PWtM-Flex: Flexible operation of plastic waste-to-methanol plants using next-generation electrolyzers

Videnbro project (Funded by Energy Cluster Denmark)
14:00–15:00 December 4th, 2024

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Link: www.energycluster.dk/projekter/pwtm-flex

Outline

The project

Modeling
(electrolyzer + gasification)

Single-stage optimization
for various electricity prices

Multi-stage optimization
for time-varying electricity prices

Mitigating fluctuations
in the feed stream

The project

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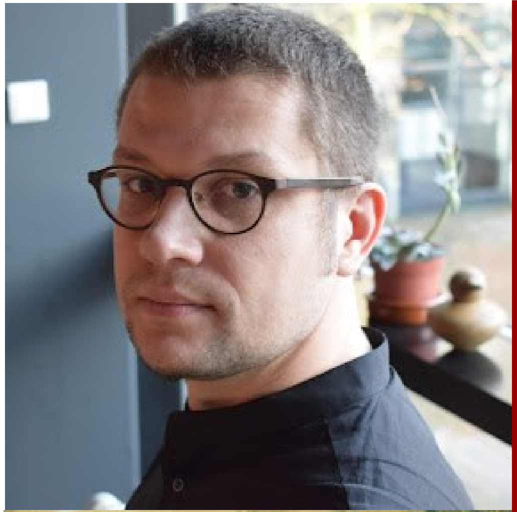






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Project

September–November, 2024

Technical University of Denmark
SemperCycle ApS
Nordic Hydrogen ApS

Videnbro Project (Funded by Energy Cluster Denmark)

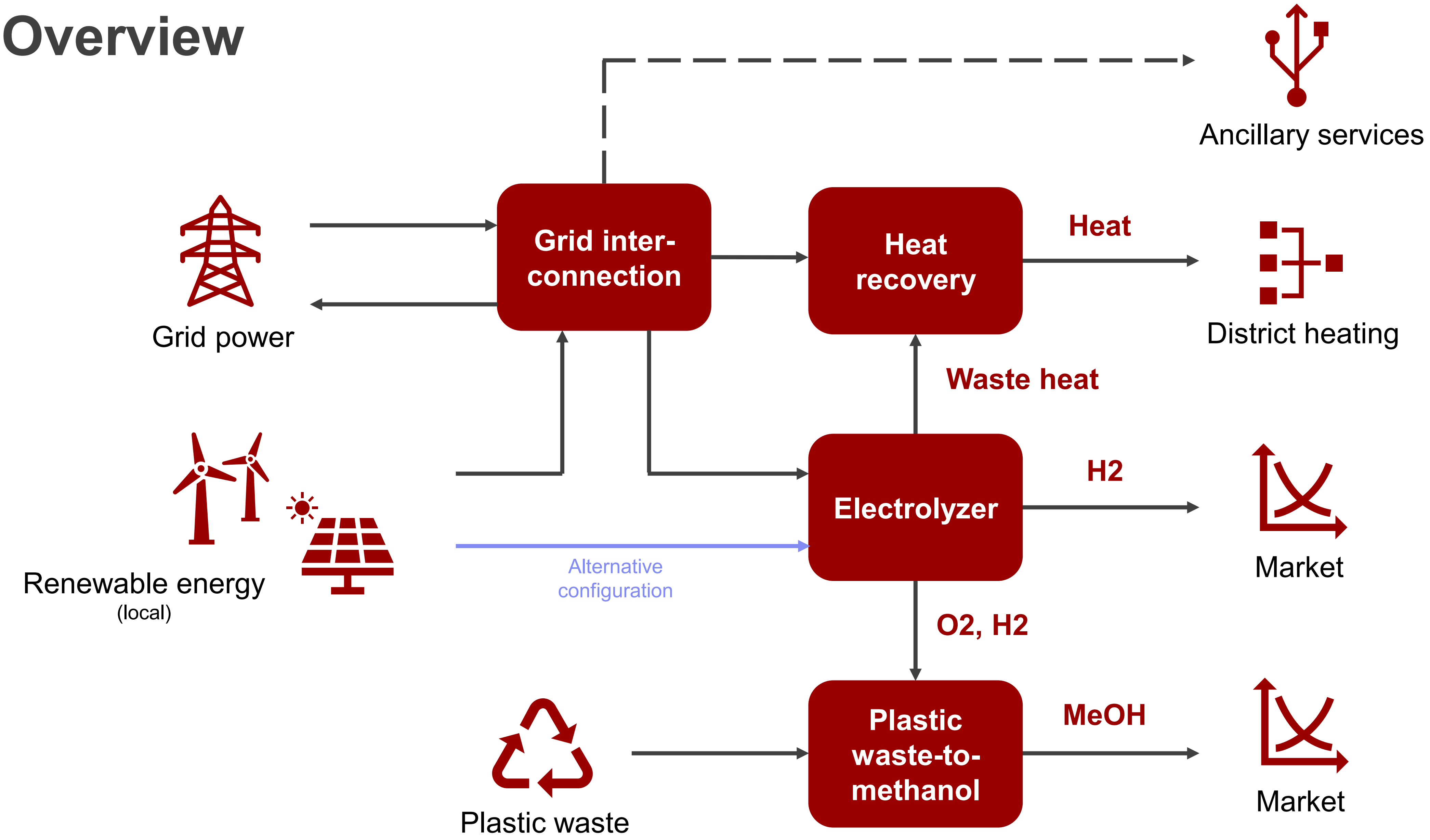
Activity 1: Model electrolyzer

Activity 2: Extend existing model of SemperCycle's plant

Activity 3: Formulate process optimization problem

Activity 4: Analyze solution to optimization problem

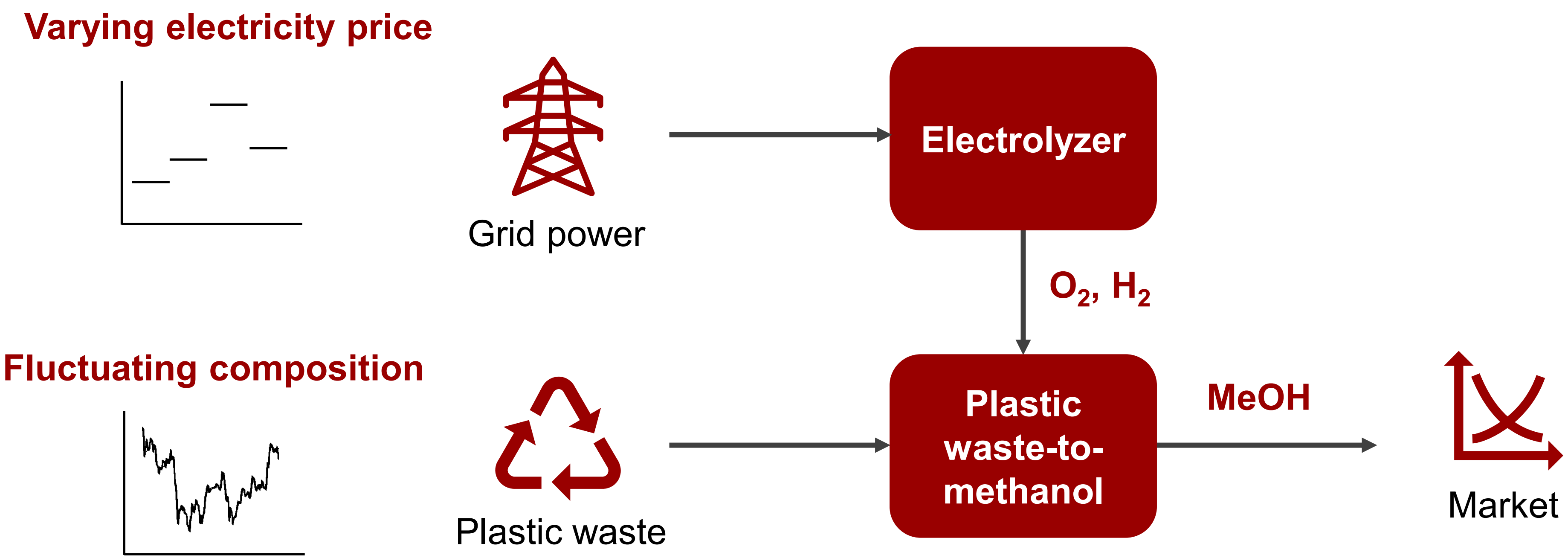
Overview



Ancillary services
Grid power
Grid inter-connection
Heat recovery
Heat
District heating
Waste heat
Renewable energy
(local)
Electrolyzer
H2
Market
Alternative configuration
O2, H2
Plastic waste
Plastic waste-to-methanol
MeOH
Market

