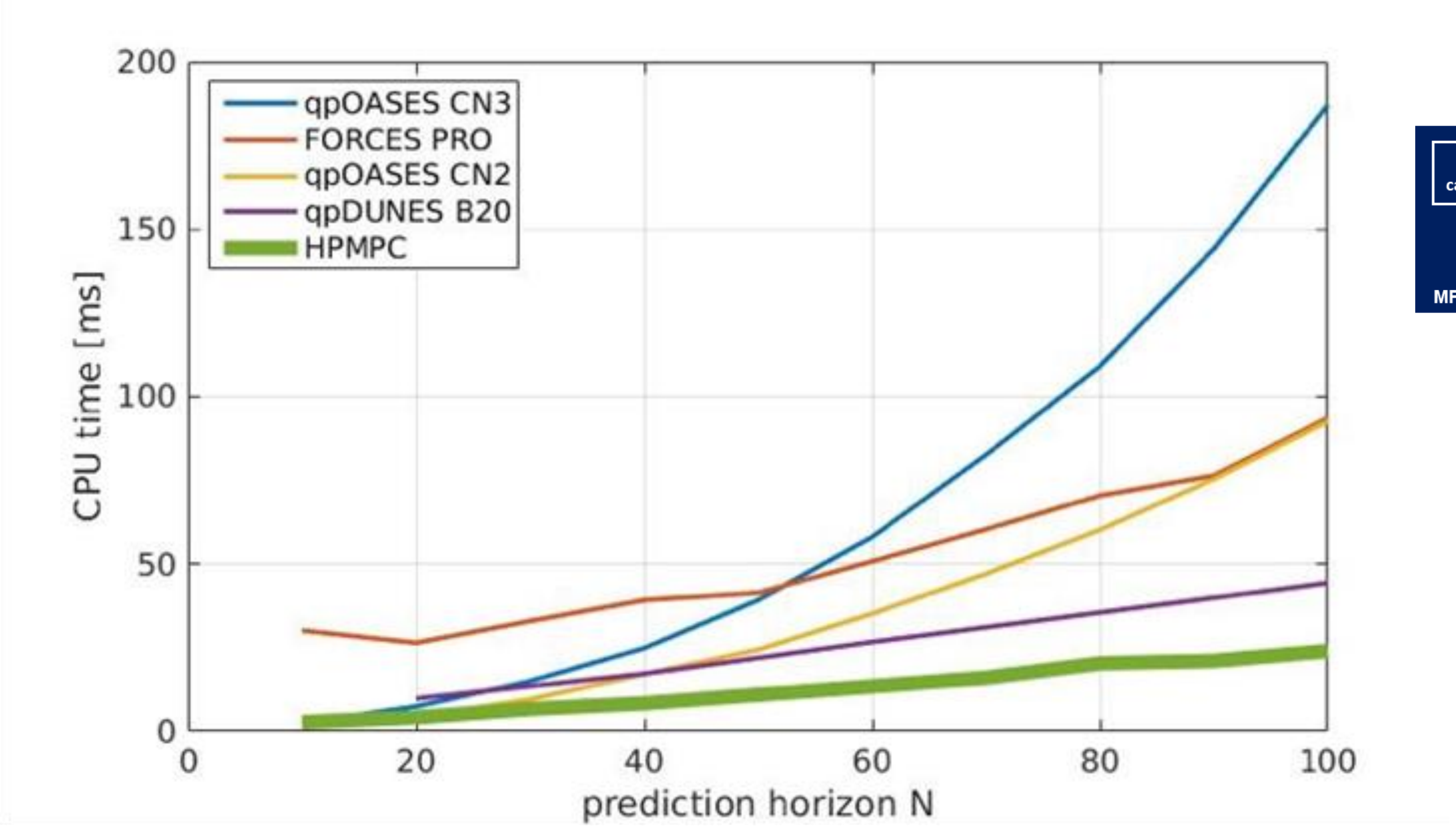
Select the future actuators of the process such that the process behaves as good as possible according to some criterion (as predicted by the model).

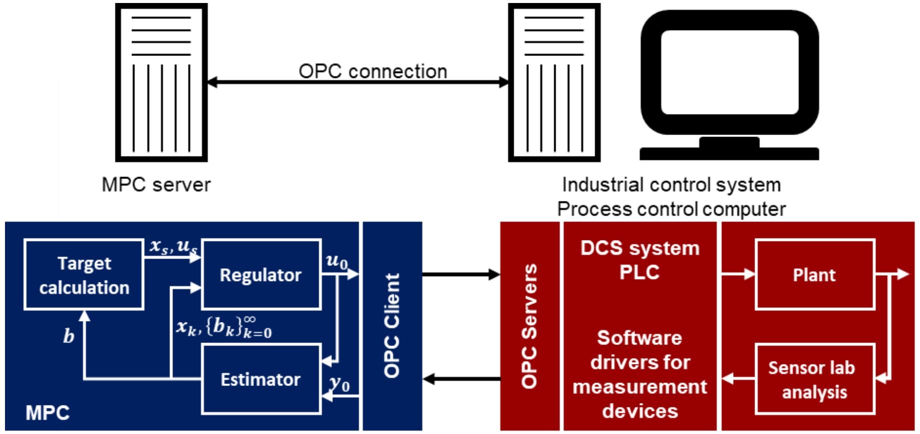
Model Predictive Controller

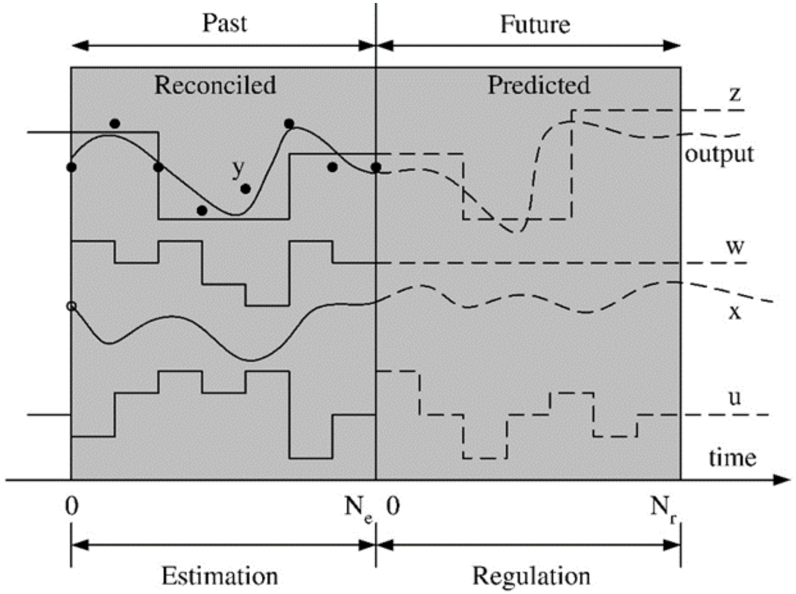




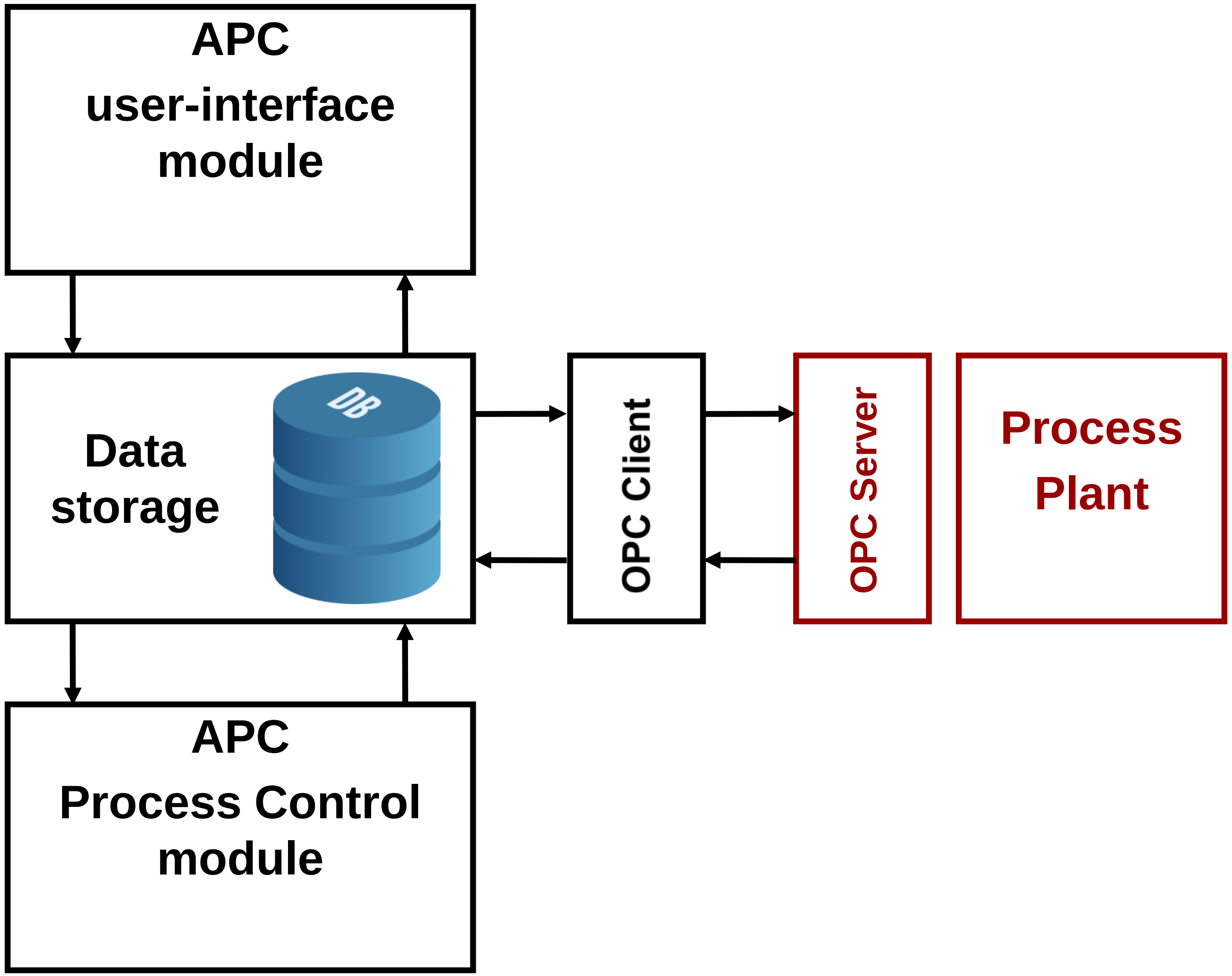
Fast Algorithms for Model Predictive Control
- enable new applications



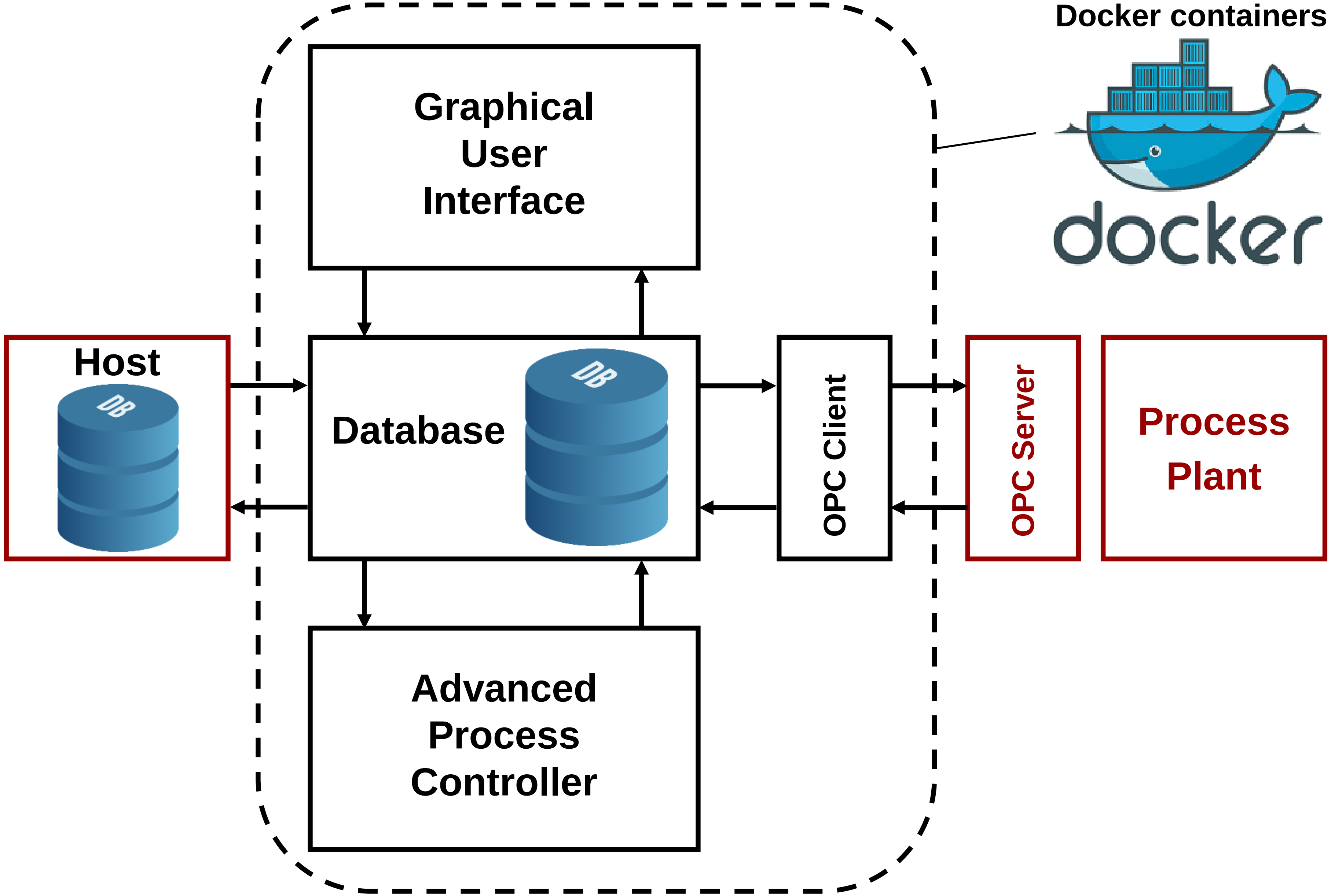




APC framework setup



APC framework setup

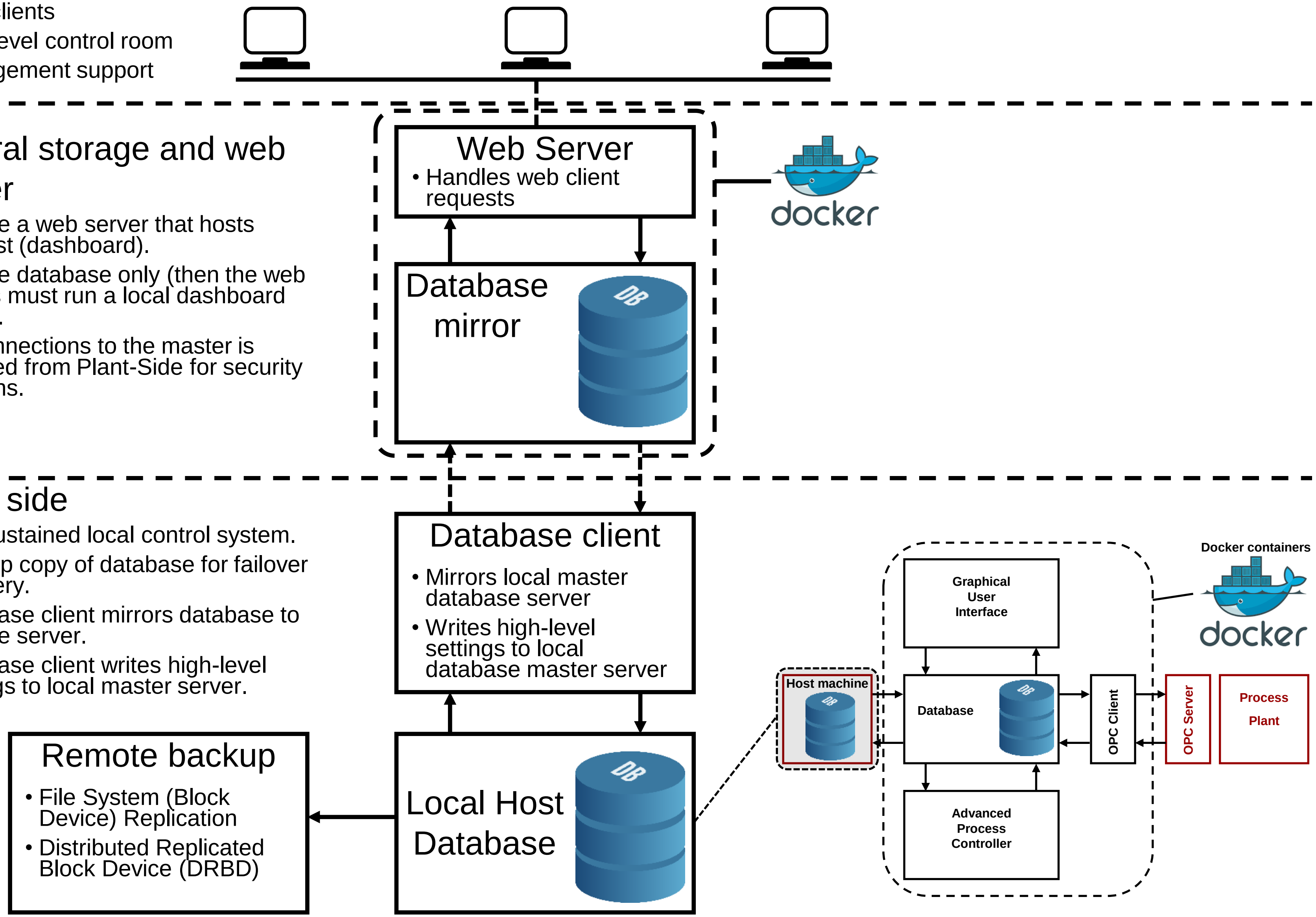


APC framework setup

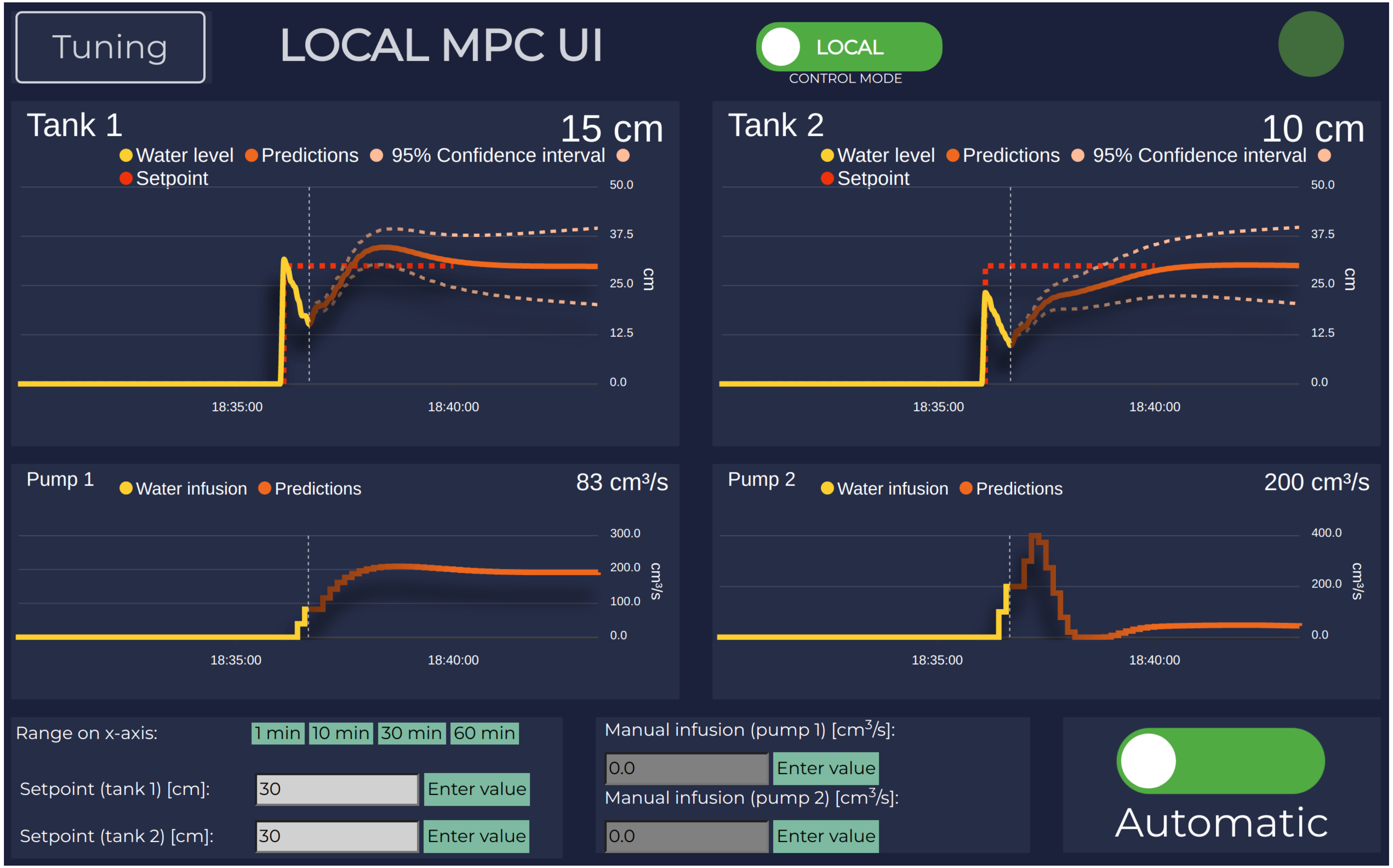
Remote monitoring
- Web clients
- High-level control room
- Management support

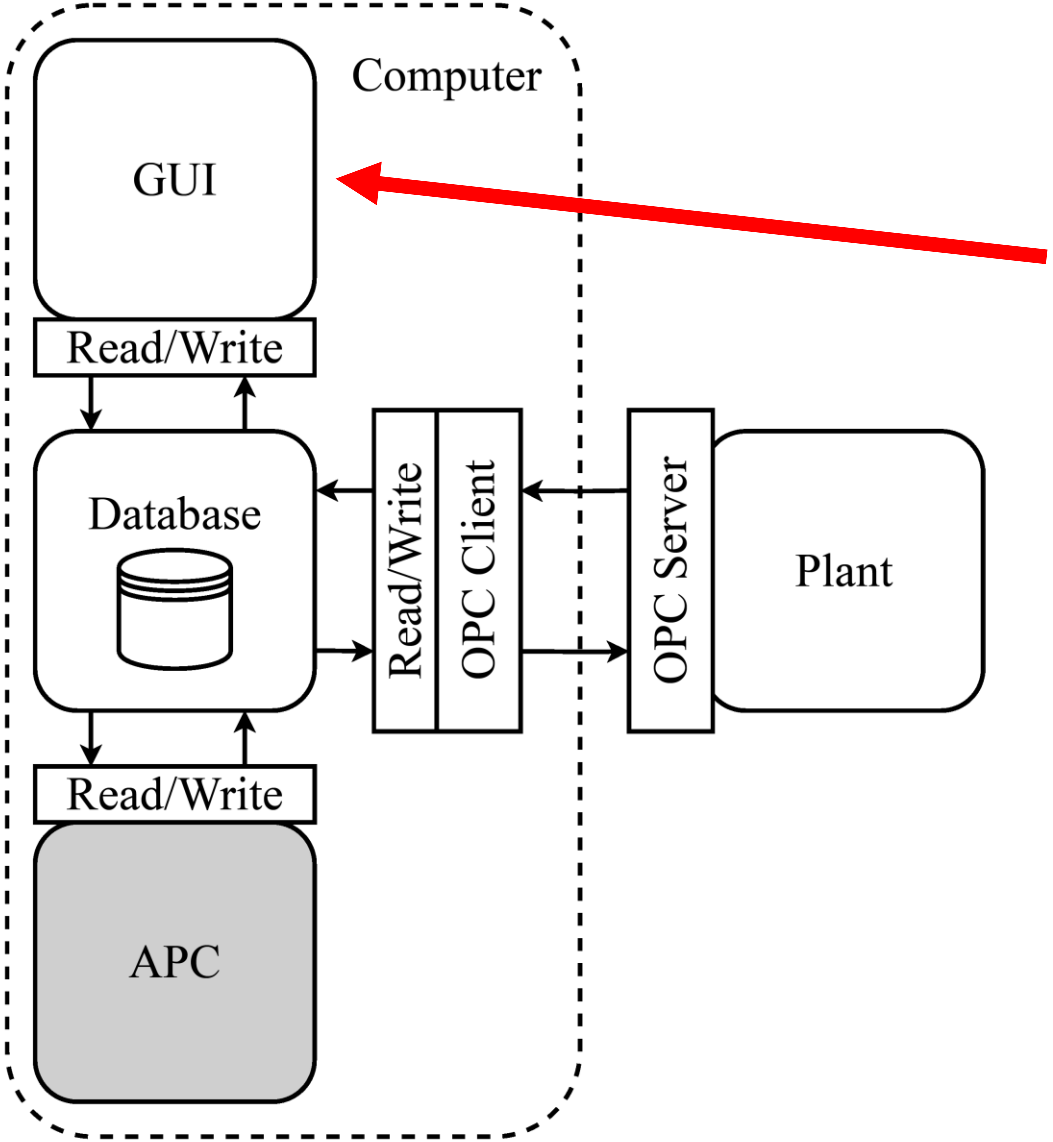
Central storage and web server
- Can be a web server that hosts request (dashboard).
- Can be database only (then the web clients must run a local dashboard client).
- All connections to the master is handled from Plant-Side for security reasons.

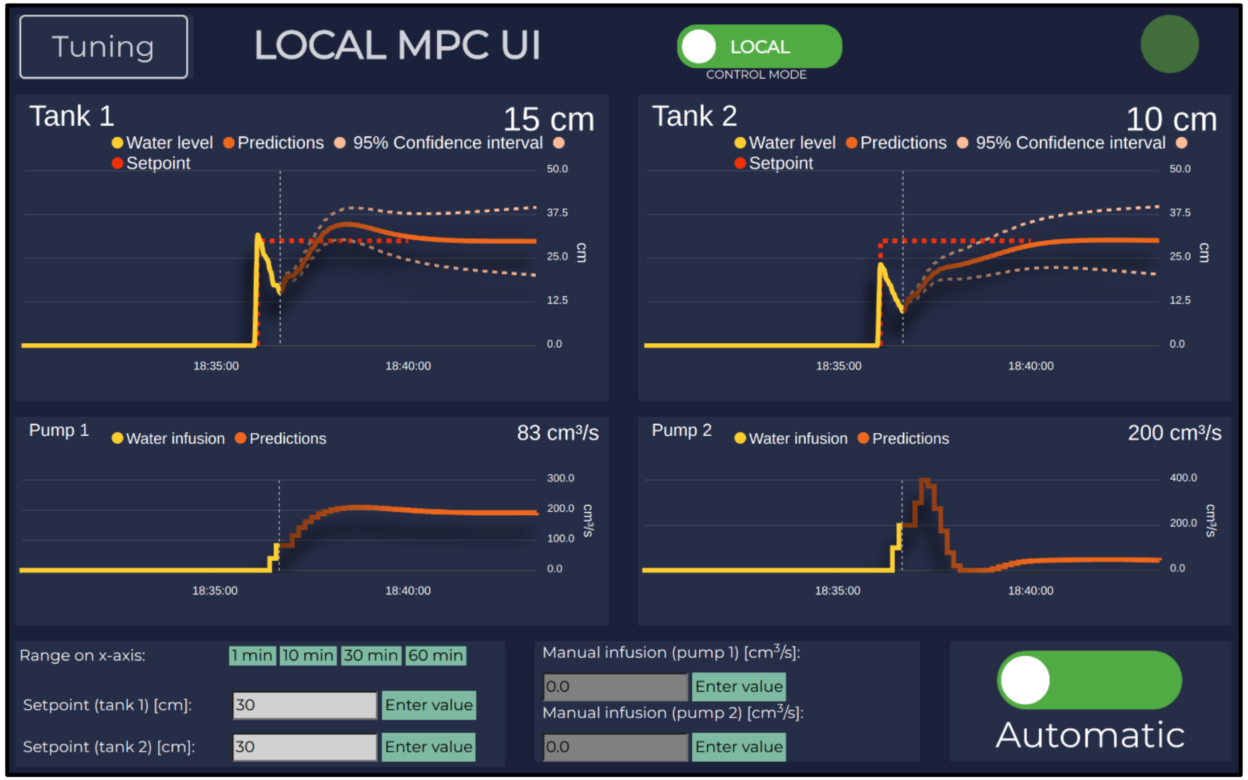
Plant side
- Self sustained local control system.
- Backup copy of database for failover recovery.
- Database client mirrors database to outside server.
- Database client writes high-level settings to local master server.



Four Tank System APC – GUI



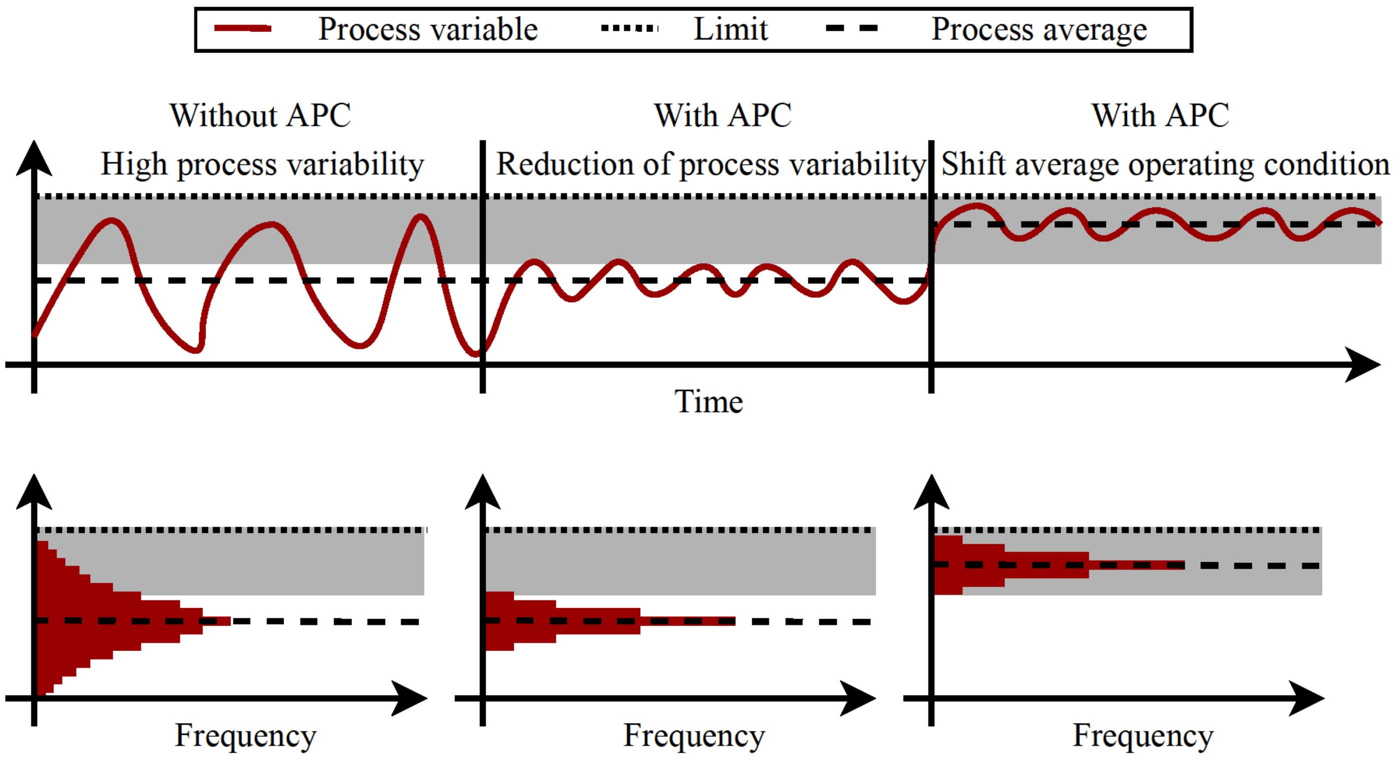

Computer
GUI
Read/Write
Database
Read/Write
APC
Read/Write
OPC Client
OPC Server
Plant

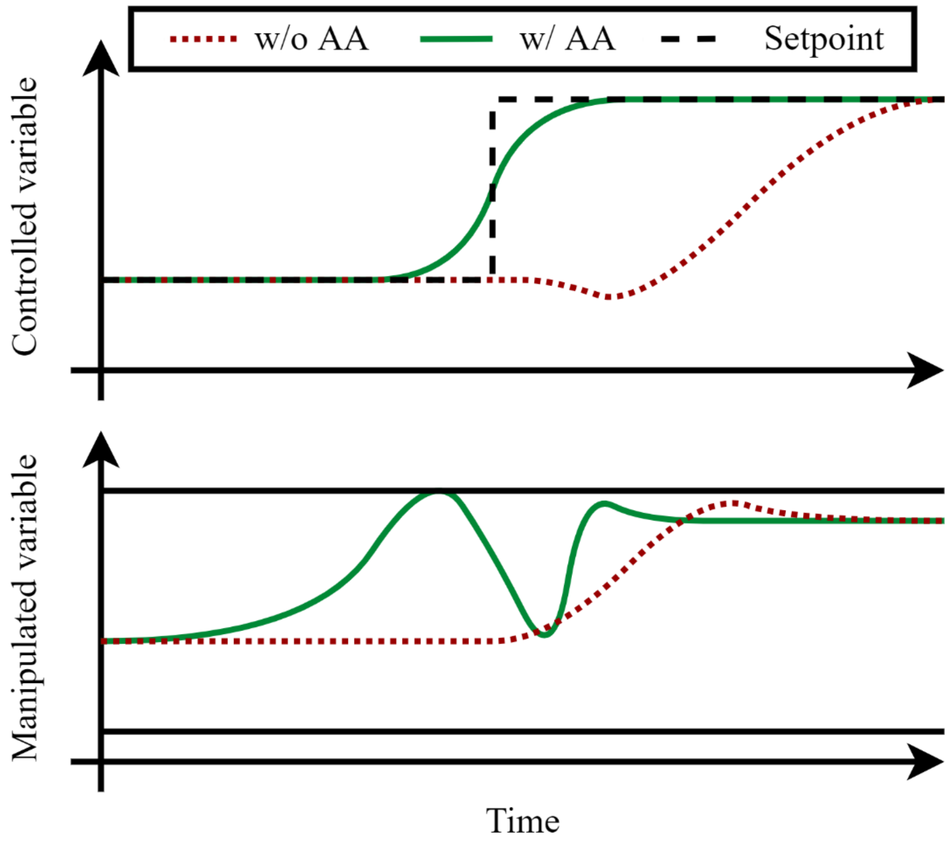

Tuning
LOCAL MPC UI
LOCAL
CONTROL MODE
Tank 1
15 cm
Water level
Predictions
95% Confidence interval
Setpoint
Tank 2
10 cm
Pump 1
83 cm³/s
Water infusion
Pump 2
200 cm³/s
Range on x-axis:
1 min
10 min
30 min
60 min
Setpoint (tank 1) [cm]:
Setpoint (tank 2) [cm]:
Enter value
Manual infusion (pump 1) [cm³/s]:
Manual infusion (pump 2) [cm³/s]:
Automatic

Advanced process control

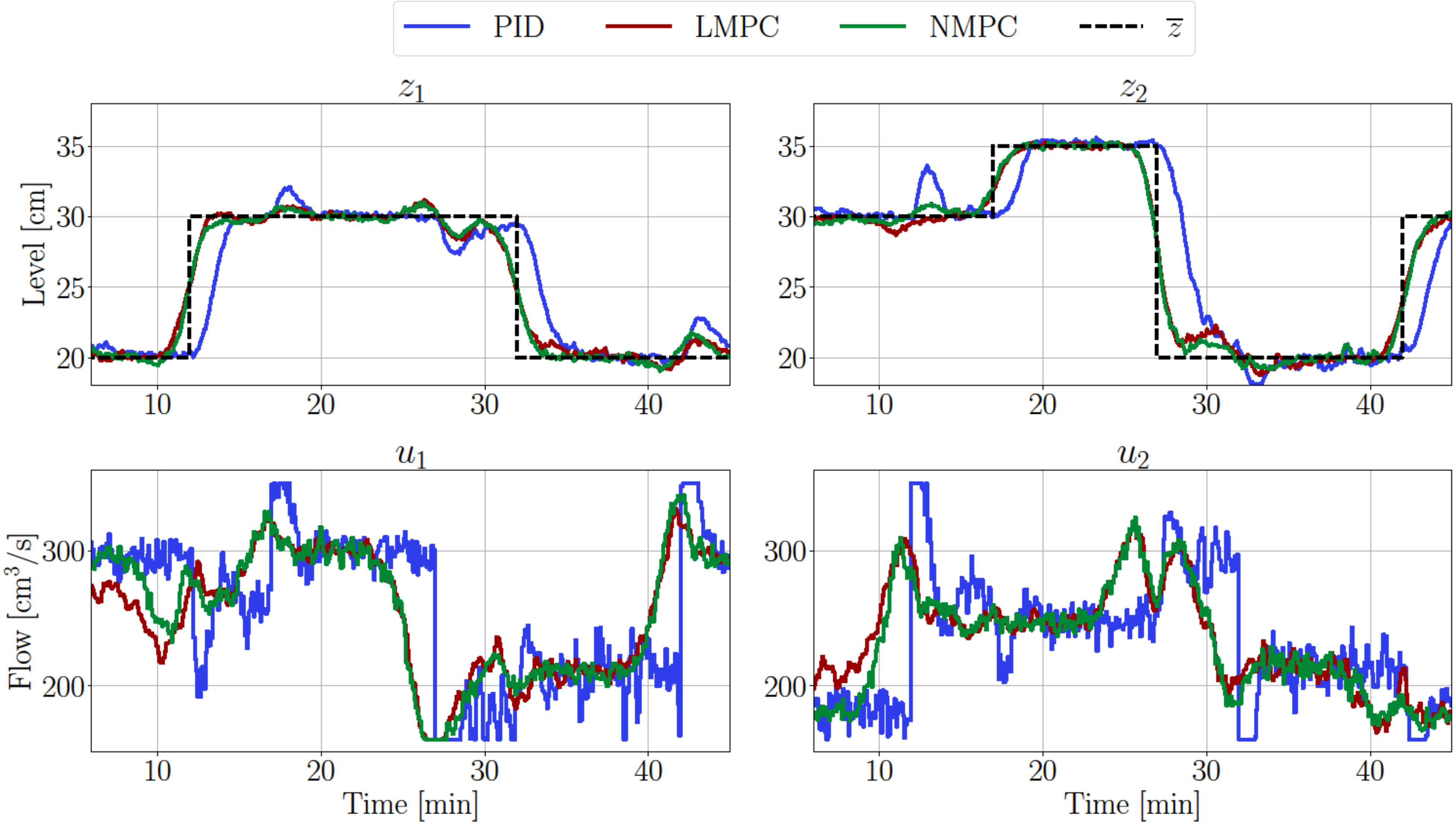
Why use advanced process control (APC)?