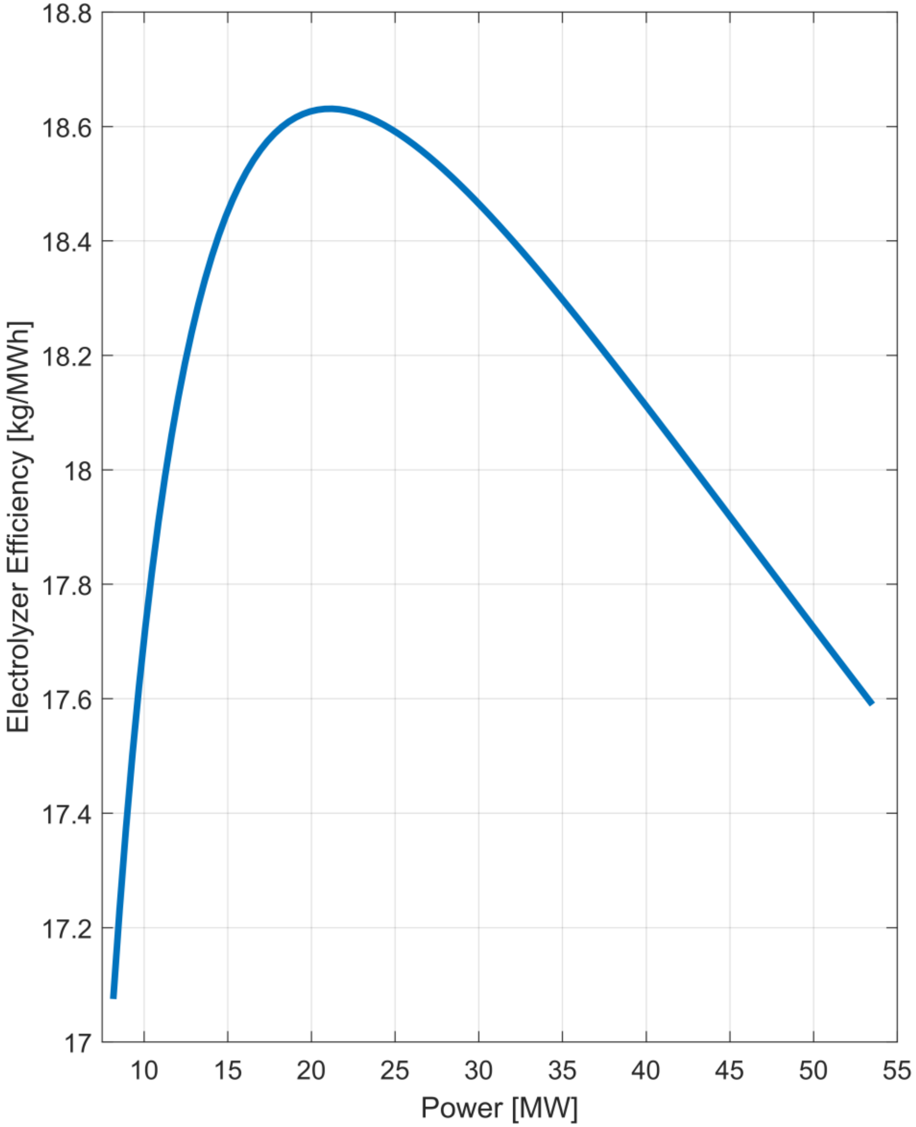
Objective

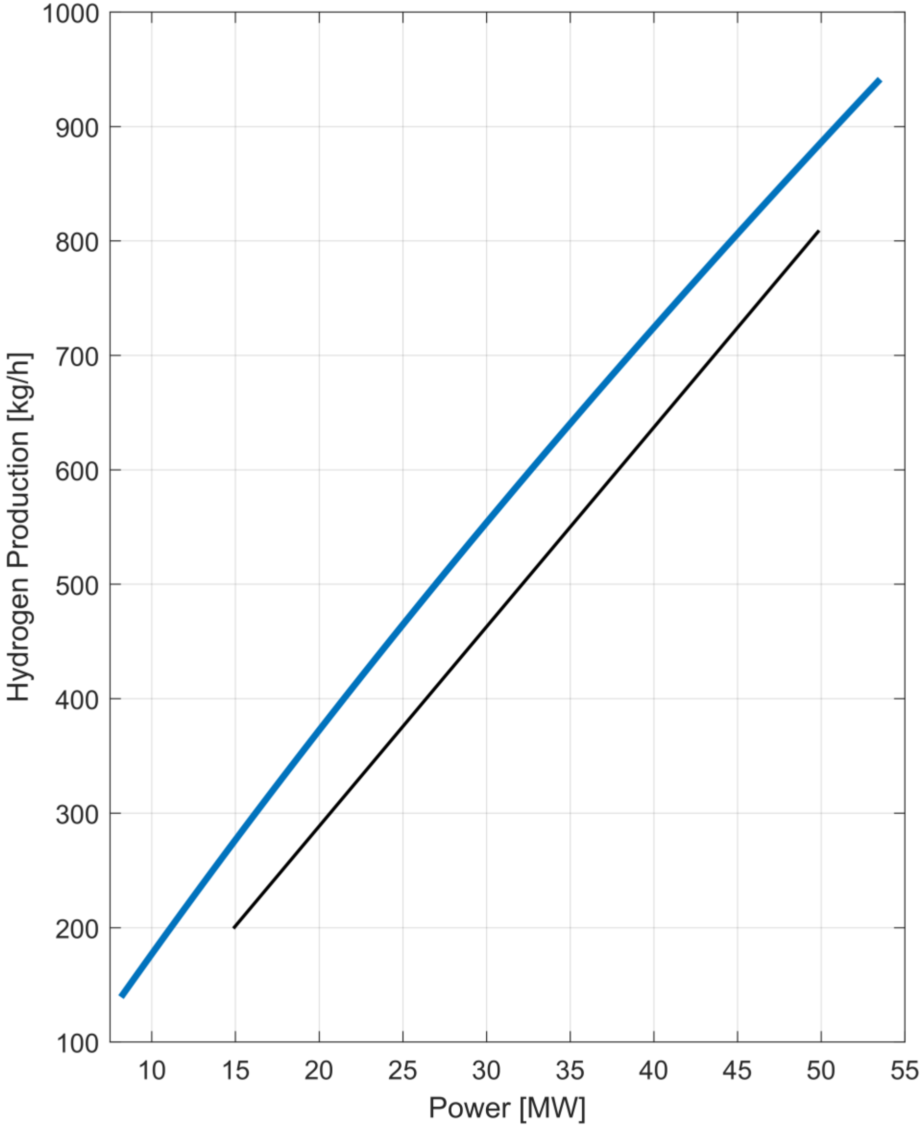
Operate plastic waste-to-methanol plant flexibly in response to dynamic electricity prices



Electrolysis

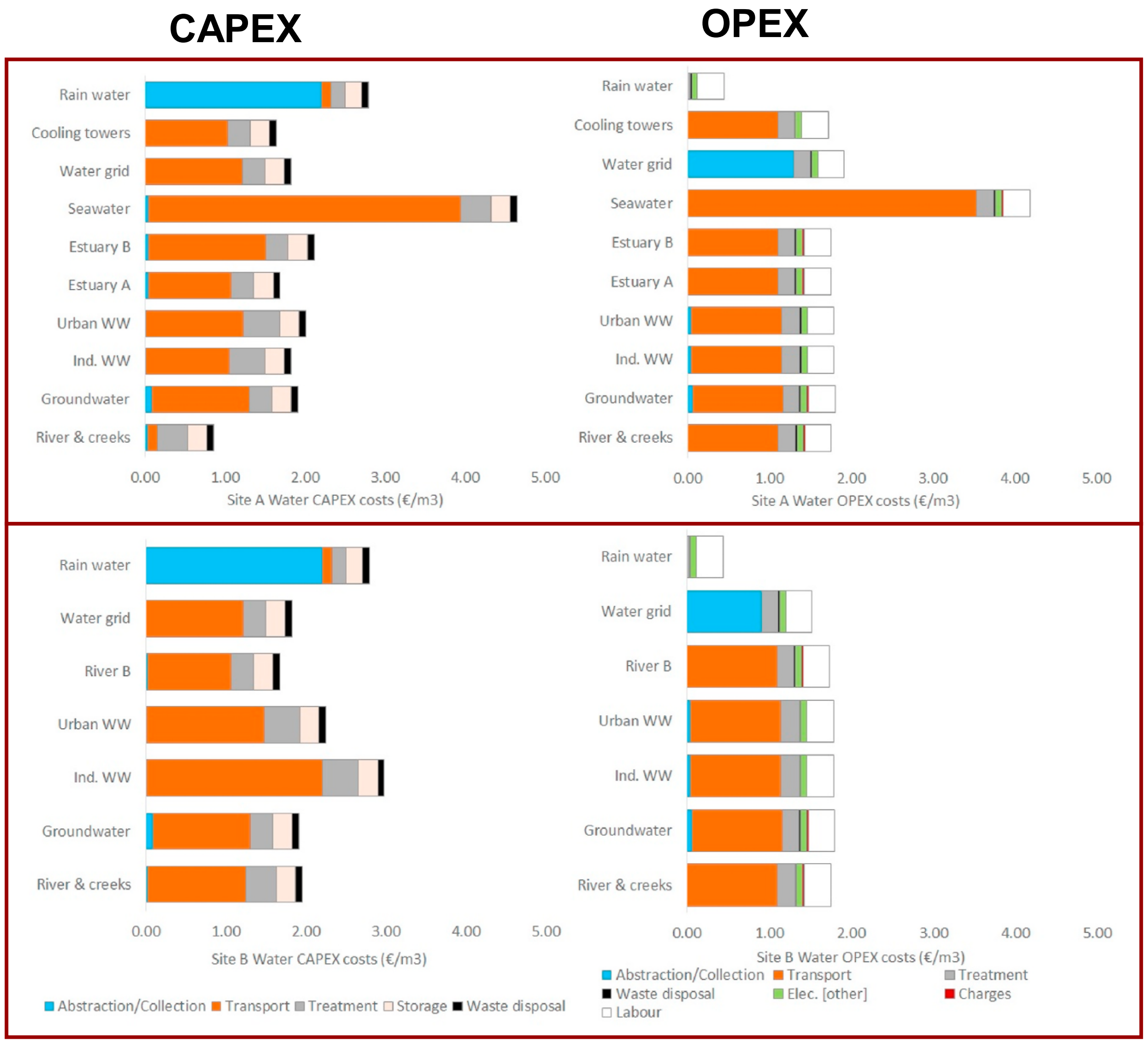
Electrolyzer efficiency





DOI: 10.1109/PowerTech55446.2023.10202860

Where should the water come from?



Site A

Site B

https://doi.org/10.1016/j.jclepro.2021.128124

Flexible/intermittent operation

Flexible operation:
Technically feasible

Flexibility => degradation?
Unclear

References

- Jolaoso, L. A., Bello, I. T., Ojelade, O. A., Yousuf, A., Duan, C., & Kazempoor, P. (2023). Operational and scaling-up barriers of SOEC and mitigation strategies to boost H2 production - a comprehensive review. International Journal of Hydrogen Energy, 48, 33017–33041.

- Lange, H., Klose, A., Lippmann, W., & Urbas, L. (2023). Technical evaluation of the flexibility of water electrolysis systems to increase energy flexibility: A review. *International Journal of Hydrogen Energy*, *48*, 15771–15783.

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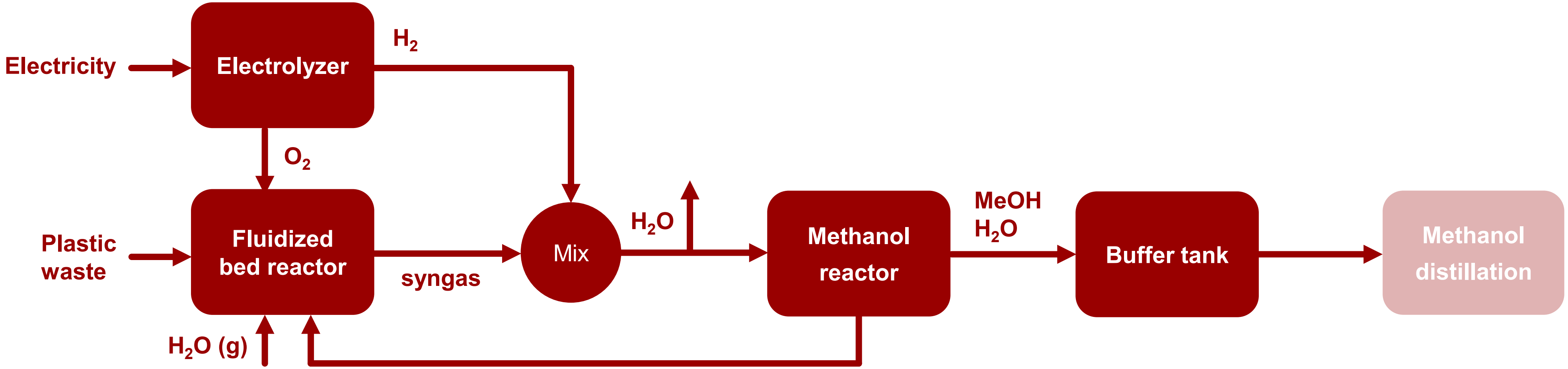
- Nguyen, E., Olivier, P., Pera, M.-C., Pahon, E., & Roche, R. (2024). Impacts of intermittency on low-temperature electrolysis technologies: A comprehensive review. *International Journal of Hydrogen Energy*, *70*, 474–492.