- Squeeze and shift
- Anticipatory action (AA)

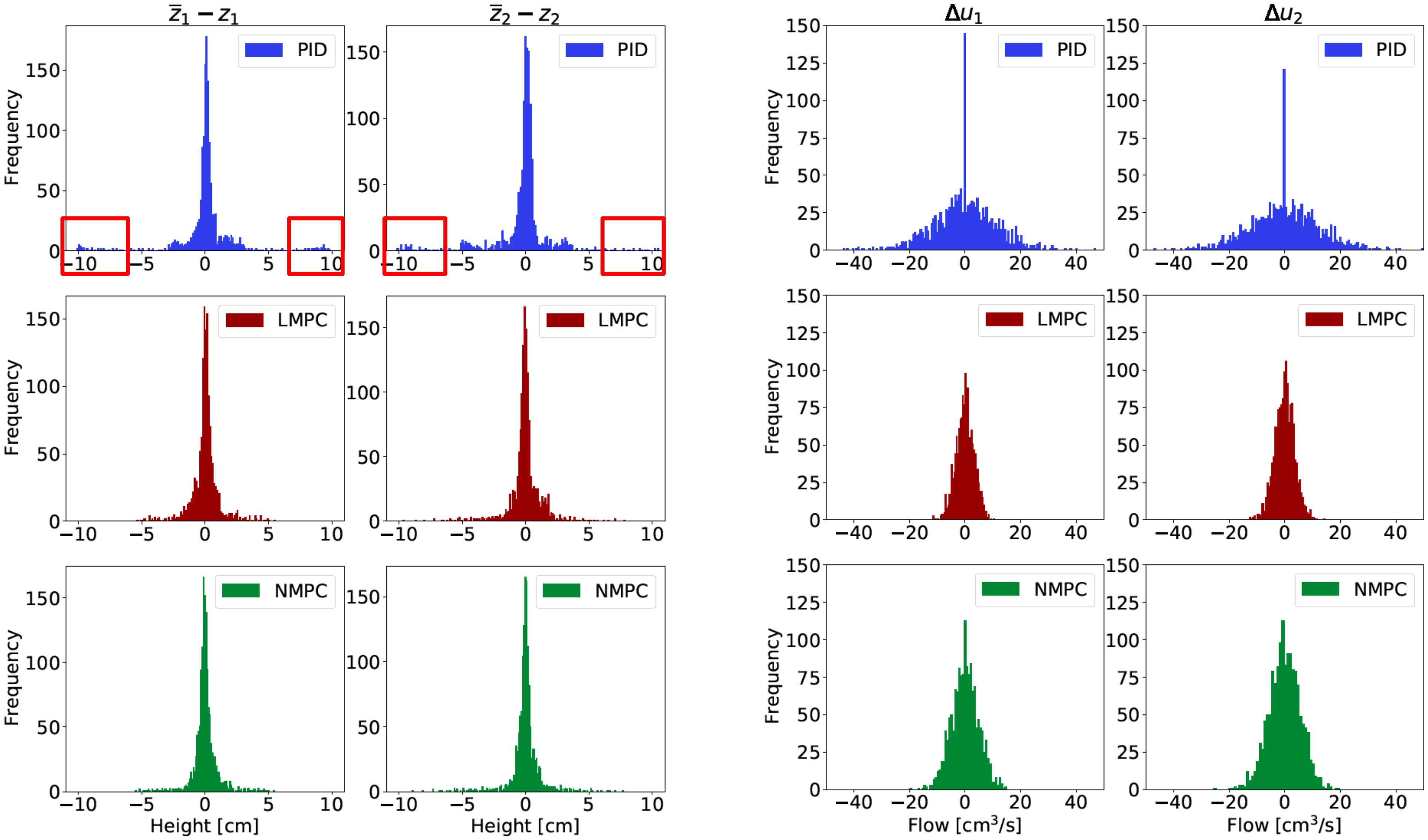




Experimental data

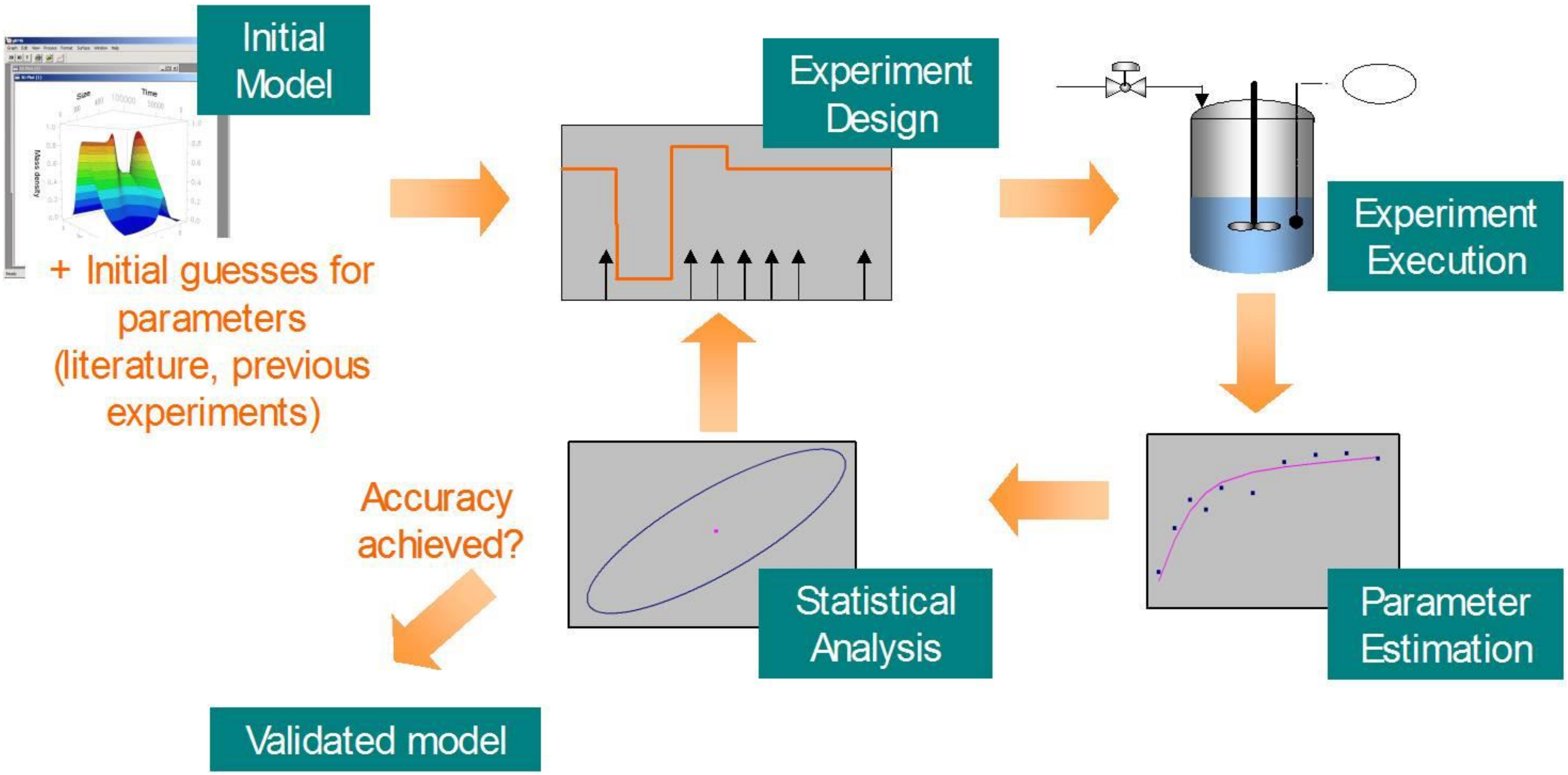


Analyzing the data

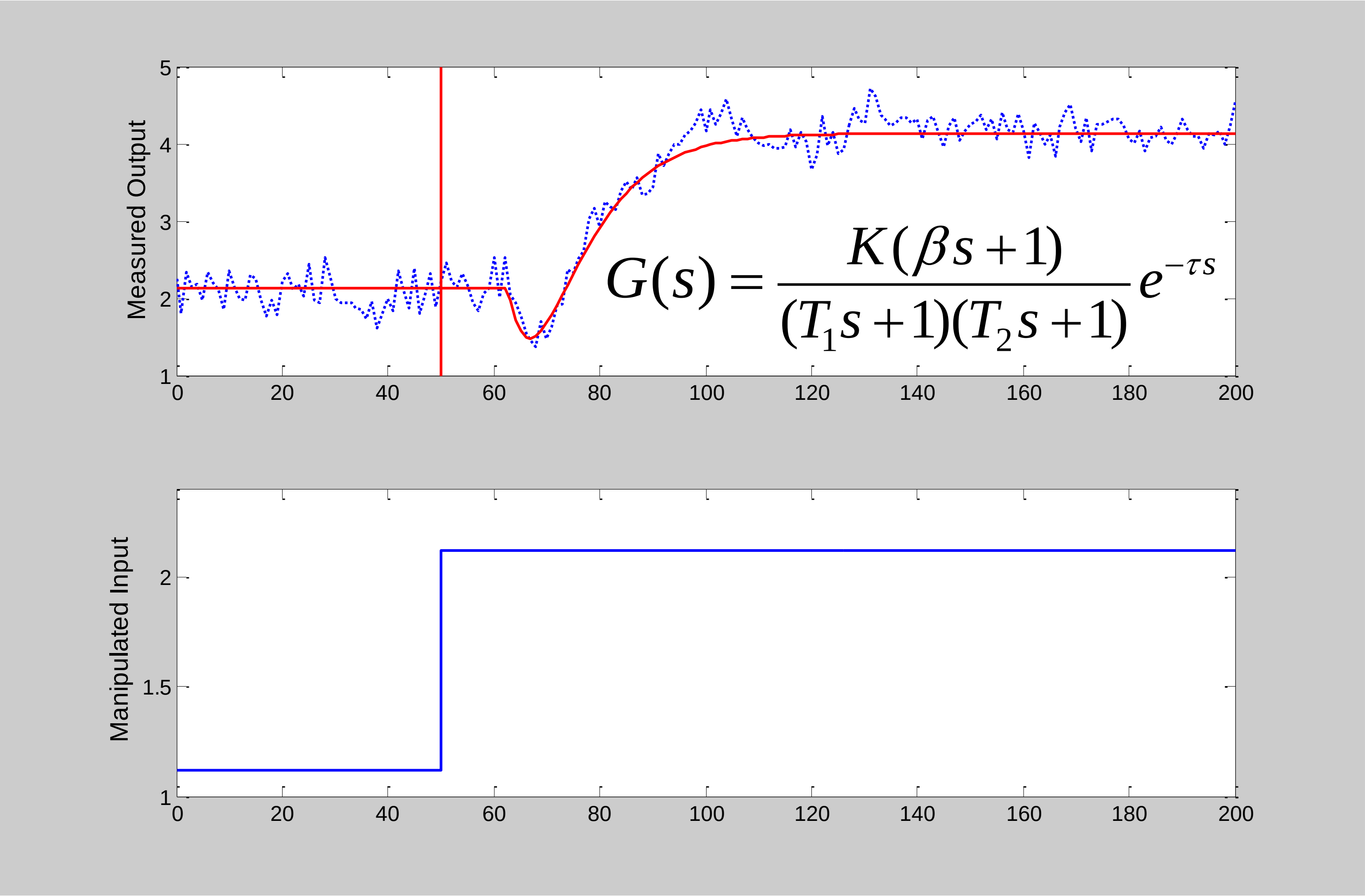


Online Optimization and Control Room
– Center Denmark for Smart Energy System Optimization and Control

Systematic Model Building

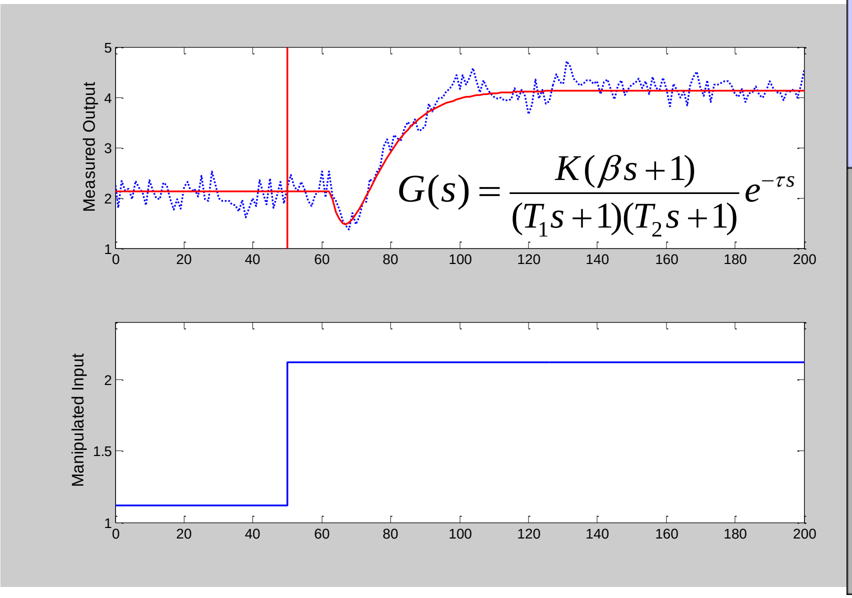


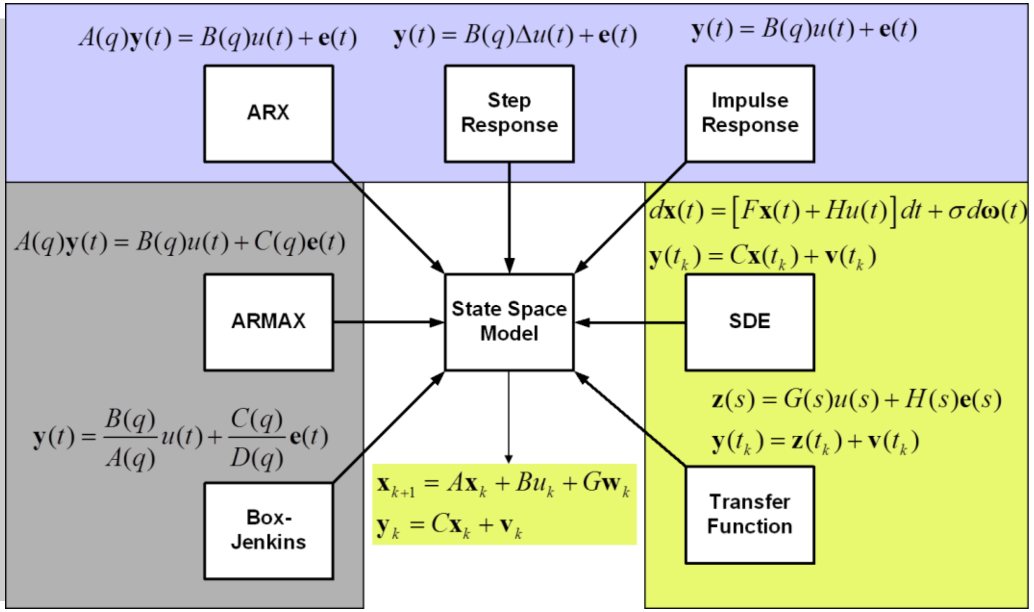
LMPC - Step Response Experiments and Transfer Functions



$$G(s) = \frac{K(\beta s + 1)}{(T_1 s + 1)(T_2 s + 1)} e^{-\tau s}$$

LMPC - Data based prediction models

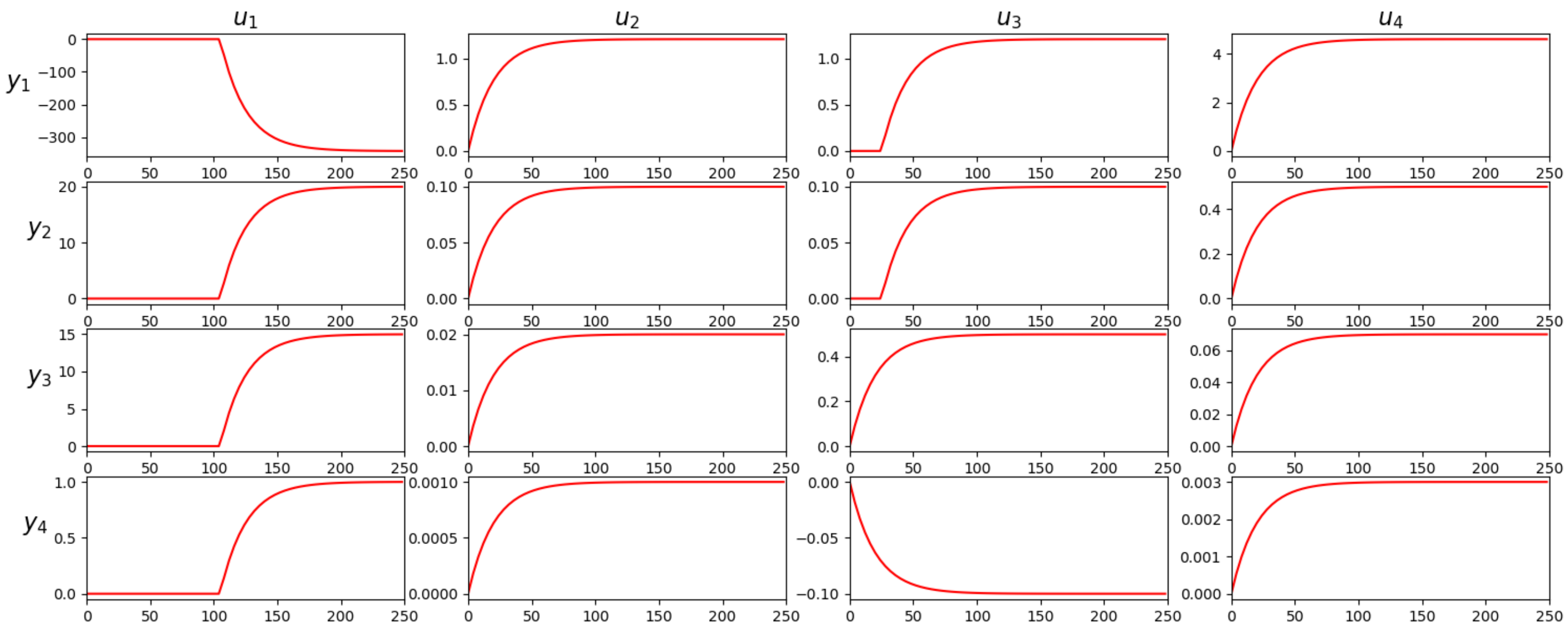




The models for filtering and prediction are

- Adaptive
- Data-based
- Combines a-priori (model) and a-posterior (data) information
- Able to predict the mean values and the uncertainties

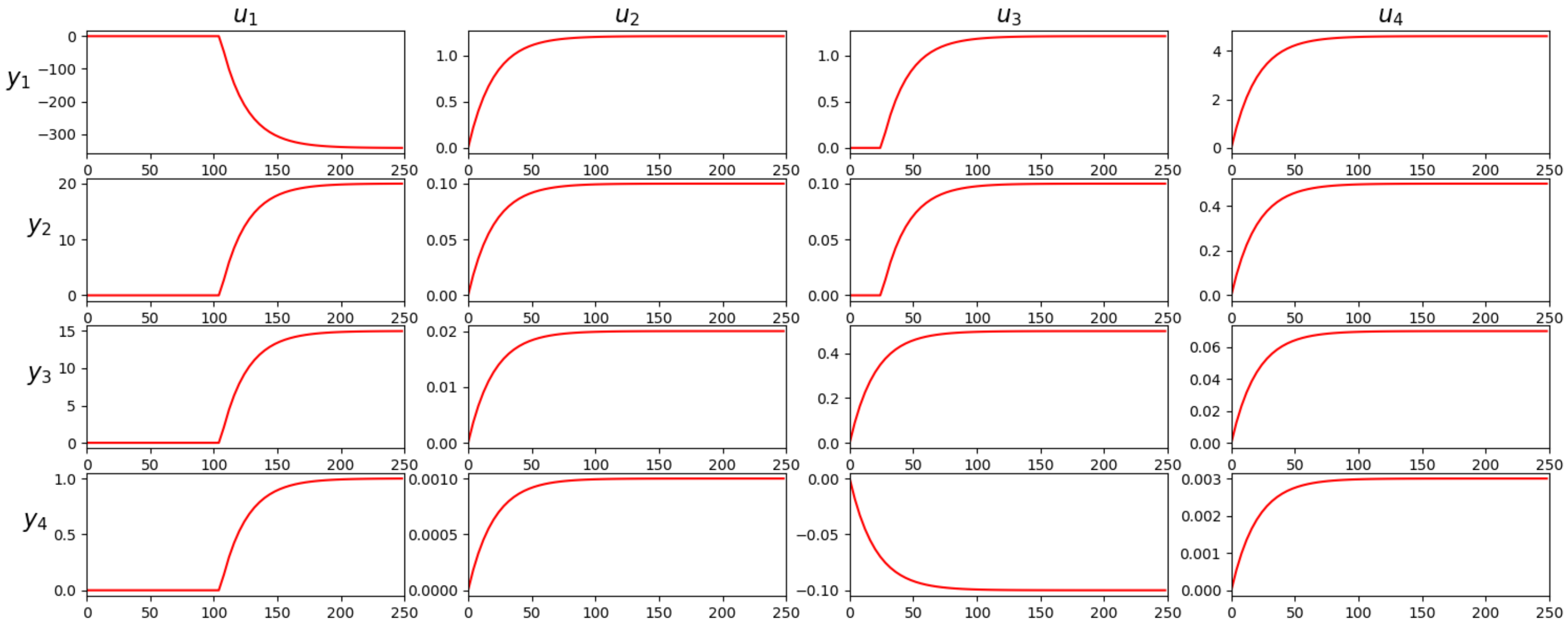
Multivariate step responses



Multivariate step responses

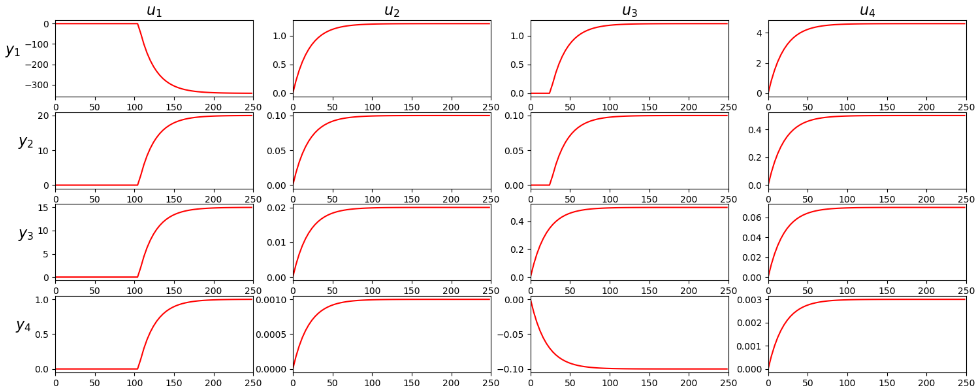
$$G(s) = \begin{bmatrix} \frac{-342.0e^{-105.0s}}{20.0s+1} & \frac{1.21}{20.0s+1} & \frac{1.21e^{-25.0s}}{20.0s+1} & \frac{4.6}{20.0s+1} \\ \frac{20.0e^{-105.0s}}{20.0s+1} & \frac{0.1}{20.0s+1} & \frac{0.1e^{-25.0s}}{20.0s+1} & \frac{0.5}{20.0s+1} \\ \frac{15.0e^{-105.0s}}{20.0s+1} & \frac{0.02}{20.0s+1} & \frac{0.5}{20.0s+1} & \frac{0.07}{20.0s+1} \\ \frac{1.0e^{-105.0s}}{20.0s+1} & \frac{0.001}{20.0s+1} & \frac{-0.1}{20.0s+1} & \frac{0.003}{20.0s+1} \end{bmatrix}$$

$$G_{i,j}(s) = \frac{K(\beta s + 1)e^{-\tau_d s}}{(\tau_1 s + 1)(\tau_2 s + 1)}$$



Multivariate step responses

$$G(s) = \begin{bmatrix} \frac{-342.0e^{-105.0s}}{20.0s+1} & \frac{1.21}{20.0s+1} & \frac{1.21e^{-25.0s}}{20.0s+1} & \frac{4.6}{20.0s+1} \\ \frac{20.0e^{-105.0s}}{20.0s+1} & \frac{0.1}{20.0s+1} & \frac{0.1e^{-25.0s}}{20.0s+1} & \frac{0.5}{20.0s+1} \\ \frac{15.0e^{-105.0s}}{20.0s+1} & \frac{0.02}{20.0s+1} & \frac{0.5}{20.0s+1} & \frac{0.07}{20.0s+1} \\ \frac{1.0e^{-105.0s}}{20.0s+1} & \frac{0.001}{20.0s+1} & \frac{-0.1}{20.0s+1} & \frac{0.003}{20.0s+1} \end{bmatrix}$$



$$G_{i,j}(s) = \frac{K(\beta s + 1)e^{-\tau_d s}}{(\tau_1 s + 1)(\tau_2 s + 1)}$$

G(s)	K	beta	tau1	tau2	tauD
G11	-342,000	0	20,000	0	105,000
G12	1,210	0	20,000	0	0
G13	1,210	0	20,000	0	25,000
G14	4,600	0	20,000	0	0
G21	20,000	0	20,000	0	105,000
G22	0,100	0	20,000	0	0
G23	0,100	0	20,000	0	25,000
G24	0,500	0	20,000	0	0
G31	15,000	0	20,000	0	105,000
G32	0,020	0	20,000	0	0
G33	0,500	0	20,000	0	0
G34	0,070	0	20,000	0	0
G41	1,000	0	20,000	0	105,000
G42	0,001	0	20,000	0	0
G43	-0,100	0	20,000	0	0
G44	0,003	0	20,000	0	0

Process inputs and outputs

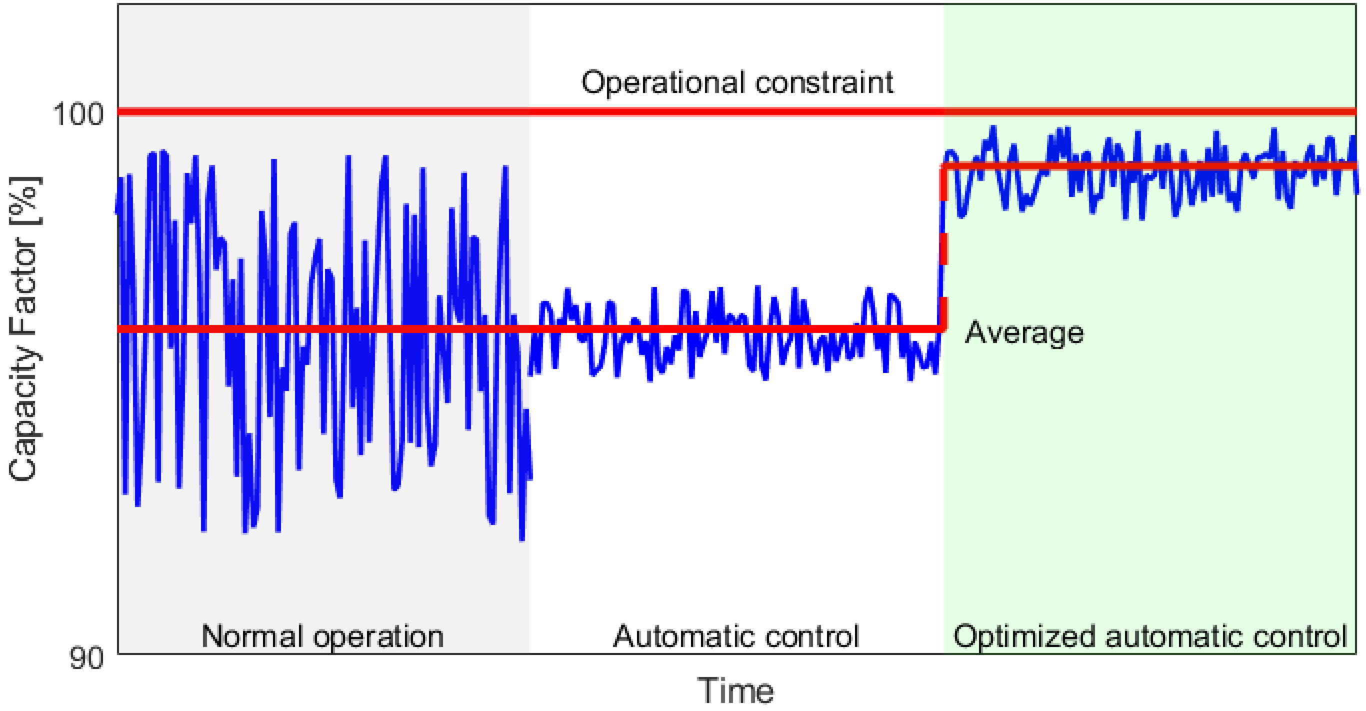
$$
\begin{aligned}
\min_{\{u_{k+n-1}, s_{k+n}, t_{k+n}\}_{n=1}^{N}} \quad & \phi = \phi_z + \phi_{\Delta u} + \phi_s + \phi_t \\
\text{s.t.} \quad & x_0 = \hat{x}_{k|k}, \\
& x_{k+n+1} = A x_{k+n} + B u_{k+n}, && n \in [0, N-1], \\
& z_{k+n} = C x_{k+n}, && n \in [0, N], \\
& u_{\min} \le u_{k+n} \le u_{\max}, && n \in [0, N-1], \\
& -\Delta u_{\max} \le \Delta u_{k+n} \le \Delta u_{\max}, && n \in [0, N-1], \\
& z_{k+n} + s_{k+n} \ge z_{\min}, && n \in [0, N], \\
& -z_{k+n} + t_{k+n} \ge -z_{\max}, && n \in [0, N], \\
& (s_{k+n}, t_{k+n}) \ge 0. && n \in [0, N],
\end{aligned}
$$

$$
G_{i,j}(s) = \frac{K(\beta s + 1)\mathrm{e}^{-\tau_d s}}{(\tau_1 s + 1)(\tau_2 s + 1)}
$$

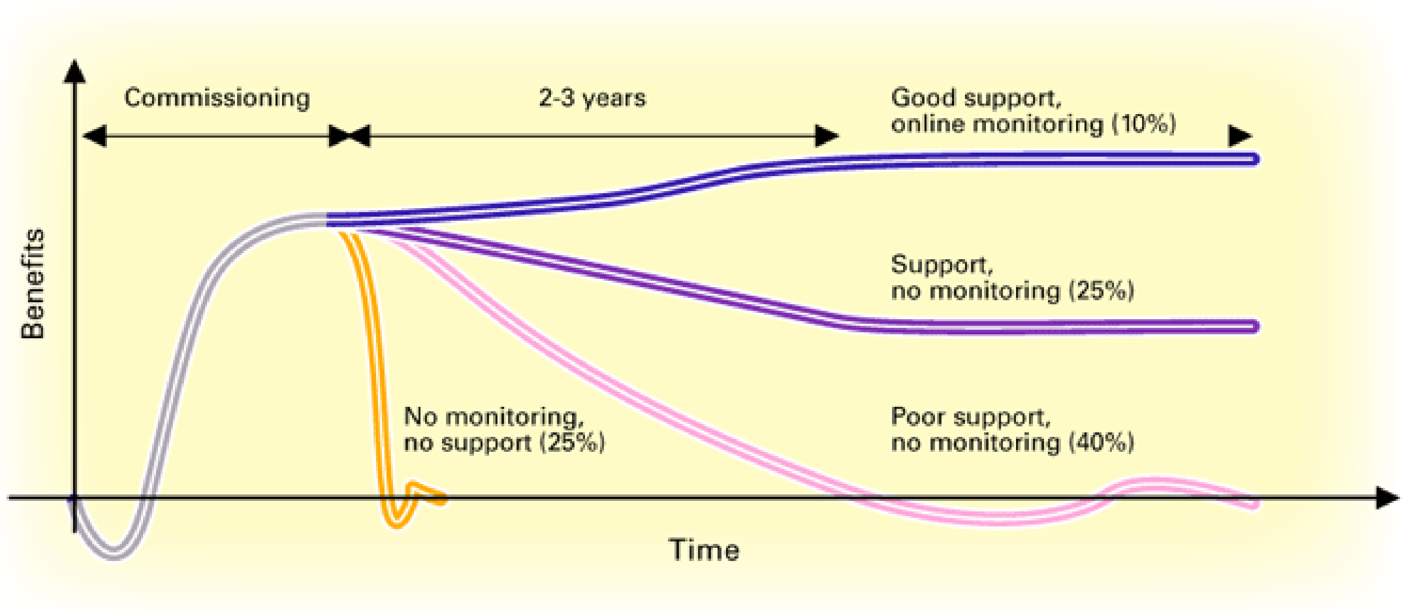
G(s)	K	beta	tau1	tau2	tauD
G11	-342,000	0	20,000	0	105,000
G12	1,210	0	20,000	0	0
G13	1,210	0	20,000	0	25,000
G14	4,600	0	20,000	0	0
G21	20,000	0	20,000	0	105,000
G22	0,100	0	20,000	0	0
G23	0,100	0	20,000	0	25,000
G24	0,500	0	20,000	0	0
G31	15,000	0	20,000	0	105,000
G32	0,020	0	20,000	0	0
G33	0,500	0	20,000	0	0
G34	0,070	0	20,000	0	0
G41	1,000	0	20,000	0	105,000
G42	0,001	0	20,000	0	0
G43	-0,100	0	20,000	0	0
G44	0,003	0	20,000	0	0

	A	B	C	D	E	F	G	H	I	J	K	L
4	--											
5	Controller info	N	T_s	nu	ny	nz	Memory					
6	value	30	30	4	4	4	20					
7	--											
8	Process inputs	Name	Unit	u_s	u_min	u_max	du_max	Q_du				
9	F_g,s	Gas flow rate	m3/h	2200.00	0.00	3000.00	150.00	1.00				
10	F_o,s	Oil flow rate	m3/h	1800.00	0.00	2500.00	90.00	1.00				
11	F_w,s	Water flow rate	m3/h	280.00	0.00	500.00	30.00	1.00				
12	F_m,rec	Recycled fluid flow rate	m3/h	2.00	0.00	10.00	1.00	1.00				
13	--											
14	Process outputs	Name	Unit	z_s	z_min	z_bar	z_max	Q_z	q_zmin	Q_zmin	q_zmax	Q_zmax
15	P_g	Separator gas pressure	bar	8.00	4.00	8.00	4.00	100.00	1.00	100.00	1.00	100.00
16	L_o	Separator oil level	m	2.20	0.20	2.20	0.30	100.00	1.00	100.00	1.00	100.00
17	L_w	Separator water level	m	1.50	1.40	1.50	0.30	100.00	1.00	100.00	1.00	100.00
18	C_o,h	Oil-in-water concentration	ppm	30.00	5.00	30.00	5.00	100.00	1.00	100.00	1.00	100.00

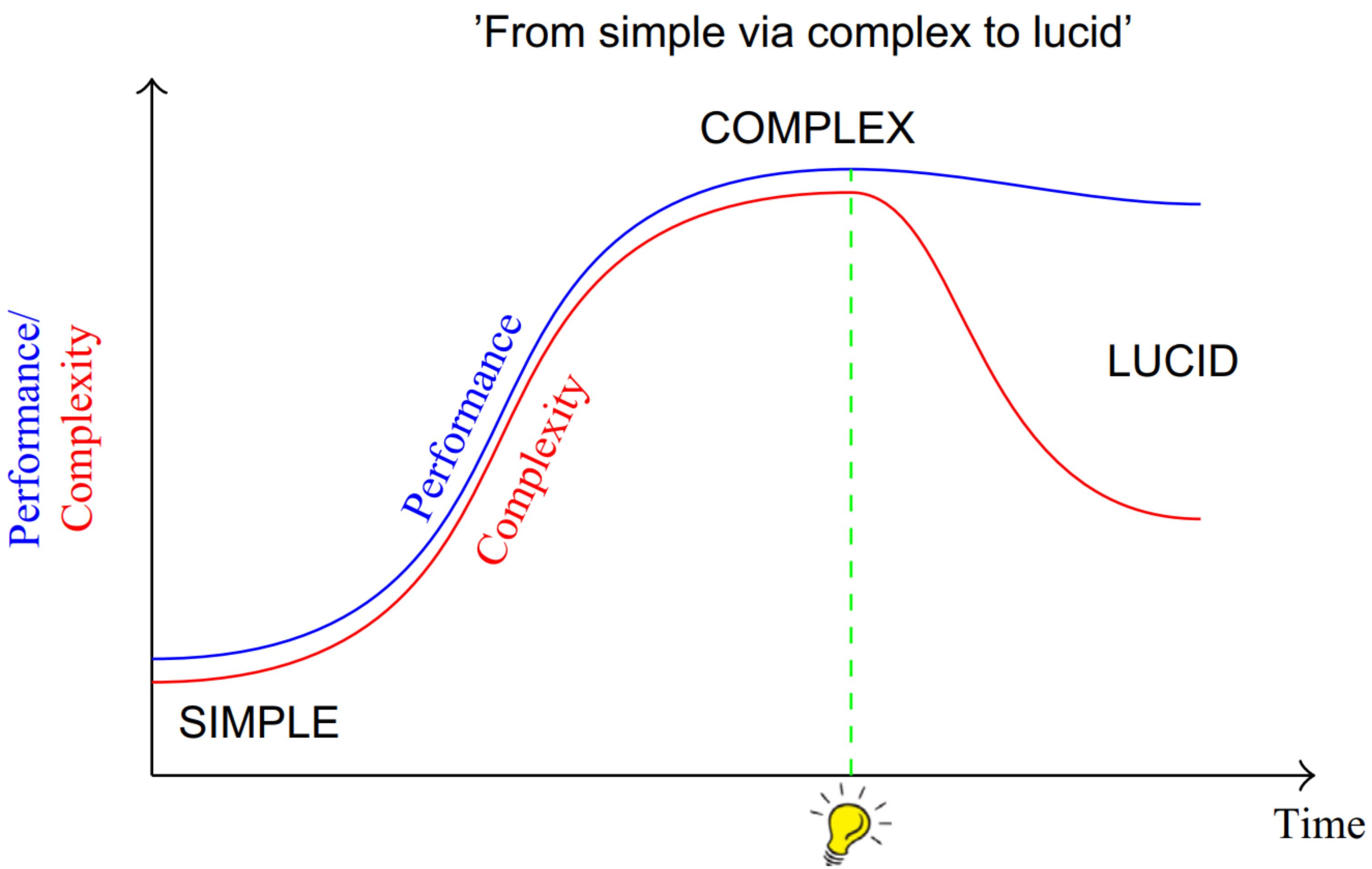
Squeeze and Shift



Long-term Benefits

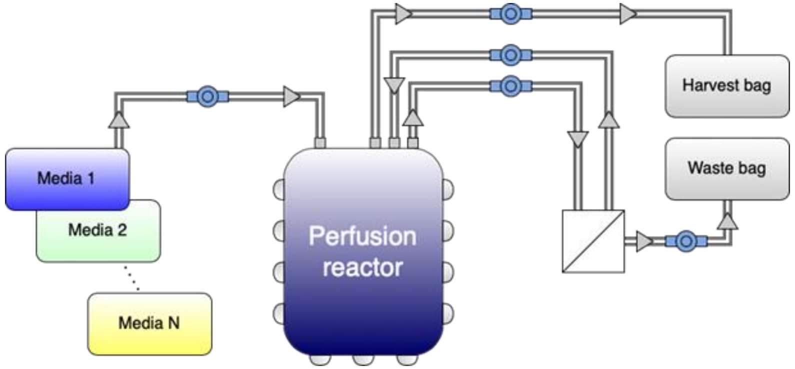


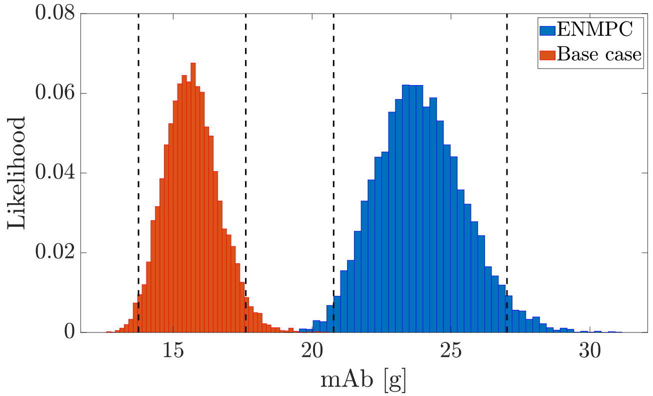
Implementation of optimizing control – NMPC – can be implemented as simplified controllers

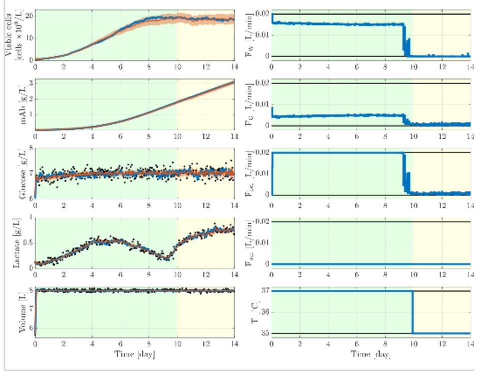


Stoustrup (2013)

mAb production in a perfusion reactor







- 10,000 simulations of the fermentation process with Economic Nonlinear Model Predictive Control (ENMPC) and a base case strategy
- Increased mean production
- Non-overlapping confidence intervals

mAb production

	Mean		min		max		Range		Std		95% CI	
ENMPC	23.89	[g]	18.83	[g]	31.13	[g]	12.29	[g]	1.59	[g]	[20.78, 27.04]	[g]
Base case	15.68	[g]	12.69	[g]	20.56	[g]	7.87	[g]	0.99	[g]	[13.75, 17.61]	[g]
Increase	52	[%]	48	[%]	51	[%]	56	[%]	62	[%]	[51, 53]	[%]

Model-based control
- and scientific computing

Continuous-Discrete System - Stochastic Differential Equation System

$$\boldsymbol{x}(t_0) = \hat{\boldsymbol{x}}_0 \qquad \hat{\boldsymbol{x}}_0 \sim N(\hat{x}_0, \hat{P}_0)$$

$$d\boldsymbol{x}(t) = \overbrace{f(\boldsymbol{x}(t), u(t), d(t), \theta)dt}^{=\text{drift}} + \overbrace{\sigma(\boldsymbol{x}(t), u(t), d(t), \theta)d\boldsymbol{\omega}(t)}^{=\text{diffusion}} \qquad d\boldsymbol{\omega}(t) \sim N_{iid}(0, Idt)$$

$$\boldsymbol{y}(t_k) = g(\boldsymbol{x}(t_k), \theta) + \boldsymbol{v}(t_k) \qquad \boldsymbol{v}(t_k) \sim N_{iid}(0, R(\theta))$$

$$\boldsymbol{z}(t) = h(\boldsymbol{x}(t), \theta)$$

Stochastic Continuous-Discrete Dynamical Model

- Ordinary Differential Equations (ODEs) and output equation

$$
\begin{aligned}
x(t_0) &= \hat{x}_0 \\
dx(t) &= f(x(t), u(t), d(t), \theta)dt \\
y(t_k) &= g(x(t_k), \theta)
\end{aligned}
$$

- Stochastic Differential Equations (SDEs) and output equation

$$
\begin{aligned}
\boldsymbol{x}(t_0) &= \hat{\boldsymbol{x}}_0 & \hat{\boldsymbol{x}}_0 &\sim N(\hat{x}_0, \hat{P}_0) \\
d\boldsymbol{x}(t) &= \overbrace{f(\boldsymbol{x}(t), u(t), d(t), \theta)dt}^{=\text{drift}} + \overbrace{\sigma(\boldsymbol{x}(t), u(t), d(t), \theta)d\boldsymbol{\omega}(t)}^{=\text{diffusion}} & d\boldsymbol{\omega}(t) &\sim N_{iid}(0, Idt) \\
\boldsymbol{y}(t_k) &= g(\boldsymbol{x}(t_k), \theta) + \boldsymbol{v}(t_k) & \boldsymbol{v}(t_k) &\sim N_{iid}(0, R(\theta))
\end{aligned}
$$

- Euler-Maruyama Discretization (Explicit-Explicit)

$$
\begin{aligned}
\boldsymbol{x}_0 &= \hat{\boldsymbol{x}}_0 & \hat{\boldsymbol{x}}_0 &\sim N(\hat{x}_0, \hat{P}_0) \\
\boldsymbol{x}_{k+1} &= \boldsymbol{x}_k + f(\boldsymbol{x}_k, u_k, d_k, \theta)\Delta t + \sigma(\boldsymbol{x}_k, u_k, d_k, \theta)\Delta\boldsymbol{\omega}_k & \Delta\boldsymbol{\omega}_k &\sim N_{iid}(0, I\Delta t) \\
\boldsymbol{y}_k &= g(\boldsymbol{x}_k, \theta) + \boldsymbol{v}_k & \boldsymbol{v}_k &\sim N_{iid}(0, R(\theta))
\end{aligned}
$$

Continuous-Discrete Extended Kalman Filter (CDEKF)

- Continuous-Discrete Stochastic Model

$$
\begin{aligned}
\boldsymbol{x}(t_0) &= \hat{\boldsymbol{x}}_0 & \hat{\boldsymbol{x}}_0 &\sim N(\hat{x}_0, \hat{P}_0) \\
d\boldsymbol{x}(t) &= f(\boldsymbol{x}(t), u(t), d(t), \theta)dt + \sigma(\boldsymbol{x}(t), u(t), d(t), \theta)d\boldsymbol{\omega}(t) & d\boldsymbol{\omega}(t) &\sim N_{iid}(0, Idt) \\
\boldsymbol{y}(t_k) &= g(\boldsymbol{x}(t_k), \theta) + \boldsymbol{v}(t_k) & \boldsymbol{v}(t_k) &\sim N_{iid}(0, R(\theta))
\end{aligned}
$$

- Continuous-Discrete Extended Kalman Filter Algorithm ($\hat{x}_{0|-1} = \hat{x}_0$, $P_{0|-1} = \hat{P}_0$)
  - Measurement update

$$
\begin{aligned}
\hat{y}_{k|k-1} &= g(\hat{x}_{k|k-1}, \theta) & C_k &= \frac{\partial g}{\partial x}(\hat{x}_{k|k-1}, \theta) \\
e_k &= y_k - \hat{y}_{k|k-1} & R_{e,k} &= C_k P_{k|k-1} C_k' + R_k \\
\hat{x}_{k|k} &= \hat{x}_{k|k-1} + K_k e_k & K_k &= P_{k|k-1} C_k' R_{e,k}^{-1}
\end{aligned}
$$

$$
P_{k|k} = P_{k|k-1} - K_k R_{e,k} K_k' = (I - K_k C_k) P_{k|k-1} (I - K_k C_k)' + K_k R_k K_k'
$$

  - Time update - compute $\hat{x}_{k+1|k} = \hat{x}_k(t_{k+1})$ and $P_{k+1|k} = P_k(t_{k+1})$ by solving

$$
\begin{aligned}
\frac{d}{dt}\hat{x}_k(t) &= f(\hat{x}_k(t), u_k, d_k, \theta) & \hat{x}_k(t_k) &= \hat{x}_{k|k} \\
\frac{d}{dt}P_k(t) &= A_k(t)P_k(t) + P_k(t)A_k(t)' + \sigma_k(t)\sigma_k(t)' & P_k(t_k) &= P_{k|k} \\
A_k(t) &= \frac{\partial f}{\partial x}(\hat{x}_k(t), u_k, d_k, \theta) \\
\sigma_k(t) &= \sigma(\hat{x}_k(t), u_k, d_k, \theta)
\end{aligned}
$$

Filters and Predictors

- Discrete Stochastic Model

$$
\begin{aligned}
\boldsymbol{x}_0 &= \hat{\boldsymbol{x}}_0 & \hat{\boldsymbol{x}}_0 &\sim N(\hat{x}_0, \hat{P}_0) \\
\boldsymbol{x}_{k+1} &= F(\boldsymbol{x}_k, u_k, d_k, \theta) + \boldsymbol{w}_k, & \boldsymbol{w}_k &\sim N_{iid}(0, Q_k) \quad Q_k = Q_k(\theta) \\
\boldsymbol{y}_k &= g(\boldsymbol{x}_k, \theta) + \boldsymbol{v}_k & \boldsymbol{v}_k &\sim N_{iid}(0, R_k) \quad R_k = R(\theta)
\end{aligned}
$$

  - Extended Kalman Filter (EKF)
  - Unscented Kalman Filter (UKF)
  - Ensemble Kalman Filter (EnKF)
  - Particle Filter (PF)
- Continuous-Discrete Stochastic Model

$$
\begin{aligned}
\boldsymbol{x}(t_0) &= \hat{\boldsymbol{x}}_0 & \hat{\boldsymbol{x}}_0 &\sim N(\hat{x}_0, \hat{P}_0) \\
d\boldsymbol{x}(t) &= f(\boldsymbol{x}(t), u(t), d(t), \theta)dt + \sigma(\boldsymbol{x}(t), u(t), d(t), \theta)d\boldsymbol{\omega}(t) & d\boldsymbol{\omega}(t) &\sim N_{iid}(0, Idt) \\
\boldsymbol{y}(t_k) &= g(\boldsymbol{x}(t_k), \theta) + \boldsymbol{v}(t_k) & \boldsymbol{v}(t_k) &\sim N_{iid}(0, R(\theta))
\end{aligned}
$$

  - Continuous-Discrete Extended Kalman Filter (CDEKF)
  - Continuous-Discrete Unscented Kalman Filter (CDUKF)
  - Continuous-Discrete Ensemble Kalman Filter (CDEnKF)
  - Continuous-Discrete Particle Filter (CDPF)

Innovation

In the measurement update of the filters, we compute the innovation and its covariance

$$e_k = e_k(\theta)$$
$$R_{e,k} = R_{e,k}(\theta)$$

The innovation is assumed to be distributed as

$$\boldsymbol{e}_k \sim N_{iid}(0, R_{e,k})$$

Statistical analysis is based on statistical tests assuming that the innovation has this distribution

System Identification Methods

- Prediction-Error-Method (PEM)
  - Assume a stochastic model (discrete or continuous-discrete)
  - Compute the innovation and its covariance by a filter and prediction algorithm

$$e_k = e_k(\theta)$$
$$R_{e,k} = R_{e,k}(\theta)$$

  - Assume that $\boldsymbol{e}_k \sim N_{iid}(0, R_{e,k})$ such that

$$V_{ML}(\theta) = \frac{1}{2}\sum_{k=0}^{N_d} \ln(\det R_{e,k}(\theta)) + e_k(\theta)' \left[R_{e,k}(\theta)\right]^{-1} e_k(\theta) + \frac{(N_d+1)n_y}{2}\ln(2\pi)$$

- Output-Error (OE)
  - Assume a deterministic model, but with measurement noise.
  - This is equivalent to a stochastic model with no process noise (diffusion) and perfectly known initial conditions. A PEM can be applied to such a system.
  - This is also know as a **simulation** model.

Parameter Estimation

$$\min_{\theta} \quad V(\theta)$$
$$s.t. \quad \theta_{\min} \leq \theta \leq \theta_{\max}$$

Innovation (computed from model and data using a filter and predictor)

$$e_k(\theta) = e_k$$
$$R_{e,k}(\theta) = R_{e,k}$$

Least squares (LS) objective function

$$V_{LS}(\theta) = \frac{1}{2}\sum_{k=0}^{N_d} \|e_k(\theta)\|_2^2$$

Maximum likelihood (ML) objective function

$$V_{ML}(\theta) = \frac{1}{2}\sum_{k=0}^{N_d} \ln(\det R_{e,k}(\theta)) + e_k(\theta)' \left[R_{e,k}(\theta)\right]^{-1} e_k(\theta) + \frac{(N_d+1)n_y}{2}\ln(2\pi)$$

Maximum a posteriori (MAP) objective function

$$V_{MAP}(\theta) = V_{ML}(\theta) + \frac{1}{2}(\theta-\theta_0)'P_{\theta_0}^{-1}(\theta-\theta_0) + \frac{1}{2}\ln(\det P_{\theta_0}) + \frac{n_\theta}{2}\ln(2\pi)$$

Continuous-Discrete Extended Kalman Filter (CDEKF)

- Continuous-Discrete Stochastic Model

$$\begin{aligned} \boldsymbol{x}(t_0) &= \hat{\boldsymbol{x}}_0 & \hat{\boldsymbol{x}}_0 &\sim N(\hat{x}_0, \hat{P}_0) \\ d\boldsymbol{x}(t) &= f(\boldsymbol{x}(t), u(t), d(t), \theta)dt + \sigma(\boldsymbol{x}(t), u(t), d(t), \theta)d\boldsymbol{\omega}(t) & d\boldsymbol{\omega}(t) &\sim N_{iid}(0, Idt) \\ \boldsymbol{y}(t_k) &= g(\boldsymbol{x}(t_k), \theta) + \boldsymbol{v}(t_k) & \boldsymbol{v}(t_k) &\sim N_{iid}(0, R(\theta)) \end{aligned}$$

- Continuous-Discrete Extended Kalman Filter Algorithm ($\hat{x}_{0|-1} = \hat{x}_0$, $P_{0|-1} = \hat{P}_0$)
  - Measurement update

$$\begin{aligned} \hat{y}_{k|k-1} &= g(\hat{x}_{k|k-1}, \theta) & C_k &= \frac{\partial g}{\partial x}(\hat{x}_{k|k-1}, \theta) \\ e_k &= y_k - \hat{y}_{k|k-1} & R_{e,k} &= C_k P_{k|k-1} C_k' + R_k \\ \hat{x}_{k|k} &= \hat{x}_{k|k-1} + K_k e_k & K_k &= P_{k|k-1} C_k' R_{e,k}^{-1} \end{aligned}$$
$$P_{k|k} = P_{k|k-1} - K_k R_{e,k} K_k' = (I - K_k C_k) P_{k|k-1} (I - K_k C_k)' + K_k R_k K_k'$$

  - Time update - compute $\hat{x}_{k+1|k} = \hat{x}_k(t_{k+1})$ and $P_{k+1|k} = P_k(t_{k+1})$ by solving

$$\begin{aligned} \frac{d}{dt}\hat{x}_k(t) &= f(\hat{x}_k(t), u_k, d_k, \theta) & \hat{x}_k(t_k) &= \hat{x}_{k|k} \\ \frac{d}{dt}P_k(t) &= A_k(t)P_k(t) + P_k(t)A_k(t)' + \sigma_k(t)\sigma_k(t)' & P_k(t_k) &= P_{k|k} \\ A_k(t) &= \frac{\partial f}{\partial x}(\hat{x}_k(t), u_k, d_k, \theta) \\ \sigma_k(t) &= \sigma(\hat{x}_k(t), u_k, d_k, \theta) \end{aligned}$$

Filters and Predictors

- Discrete Stochastic Model

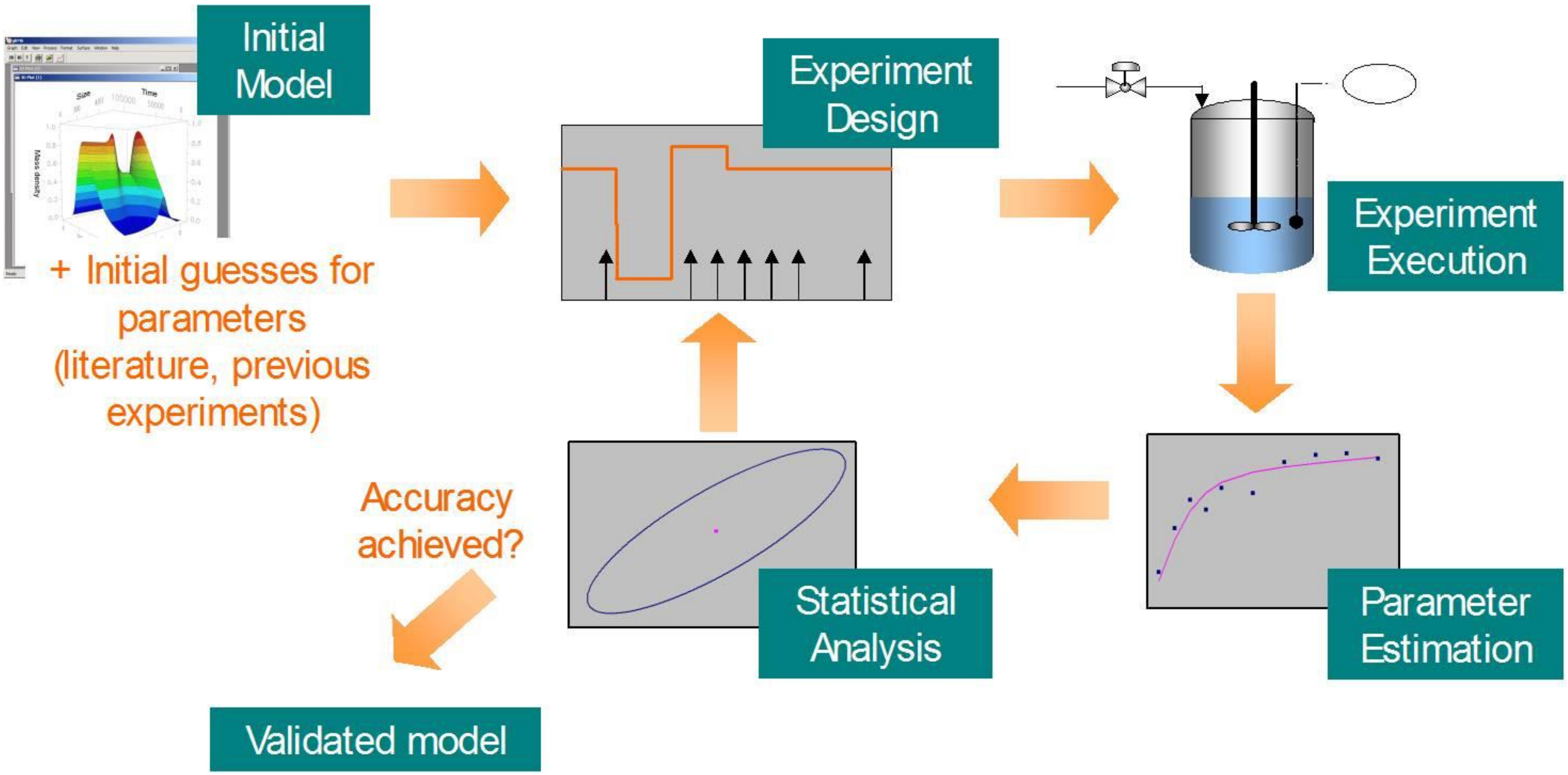
$$\begin{aligned} \boldsymbol{x}_0 &= \hat{\boldsymbol{x}}_0 & \hat{\boldsymbol{x}}_0 &\sim N(\hat{x}_0, \hat{P}_0) \\ \boldsymbol{x}_{k+1} &= F(\boldsymbol{x}_k, u_k, d_k, \theta) + \boldsymbol{w}_k, & \boldsymbol{w}_k &\sim N_{iid}(0, Q_k) \quad Q_k = Q_k(\theta) \\ \boldsymbol{y}_k &= g(\boldsymbol{x}_k, \theta) + \boldsymbol{v}_k & \boldsymbol{v}_k &\sim N_{iid}(0, R_k) \quad R_k = R(\theta) \end{aligned}$$

  - Extended Kalman Filter (EKF)
  - Unscented Kalman Filter (UKF)
  - Ensemble Kalman Filter (EnKF)
  - Particle Filter (PF)
- Continuous-Discrete Stochastic Model

$$\begin{aligned} \boldsymbol{x}(t_0) &= \hat{\boldsymbol{x}}_0 & \hat{\boldsymbol{x}}_0 &\sim N(\hat{x}_0, \hat{P}_0) \\ d\boldsymbol{x}(t) &= f(\boldsymbol{x}(t), u(t), d(t), \theta)dt + \sigma(\boldsymbol{x}(t), u(t), d(t), \theta)d\boldsymbol{\omega}(t) & d\boldsymbol{\omega}(t) &\sim N_{iid}(0, Idt) \\ \boldsymbol{y}(t_k) &= g(\boldsymbol{x}(t_k), \theta) + \boldsymbol{v}(t_k) & \boldsymbol{v}(t_k) &\sim N_{iid}(0, R(\theta)) \end{aligned}$$

  - Continuous-Discrete Extended Kalman Filter (CDEKF)
  - Continuous-Discrete Unscented Kalman Filter (CDUKF)
  - Continuous-Discrete Ensemble Kalman Filter (CDEnKF)
  - Continuous-Discrete Particle Filter (CDPF)

Systematic model building



Regulator - Nonlinear Model Predictive Control

Optimal control problem

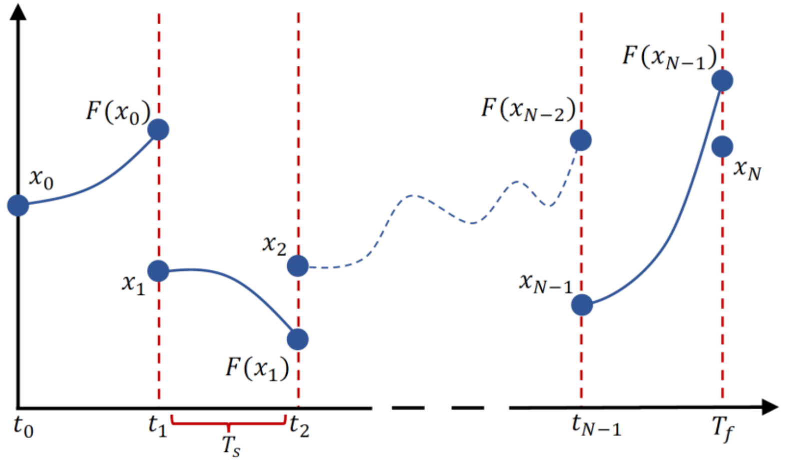
$$
\begin{aligned}
\min_{x,u} \quad & \phi_k = \phi_{z,k} + \phi_{u,k} + \phi_{\Delta u,k}, & \\
s.t. \quad & x(t_k) = \hat{x}_{k|k}, & \\
& \dot{x}(t) = f(x(t), u(t), \theta), & t_k \le t \le t_k + T_p, \\
& z(t) = h(x(t), \theta), & t_k \le t \le t_k + T_p, \\
& u(t) = u_{k+j|k}, \quad j \in \mathcal{N}, & t_{k+j} \le t < t_{k+j+1}, \\
& u_{\min} \le u_{k+j|k} \le u_{\max}, & j \in \mathcal{N}, \\
& \Delta u_{\min} \le \Delta u_{k+j|k} \le \Delta u_{\max}, & j \in \mathcal{N}
\end{aligned}
$$

$$
\phi_{z,k} = \frac{1}{2} \int_{t_k}^{t_k+T_p} \|z(t) - \bar{z}(t)\|_{Q_z}^2 \, \mathrm{d}t,
$$

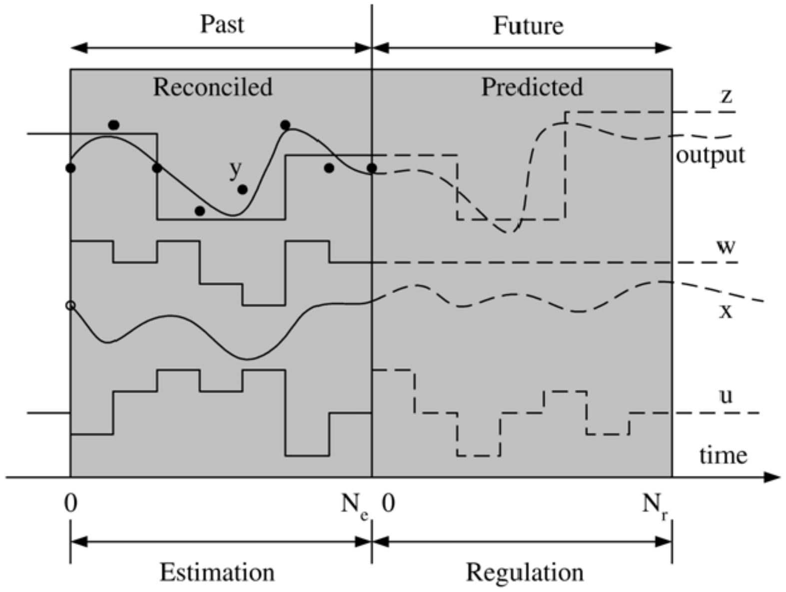
$$
\phi_{u,k} = \frac{1}{2} \int_{t_k}^{t_k+T_p} \|u(t) - \bar{u}(t)\|_{Q_u}^2 \, \mathrm{d}t,
$$

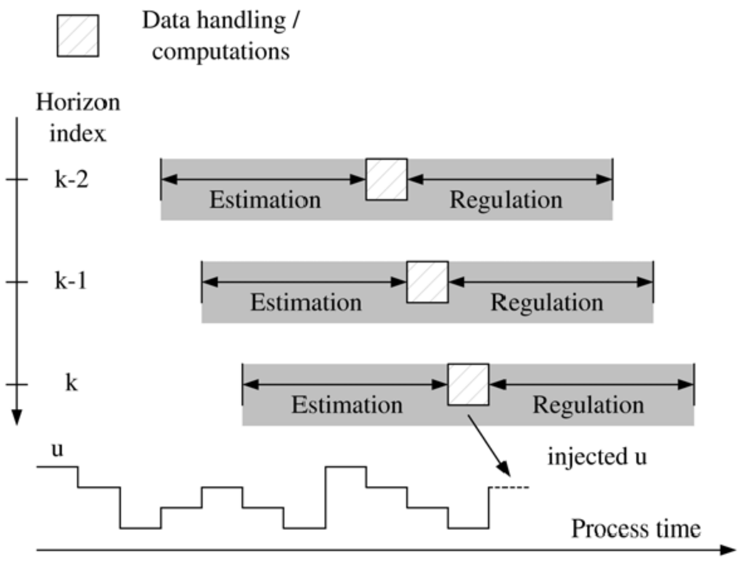
$$
\phi_{\Delta u,k} = \frac{1}{2} \sum_{j=0}^{N-1} \|\Delta u_{k+j}\|_{\bar{Q}_{\Delta u}}^2 .
$$

Multiple-shooting (with sensitivities)



Moving horizon principle





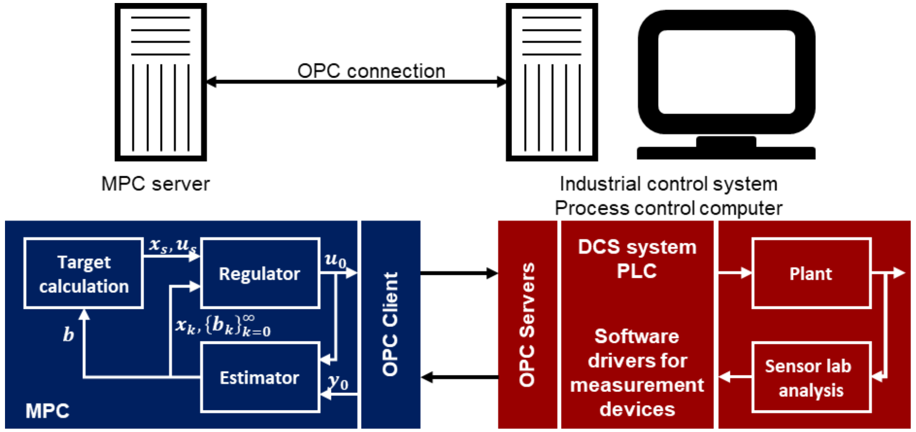
$$\min_{\{u_k, x_{k+1}\}_{k=0}^{N-1}} \quad \phi = \phi(\{u_k, x_{k+1}\}_{k=0}^{N-1}; x_0, \theta)$$

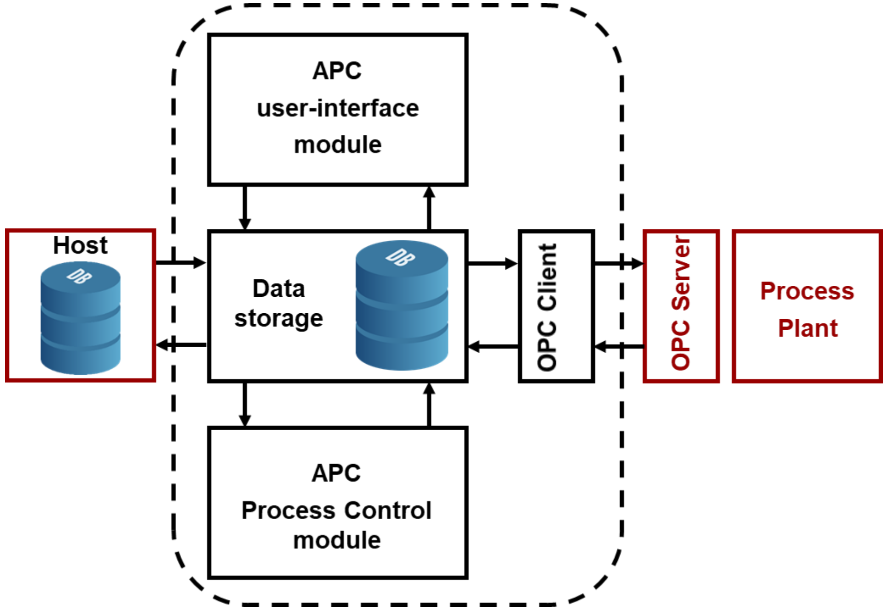
$$s.t. \quad x_{k+1} = F_k(x_k, u_k, \theta) \qquad k = 0, 1, \ldots, N-1$$

$$u_k \in \mathcal{U}$$

Adiabatic CSTR
with an exothermic reaction

Adiabatic CSTR with an Exothermic Reaction





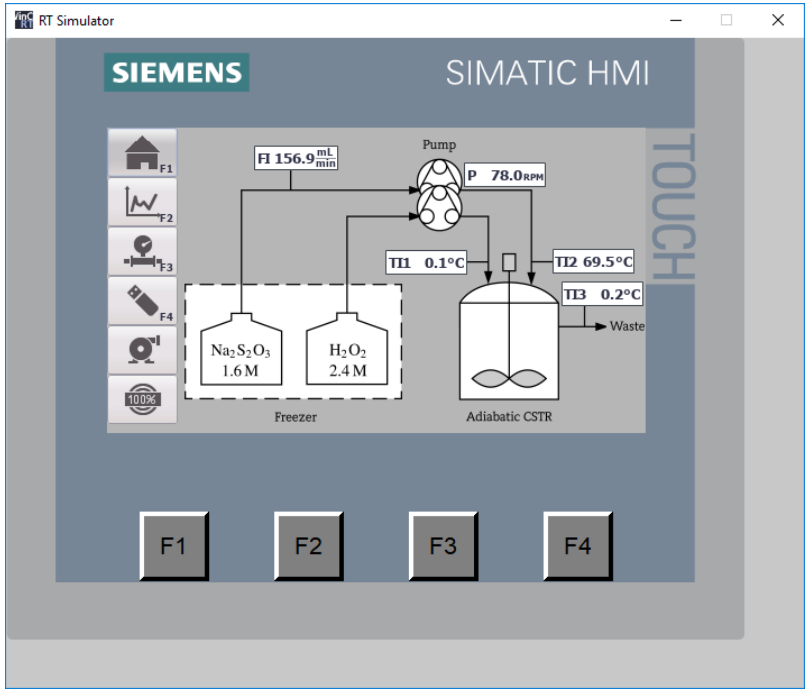
(a) Overview of the experimental setup.

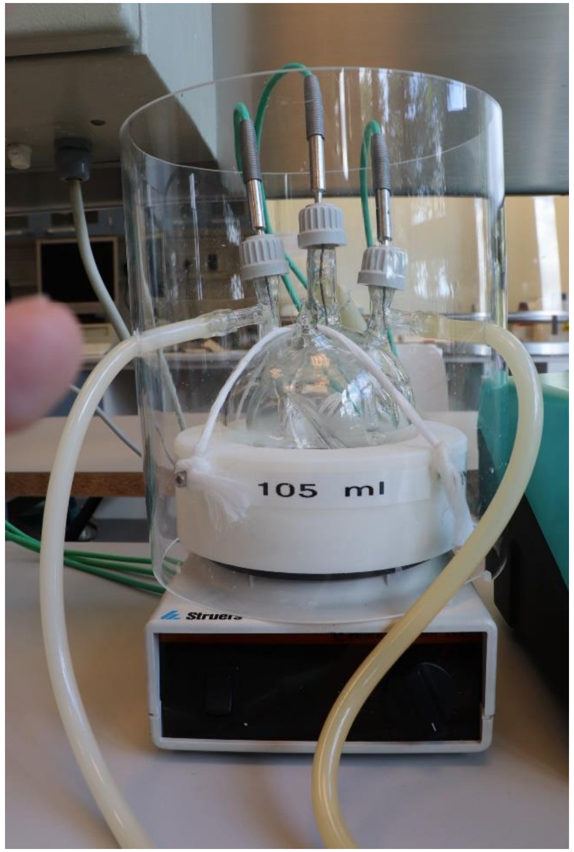
(b) Laboratory-scale adiabatic CSTR.

(c) Low level control system based on the Siemens S7-1200 platform.

(d) Human Machine Interface (HMI) showing mimic diagram.

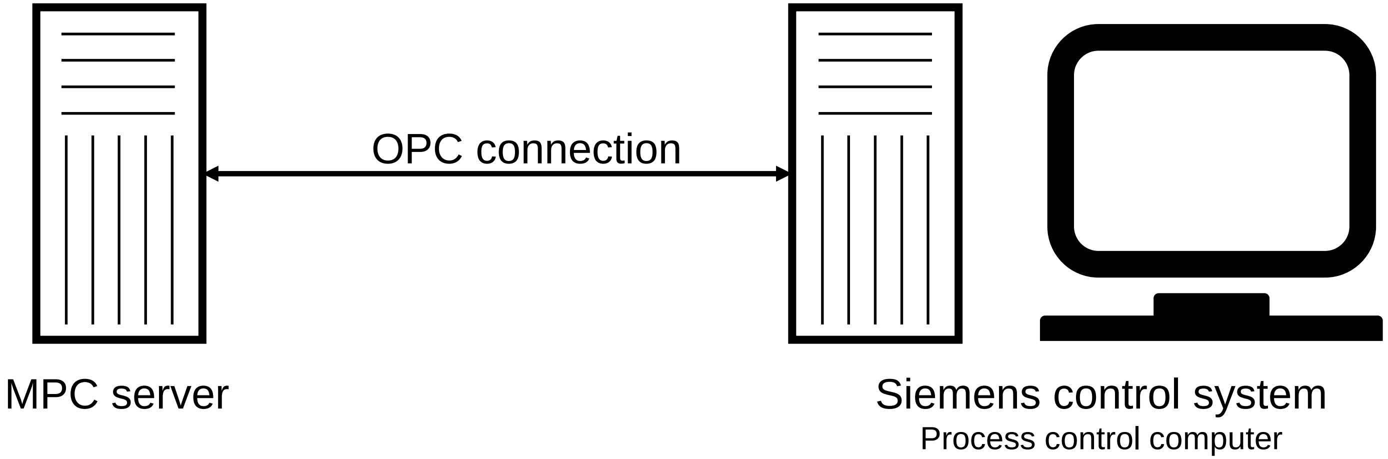
Adiabatic CSTR with an Exothermic Reaction

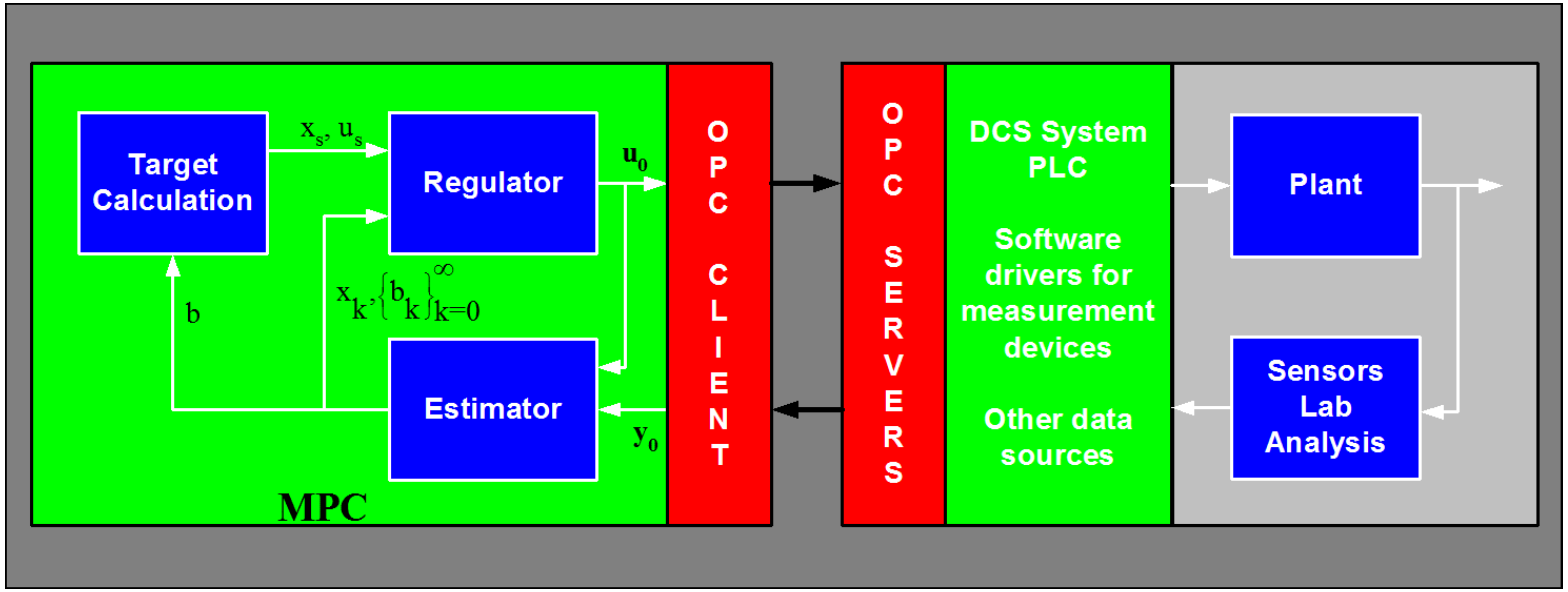




$$\mathrm{Na_2S_2O_3(aq)+2H_2O_2(aq)} \rightarrow \frac{1}{2}\mathrm{Na_2SO_4(aq)}+\frac{1}{2}\mathrm{Na_2S_3O_6(aq)+2H_2O(aq)},$$

Model Predictive Controller





Adiabatic CSTR with an Exothermic Reaction

Adiabatic CSTR with an Exothermic Reaction

(a) Overview of the experimental setup.

(b) Laboratory-scale adiabatic CSTR.

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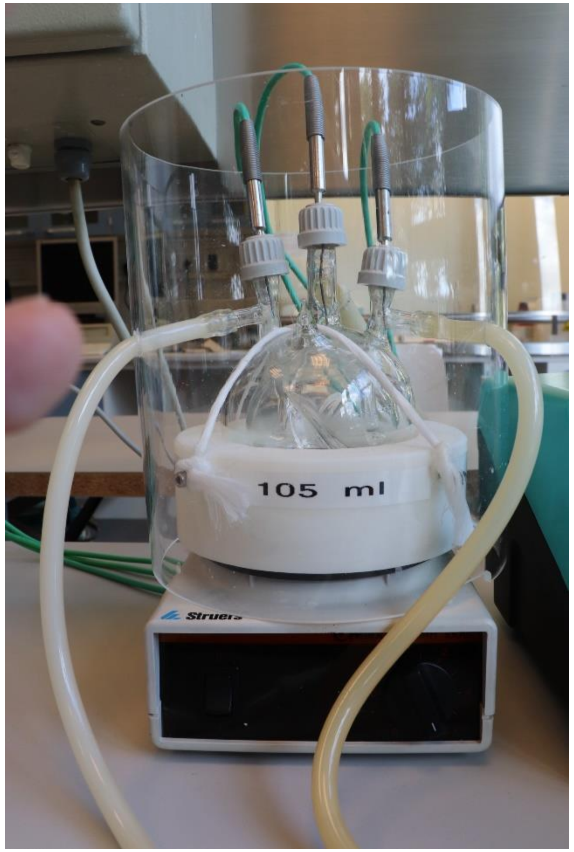
Adiabatic CSTR with an Exothermic Reaction



Mass and Energy Balance - SDE

$$dC_A = \left[\frac{F}{V}(C_{A,in} - C_A) + R_A(C_A, C_B, T)\right] dt,$$

$$dC_B = \left[\frac{F}{V}(C_{B,in} - C_B) + R_B(C_A, C_B, T)\right] dt,$$

$$dT = \left[\frac{F}{V}(T_{in} - T) + R_T(C_A, C_B, T)\right] dt + \frac{F}{V}\sigma_T d\omega.$$

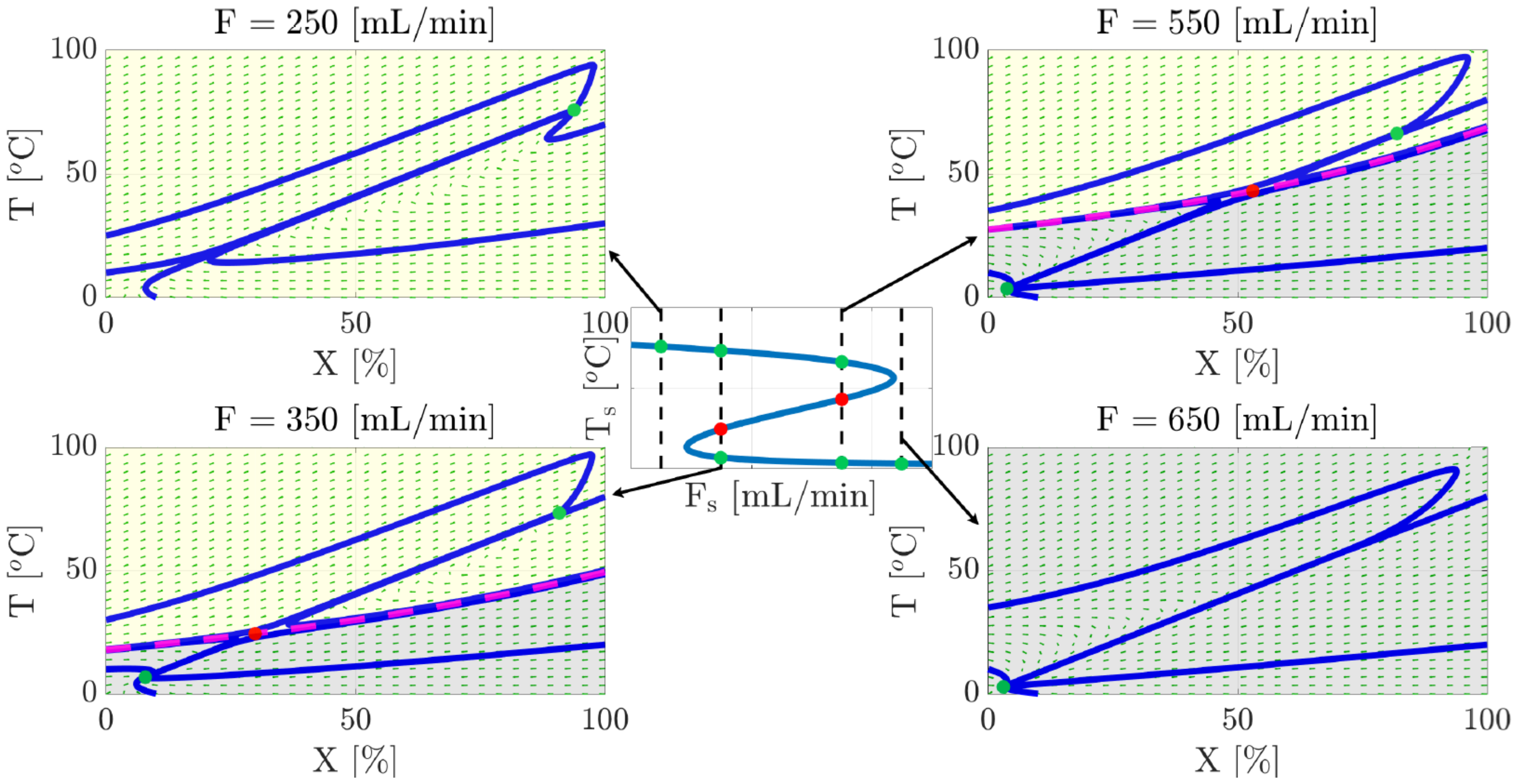
Continuous-Discrete System

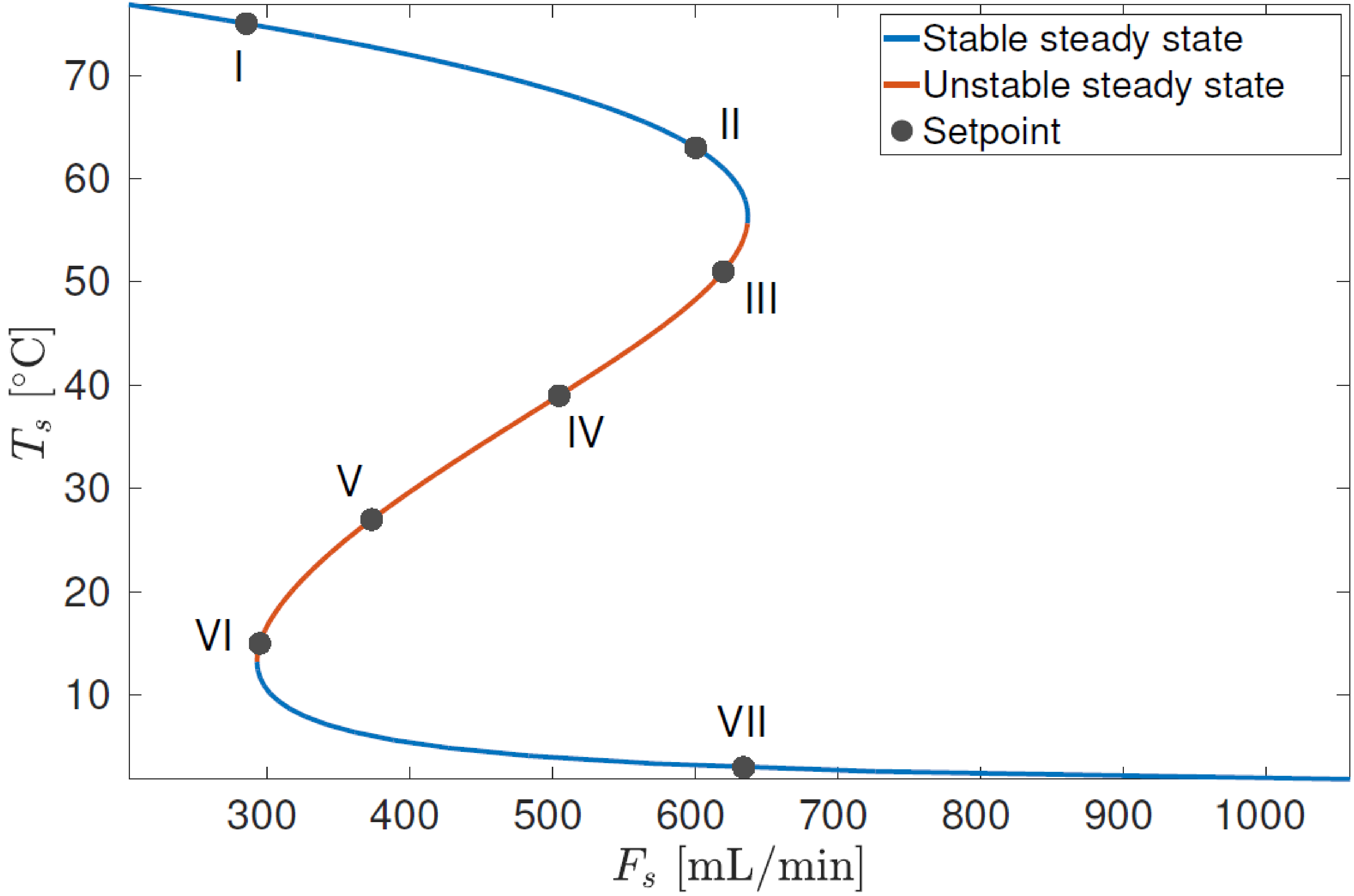
$$d\boldsymbol{x}(t) = f(\boldsymbol{x}(t), u(t), p)dt + \sigma(\boldsymbol{x}(t), u(t), p)d\boldsymbol{\omega}(t),$$

$$\boldsymbol{y}(t_k) = g(\boldsymbol{x}(t_k), p) + \boldsymbol{v}(t_k; p),$$

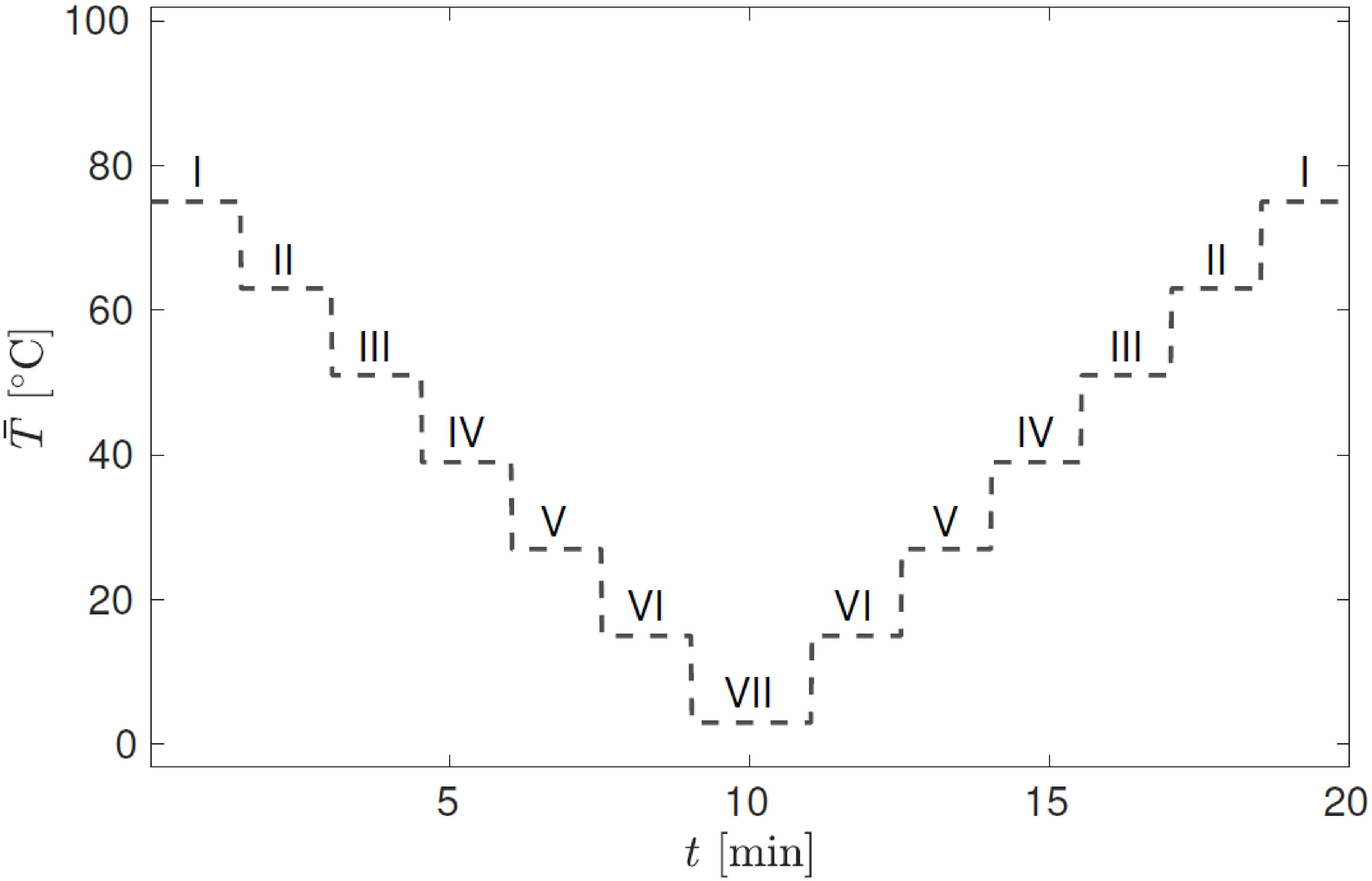
$$\boldsymbol{z}(t) = h(\boldsymbol{x}(t), p),$$

Bifurcations and nonlinear dynamics

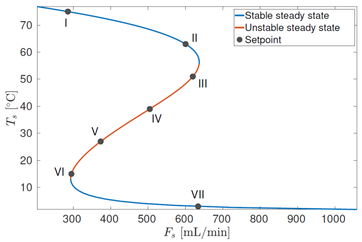


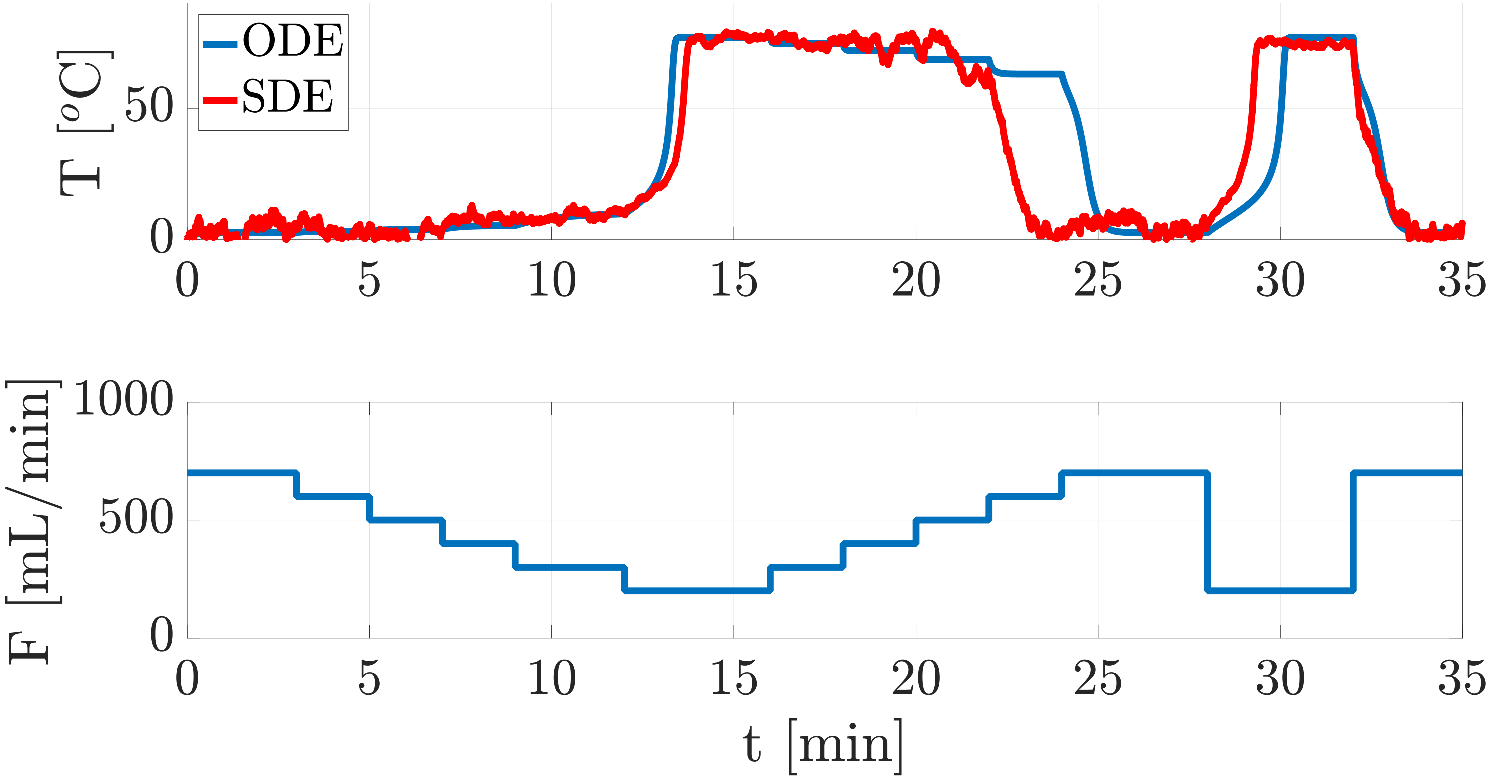


Stable steady state
Unstable steady state
Setpoint
I
II
III
IV
V
VI
VII
70
60
50
40
30
20
10
300
400
500
600
700
800
900
1000
T_s [°C]
F_s [mL/min]