CANSI (ECD): www.energycluster.dk/en/cansi

Plastic waste to methanol

Plastic waste-to-methanol plant



Chemical reactions

Fluidized bed reactor and partial oxidation reactor

- Depolymerization and hydrogenation

$$[CH_2]_n \rightleftharpoons n/2\, C_2H_4,$$
$$C_2H_4 + H_2 \rightleftharpoons C_2H_6$$

- Combustion reactions

$$2\,C + O_2 \rightleftharpoons 2\,CO,$$
$$2\,CO + O_2 \rightleftharpoons 2\,CO_2,$$
$$2\,H_2 + O_2 \rightleftharpoons 2\,H_2O$$

- The water-gas and water-gas shift reactions

$$C + H_2O \rightleftharpoons CO + H_2,$$
$$CO + H_2O \rightleftharpoons CO_2 + H_2$$

- The Boudouard reaction

$$C + CO_2 \rightleftharpoons 2\,CO$$

See also the book by Higman and van der Burgt [2] and the website by the National Energy Technology Laboratory [3, Sec. 5.1.2–5.1.3 and 10.3].

- The methanation/hydrogasification reaction

$$C + 2\,H_2 \rightleftharpoons CH_4$$

- Partial oxidation

$$C_2H_4 + O_2 \rightleftharpoons 2CO + 2H_2$$

- Steam reforming

$$C_2H_4 + 2H_2O \rightleftharpoons 2CO + 4H_2$$

- Involved components: C, O_2, CO, CO_2, H_2, H_2O, CH_4, C_2H_4, C_2H_6.

Methanol reactor

- Syngas conversion to methanol

$$CO + 2\,H_2 \rightleftharpoons CH_3OH,$$
$$CO_2 + 3\,H_2 \rightleftharpoons CH_3OH + H_2O,$$
$$CO + H_2O \rightleftharpoons CO_2 + H_2$$

- Involved components: CO, CO_2, H_2, H_2O, CH_3OH.

[2] C. Higman and M. van der Burgt, *Gasification*. Elsevier, 2nd ed., 2008.

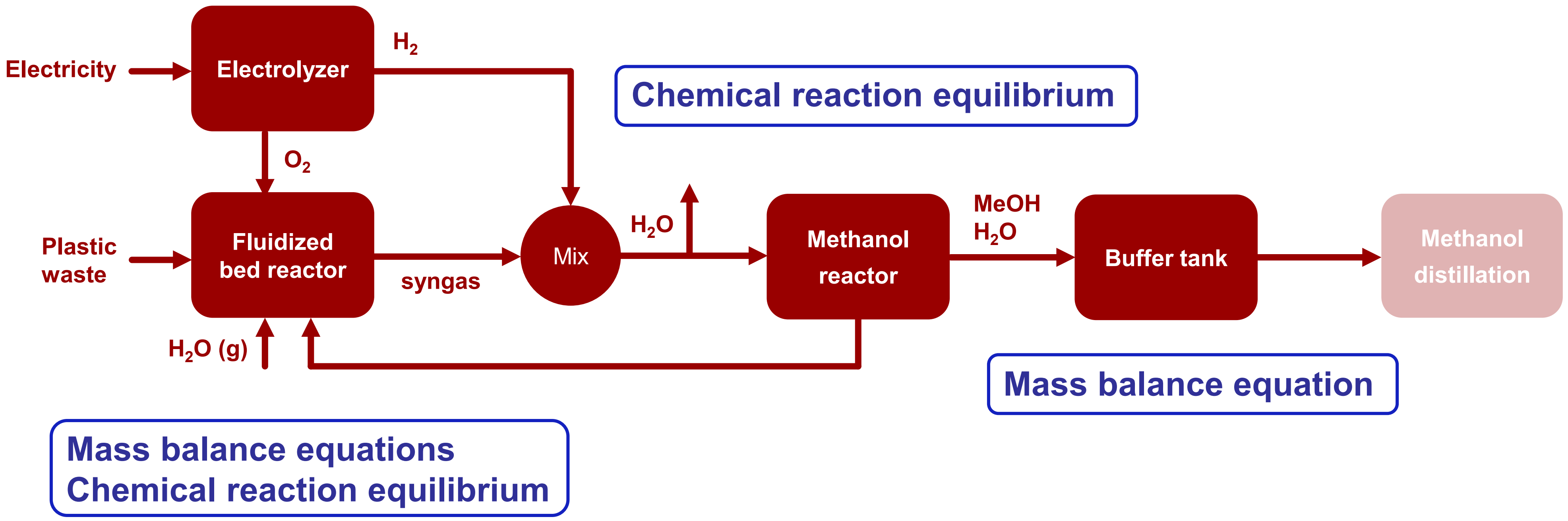
[3] U.S. Department of Energy, “Gasifipedia.” `https://netl.doe.gov/carbon-management/energy-systems/gasification/gasifipedia`.

Process model

$$0 = F(y, u, d),$$ Mass balances (FBR)

$$0 = G(x, y, z),$$ Chemical reaction equilibria (FBR + MeOH)

$$\dot{w} = H(y, u, d),$$ Storage



Model of profit

Key question: How much hydrogen do we need?