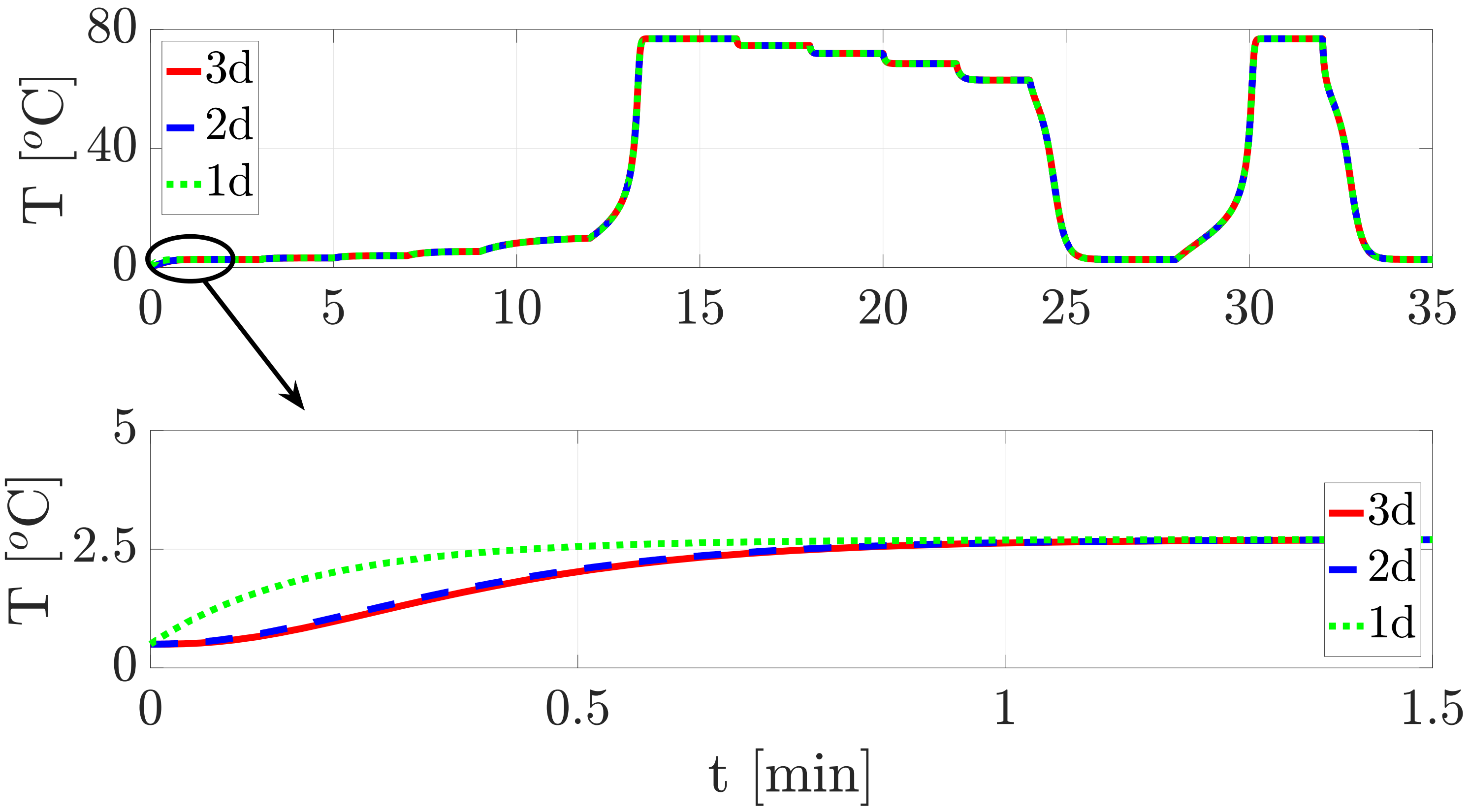

100
80
60
40
20
0
$\bar{T}$ [°C]
I
II
III
IV
V
VI
VII
VI
V
IV
III
II
I
5
10
15
20
t [min]

ODE vs SDE simulation



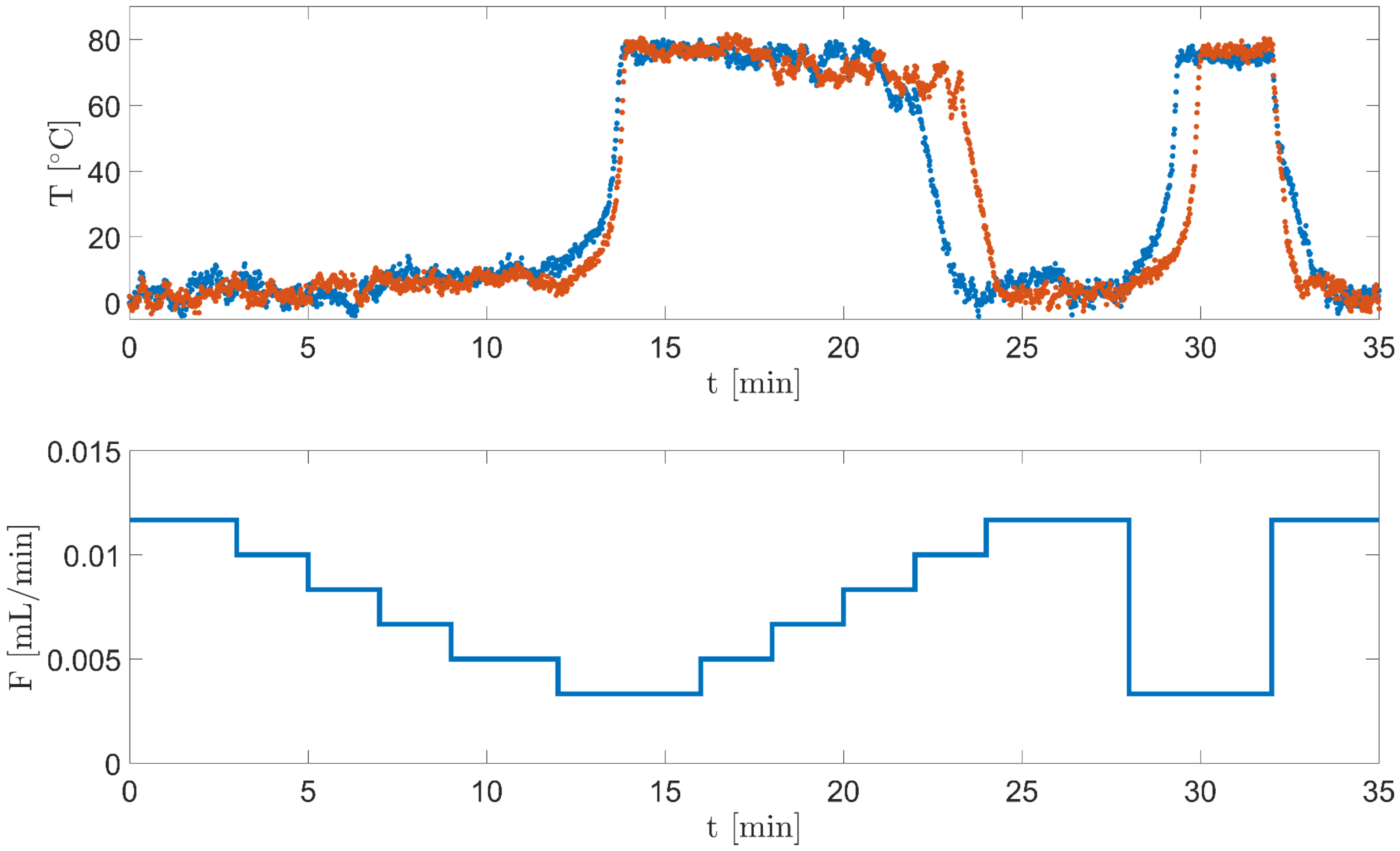


3D model and reduced-order 1D model

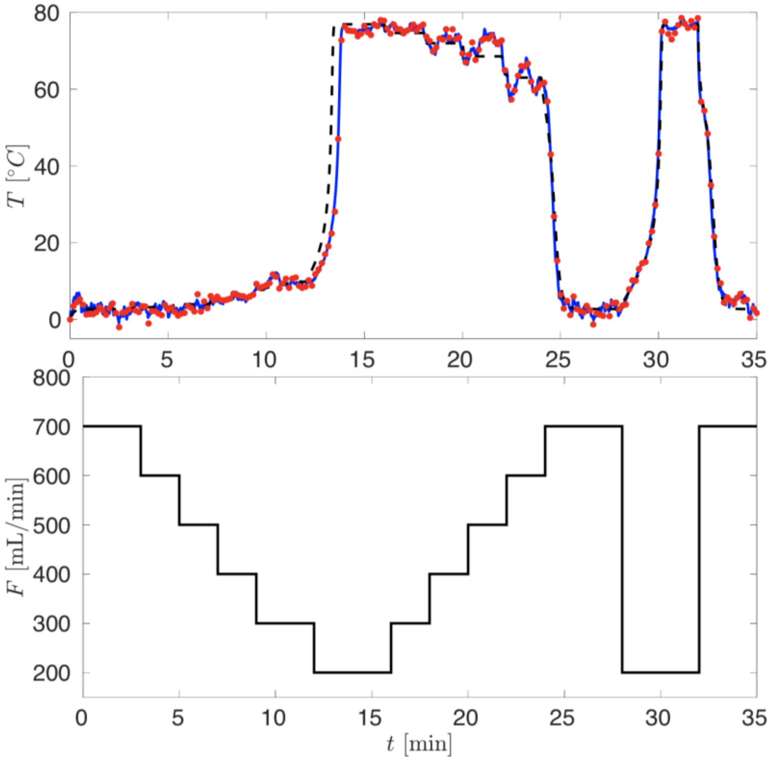


Training and validation data

Data for training and validation



System Identification
Prediction Error Method – Maximum Likelihood

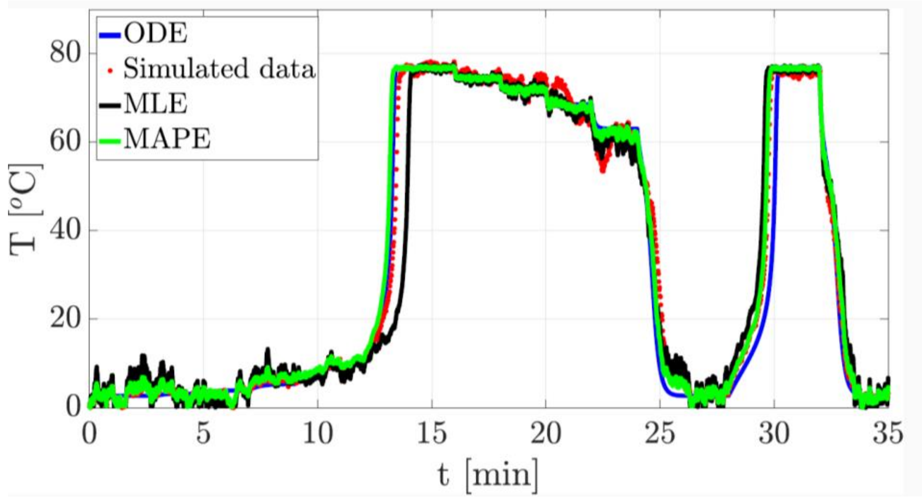


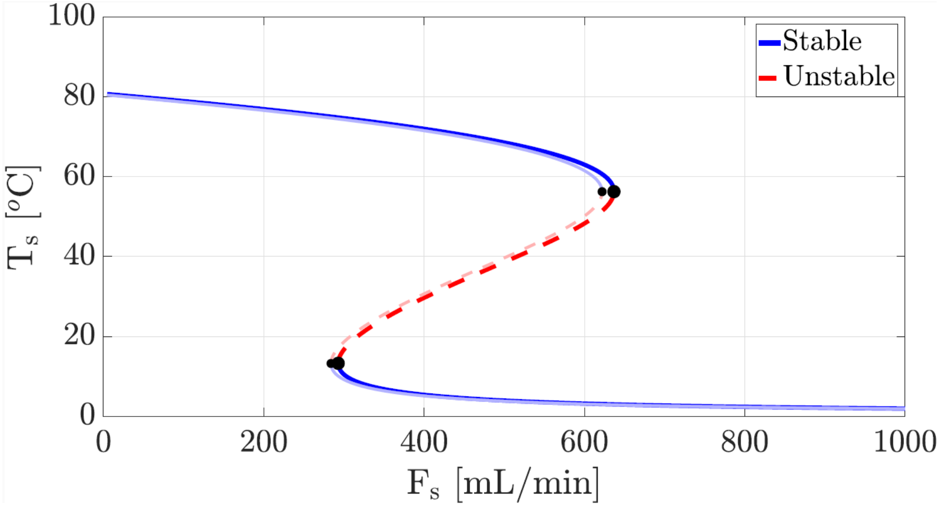
$$V_{ML}(\theta) = \frac{1}{2}(N_e+1)n_y \ln(2\pi) + \frac{1}{2}\sum_{k=0}^{N_e}\left(\ln\left[\det R_{e,k}\right] + e_k' R_{e,k}^{-1} e_k\right),$$

$$e_k = e_k(\theta) = y_k - \hat{y}_{k|k-1}(\theta),$$
$$R_{e,k} = R_{e,k}(\theta) = \bar{R}_k(\theta) + C_k(\theta)P_{k|k-1}(\theta)C_k(\theta)',$$

System Identification
Prediction Error Method – Maximum Likelihood

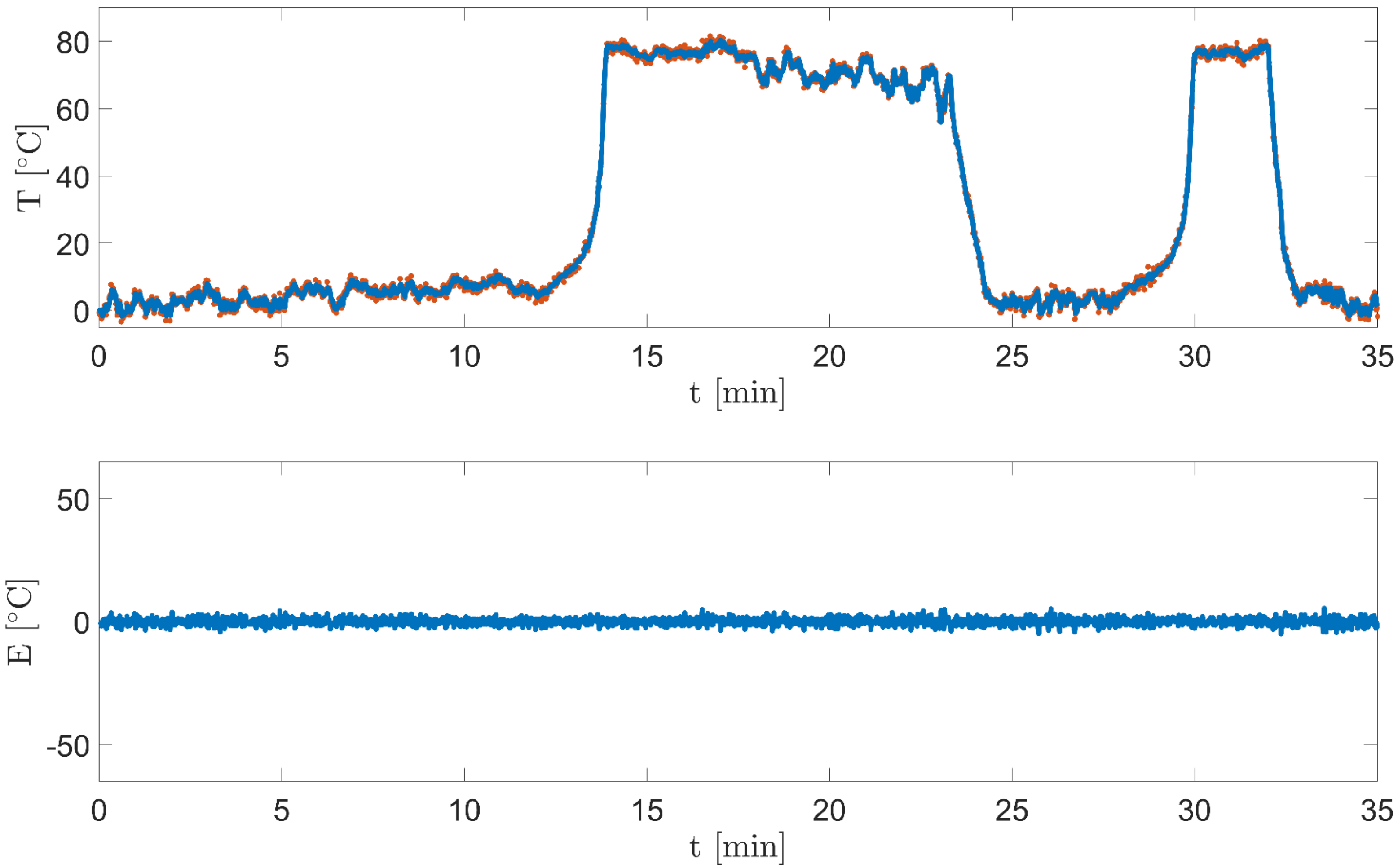
Parameter	Value	MLE value	Std	MAPE value	Std
β	133.78	133.3639	0.1384	133.4740	0.0993
$\log(k_0)$	24.6	24.7046	0.2272	24.8362	0.1431
E_a/R	8500	8537.7	74.113	8577.6	42.0107
p_v	0.15	0.0884	0.0069	0.1314	0.0061
p_w	5	11.4345	0.2694	8.7344	0.0825



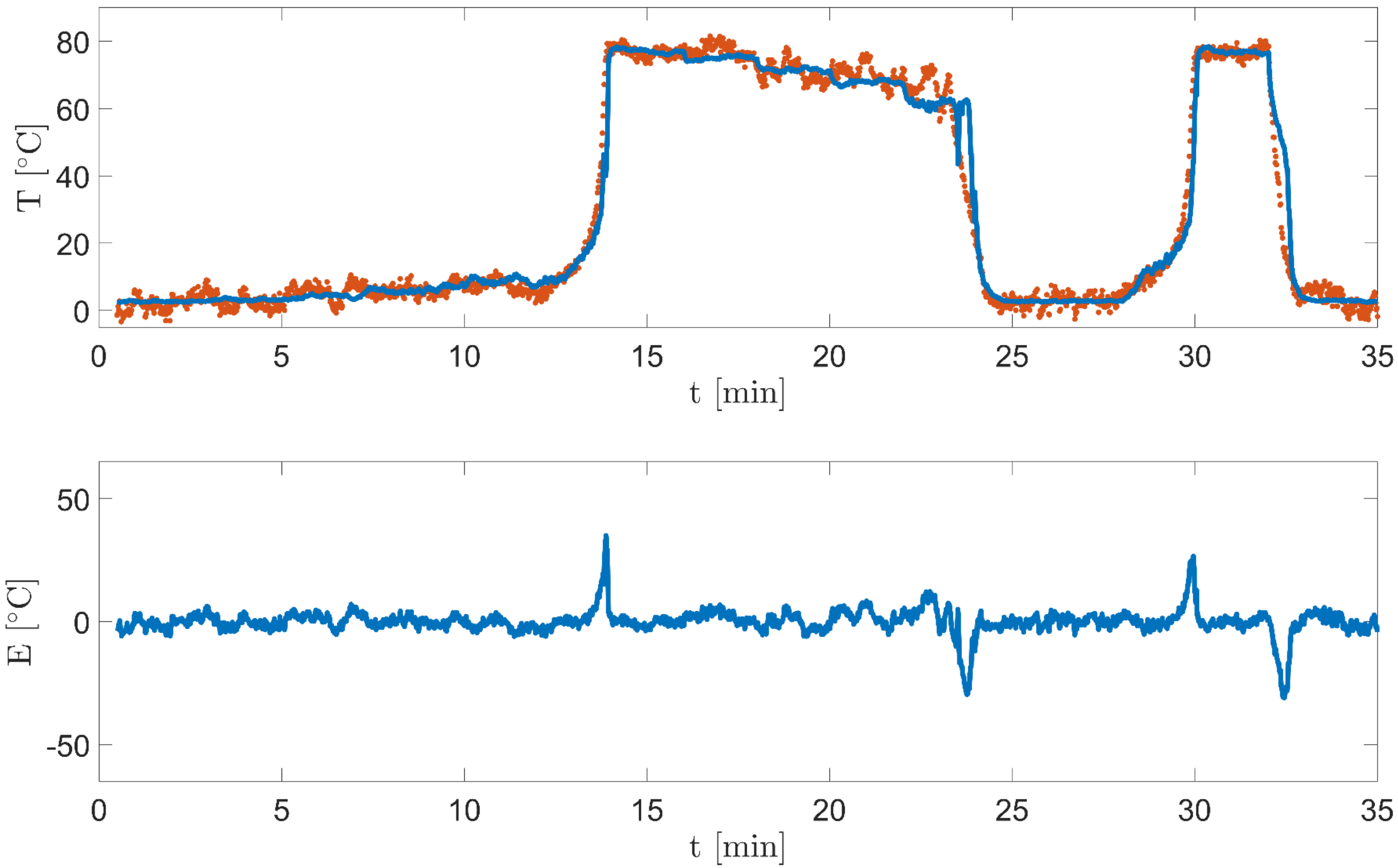


N-step predictions – MLE (3D)

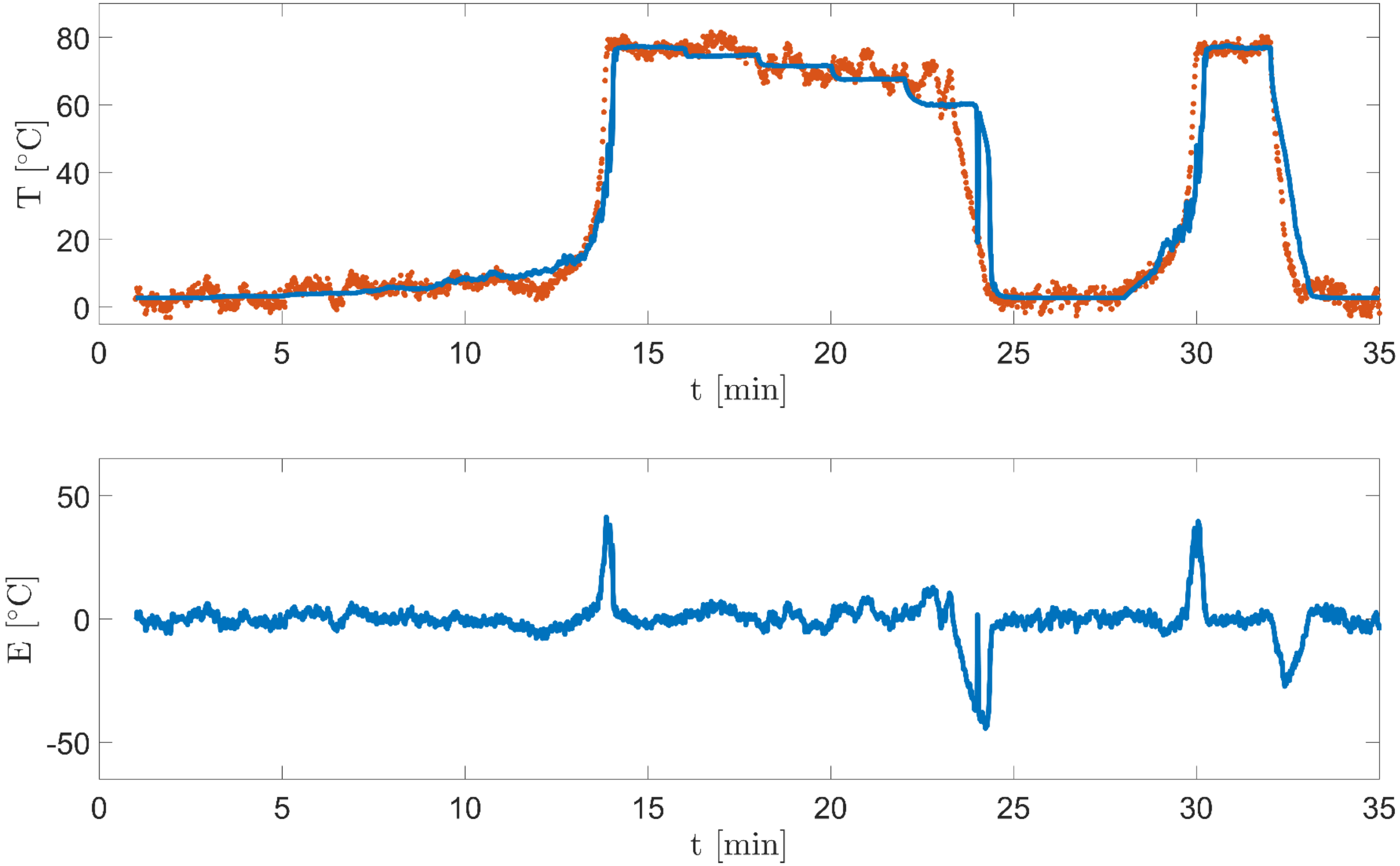
1-step predictions – MLE (3D)



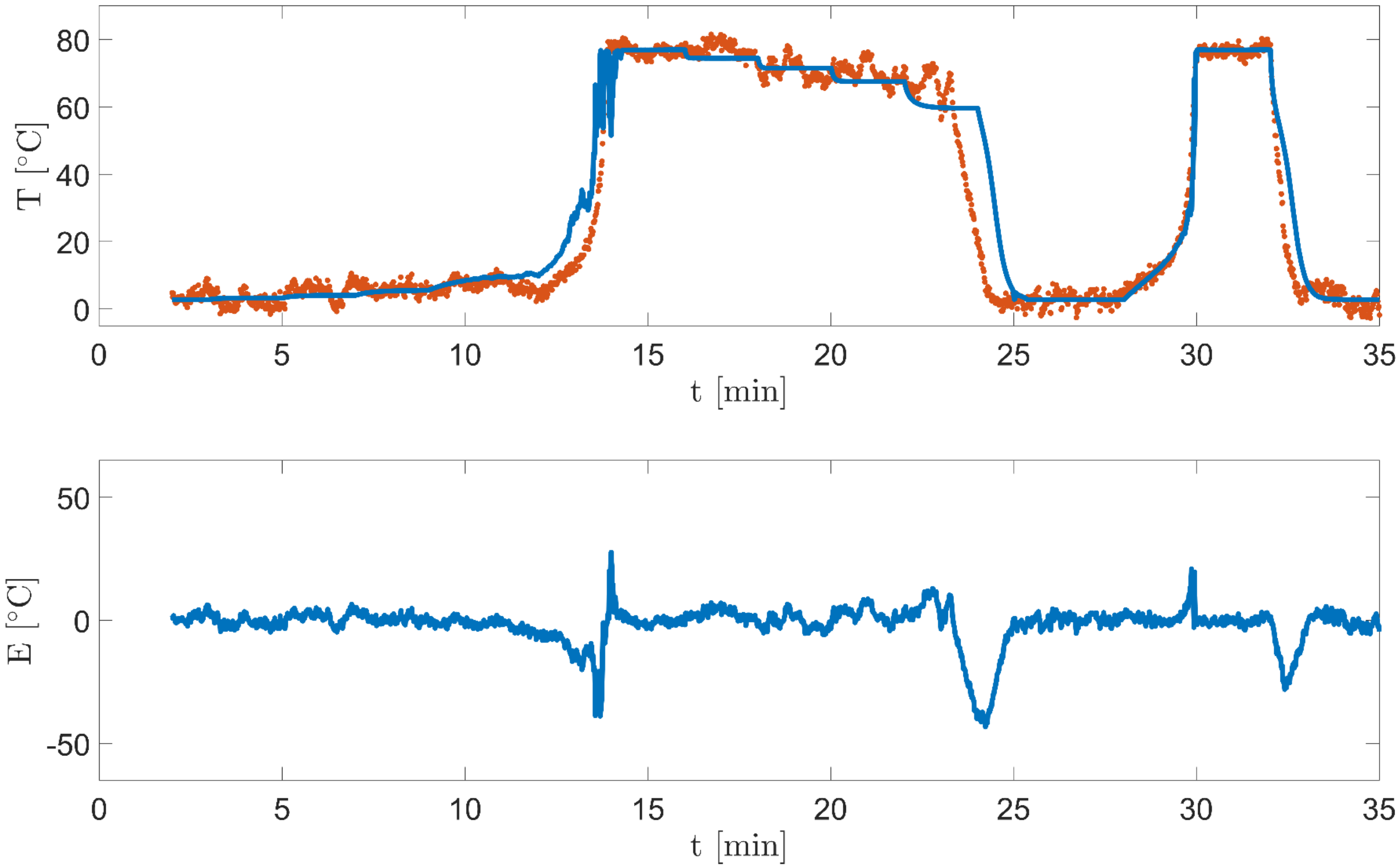
30-step predictions – MLE (3D)



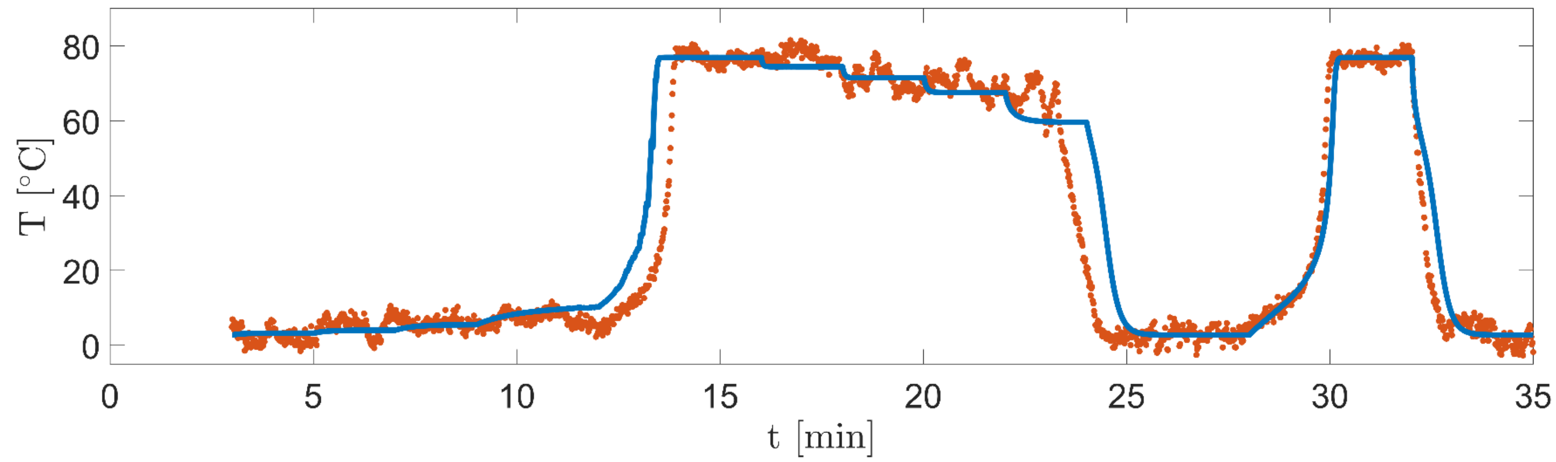
60-step predictions – MLE (3D)

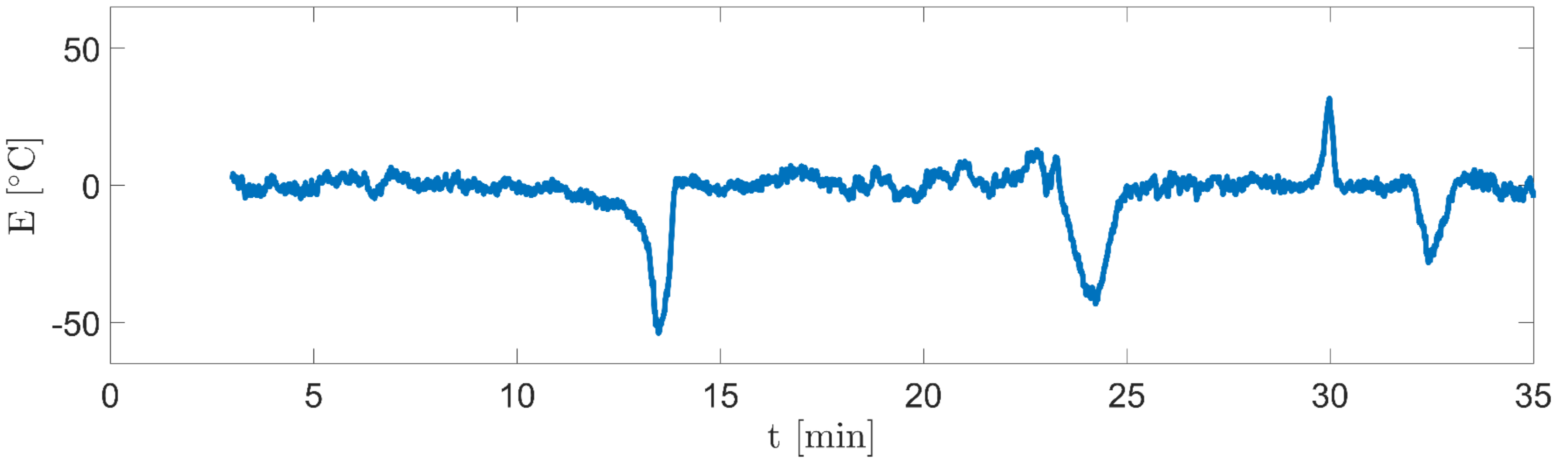


120-step predictions – MLE (3D)



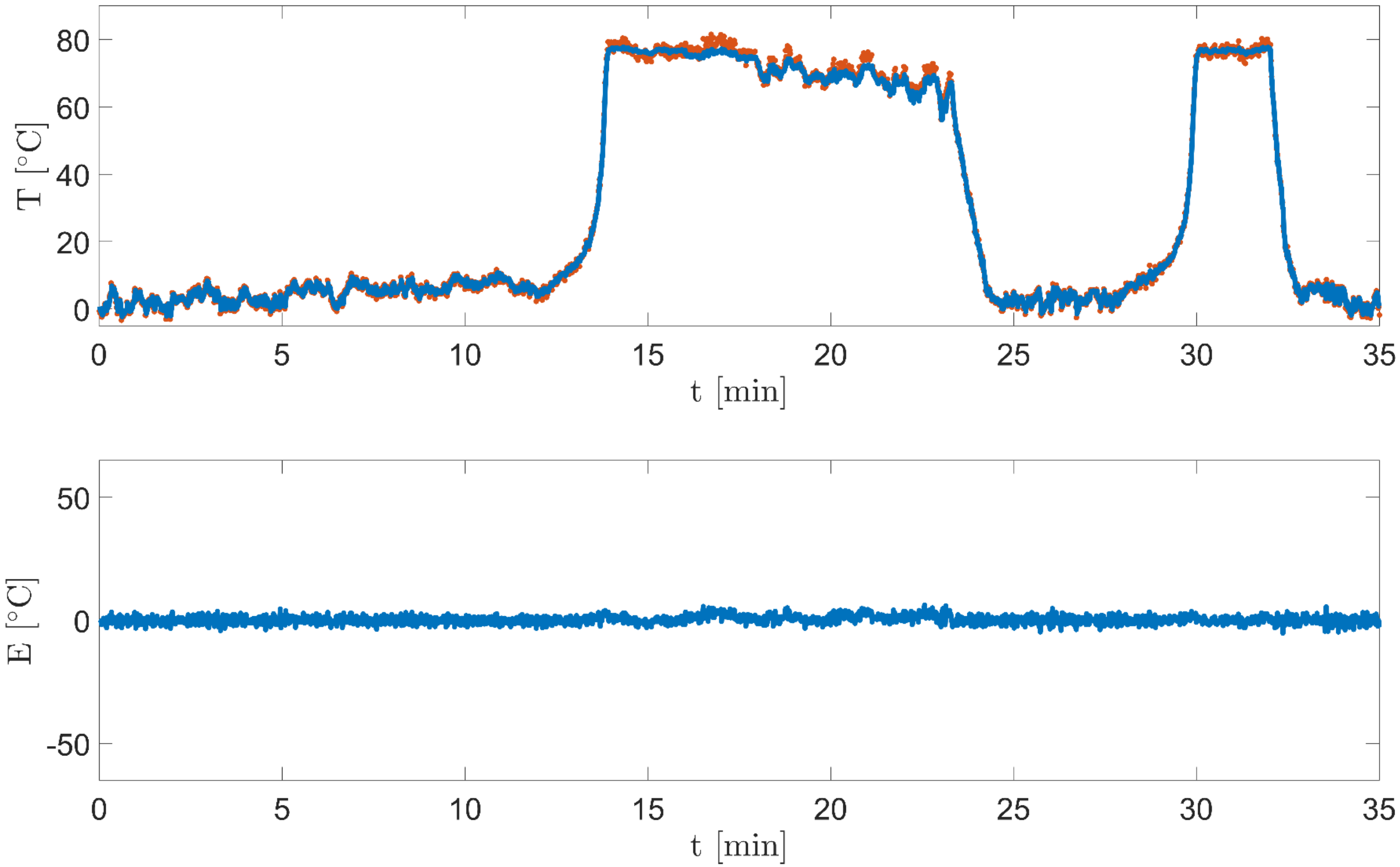
180-step predictions – MLE (3D)



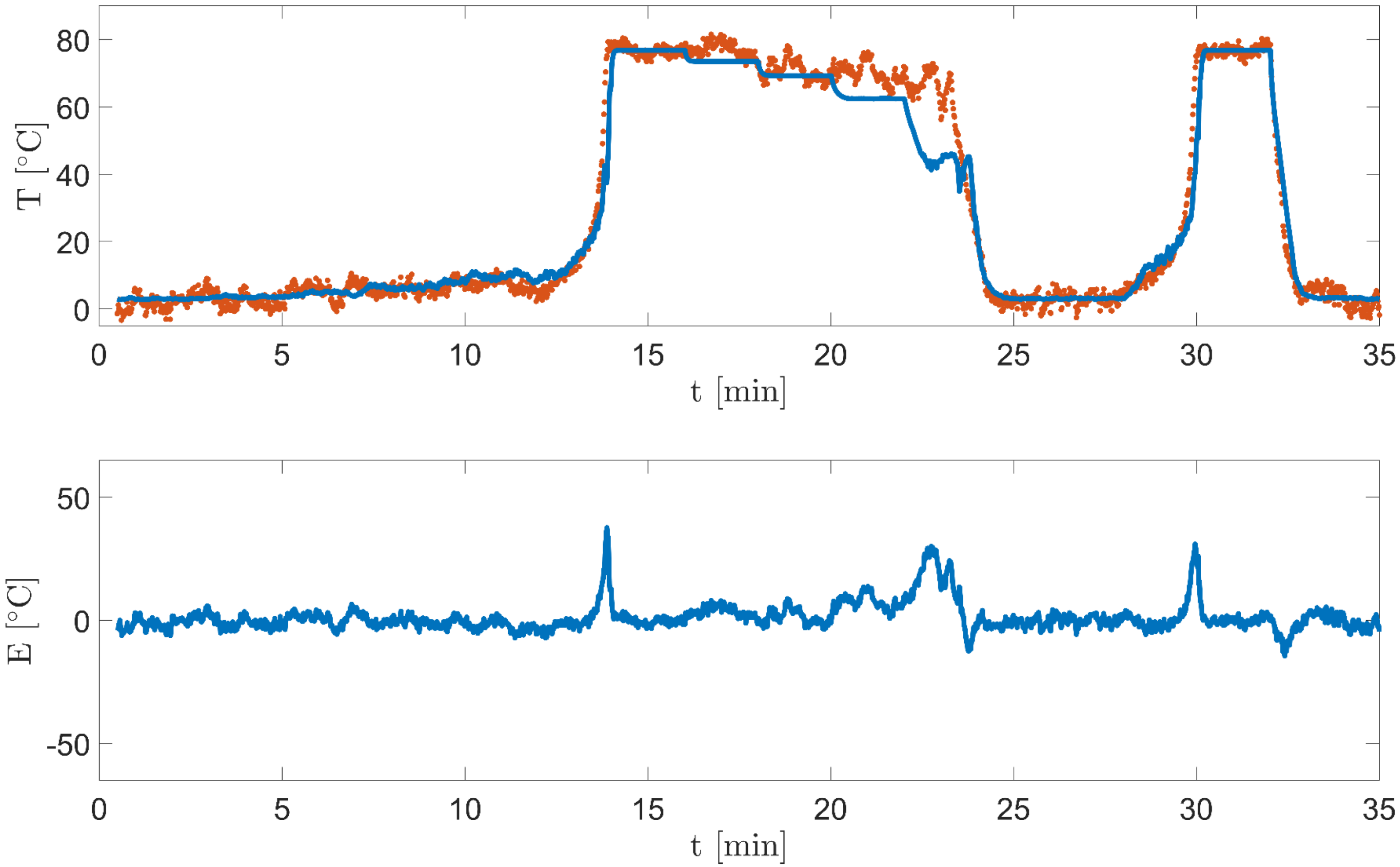


N-step predictions – MLE (1D)

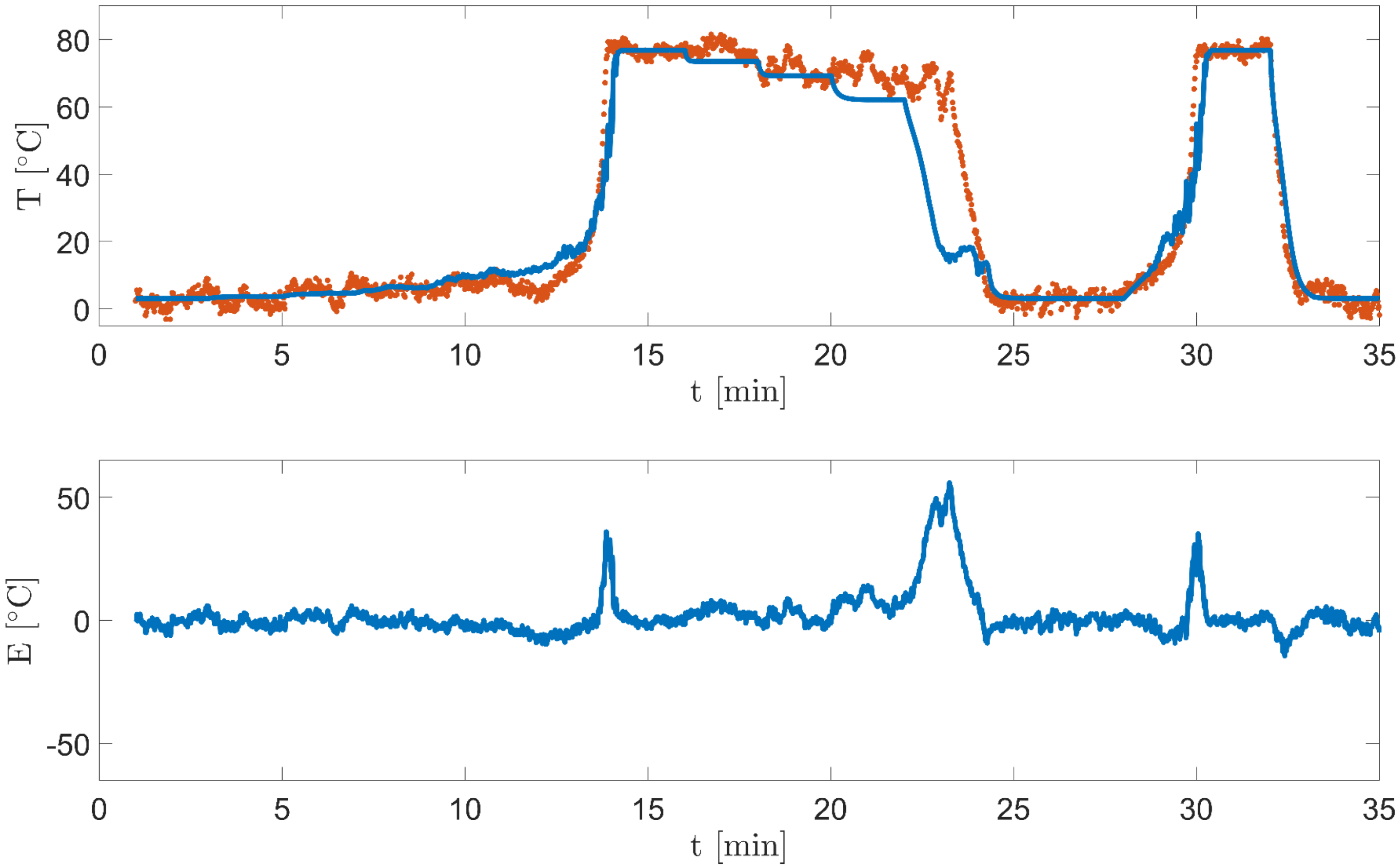
1-step predictions – MLE (1D)



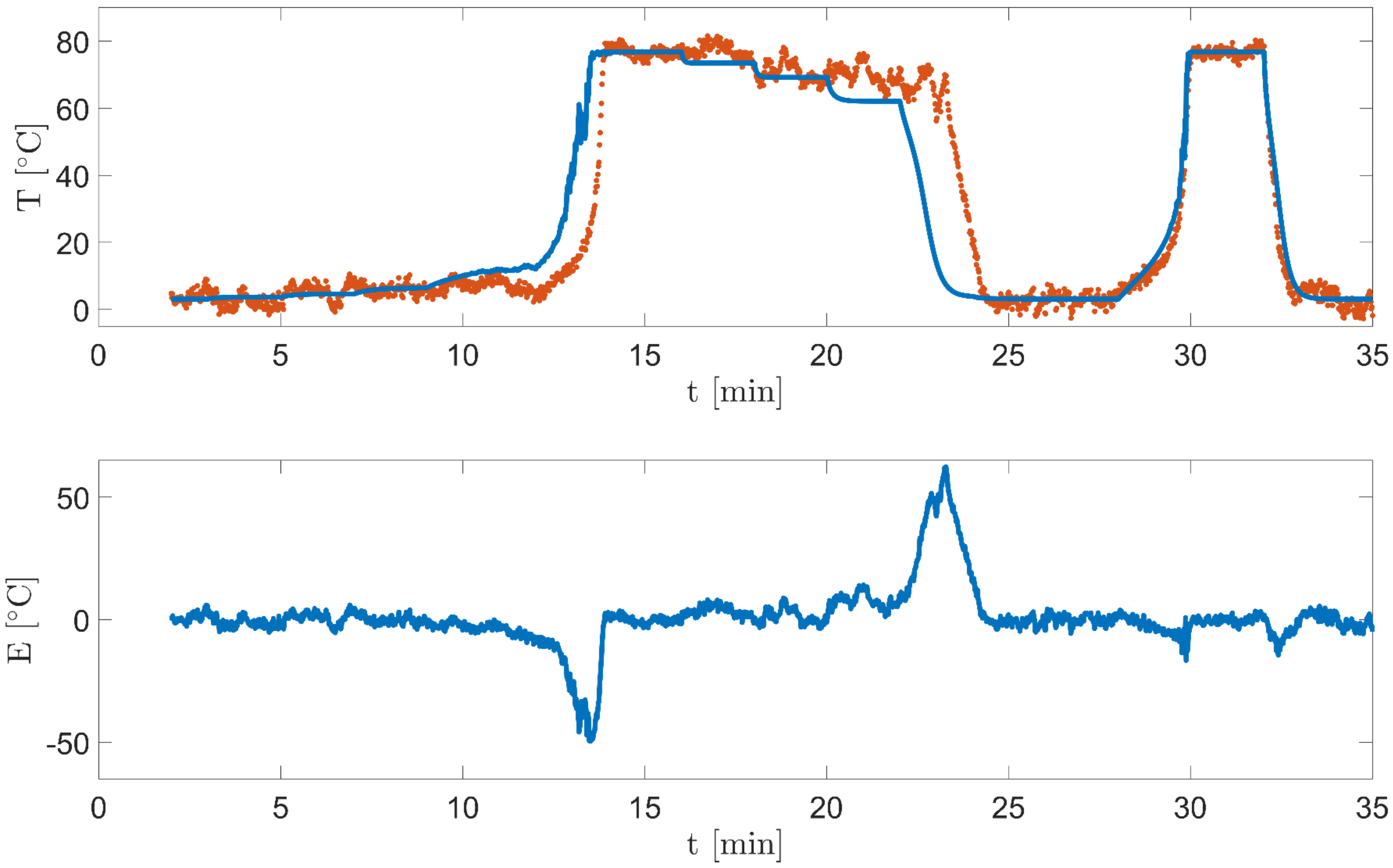
30-step predictions – MLE (1D)



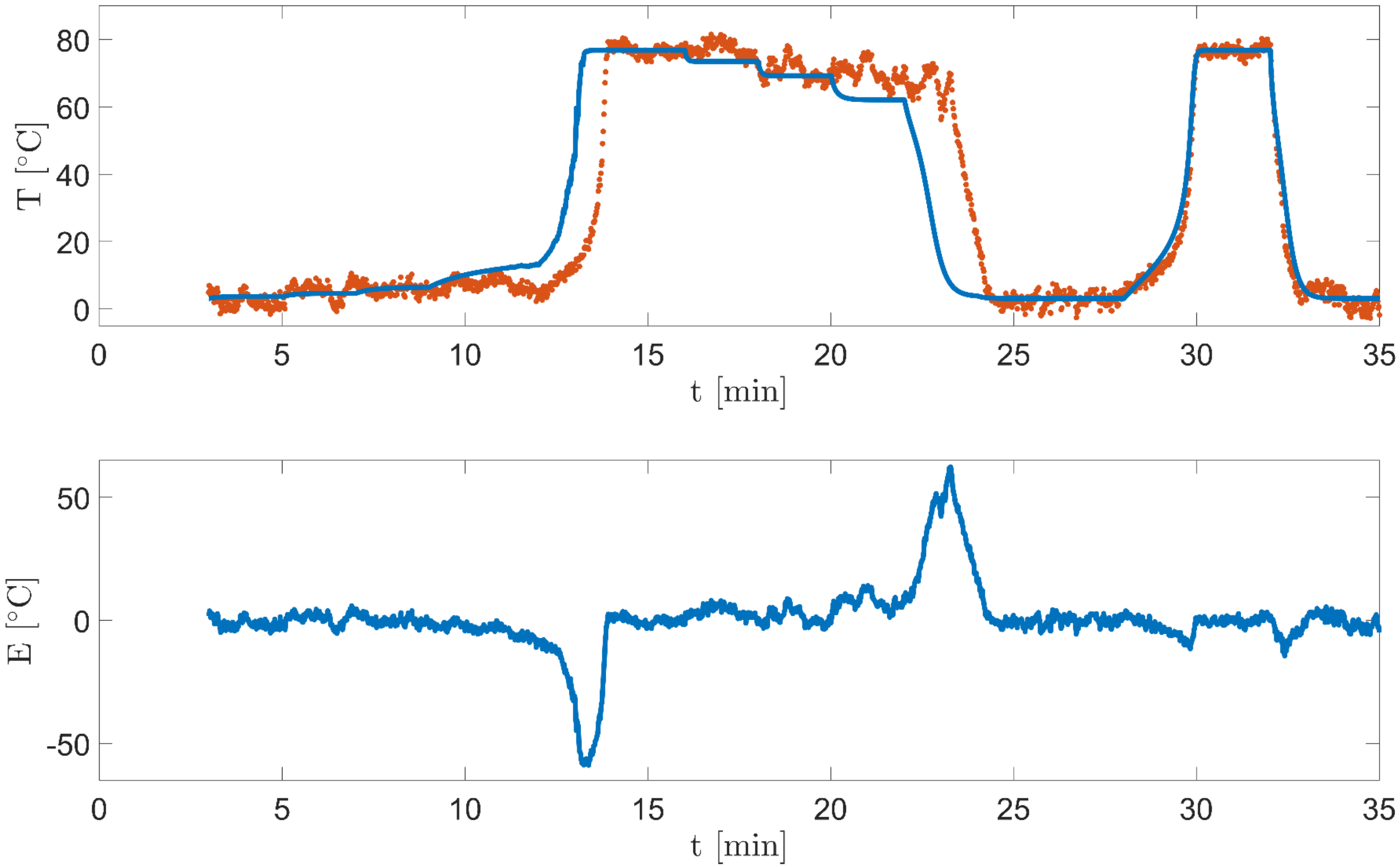
60-step predictions – MLE (1D)



120-step predictions – MLE (1D)

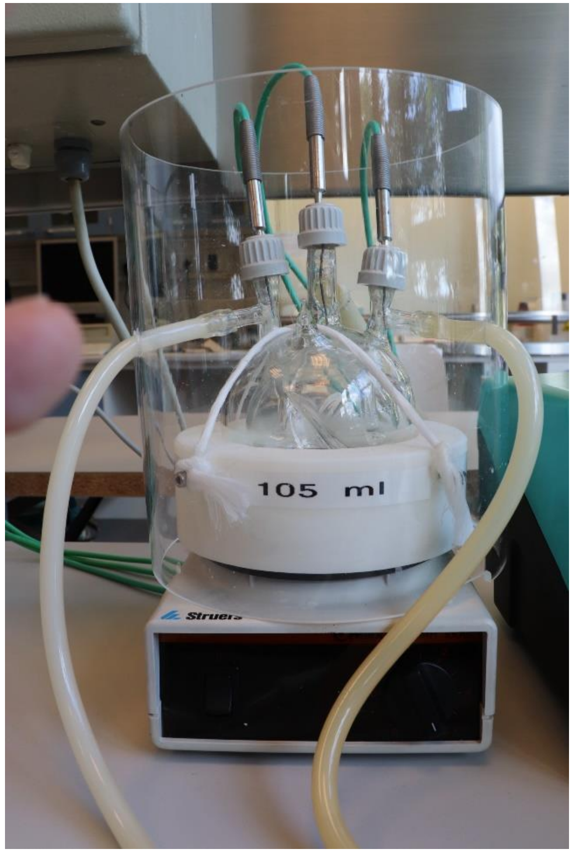


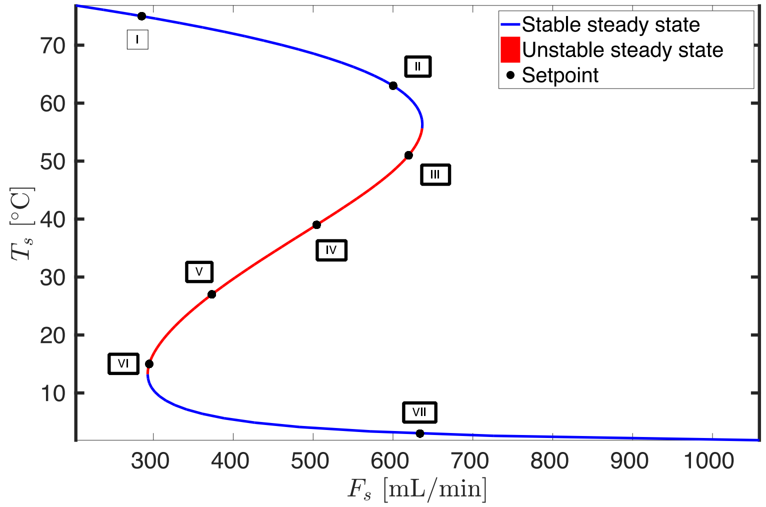
180-step predictions – MLE (1D)

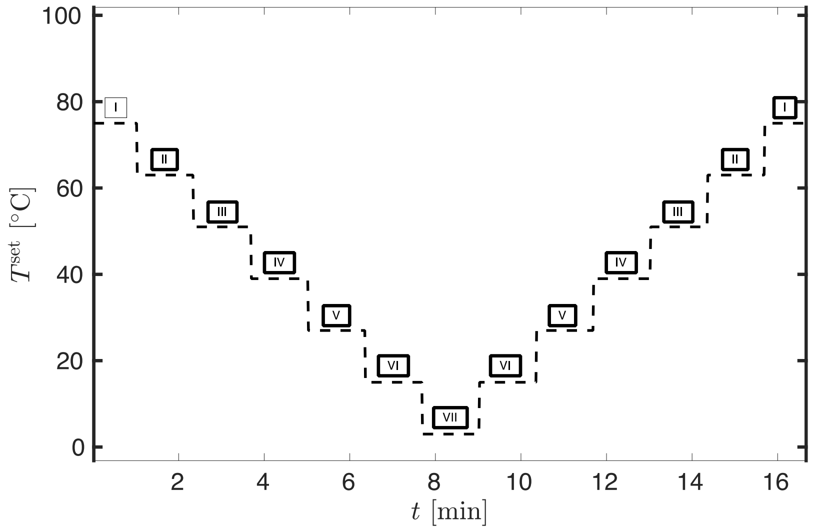


Nonlinear Model Predictive Control

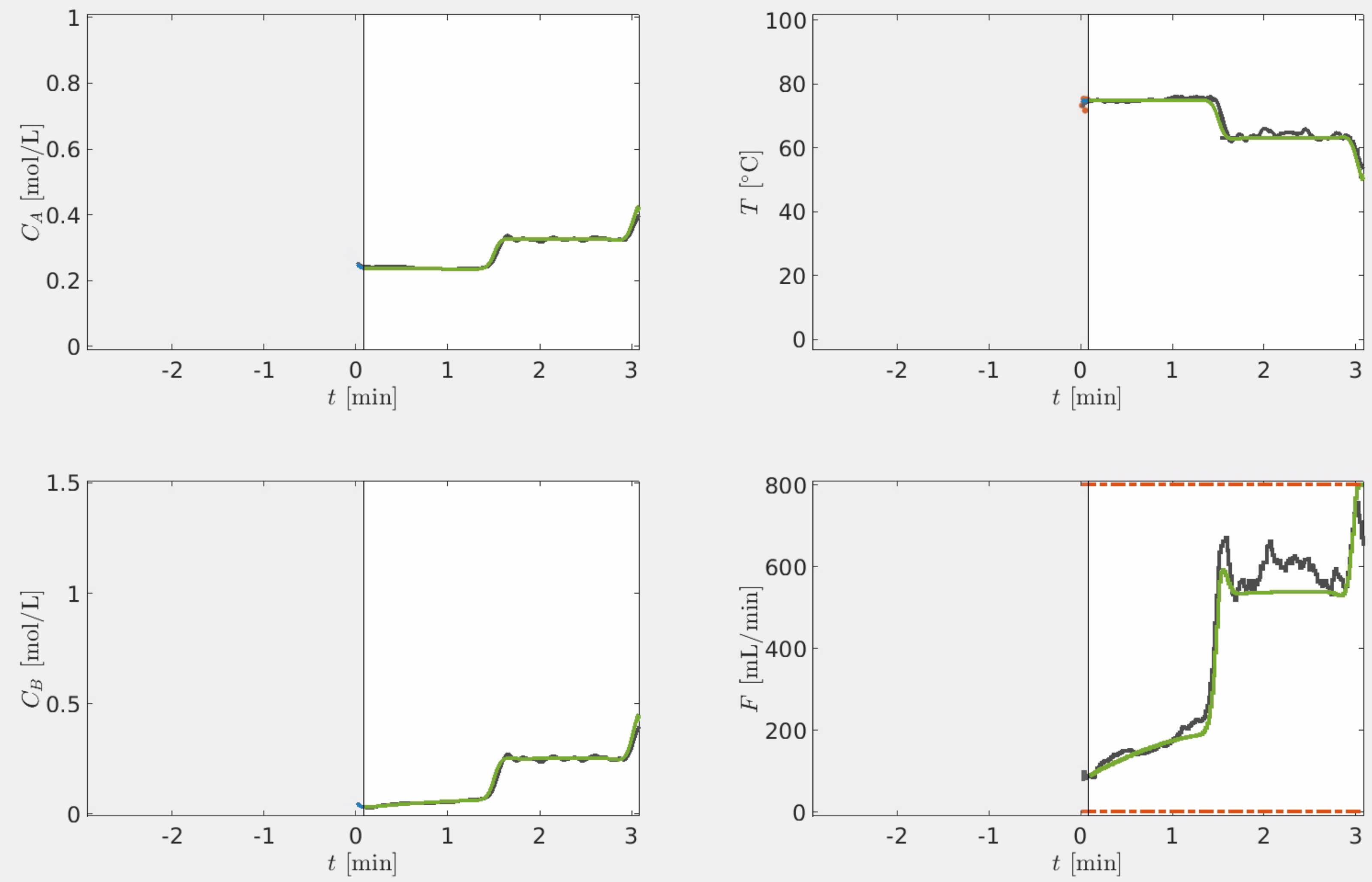
Multiple Steady States



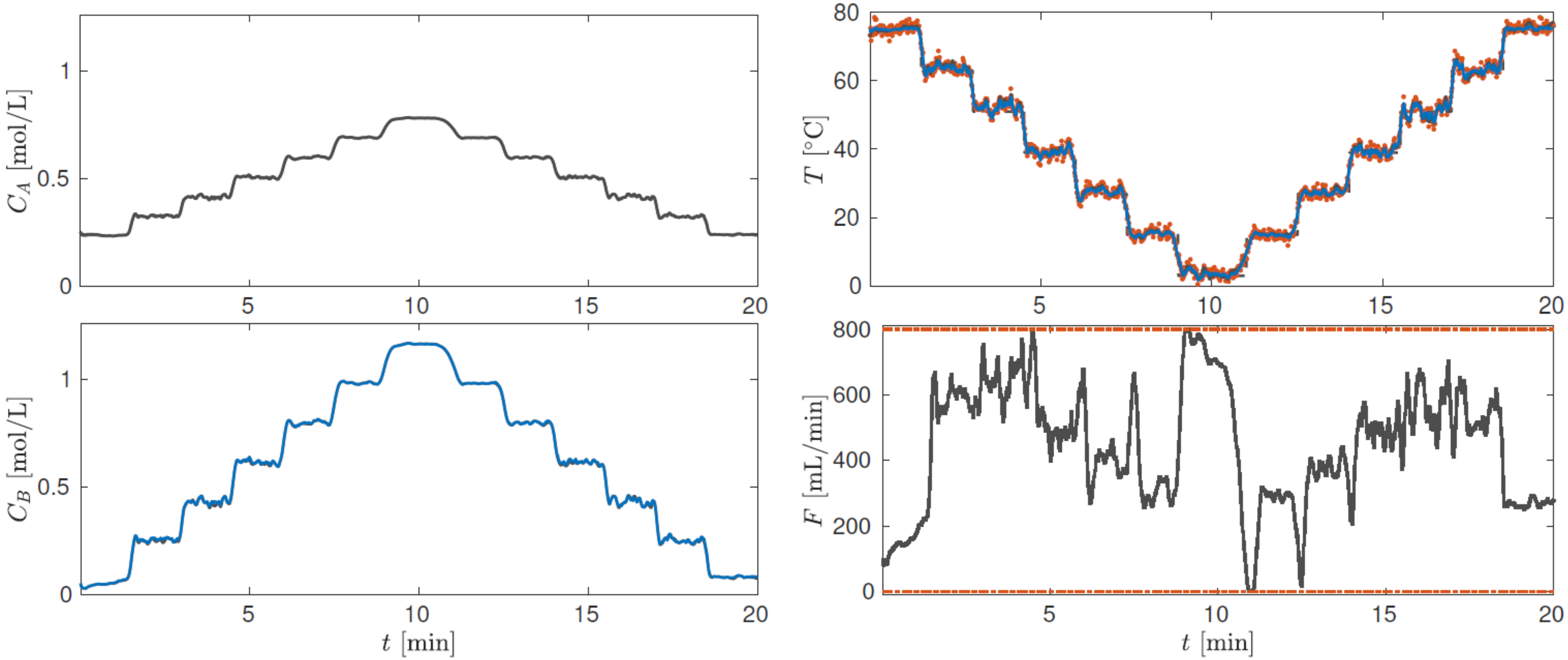




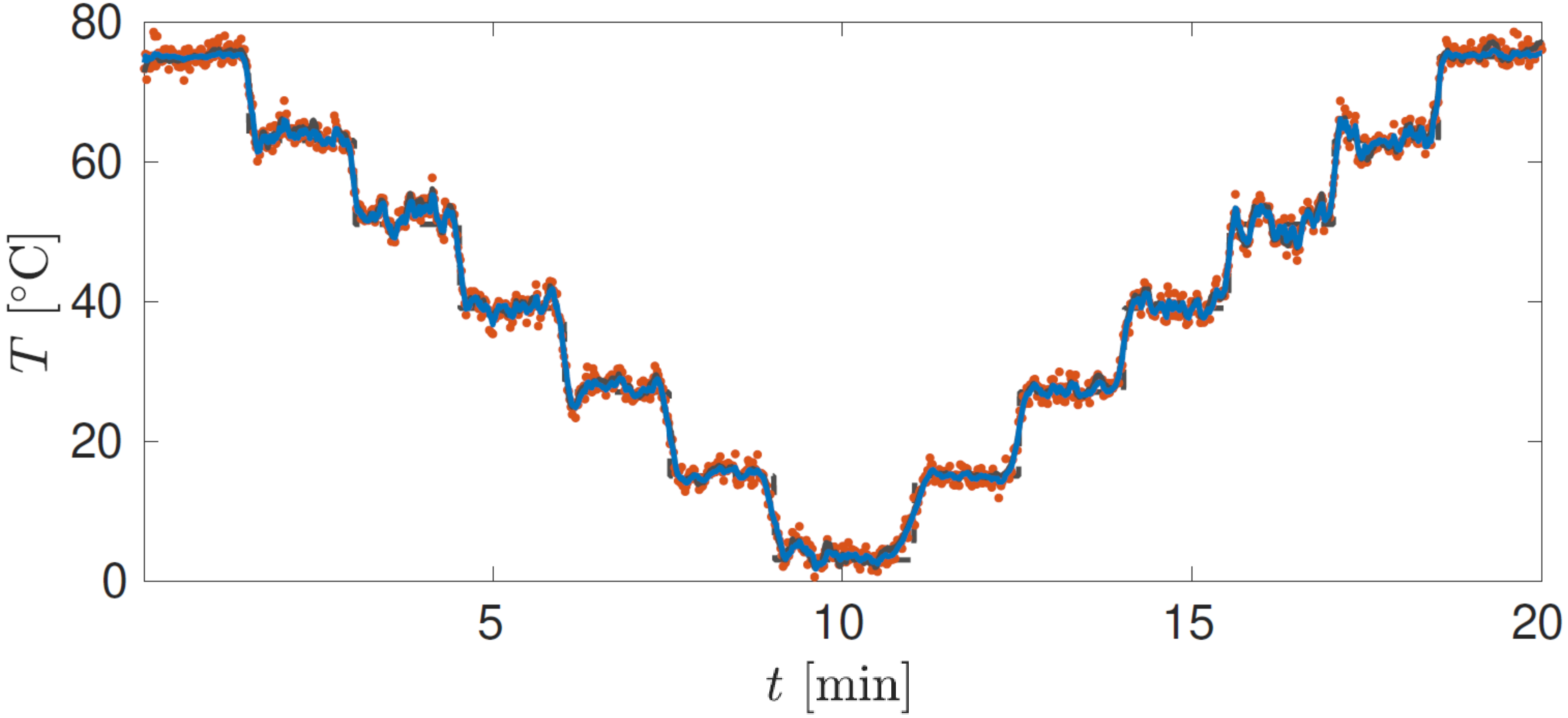
Movie of NMPC
(with true profiles in the prediction window)



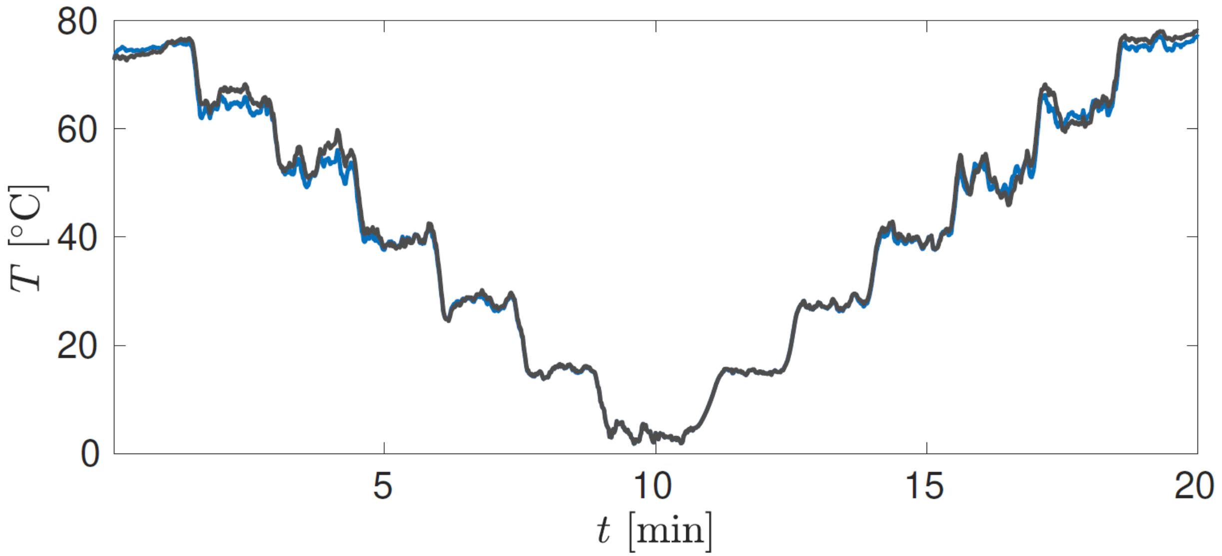
Nonlinear MPC - Closed-Loop Results

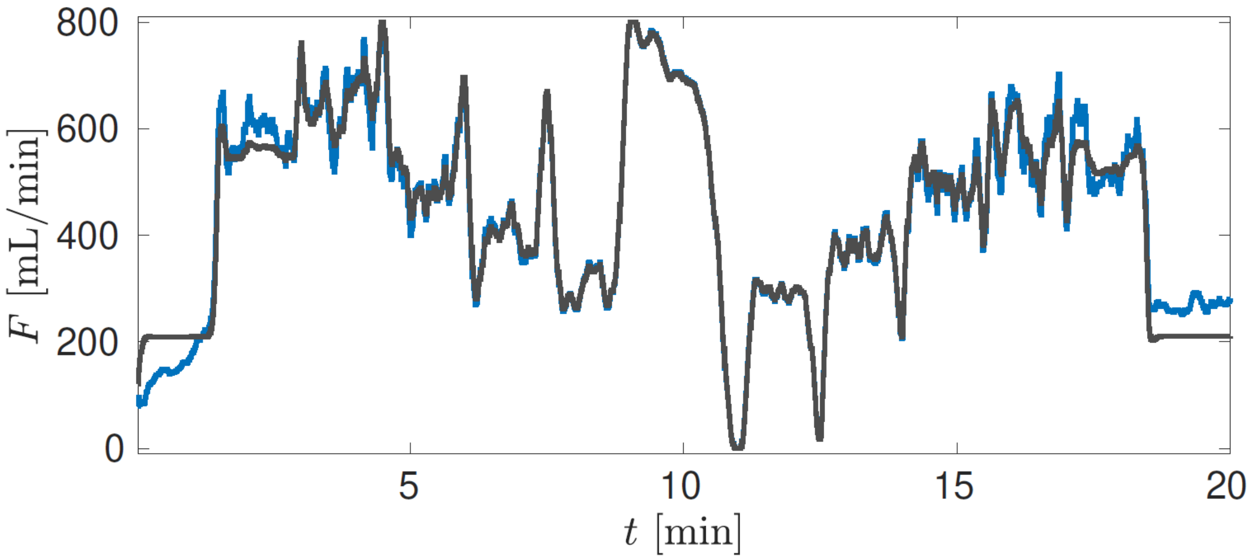


Nonlinear MPC - Closed-Loop Results (temperature)

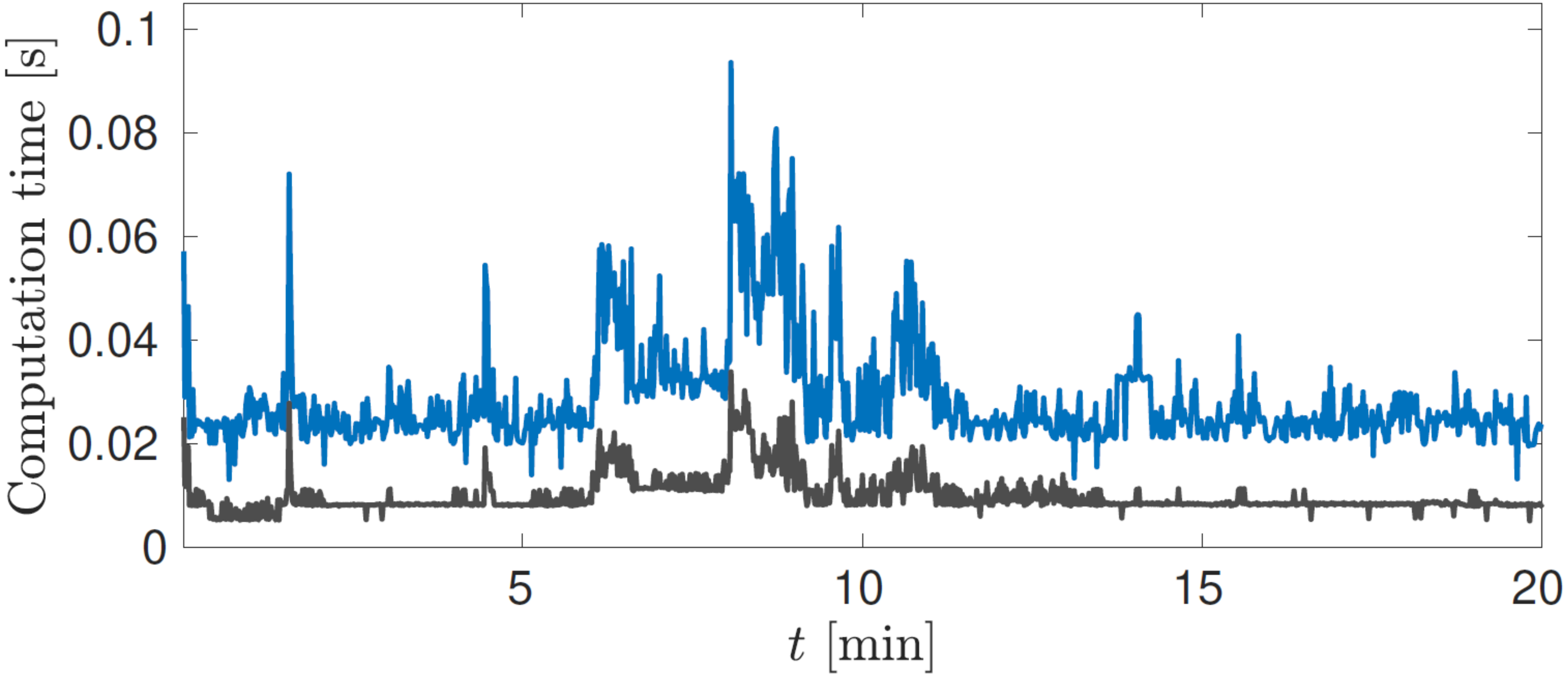


Closed-loop NMPC – 3D model – 1D model





CPU time for the NMPC – 3D model – 1D model

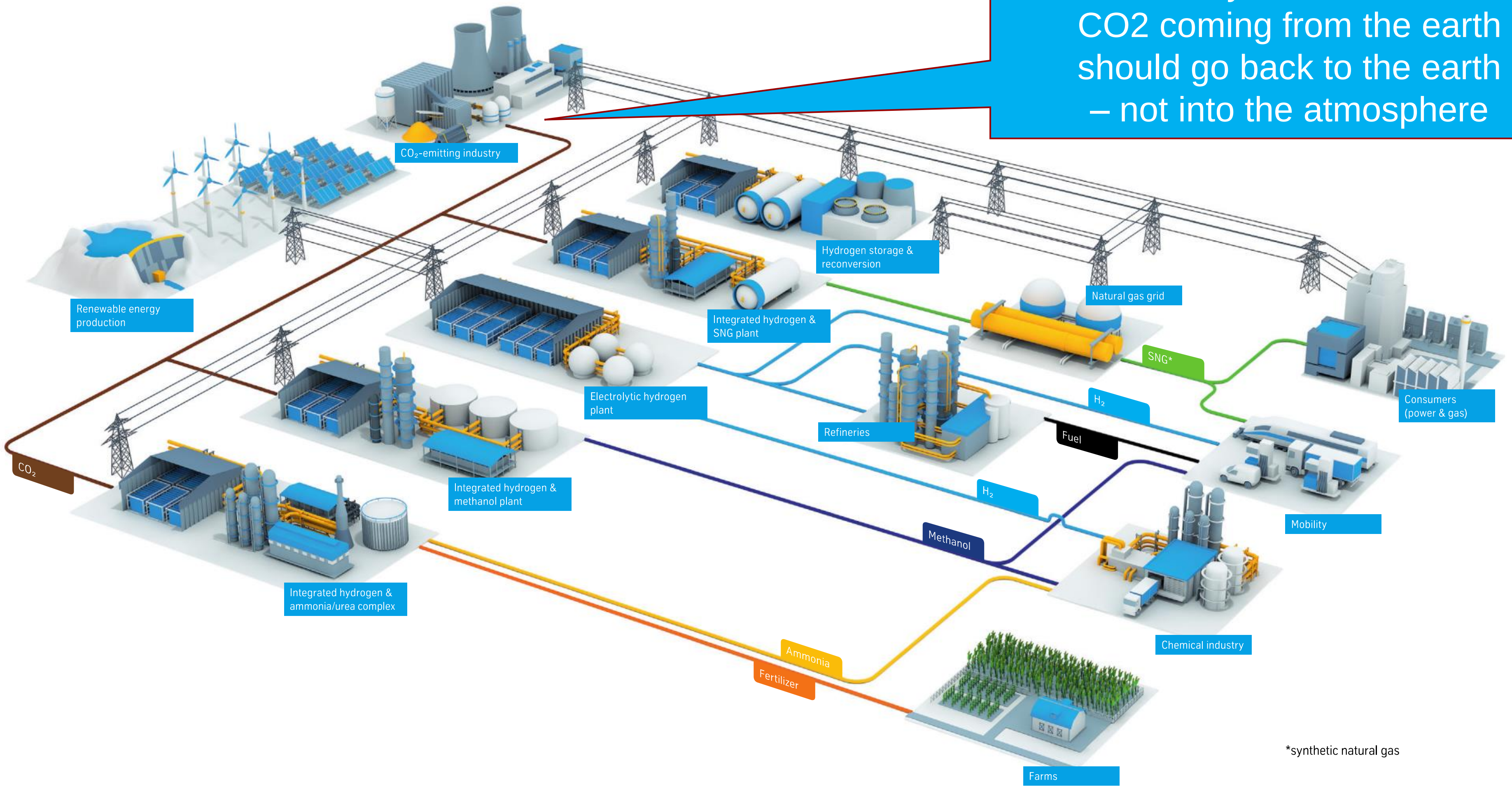


Mission Green Fuels - DYNFLEX

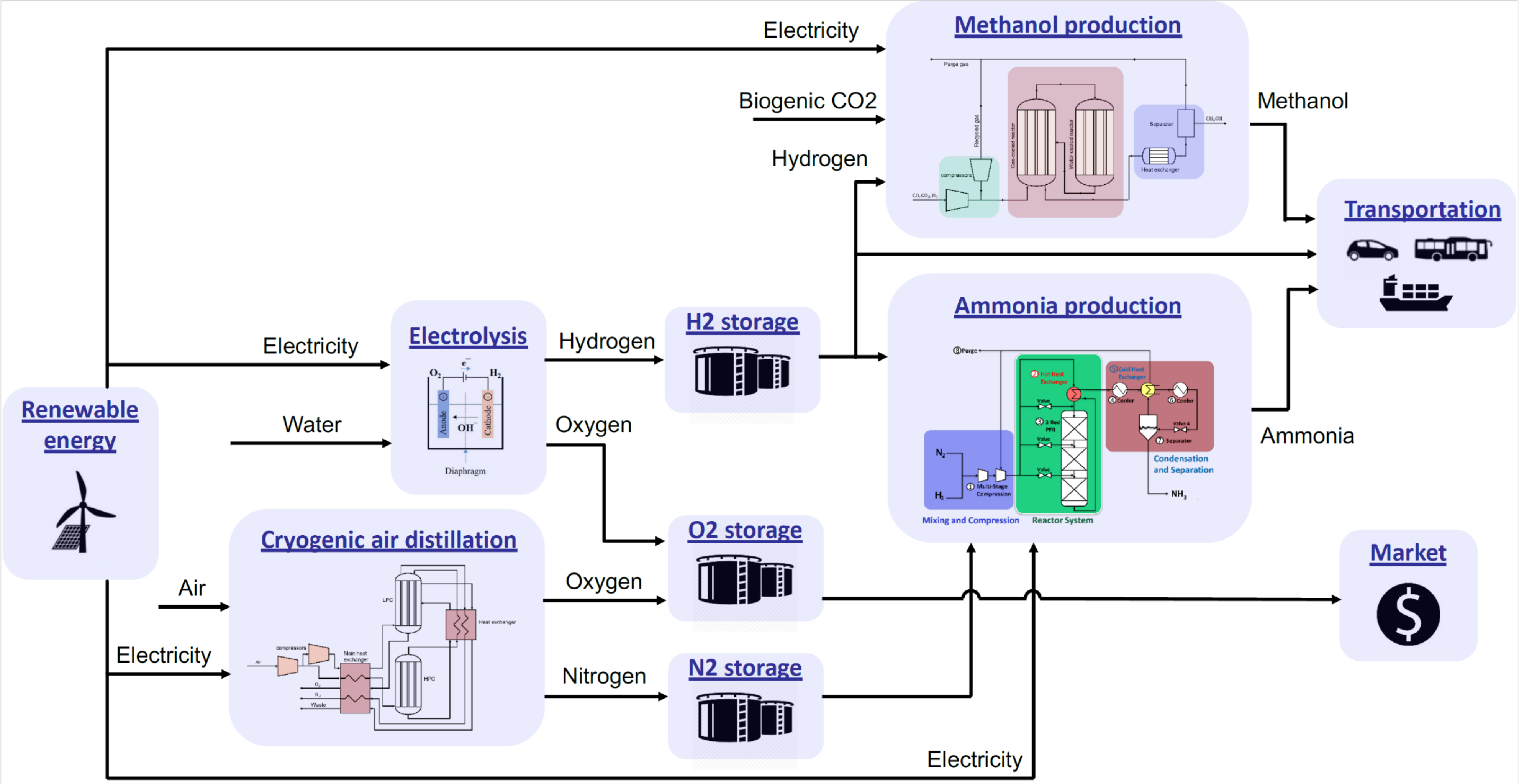
Power-2-Ammonia

Carbon Capture, Storage and Utilization (CCUS) & Power-2-X
Advanced Process Control (APC) for coordination and optimization

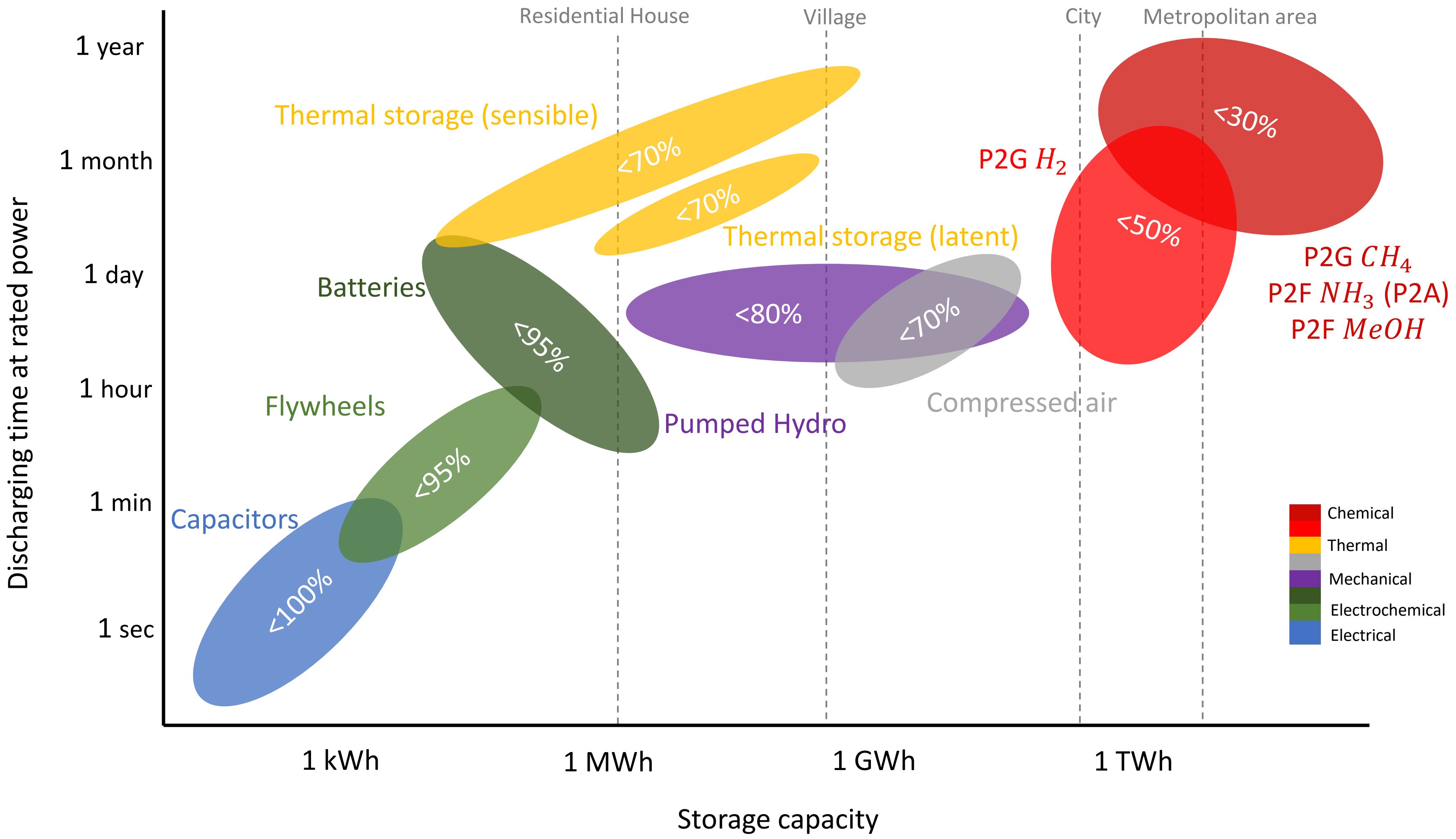
Key Problem:
CO_2 coming from the earth should go back to the earth – not into the atmosphere



Power-2-X for Green Fuels (H2, NH3, CH3OH)



Energy storage systems (ESSs) - Classification



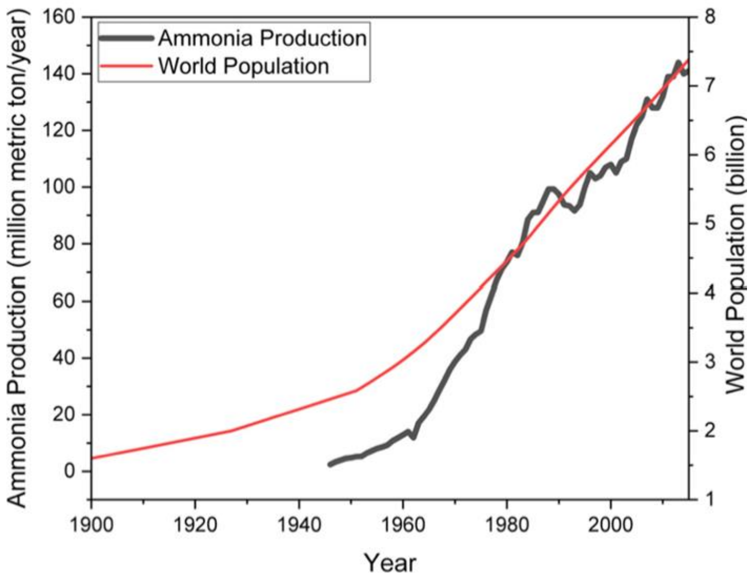
Why Power-2-Ammonia (P2A)?

- Conventional ammonia production constitutes 1-2% of the world's total CO_2 emissions.

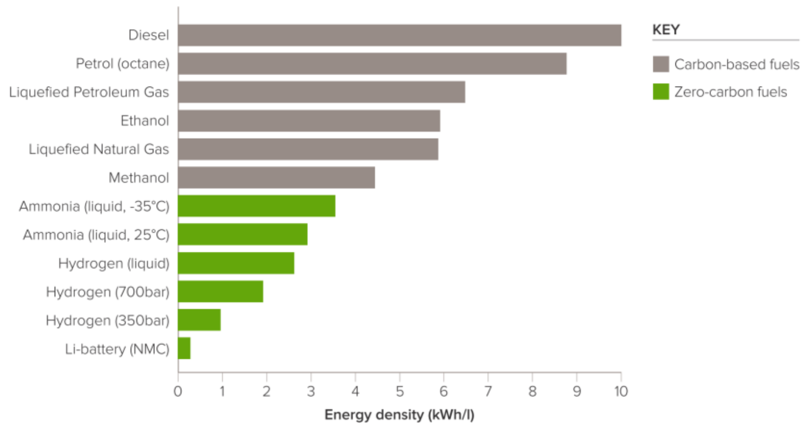
- Ammonia's main usage is as fertilizer for agriculture.