Profit

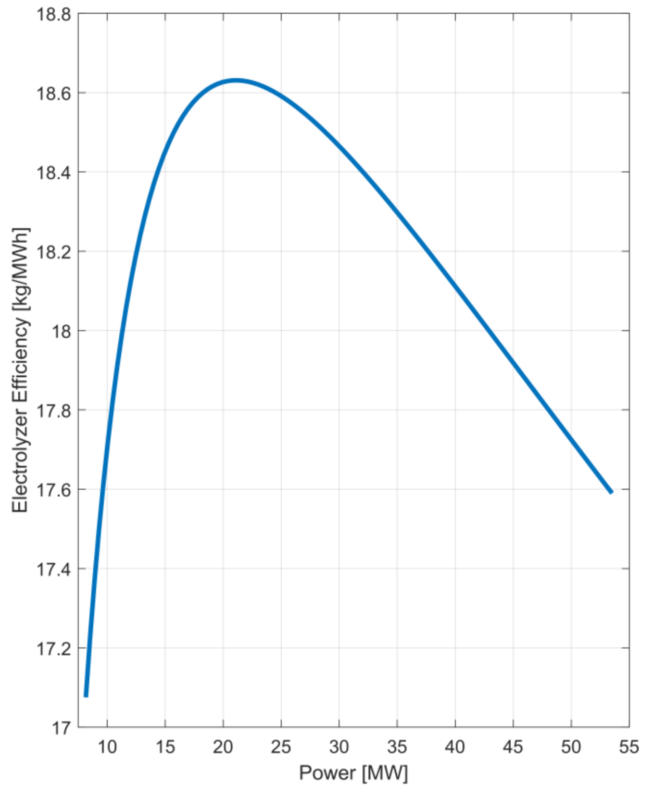
$$\phi = \phi_{rev} - \phi_{cost}$$

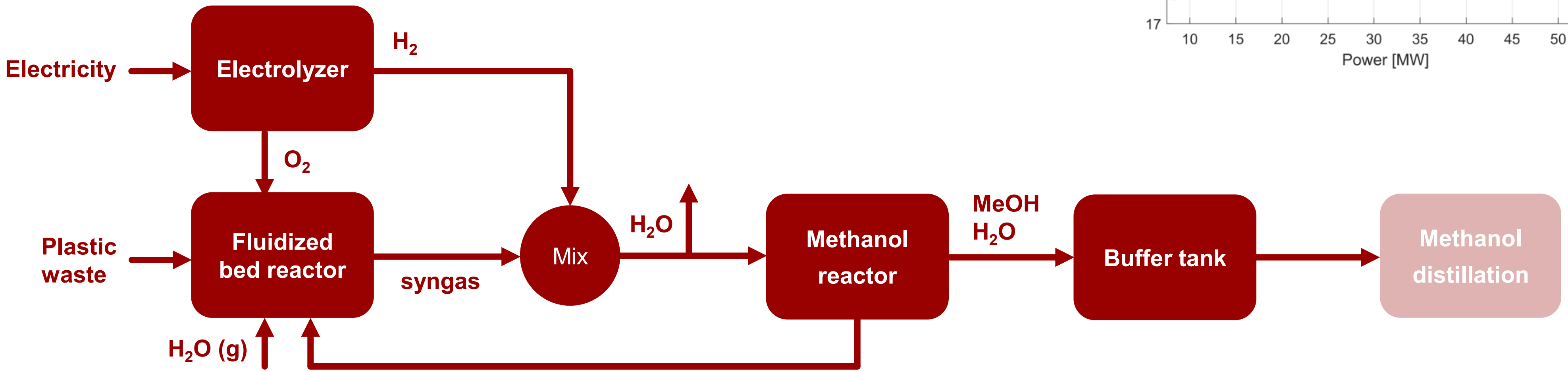
Cost

$$\phi_{cost} = \eta_{el,H_2} p_{el} f_{el,H_2},$$

Revenue

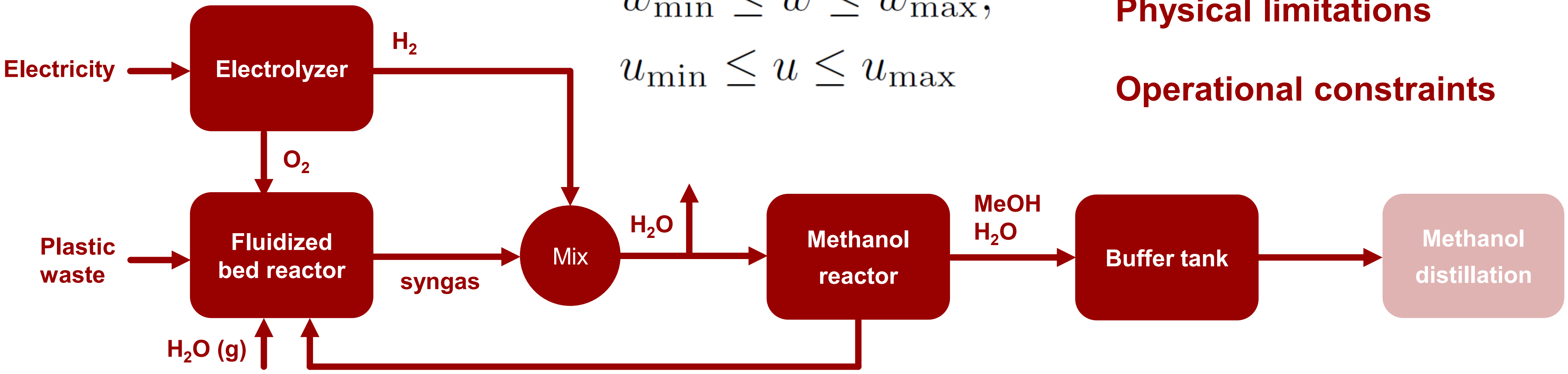
$$\phi_{rev} = p_{MeOH} f_{MeOH}$$





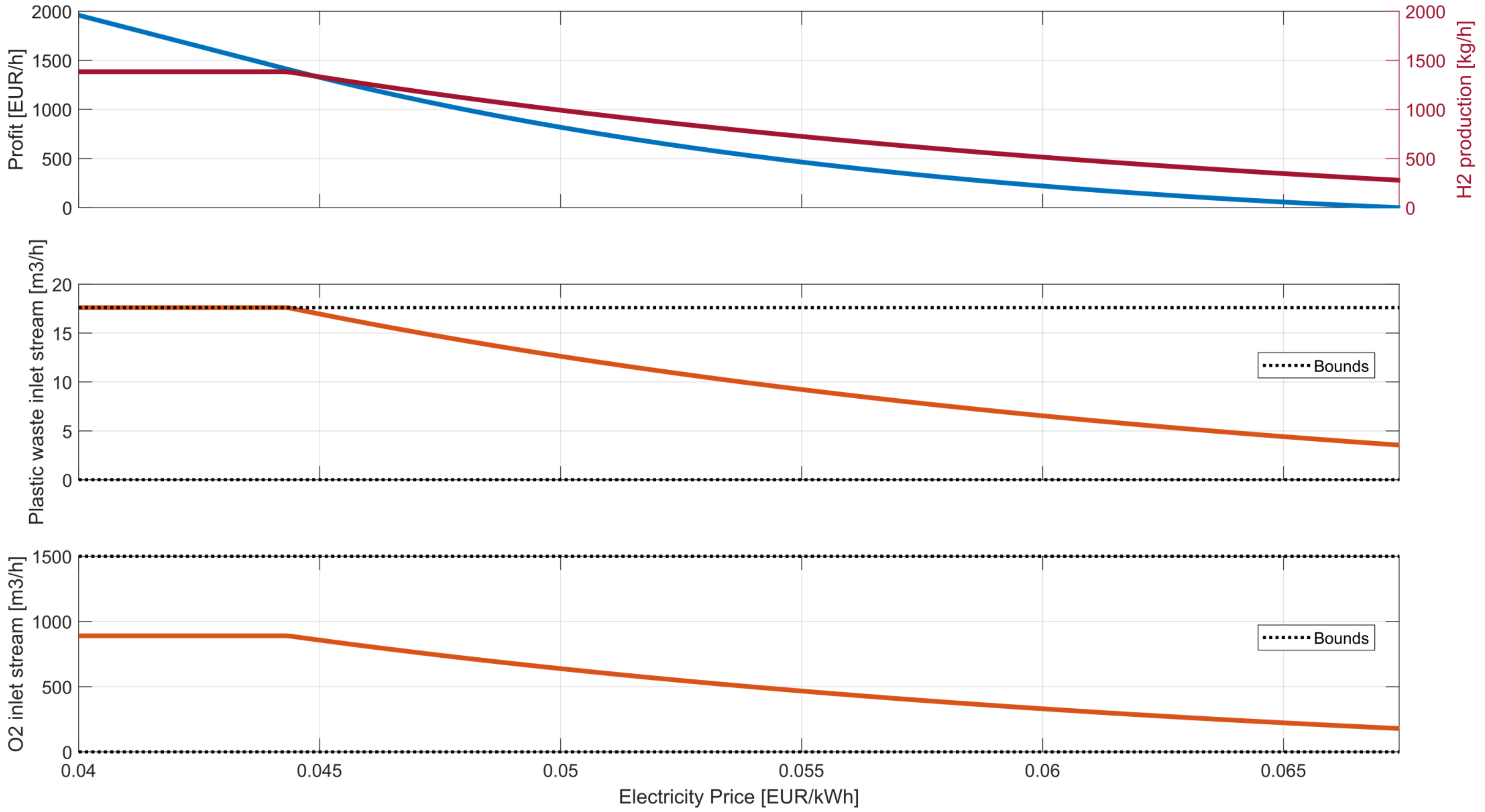
Single-stage optimization

$$
\begin{aligned}
\max_{x,y,z,w_1,u} \quad & \phi(y, w_1, u, p), && \text{Profit} \\
\text{s.t.} \quad & 0 = F(y, u, d), && \text{Mass balances (FBR)} \\
& 0 = G(x, y, z), && \text{Chemical reaction equilibria (FBR + MeOH)} \\
& w_1 = w_0 + H(y, u, d), && \text{Storage} \\
& x_{\min} \leq x \leq x_{\max}, && \text{E.g., non-negativity} \\
& y_{\min} \leq y \leq y_{\max}, && \text{No formation of solid carbon} \\
& w_{\min} \leq w \leq w_{\max}, && \text{Physical limitations} \\
& u_{\min} \leq u \leq u_{\max} && \text{Operational constraints}
\end{aligned}
$$