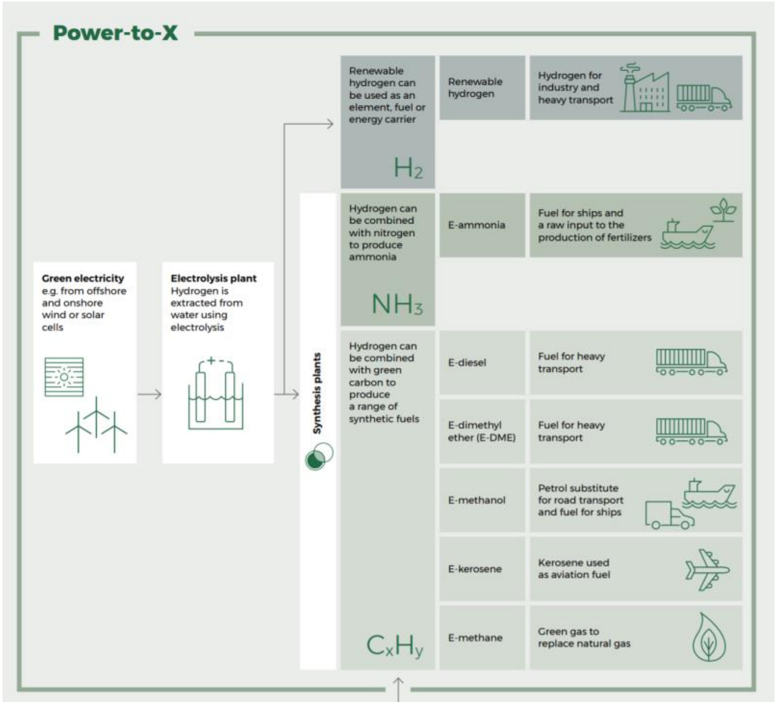
- Electrification of via intermittent energy sources: Wind, solar, ocean etc.

- Power-to-X for storage and transport of energy
  $2NH_3 + 1.5O_2 \rightarrow 3H_2O + N_2$ (382 kJ/mol)

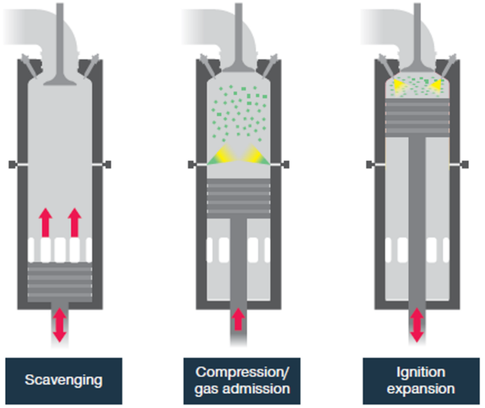


The volumetric energy density of a range of fuel options.



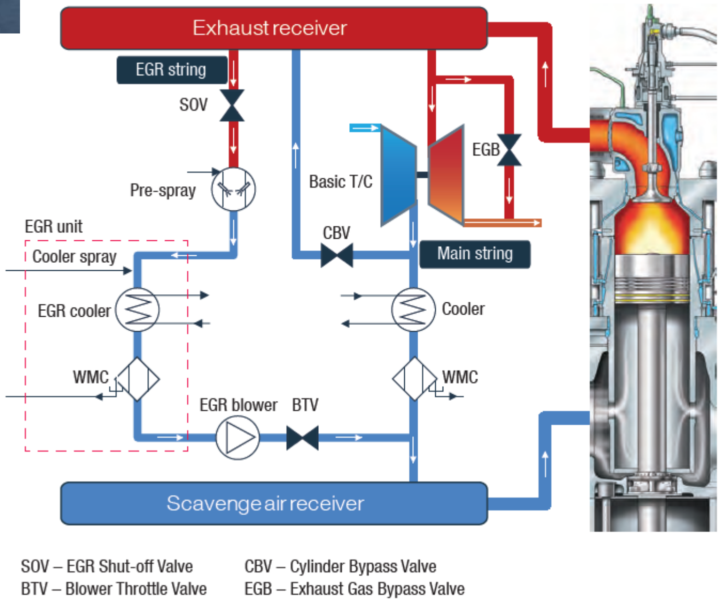


NH3 / CH3OH Ship Engines – MAN. MPC for a new generation of ship engines



Two-stroke Otto cycle (pre-mixed)

Power output ranging up to 82.4 MW



Process diagram

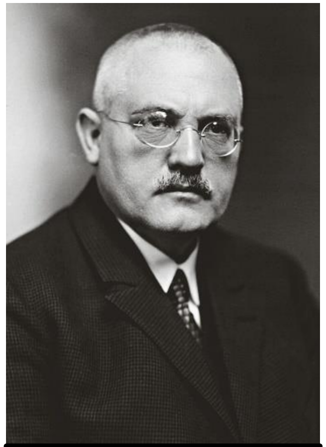
Reinventing the wheel?

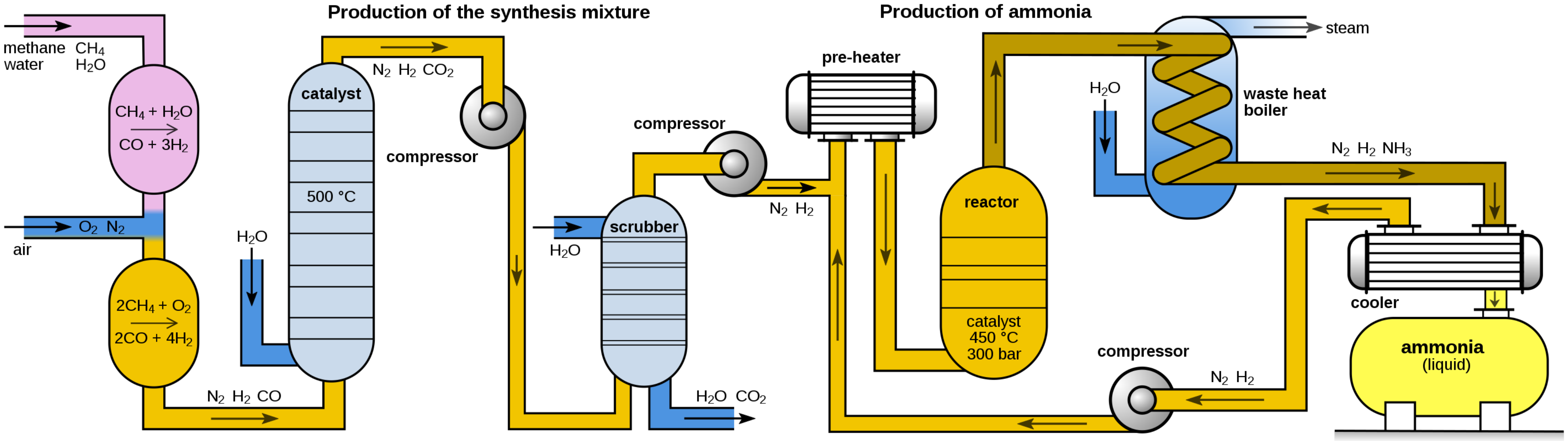
- Fritz Haber and Carl Bosch invented the Haber-Bosch process in early 1900.
- Harber-Bosch Process: Catalyst reaction at 200 bar and 650-800 K.

$$N_2 + 3H_2 \rightarrow 2NH_3$$

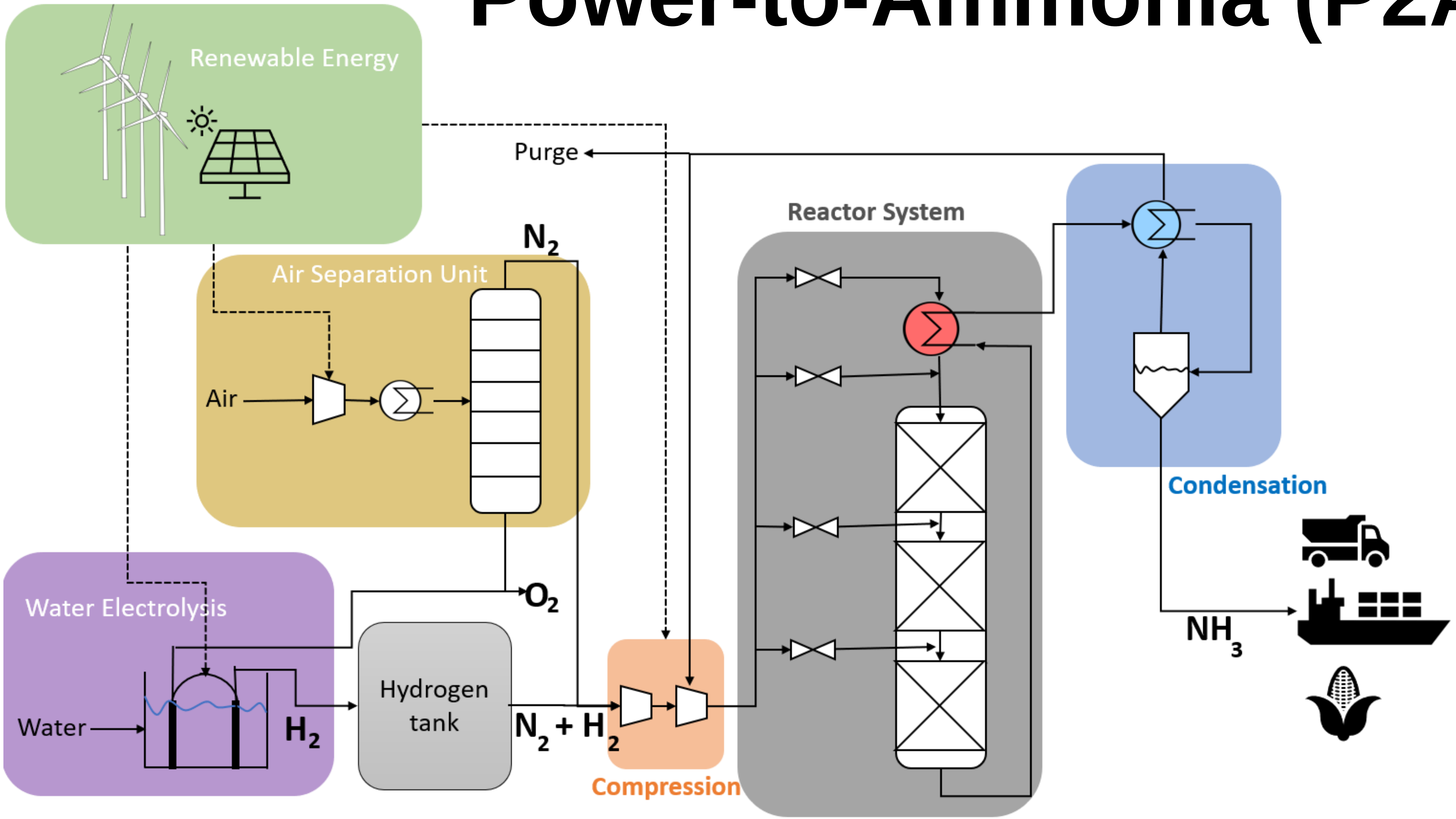
- Stable and reliable supply of reactants.


Fritz Haber


Carl Bosch

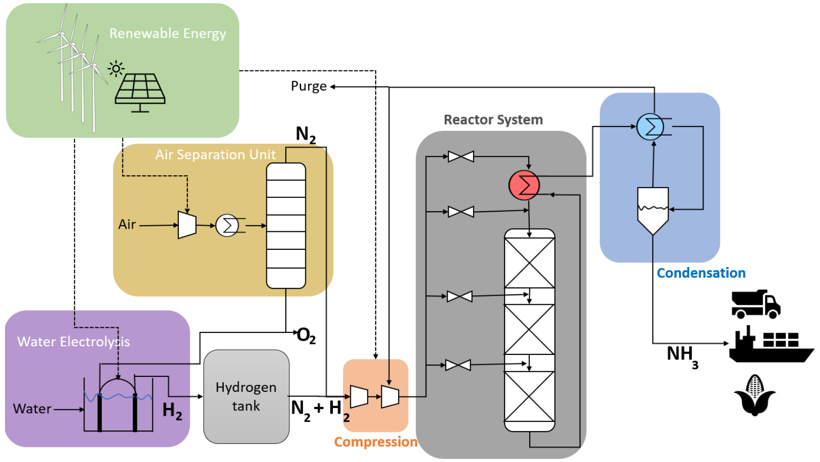


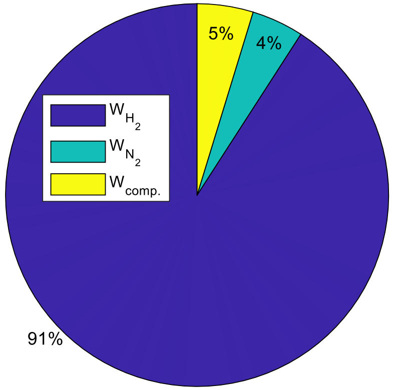
Power-to-Ammonia (P2A)

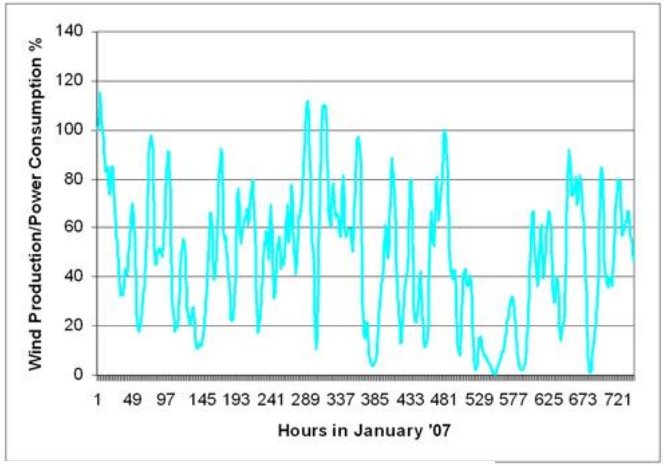


Flexible operation

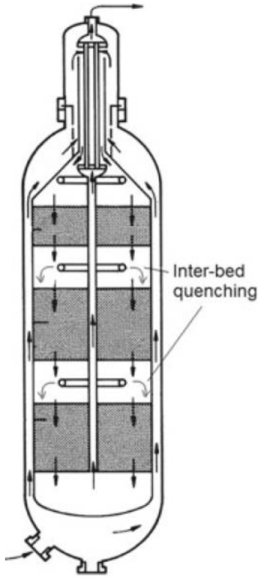
- Intermittent renewable energy sources: Wind, solar, ocean etc.
- Ammonia reactor systems are inherently oscillatory and easily become unstable.
- 91 % of power input consumed by electrolyzers for H_2 production.
- How do we ensure safe and optimal operation over an operating window from 20% - 120 % of nominal power.

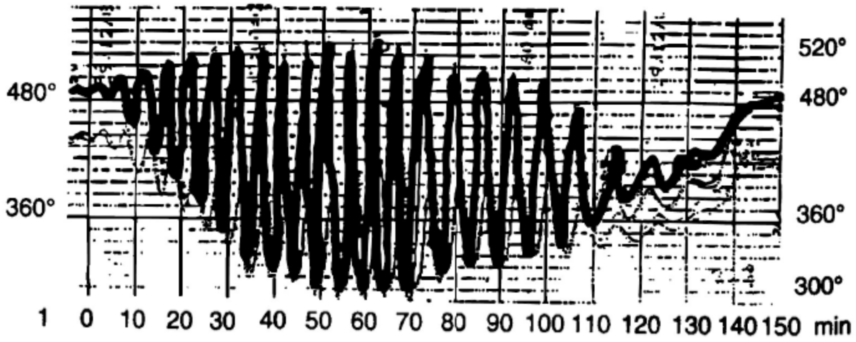






Danish wind power data





Naess et al. (1992)

Power-to-Ammonia (P2A)

Boundary 1: Reactor system

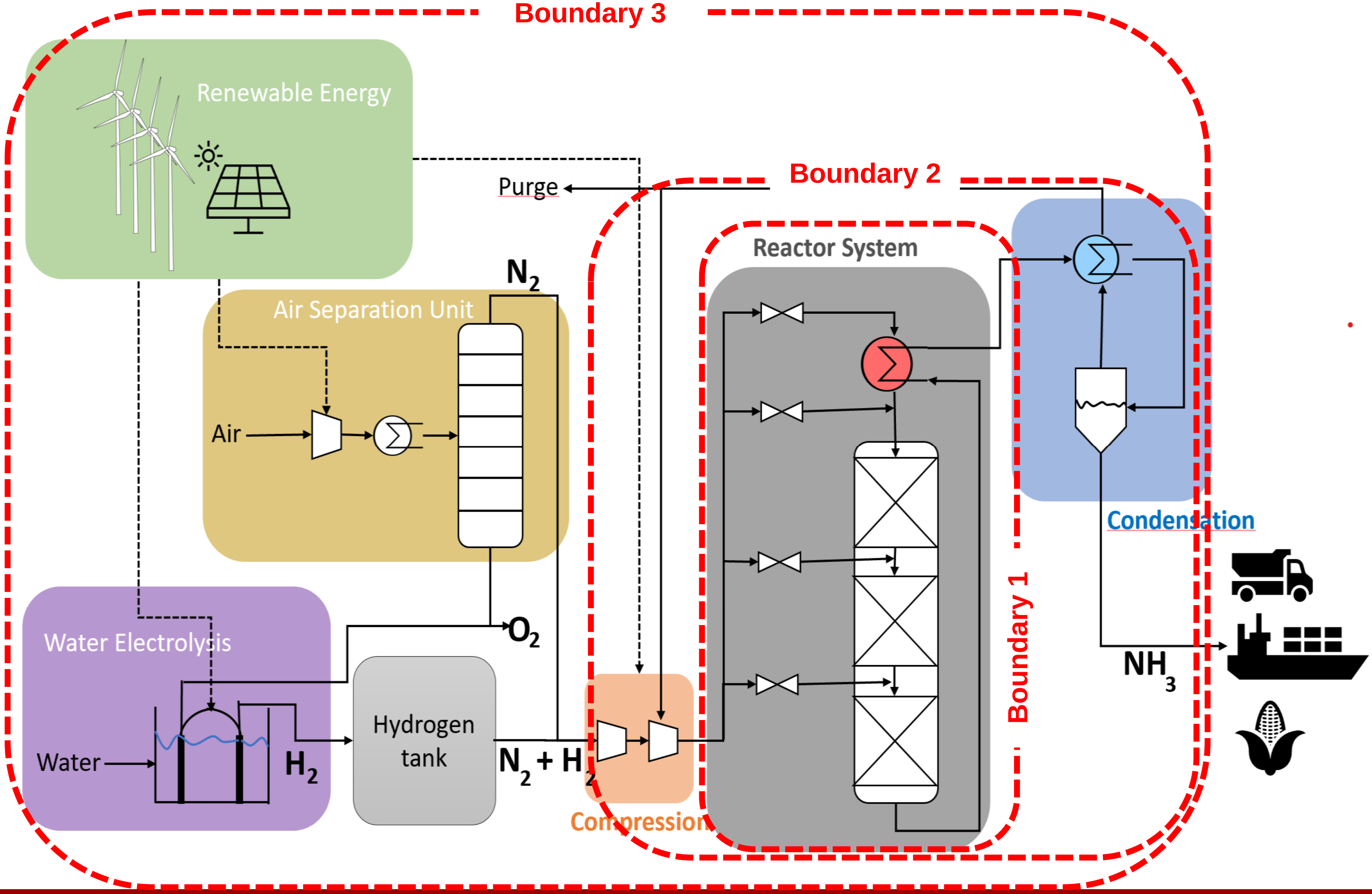
- Control and optimization of the reactor system via the quench flows.

Boundary 2: Synthesis loop

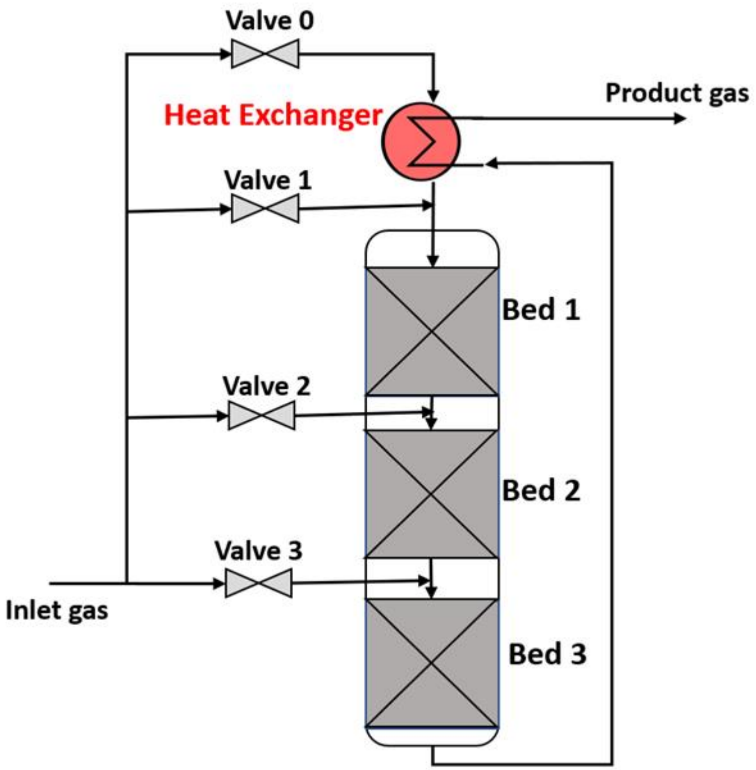
- Control compressors, NH_3 separation unit and purge fraction.

Boundary 3: P2A plant

- Forecasting of available energy (weather)
- Control and optimize production of H_2 and N_2 from electrolyser and ASU



Numerical Model



Thermophysical properties:

Enthalpy density [kJ/m^3]:

$\hat{H}_{g,k} = H(T_k, P_k, c_{g,k})$

Volume density [-]:

$\hat{V}_{g,k} = V(T_k, P_k, c_{g,k})$

Internal energy density [kJ/m^3]:

$\hat{U}_{g,k} = \hat{H}_{g,k} - P_k \hat{V}_{g,k}$

$\hat{U}_{s,k} = \rho_s c_{p,s}(T_k - T_0)$

$\hat{U}_{r,k} = U_r(T_k, P_k, c_{g,k}) = \varepsilon \hat{U}_{g,k} + (1-\varepsilon)\hat{U}_{s,k}$

Transport models:

Gas velocity [m/s]:

$\bar{v}_{g,k+\frac{1}{2}} = \pi(\Delta \bar{P}/\Delta z, \mu_{g,k+\frac{1}{2}}, \rho_{g,k+\frac{1}{2}}),$

$$v_{g,k+\frac{1}{2}} = \begin{cases} -\bar{v}_{g,k+\frac{1}{2}} & \Delta P > 0 \\ \bar{v}_{g,k+\frac{1}{2}} & \Delta P \leq 0 \end{cases}$$

Molar flux, gas [kmol/(m^2·s)]:

$N_{g,k+\frac{1}{2}} = N_{g,a,k+\frac{1}{2}} + N_{g,d,k+\frac{1}{2}},$

$N_{g,a,k+\frac{1}{2}} = v_{g,k+\frac{1}{2}} \bar{c}_{g,k+\frac{1}{2}},$

$N_{g,d,k+\frac{1}{2}} = -D_{k+\frac{1}{2}} \odot \frac{c_{g,k+1} - c_{g,k}}{\Delta z}.$

Energy flux [kJ/(m^2·s)]:

$\tilde{H}_{g,k+\frac{1}{2}} = H(\bar{T}_{k+\frac{1}{2}}, \bar{P}_{k+\frac{1}{2}}, N_{g,k+\frac{1}{2}}),$

$Q_{s,k+\frac{1}{2}} = -\kappa \frac{T_{k+1} - T_k}{\Delta z}.$

Stoichiometry and kinetics:

Reaction rate [kmol/(m^3-gas· s)]:

$r_k = r(T_k, P_k, c_{g,k})$

Production rate [kmol/(m^3-gas· s)]:

$R_k = \nu' r_k$

Mass- and energy balance:

$$\frac{\partial c_{g,k}(t)}{\partial t} = -\frac{N_{g,k+\frac{1}{2}}(t) - N_{g,k-\frac{1}{2}}(t)}{\Delta z} + R_k(t)$$

$$\frac{\partial \hat{U}_{r,k}(t)}{\partial t} = -\varepsilon \frac{\tilde{H}_{g,k+\frac{1}{2}}(t) - \tilde{H}_{g,k-\frac{1}{2}}(t)}{\Delta z} - (1-\varepsilon)\frac{Q_{s,k+1} - Q_{s,k-1}}{\Delta z}$$

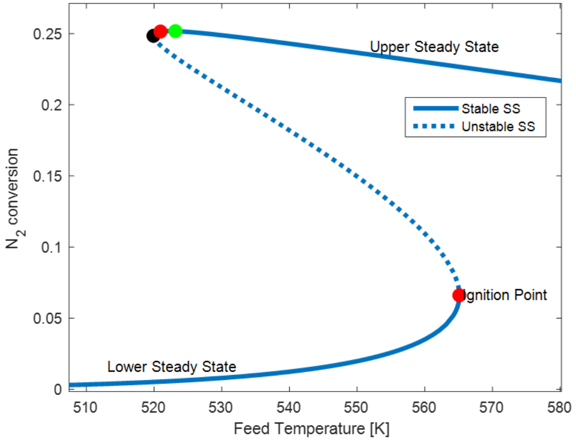
Algebraic equations:

$\hat{V}(T_k, P_k, c_{g,k}) - 1 = 0$

$U_r(T_k, P_k, c_{g,k}) - \hat{U}_{r,k} = 0$

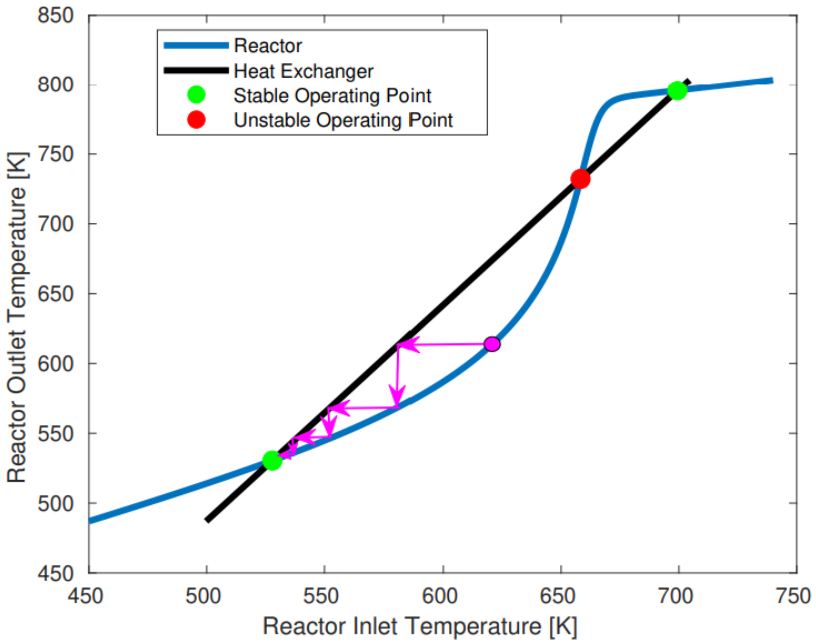
DAE Model

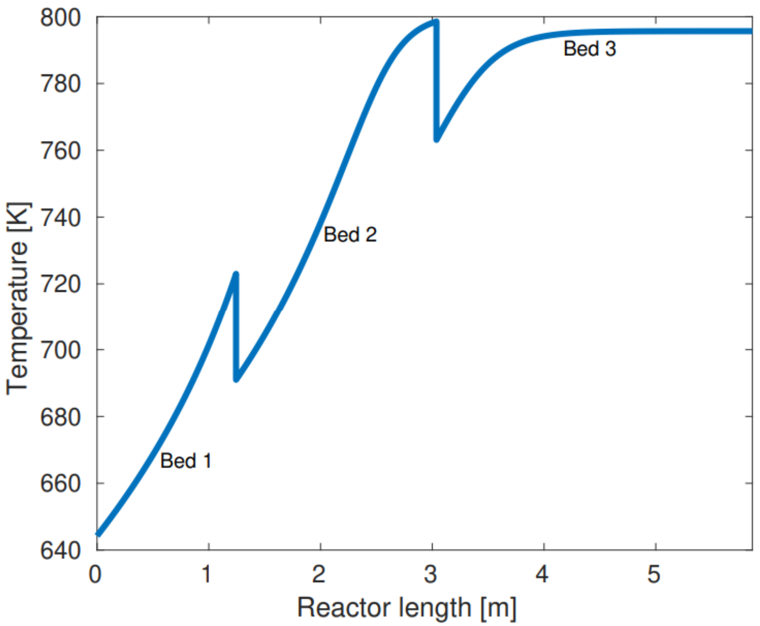
$$\dot{x}_k = f_k(x, y, u, p)$$
$$0 = g_k(x_k, y_k, p)$$

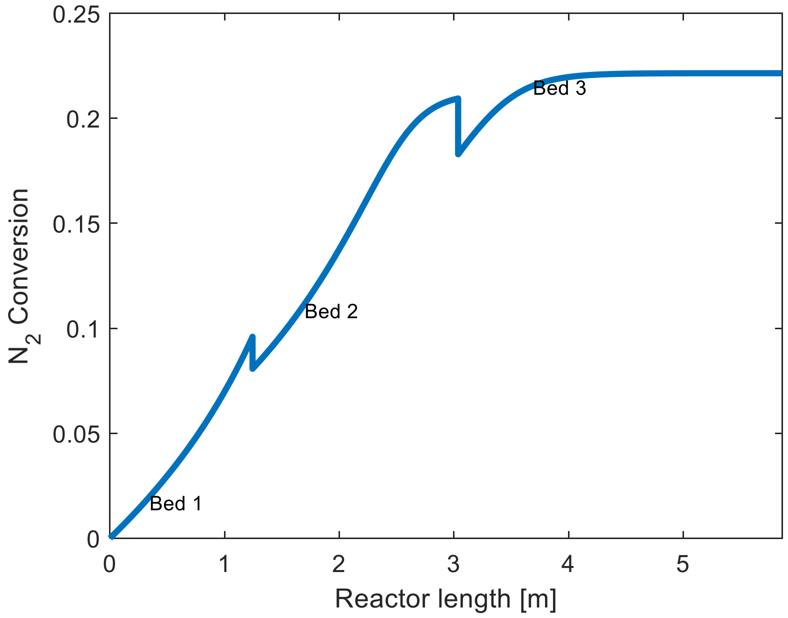


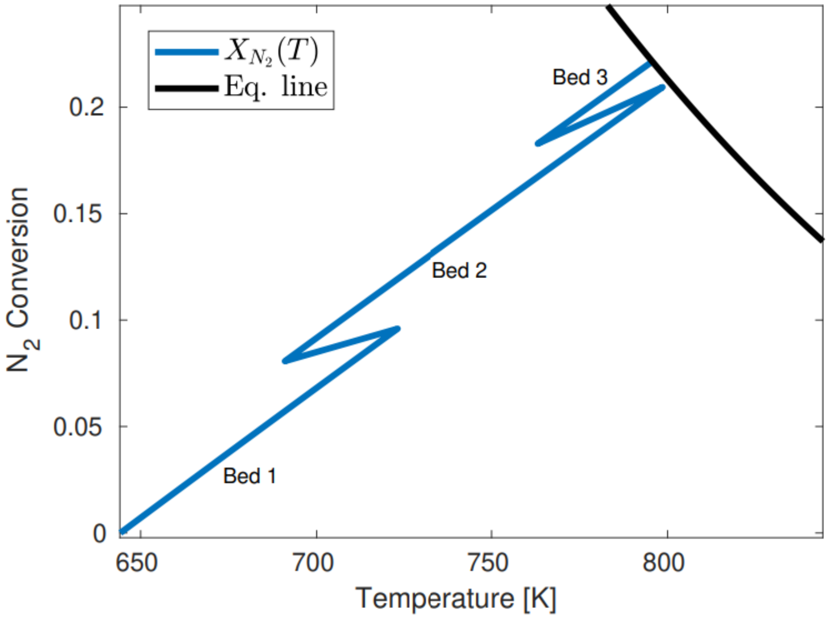
Steady state solution

- Van Heerden: 2 stable, 1 unstable OP
- Temperature: 640-800 K.
- Conversion: 22.5 % per reactor pass.



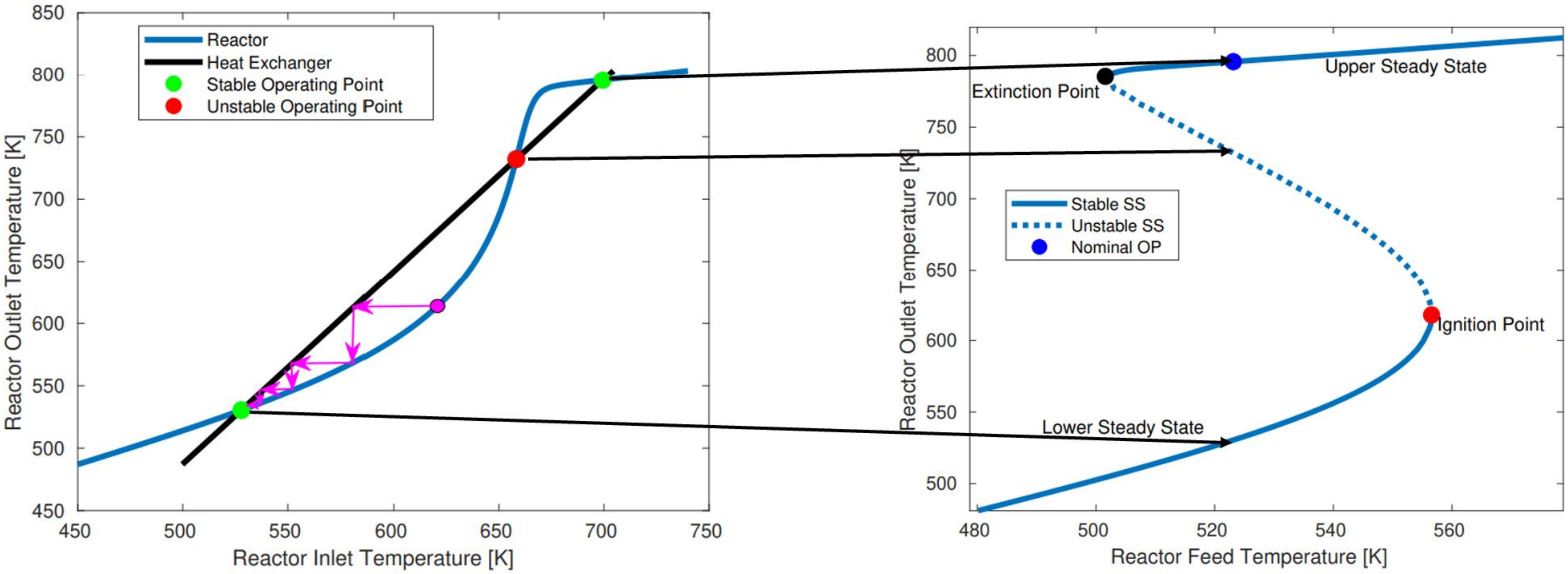






Steady state analysis

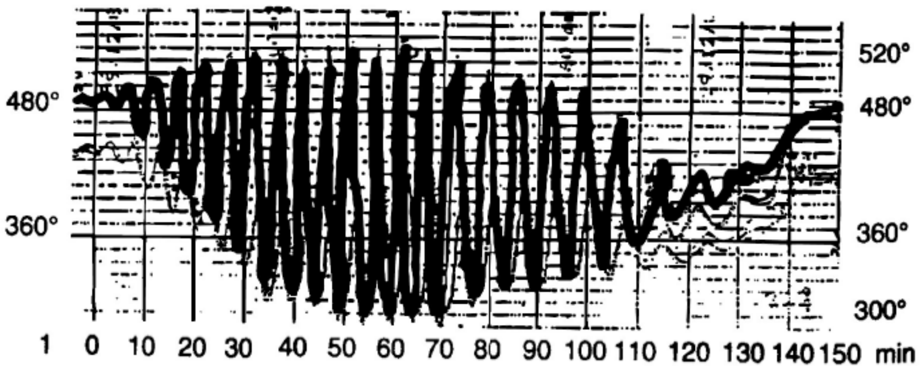
- Reactor S-Curve
- Range of multiple steady states
- Extinction and Ignition point



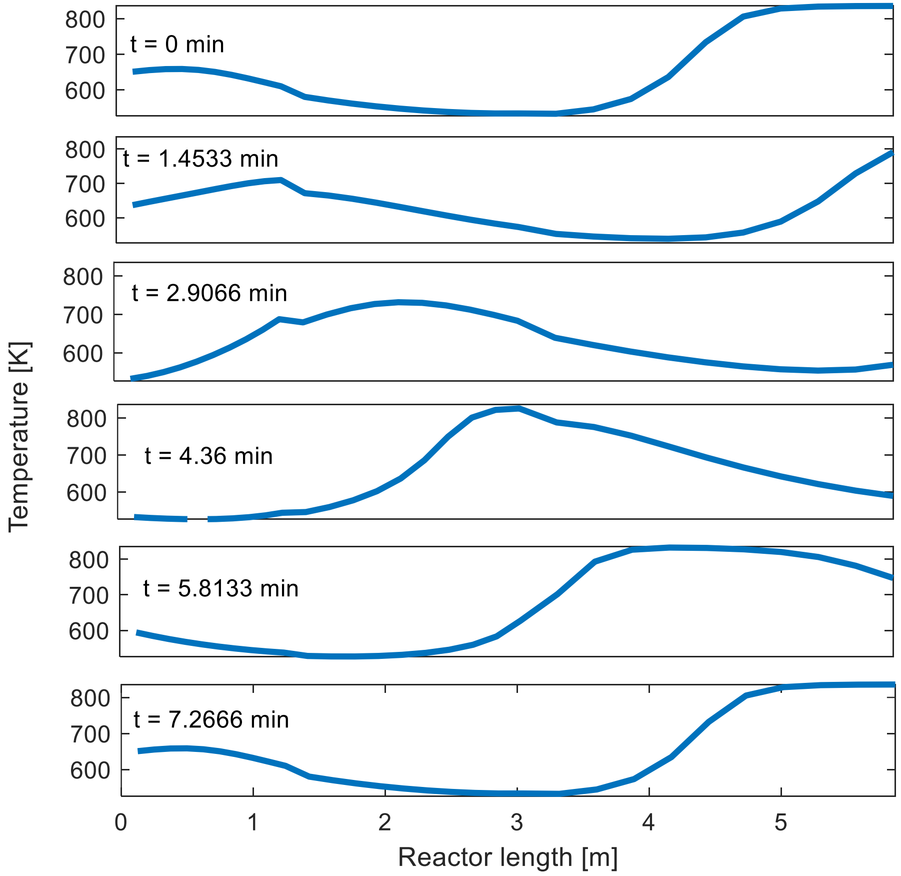
Transient simulation

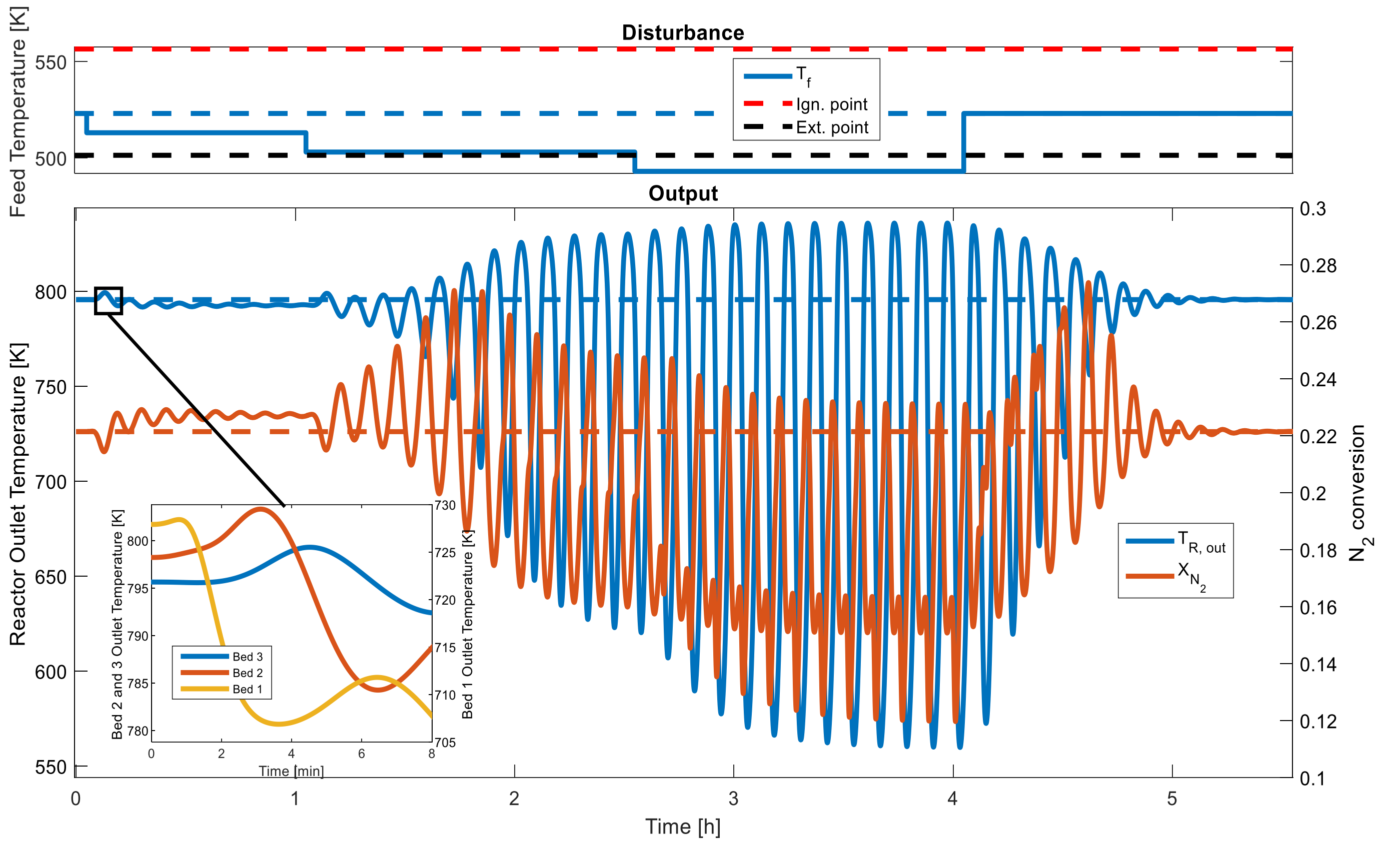
- System response to feed temperature step disturbances
- Initial inverse response.
- Differential flow of heat and matter.