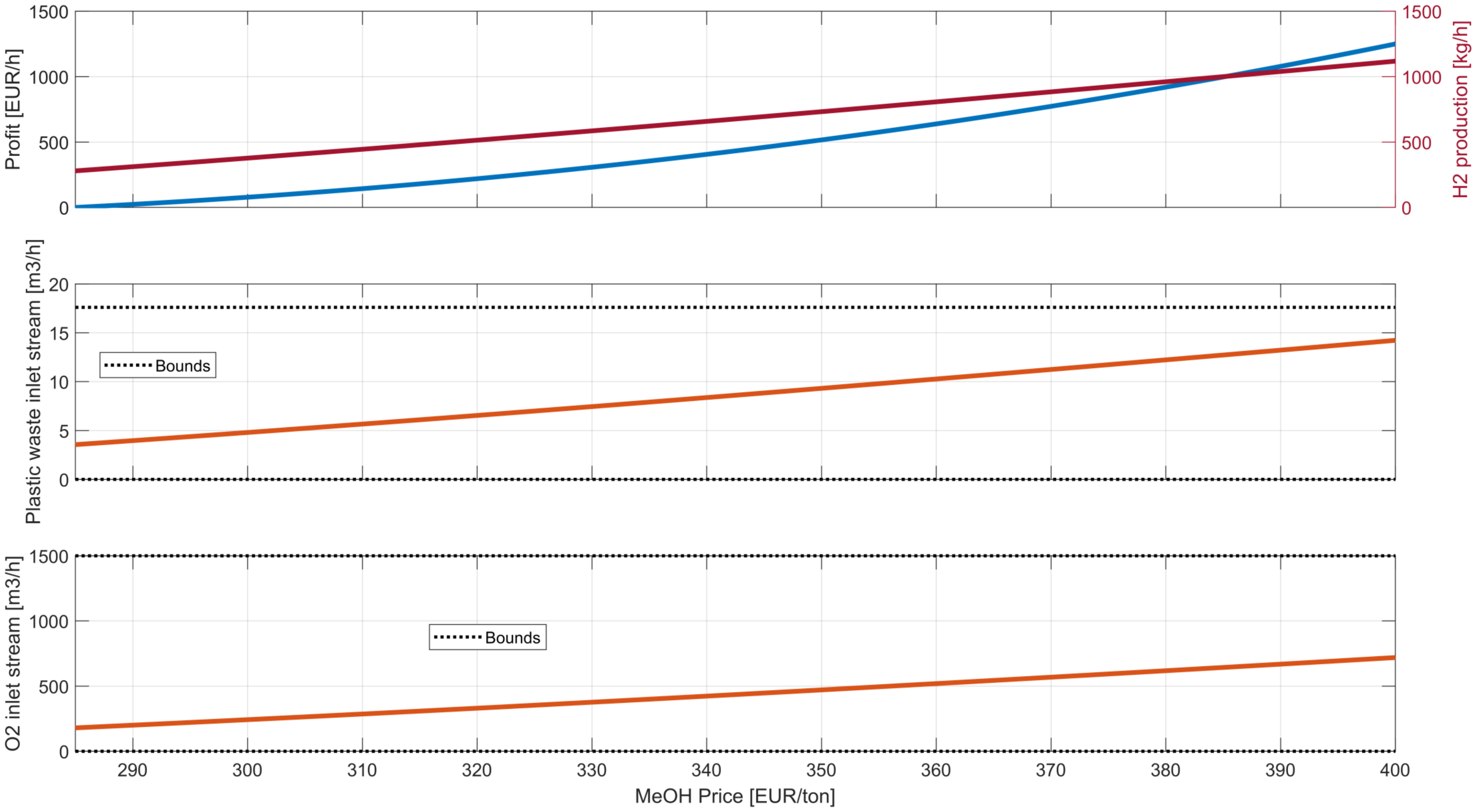
MeOH price 320 EUR/ton

Profit vs. electricity price

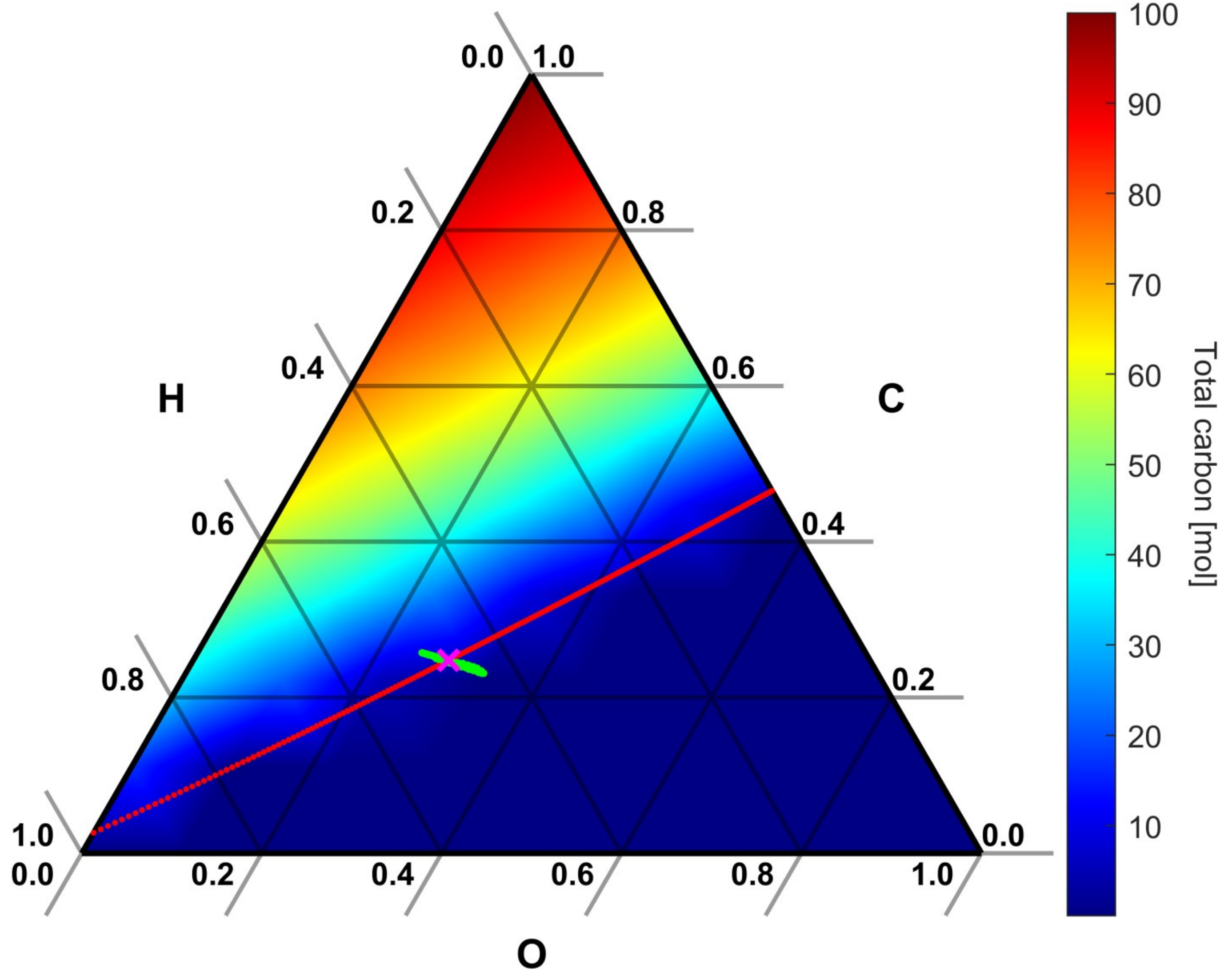


Profit vs. methanol price

Electricity price 0.06 EUR/kWh



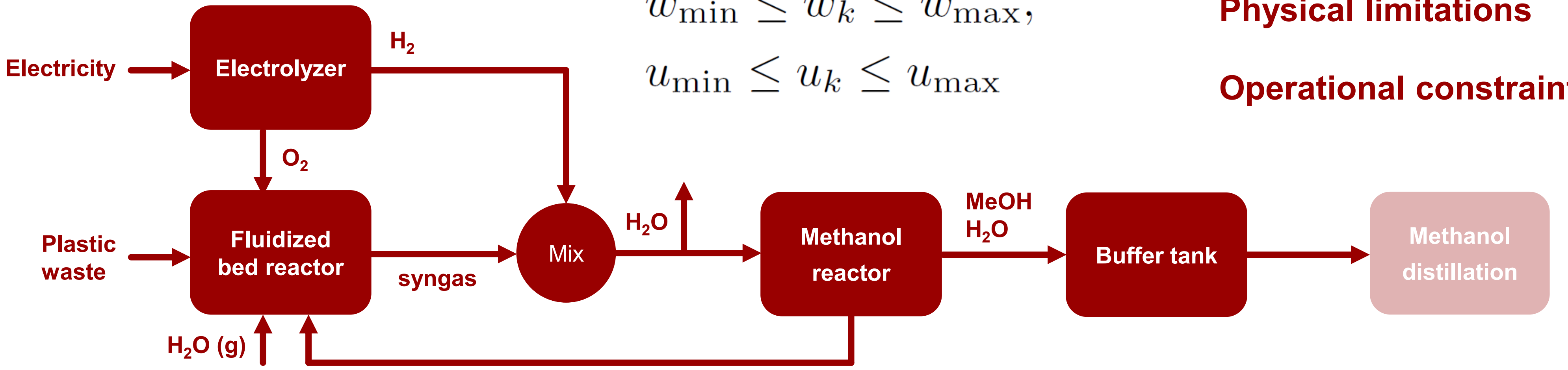
Ternary diagram



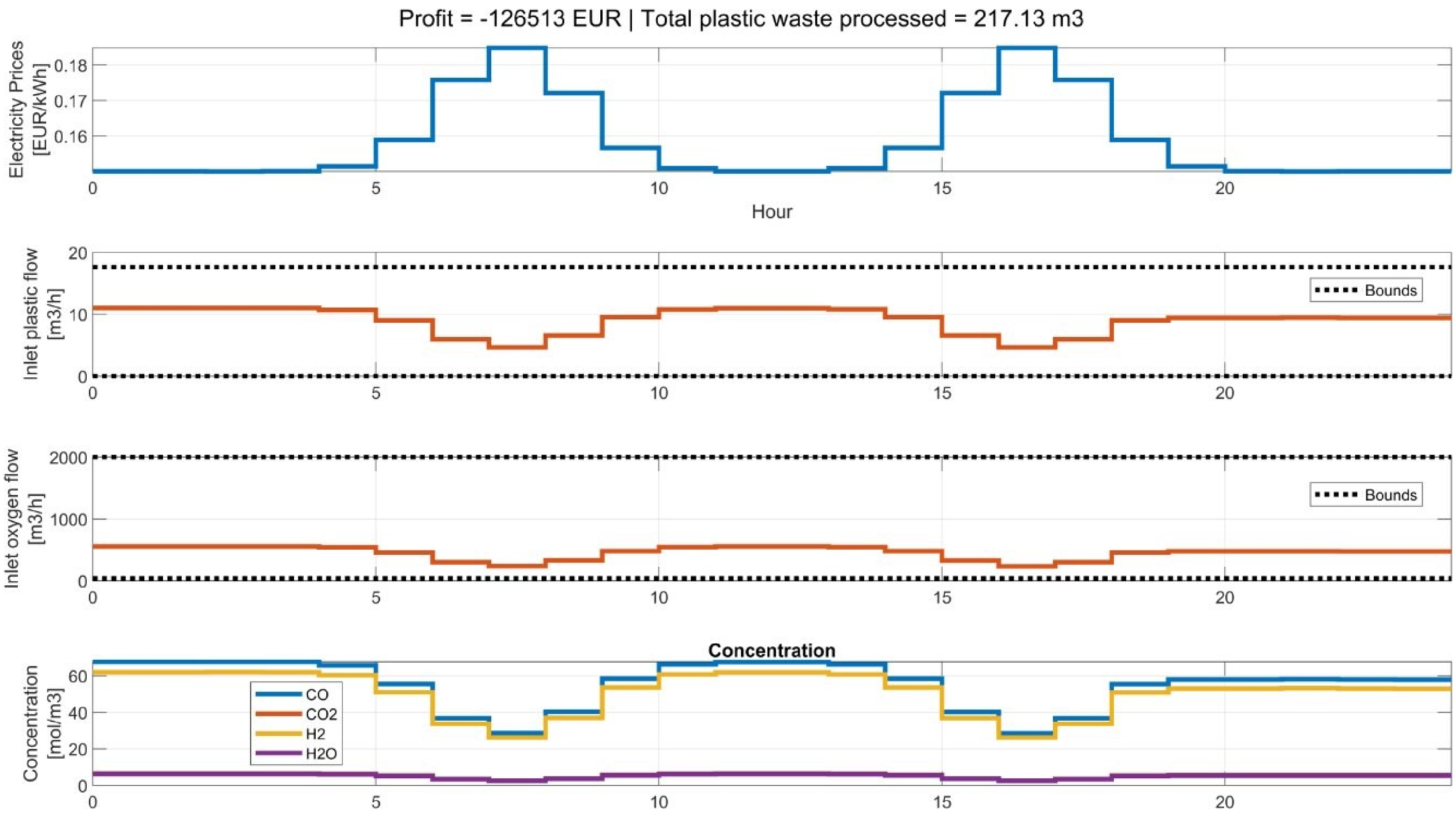
Time-varying electricity prices

Multi-stage optimization

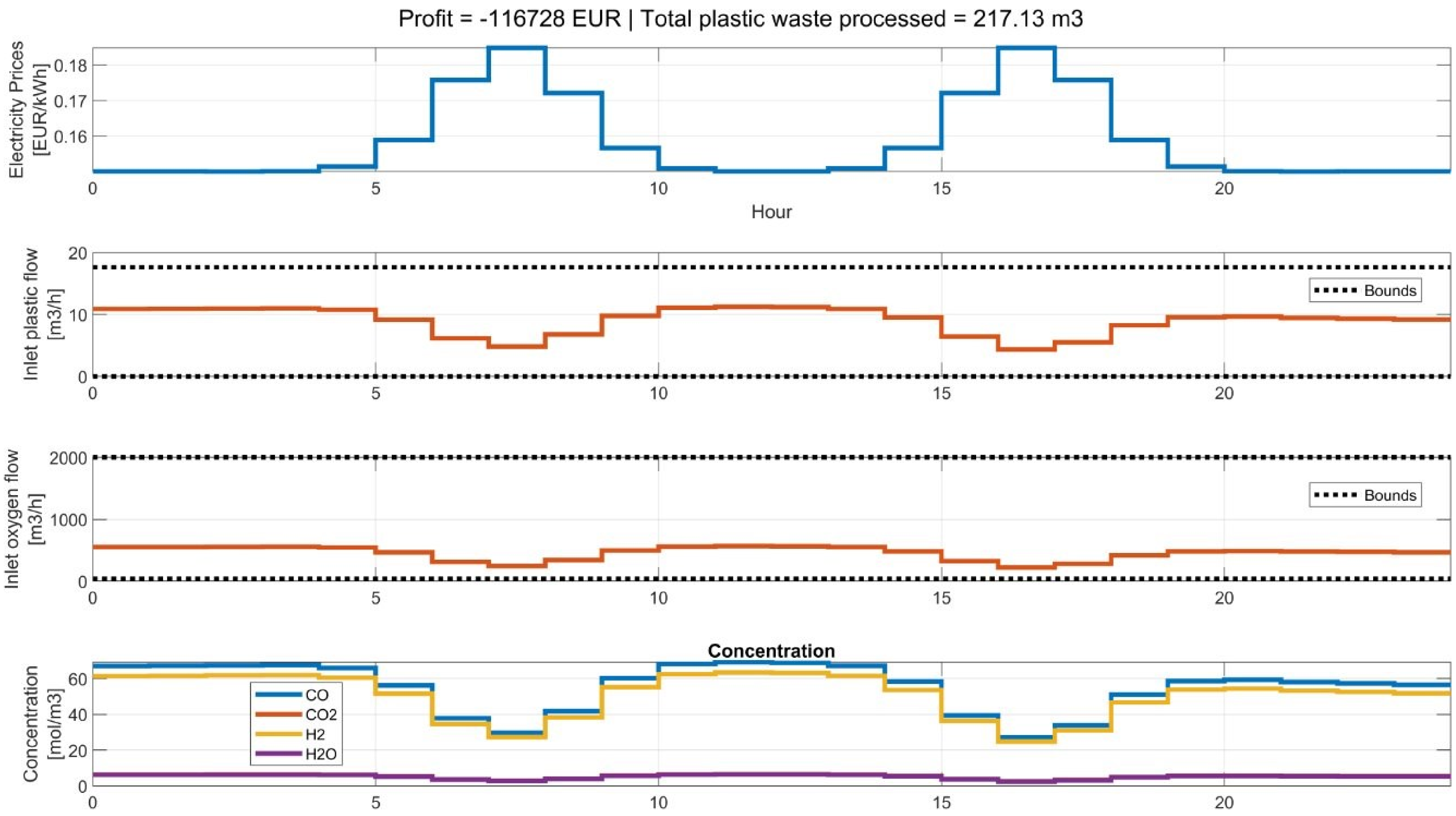