Naess et al. (1992)



Sudden reduction in pressure: 200bar → 150bar





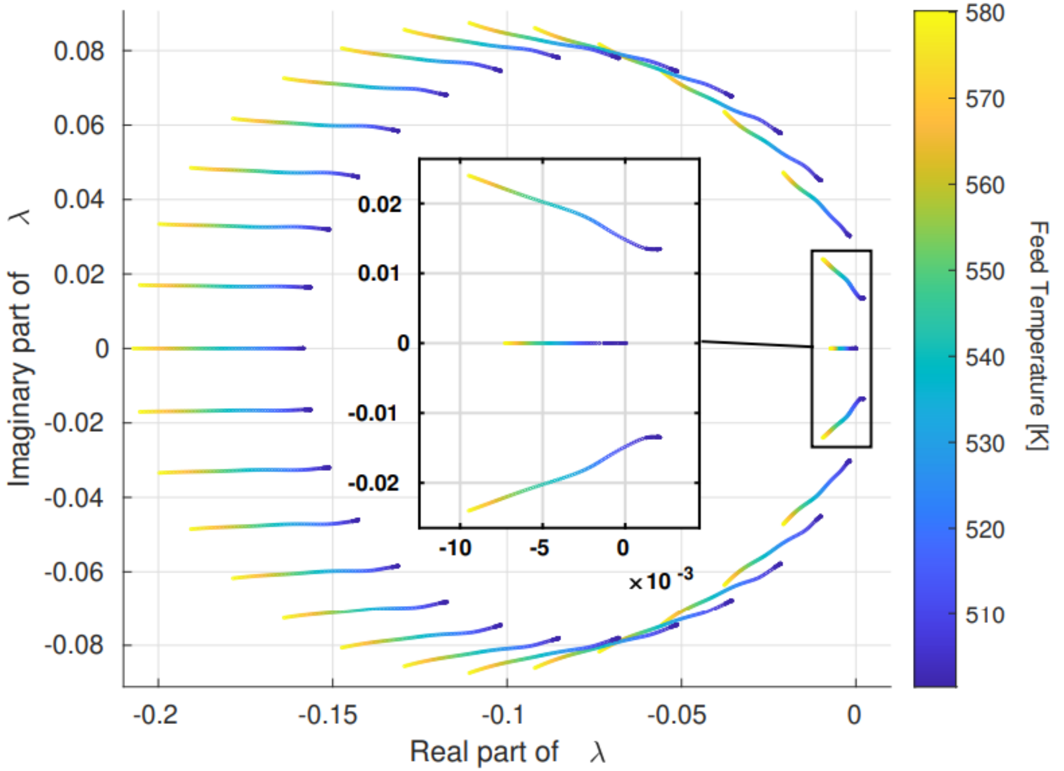
Bifurcation analysis

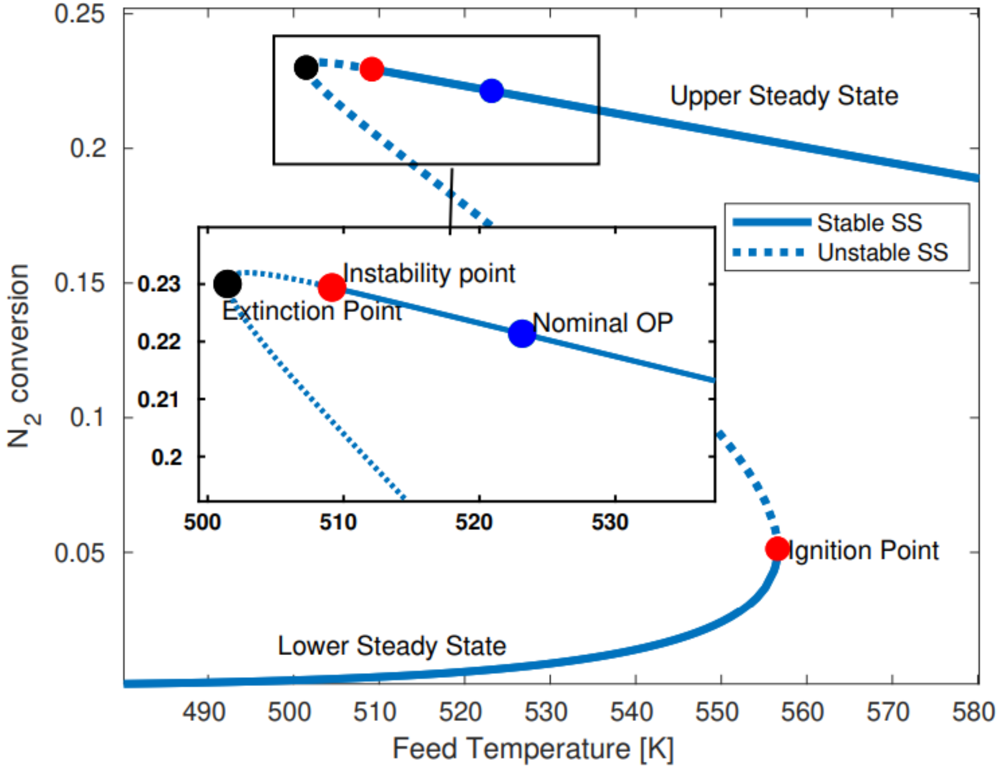
- Linearize system

$$\dot{\boldsymbol{T}} = \boldsymbol{A}\boldsymbol{T}$$

- Employ T_f as bifurcation parameter
- Hopf bifurcation point at $T_f = 510$ K with

$$\omega = \text{Im}(\lambda_{\max}) = \pm 0.0146 \text{rad/s} \qquad \tau_{osc} = \frac{2\pi}{\omega} = 430\text{s} = 7.16\text{min}$$



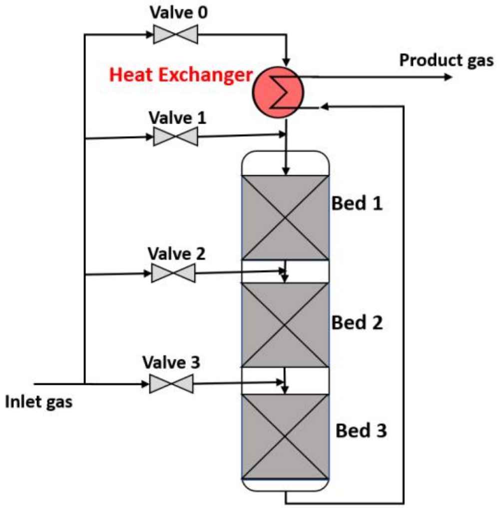


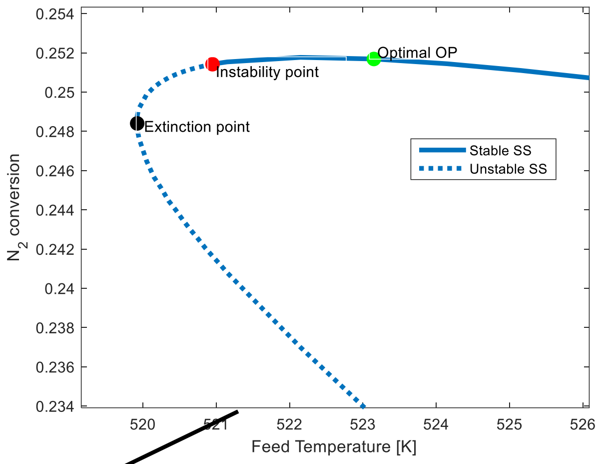
Optimization

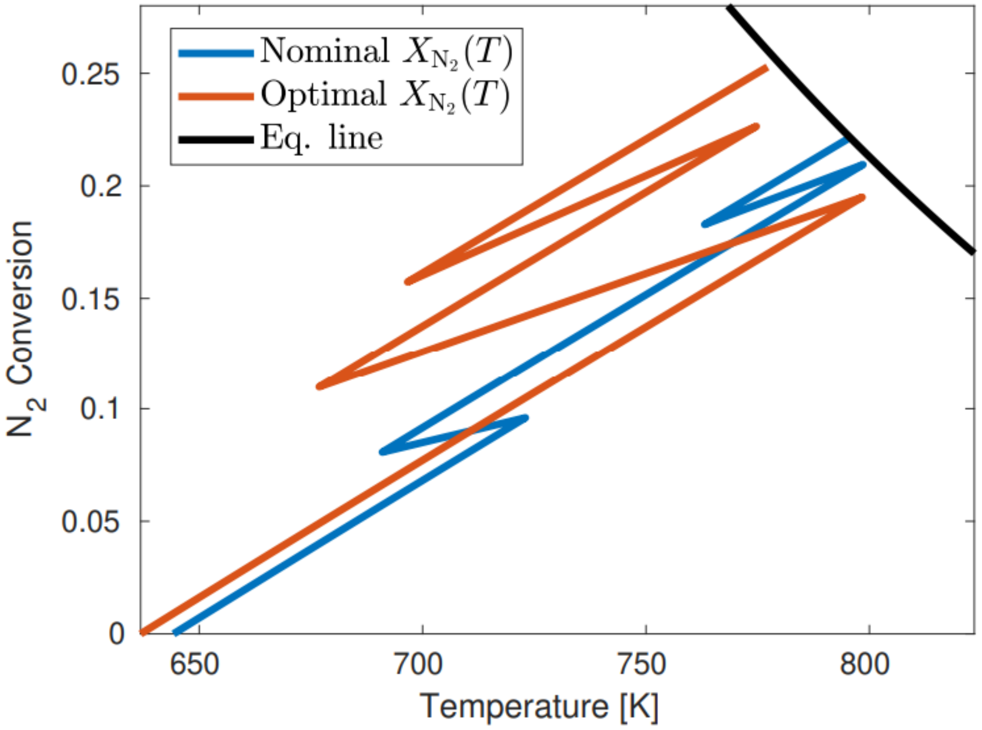
- Find optimal bed 1 inlet temperature and q_{R2}, q_{R3}
- Conversion increased from 22.2 to 25.3.

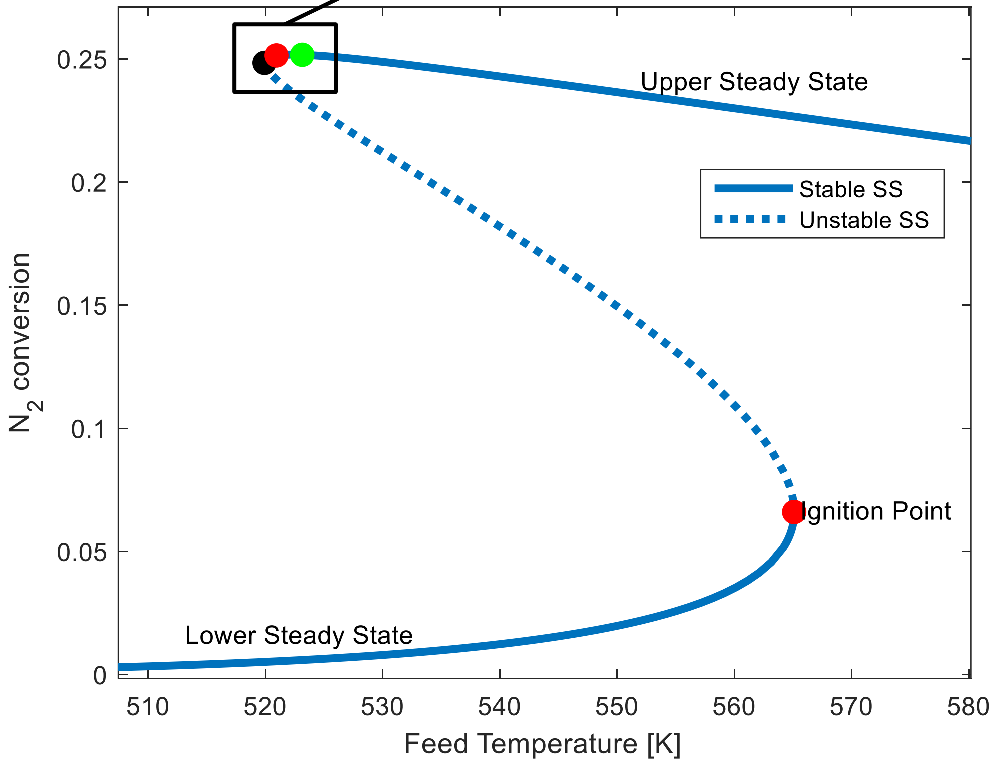
$$q_R = [0.579,\ 0.195,\ 0.118,\ 0.108]$$
$$q_R^{opt} = [0.183,\ 0.208,\ 0.304,\ 0.305]$$

- But very close to the instability point!

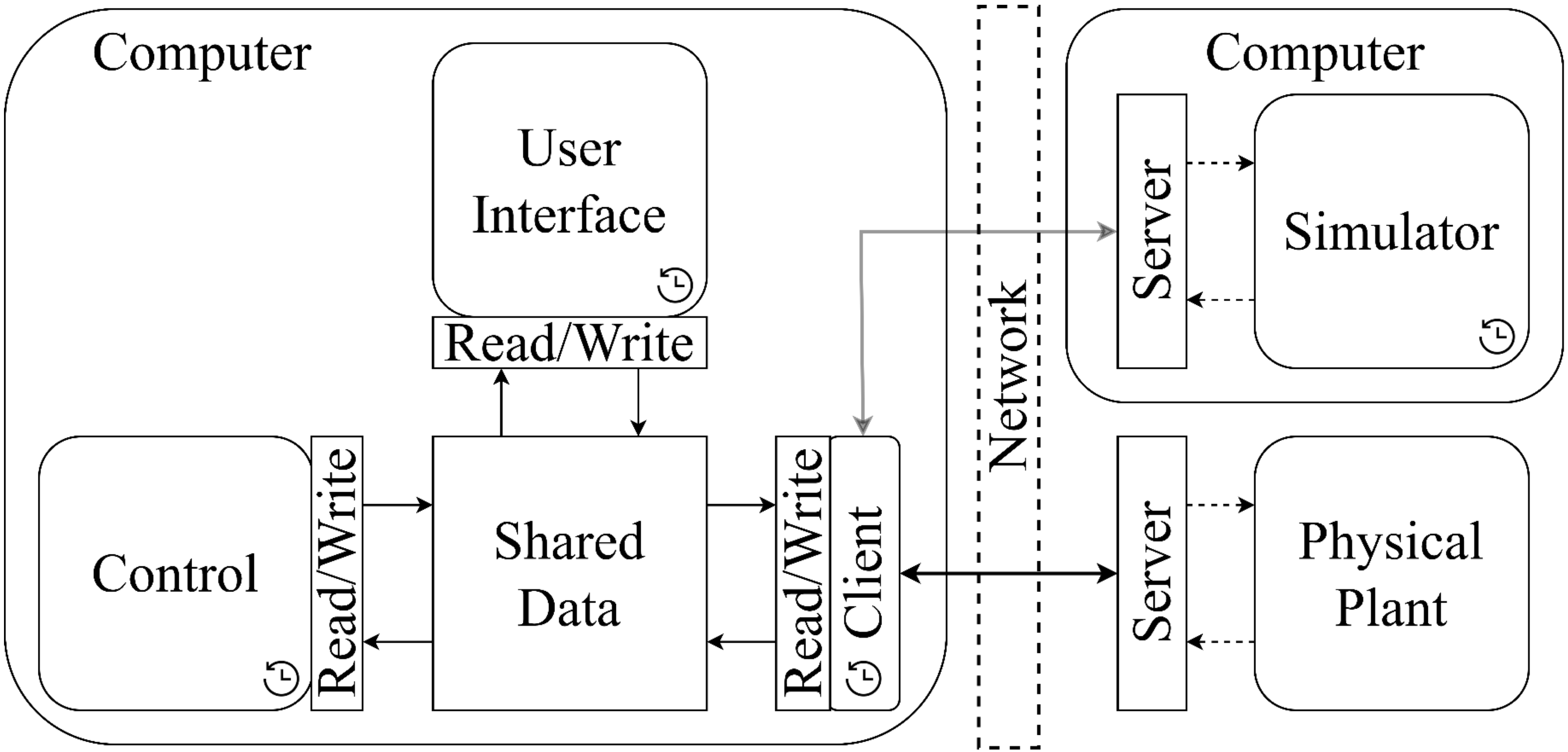




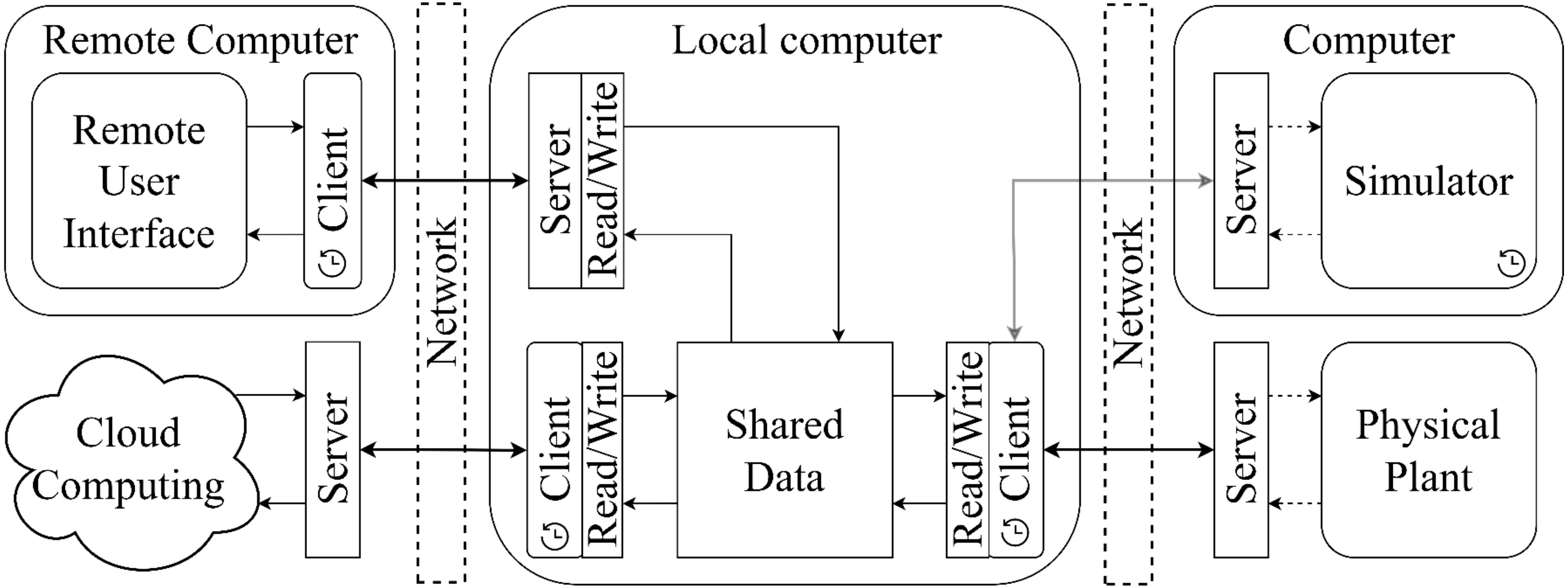




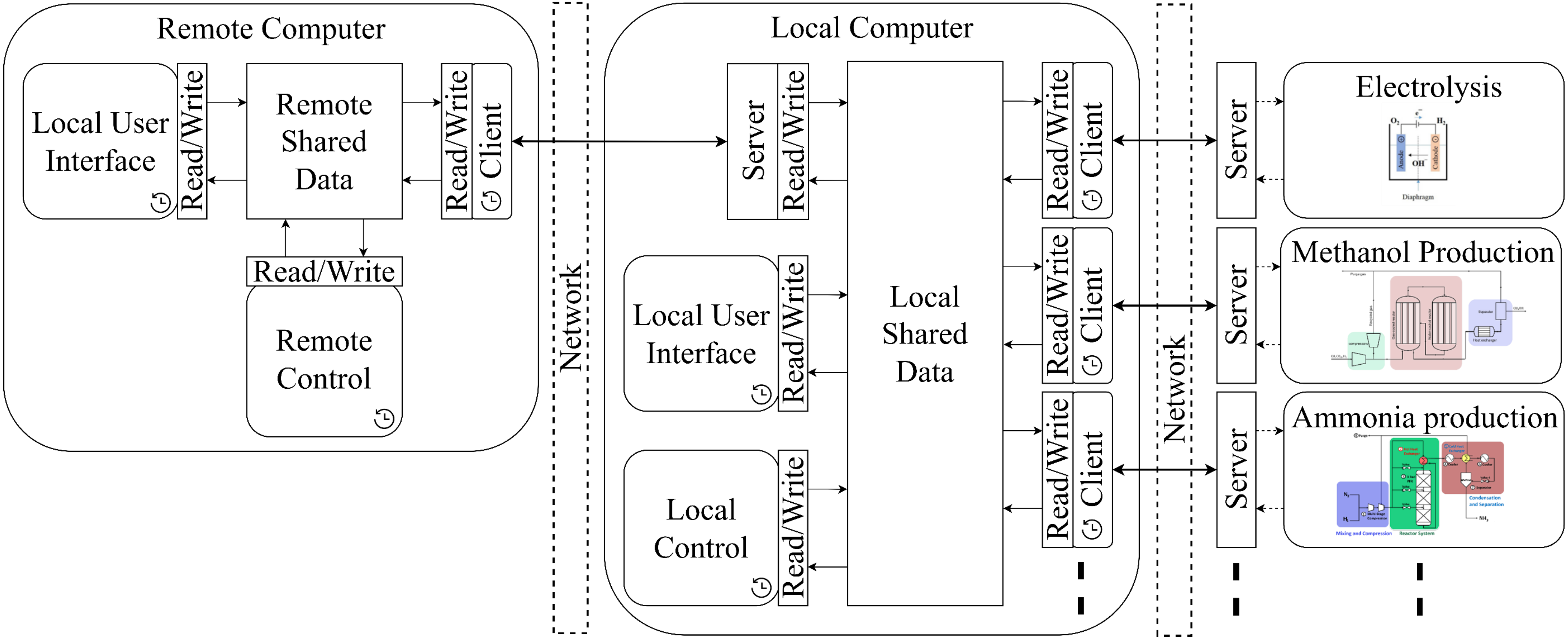
RT-APC framework for CPS



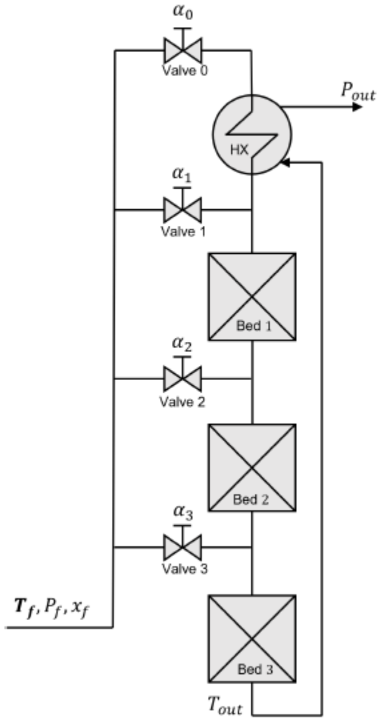
RT-APC framework for CPS

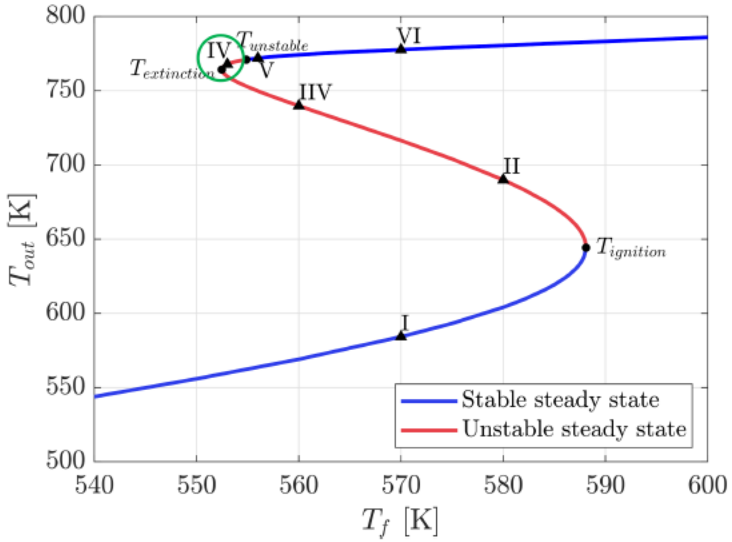


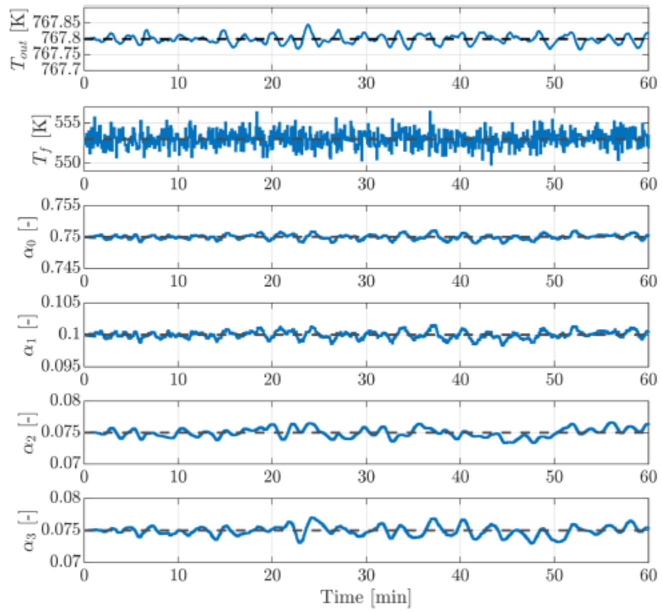
RT-APC for Power-to-X



Linear MPC for stabilization of an unstable operating point

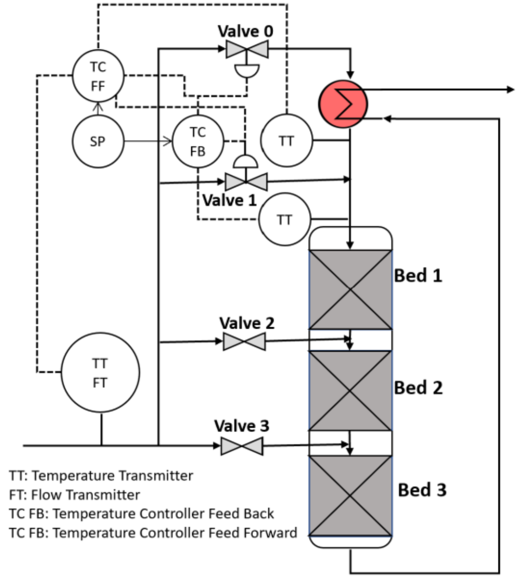


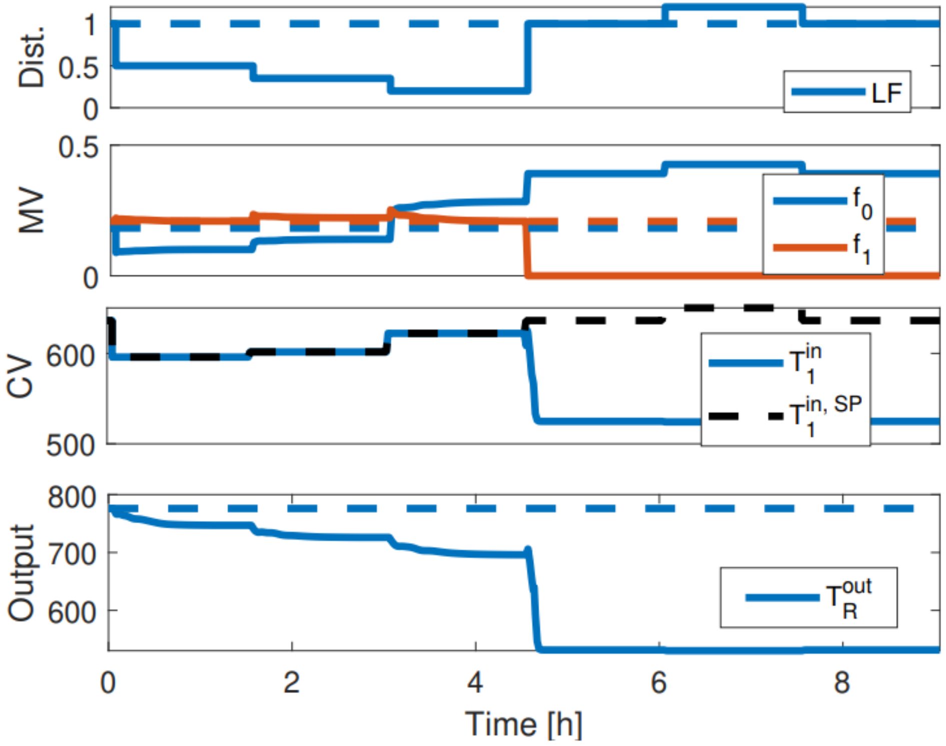


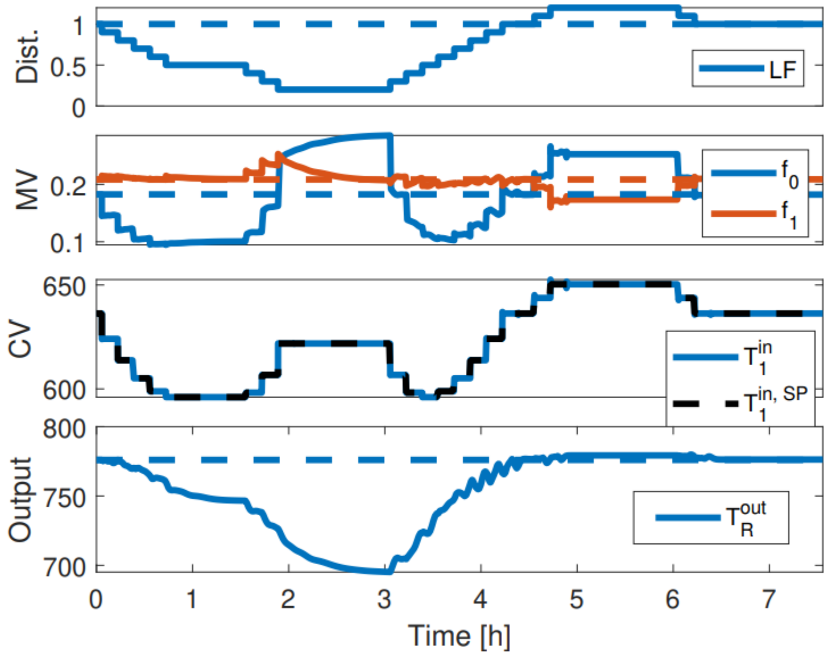


Control

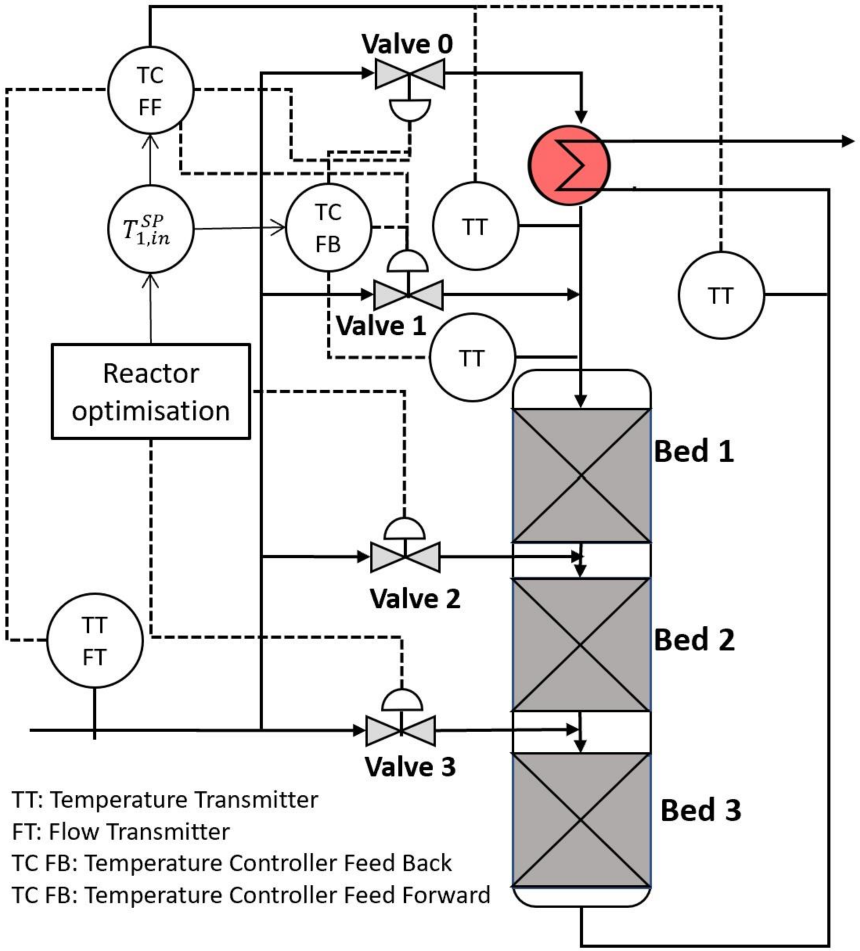
- SISO system:
  CV: $T_{1,\,in}$
  MV: Split range control on f_0 and f_1
- Feed forward + Feed back (PI), $K_p = 7.35 \cdot 10^{-4}\ \mathrm{K}^{-1},\ \tau_I = 1s$



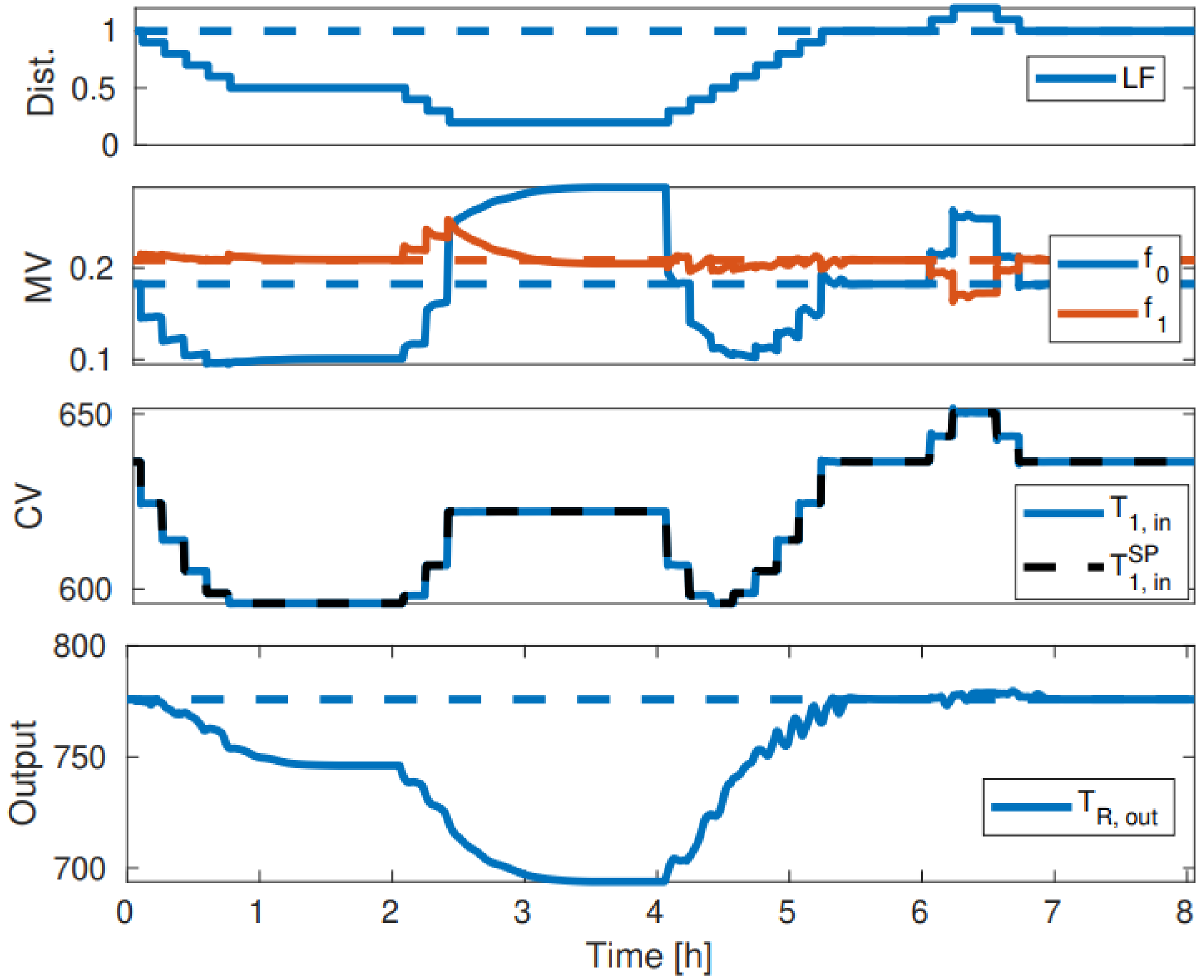




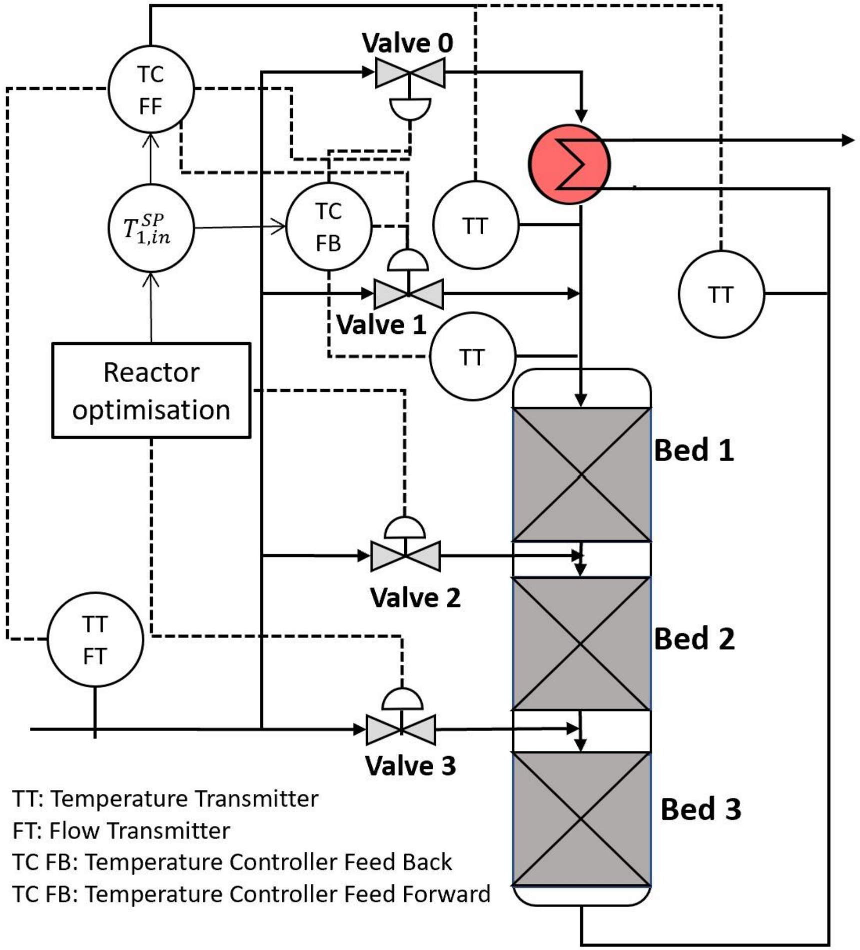
Control and Optimization for the Ammonia Reactor



TT: Temperature Transmitter
FT: Flow Transmitter
TC FB: Temperature Controller Feed Back
TC FB: Temperature Controller Feed Forward



Control and Optimization for the Ammonia Reactor



TT: Temperature Transmitter
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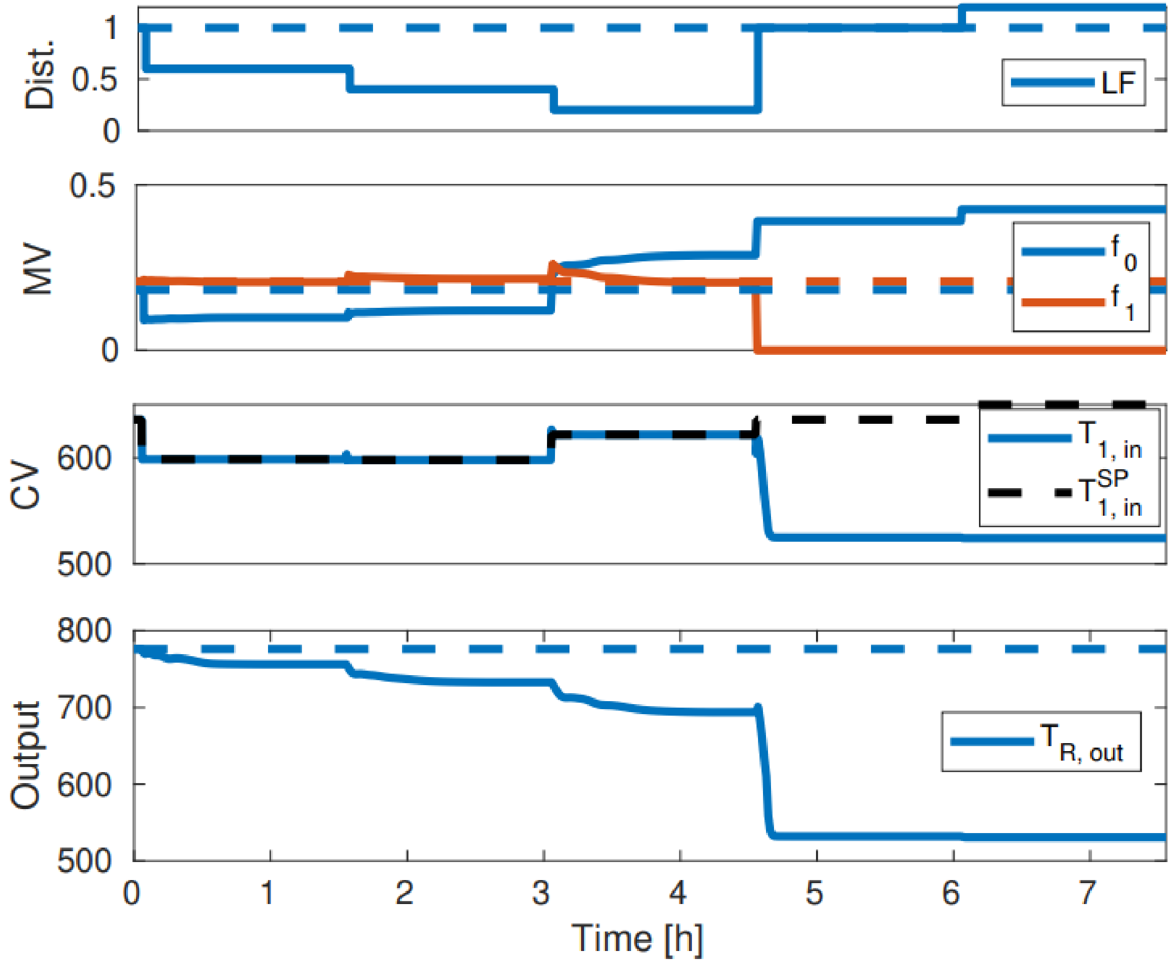


Boundary 2: Synthesis loop

- Reactor feed hydrogen flow

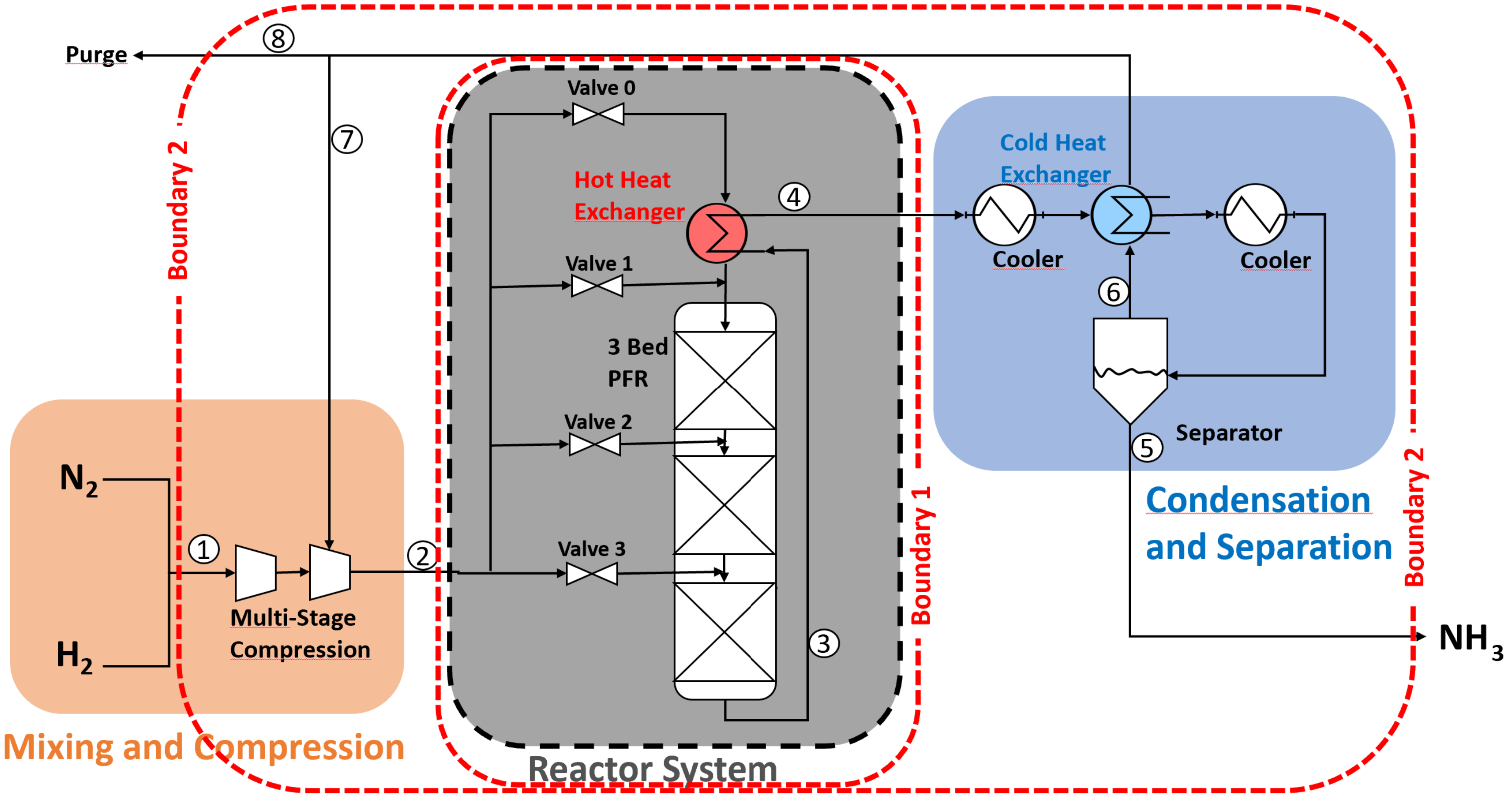
$$\frac{N_{2,\mathrm{H}_2}}{N_{2n,\mathrm{H}_2}}$$

- Stoichiometric factor

$$S_{\mathrm{N}_2/\mathrm{H}_2} = \frac{3N_{2,\mathrm{N}_2}}{N_{2,\mathrm{H}_2}}$$

- Argon to nitrogen ratio (recycle)

$$S_{\mathrm{Ar}/\mathrm{N}_2} = \frac{N_{2,\mathrm{Ar}}}{N_{2,\mathrm{H}_2}}$$



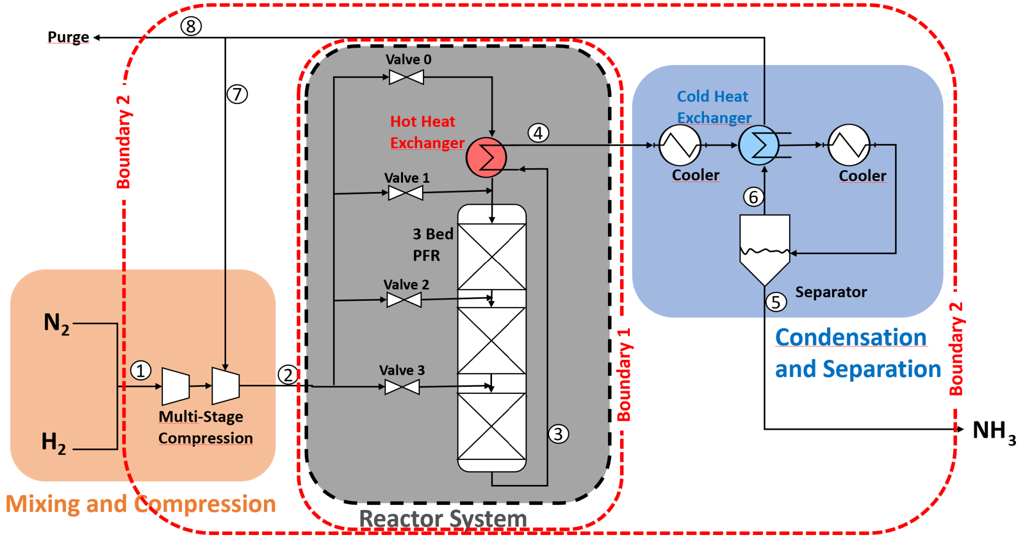
Energy input of P2A plant

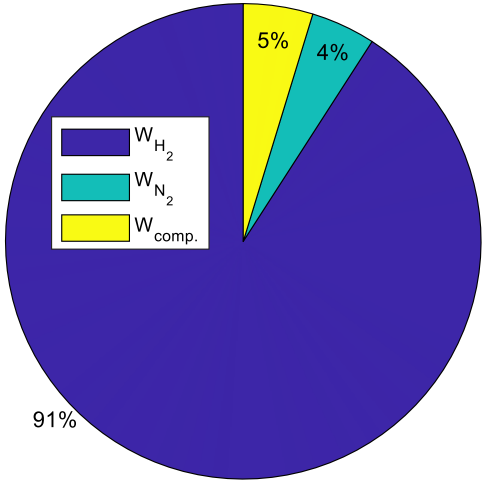
- Hydrogen production: 67% efficiency compared to LHV
  $W_{H_2} = 48 \text{ kWh/kg} \cdot \dot{m}_{H_2}$

- Nitrogen via ASU
  $W_{N_2} = 0.115 \text{ kWh/kg} \cdot \dot{m}_{N_2}$

- Compressors: Isentropic efficiency
  $$W_{comp.} = \frac{W_S}{\eta_{isen}}$$

- Energy efficiency of P2A
  $$\eta_E = \frac{LHV_{NH_3}\dot{m}_{NH_3}}{W_{tot}}$$

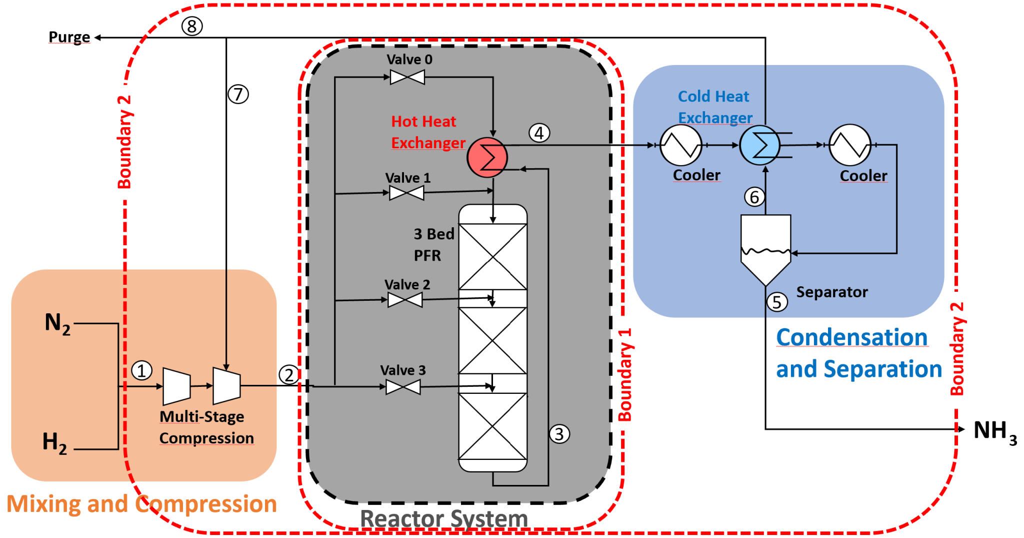


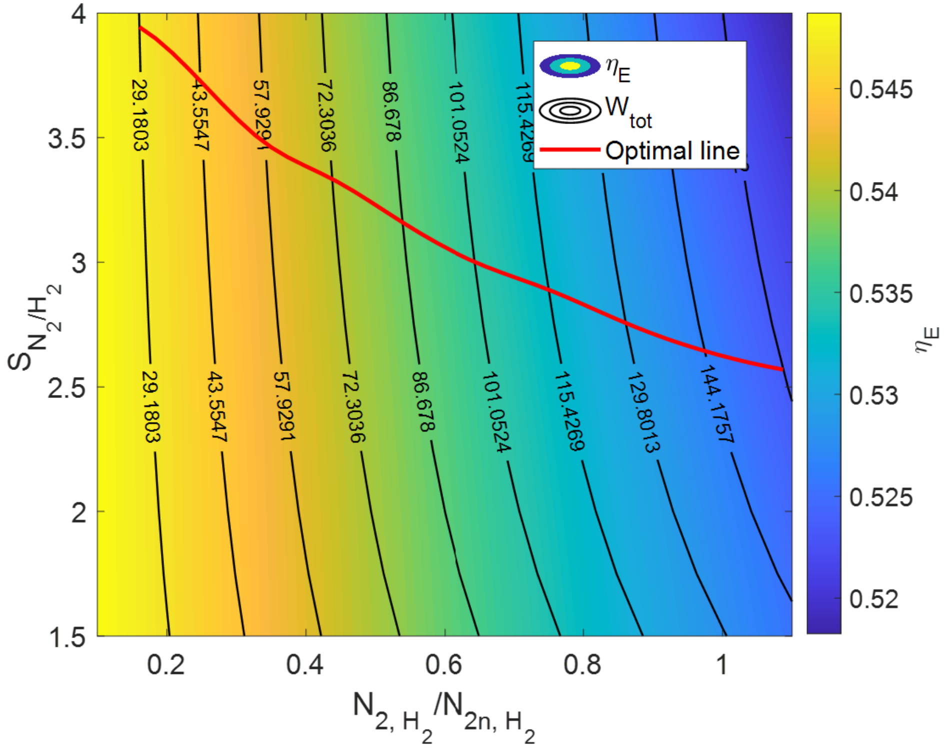


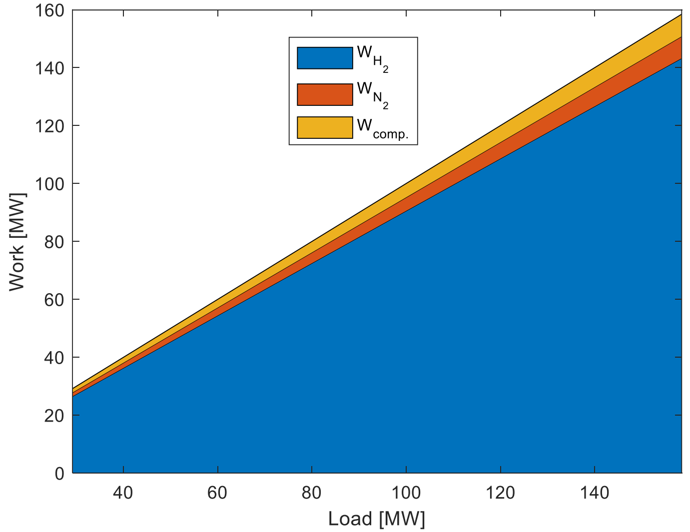
Case	W_{tot} [MW]	η_E
Nominal	104.2	50.4%
Optimal	118.1	50.5%
Opt. norm	104.2	51.3%

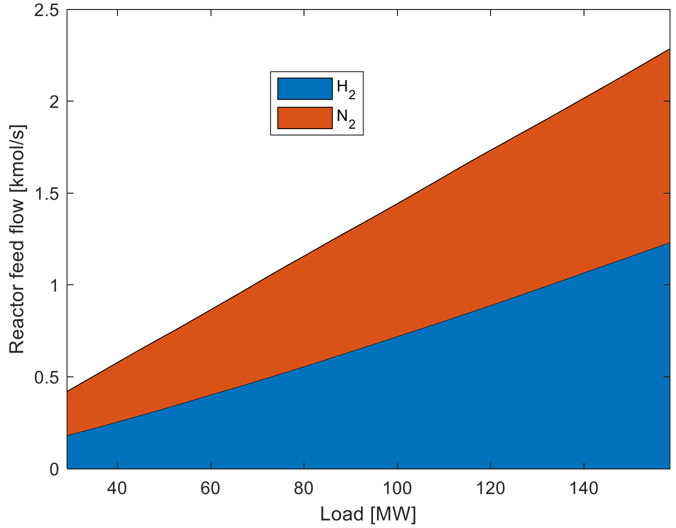
Optimal operation of P2A plants

- Vary $\frac{N_{2,H_2}}{N_{2n,H_2}}$ and S_{N_2/H_2} to the reactor.
- 2d plane of power consumption and NH_3 production
- Increased energy efficiency to 53.5% at nominal load.



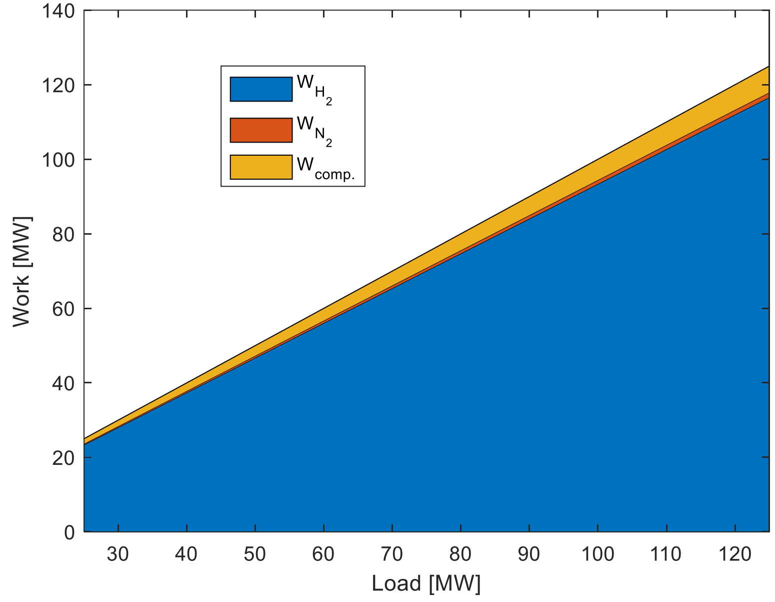


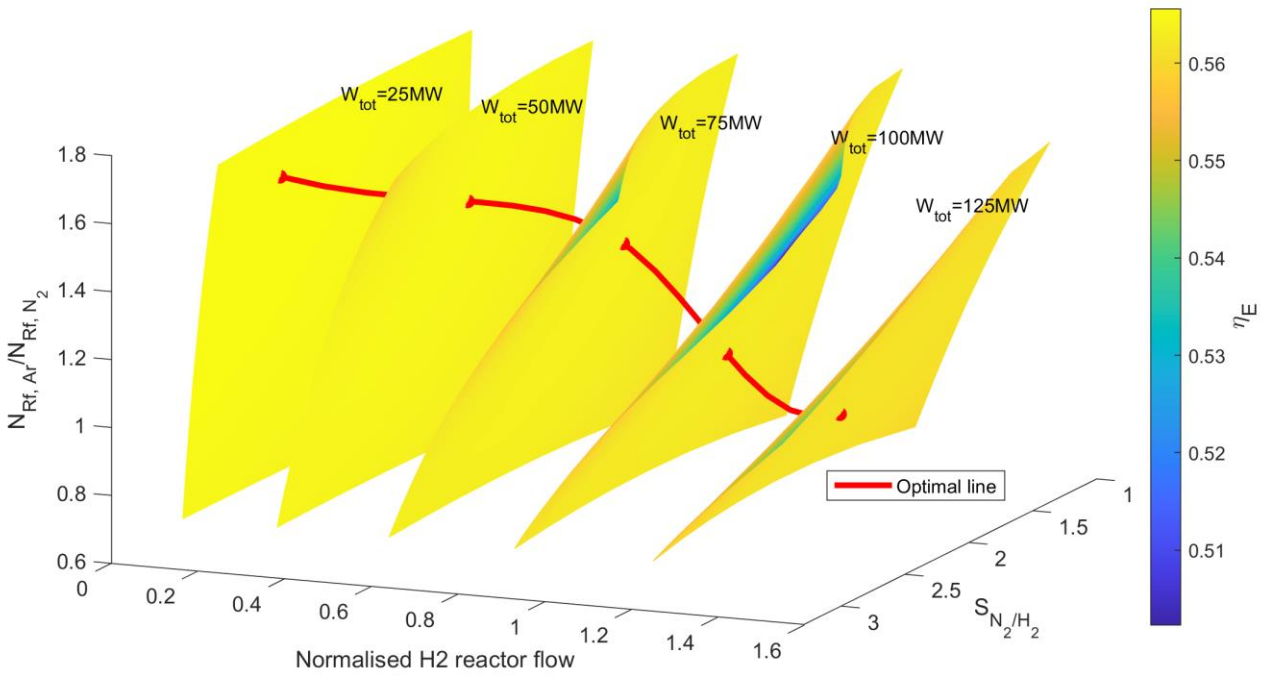


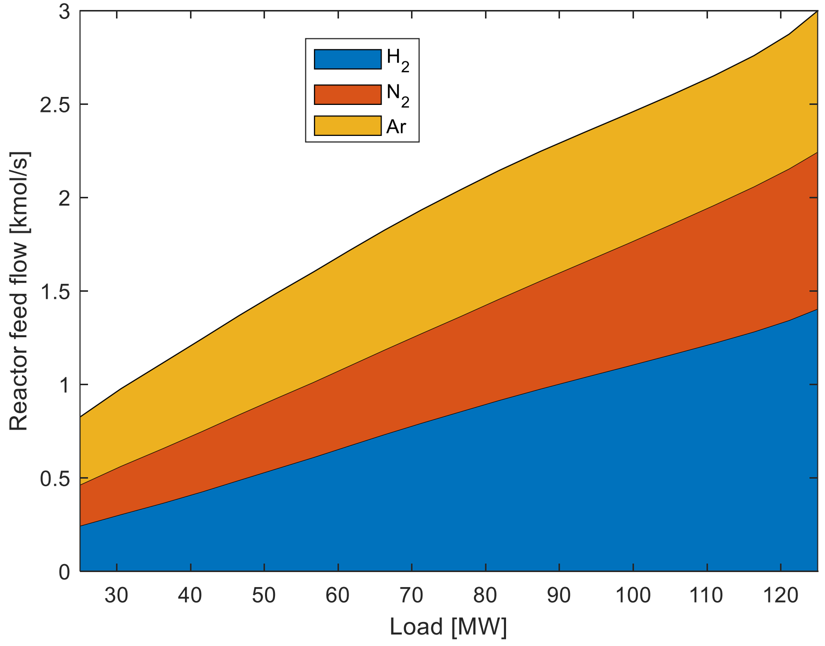


Optimal operation of P2A plants

- What about the recycling?
- 3d space of power consumption and energy efficiency
- Total energy efficiency increase: 50.3% -> 51.3% -> 53.5% -> 56.0%

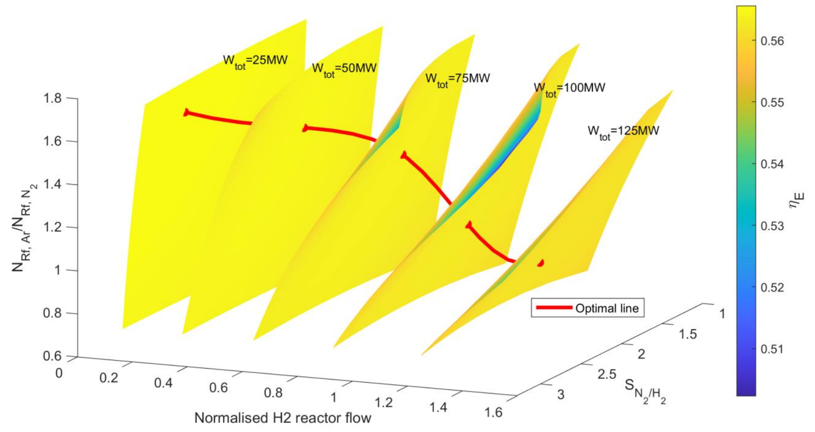


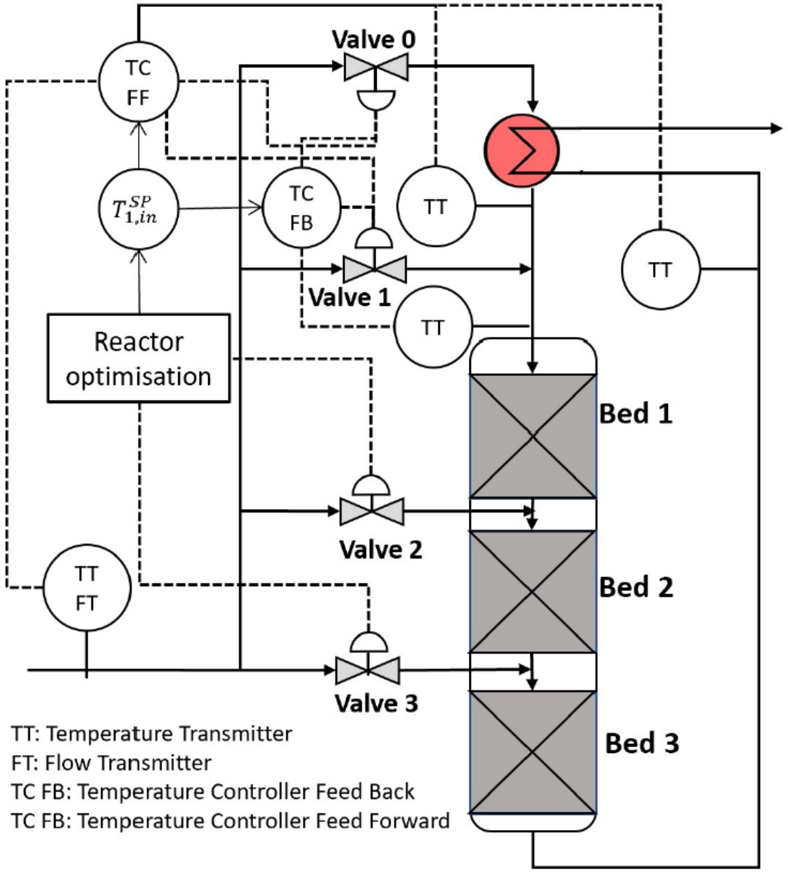


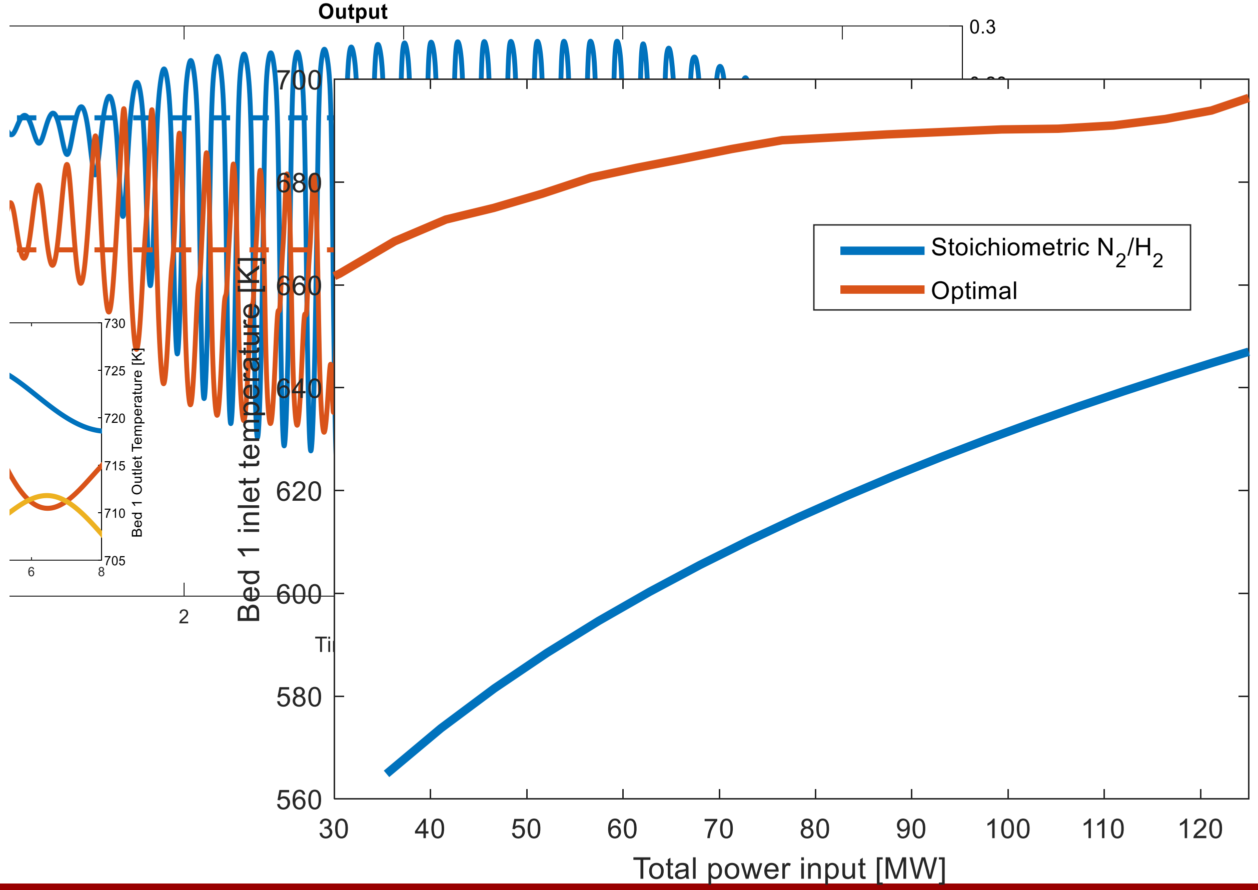


How do we operate the plant flexible?

- We don't want this!
- Supervisory layer specifying nitrogen and hydrogen production
- Simple control on the first bed inlet temperature via the quench valves.
- Relative constant temperature over the reactor beds for the optimal case.

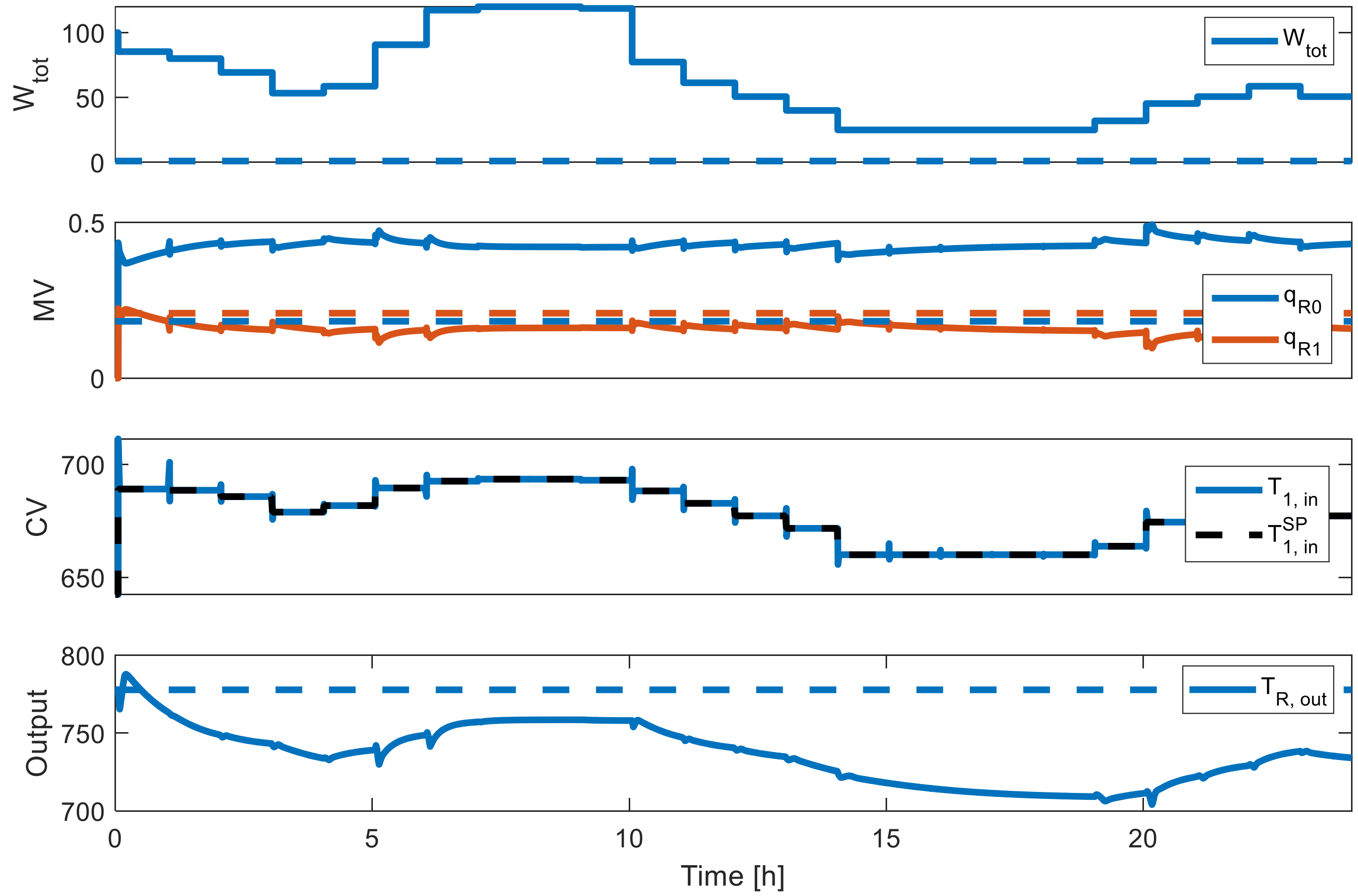


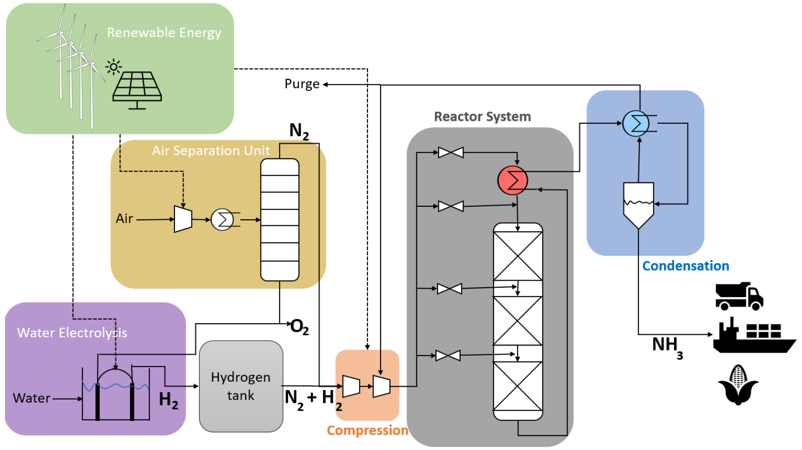


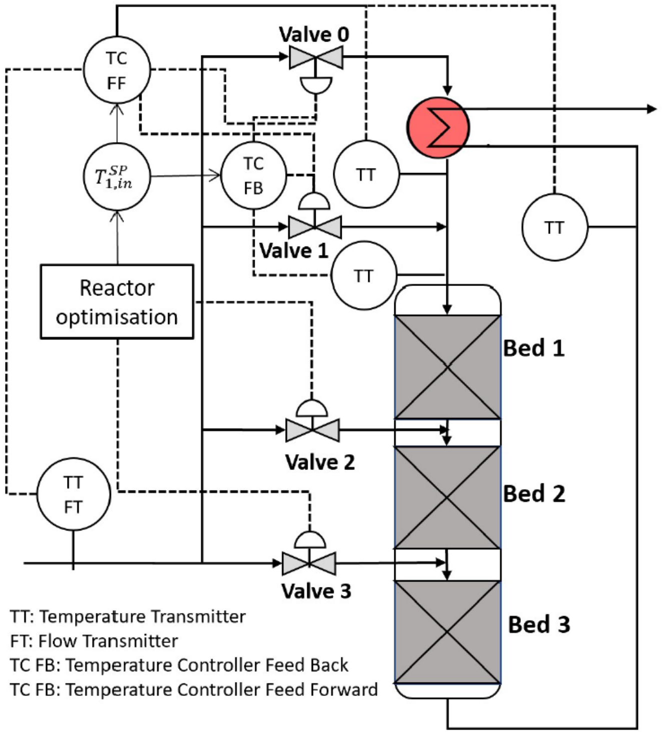


Flexible operation

- Power input for 24h operation
- Safe and flexible operation is achieved.







Near term goals

- Build and evaluate model library for all 3 reactor types
- Evaluate the applicability of the tree reactors types for P2A: Step tests, unstable operating regions and control options.
- Adapt to P2A plant in Ramme. Demonstrate control and optimization system. APC-RT.

- Dynamic compressor models
- Economic model and optimisation
- Topsoe and Skovgaard Invest P2A facility in Ramme (Operational 2023)
- Advanced control (MPC)

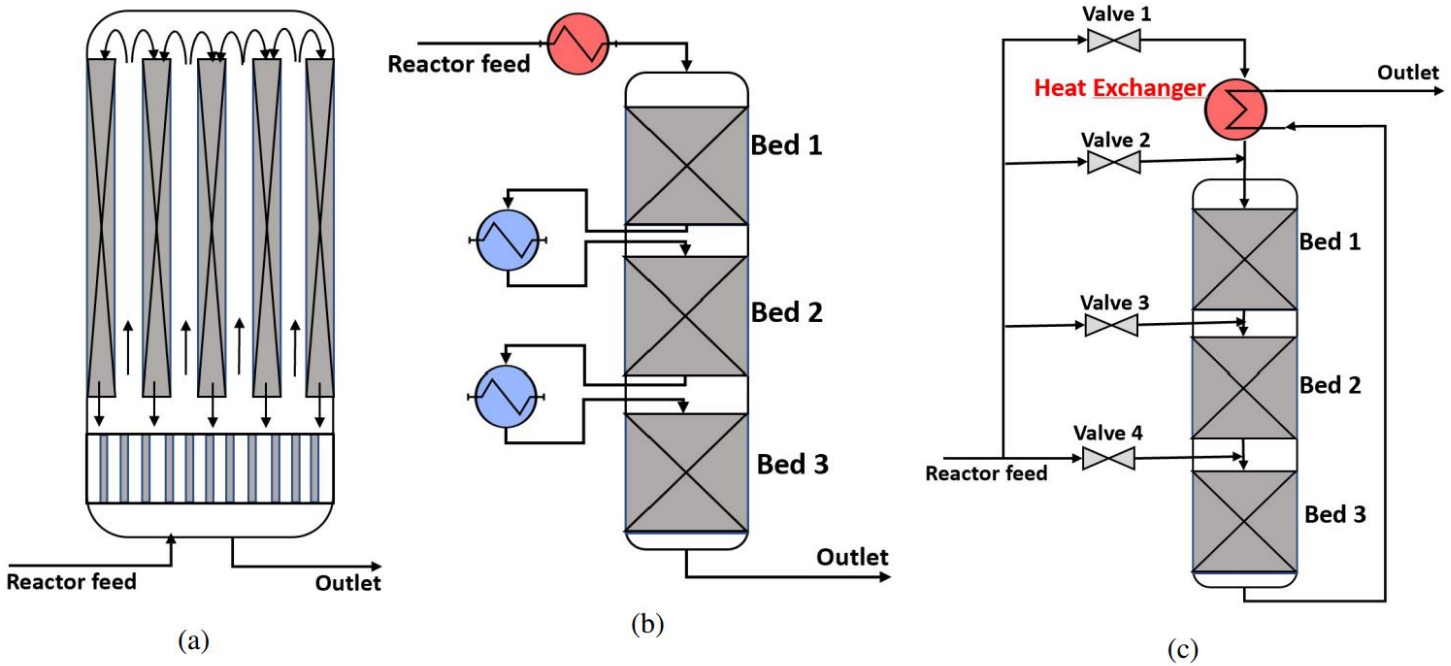


Figure 2: a) Internal Direct Cooled Reactor (IDCR), b) Adiabatic Indirect Cooled Reactor (AICR) and c) Adiabatic Quench Cooled Reactor.

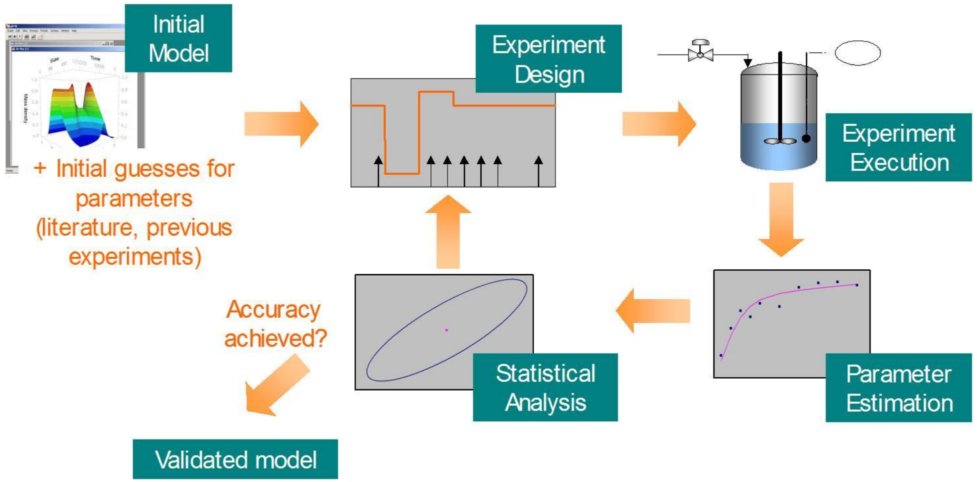
Conclusion & Summary

Conclusion

$$\boldsymbol{x}(t_0) = \hat{\boldsymbol{x}}_0 \qquad \hat{\boldsymbol{x}}_0 \sim N(\hat{x}_0, \hat{P}_0)$$

$$d\boldsymbol{x}(t) = \overbrace{f(\boldsymbol{x}(t), u(t), d(t), \theta)dt}^{=\text{drift}} + \overbrace{\sigma(\boldsymbol{x}(t), u(t), d(t), \theta)d\boldsymbol{\omega}(t)}^{=\text{diffusion}} \qquad d\boldsymbol{\omega}(t) \sim N_{iid}(0, Idt)$$

$$\boldsymbol{y}(t_k) = g(\boldsymbol{x}(t_k), \theta) + \boldsymbol{v}(t_k) \qquad \boldsymbol{v}(t_k) \sim N_{iid}(0, R(\theta))$$



Continuous-Discrete Extended Kalman Filter (CDEKF)

- Continuous-Discrete Stochastic Model

$$\boldsymbol{x}(t_0) = \hat{\boldsymbol{x}}_0 \qquad \hat{\boldsymbol{x}}_0 \sim N(\hat{x}_0, \hat{P}_0)$$
$$d\boldsymbol{x}(t) = f(\boldsymbol{x}(t), u(t), d(t), \theta)dt + \sigma(\boldsymbol{x}(t), u(t), d(t), \theta)d\boldsymbol{\omega}(t) \qquad d\boldsymbol{\omega}(t) \sim N_{iid}(0, Idt)$$
$$\boldsymbol{y}(t_k) = g(\boldsymbol{x}(t_k), \theta) + \boldsymbol{v}(t_k) \qquad \boldsymbol{v}(t_k) \sim N_{iid}(0, R(\theta))$$

- Continuous-Discrete Extended Kalman Filter Algorithm ($\hat{x}_{0|-1} = \hat{x}_0$, $P_{0|-1} = \hat{P}_0$)
  - Measurement update

$$\hat{y}_{k|k-1} = g(\hat{x}_{k|k-1}, \theta) \qquad C_k = \frac{\partial g}{\partial x}(\hat{x}_{k|k-1}, \theta)$$
$$e_k = y_k - \hat{y}_{k|k-1} \qquad R_{e,k} = C_k P_{k|k-1} C_k' + R_k$$
$$\hat{x}_{k|k} = \hat{x}_{k|k-1} + K_k e_k \qquad K_k = P_{k|k-1} C_k' R_{e,k}^{-1}$$
$$P_{k|k} = P_{k|k-1} - K_k R_{e,k} K_k' = (I - K_k C_k) P_{k|k-1} (I - K_k C_k)' + K_k R_k K_k'$$

  - Time update - compute $\hat{x}_{k+1|k} = \hat{x}_k(t_{k+1})$ and $P_{k+1|k} = P_k(t_{k+1})$ by solving

$$\frac{d}{dt}\hat{x}_k(t) = f(\hat{x}_k(t), u_k, d_k, \theta) \qquad \hat{x}_k(t_k) = \hat{x}_{k|k}$$
$$\frac{d}{dt}P_k(t) = A_k(t)P_k(t) + P_k(t)A_k(t)' + \sigma_k(t)\sigma_k(t)' \qquad P_k(t_k) = P_{k|k}$$
$$A_k(t) = \frac{\partial f}{\partial x}(\hat{x}_k(t), u_k, d_k, \theta)$$
$$\sigma_k(t) = \sigma(\hat{x}_k(t), u_k, d_k, \theta)$$

Parameter Estimation

$$\min_{\theta} \quad V(\theta)$$
$$s.t. \quad \theta_{\min} \leq \theta \leq \theta_{\max}$$

Innovation (computed from model and data using a filter and predictor)

$$e_k(\theta) = e_k$$
$$R_{e,k}(\theta) = R_{e,k}$$

Least squares (LS) objective function

$$V_{LS}(\theta) = \frac{1}{2}\sum_{k=0}^{N_d} \|e_k(\theta)\|_2^2$$

Maximum likelihood (ML) objective function

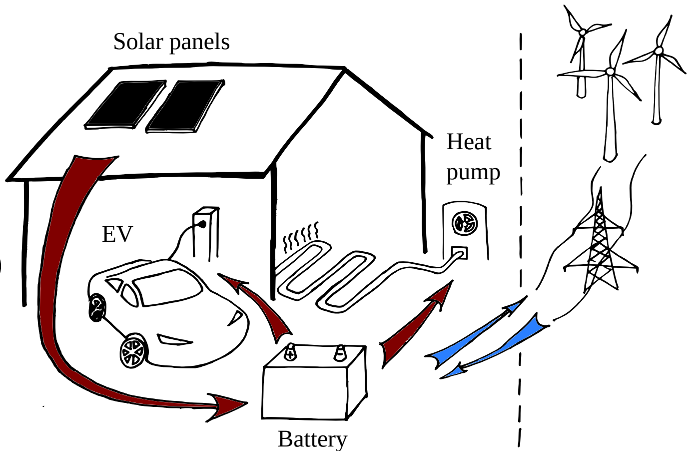
$$V_{ML}(\theta) = \frac{1}{2}\sum_{k=0}^{N_d} \ln(\det R_{e,k}(\theta)) + e_k(\theta)' \left[R_{e,k}(\theta)\right]^{-1} e_k(\theta) + \frac{(N_d+1)n_y}{2}\ln(2\pi)$$

Maximum a posteriori (MAP) objective function

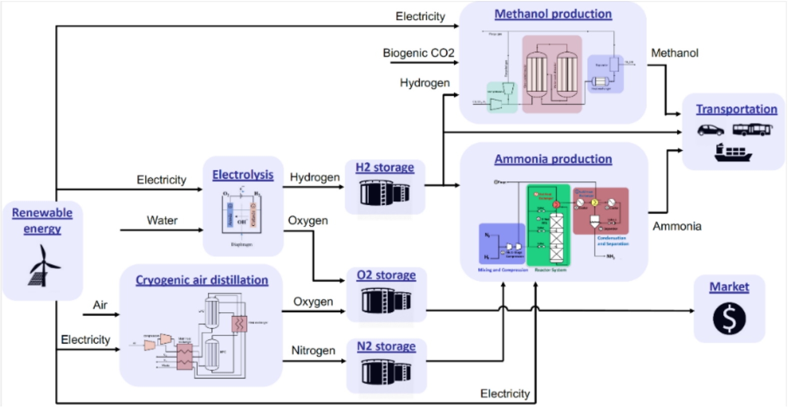
$$V_{MAP}(\theta) = V_{ML}(\theta) + \frac{1}{2}(\theta - \theta_0)' P_{\theta_0}^{-1}(\theta - \theta_0) + \frac{1}{2}\ln(\det P_{\theta_0}) + \frac{n_\theta}{2}\ln(2\pi)$$

Summary

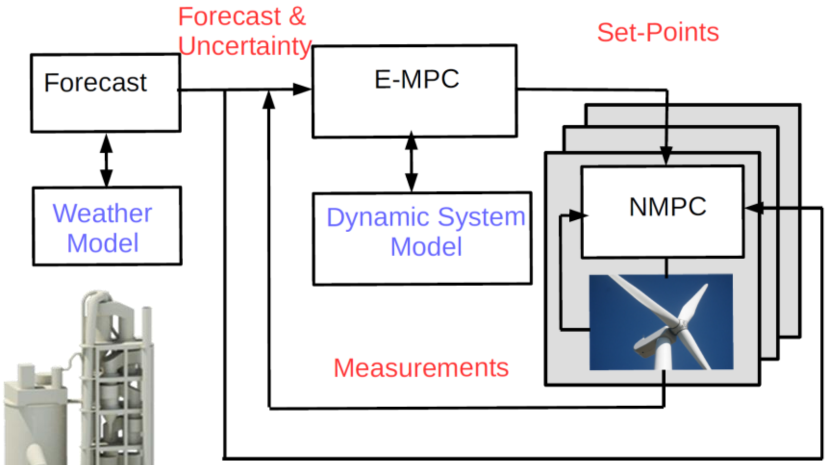
- **Key MPC technology developments**
  - MPC based on stochastic differential equations (SDEs)
  - Algorithmic
    – speed, robustness, embedded, cloud
  - Integrated Forecasting and Control
  - Integrated system identification



- **Industrial energy related processes**
  - Cement processes
  - Food processes
  - Single-cell protein production
  - Carbon capture



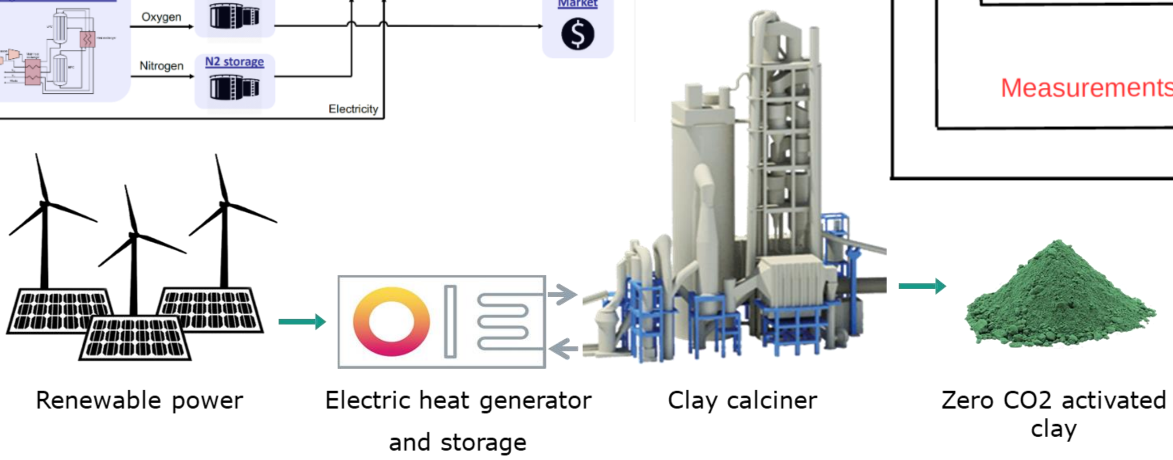
- **Energy Processes**
  - Energy system control
  - Wind turbine control
  - Refrigeration and heating systems



- **MPC technology is mature and ready**
  to be implemented on large scale for industrial facilities and buildings to enable smart zero-emission societies.

- **MPC technology is the key enabler**
  for integrated and coordinated systems.

  Implemented in many systems already
  to enable coordinated and efficient operation



Thank You – Q&A

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