$$
\begin{aligned}
\max_{\{x_k, y_k, z_k, w_{k+1}, u_k\}_{k=0}^{N-1}} \quad & \phi(\{y_k, u_k\}_{k=0}^{N-1}, w_N, p), && \text{Profit} \\
\text{s.t.} \quad & 0 = F(y_k, u_k, d_k), && \text{Mass balances (FBR)} \\
& 0 = G(x_k, y_k, z_k), && \text{Chemical reaction equilibria (FBR + MeOH)} \\
& w_{k+1} = w_k + H(y_k, u_k, d_k), && \text{Storage} \\
& x_{\min} \leq x_k \leq x_{\max}, && \text{E.g., non-negativity} \\
& y_{\min} \leq y_k \leq y_{\max}, && \text{No formation of solid carbon} \\
& w_{\min} \leq w_k \leq w_{\max}, && \text{Physical limitations} \\
& u_{\min} \leq u_k \leq u_{\max} && \text{Operational constraints}
\end{aligned}
$$



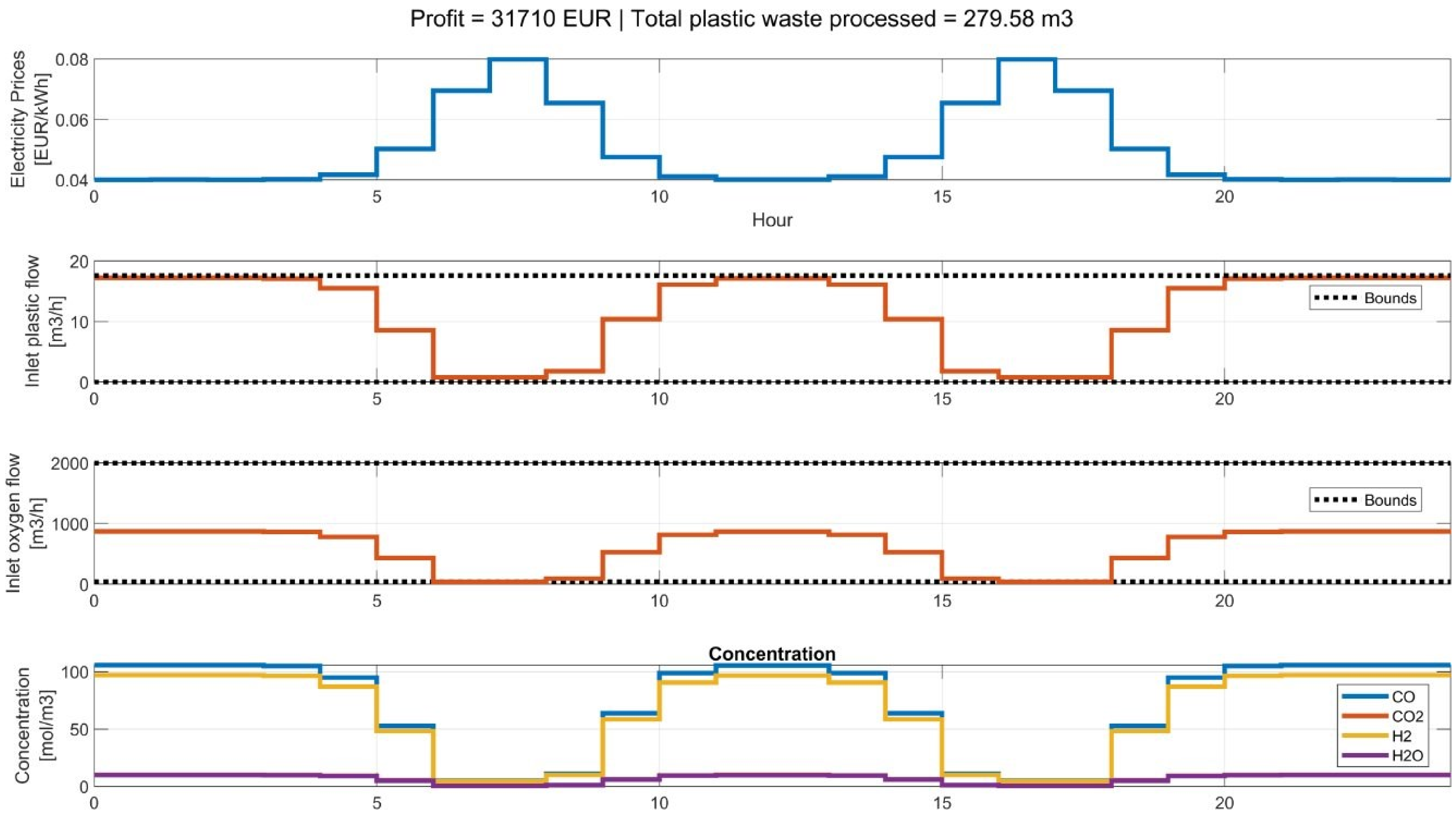
Process optimization for time-varying electricity prices



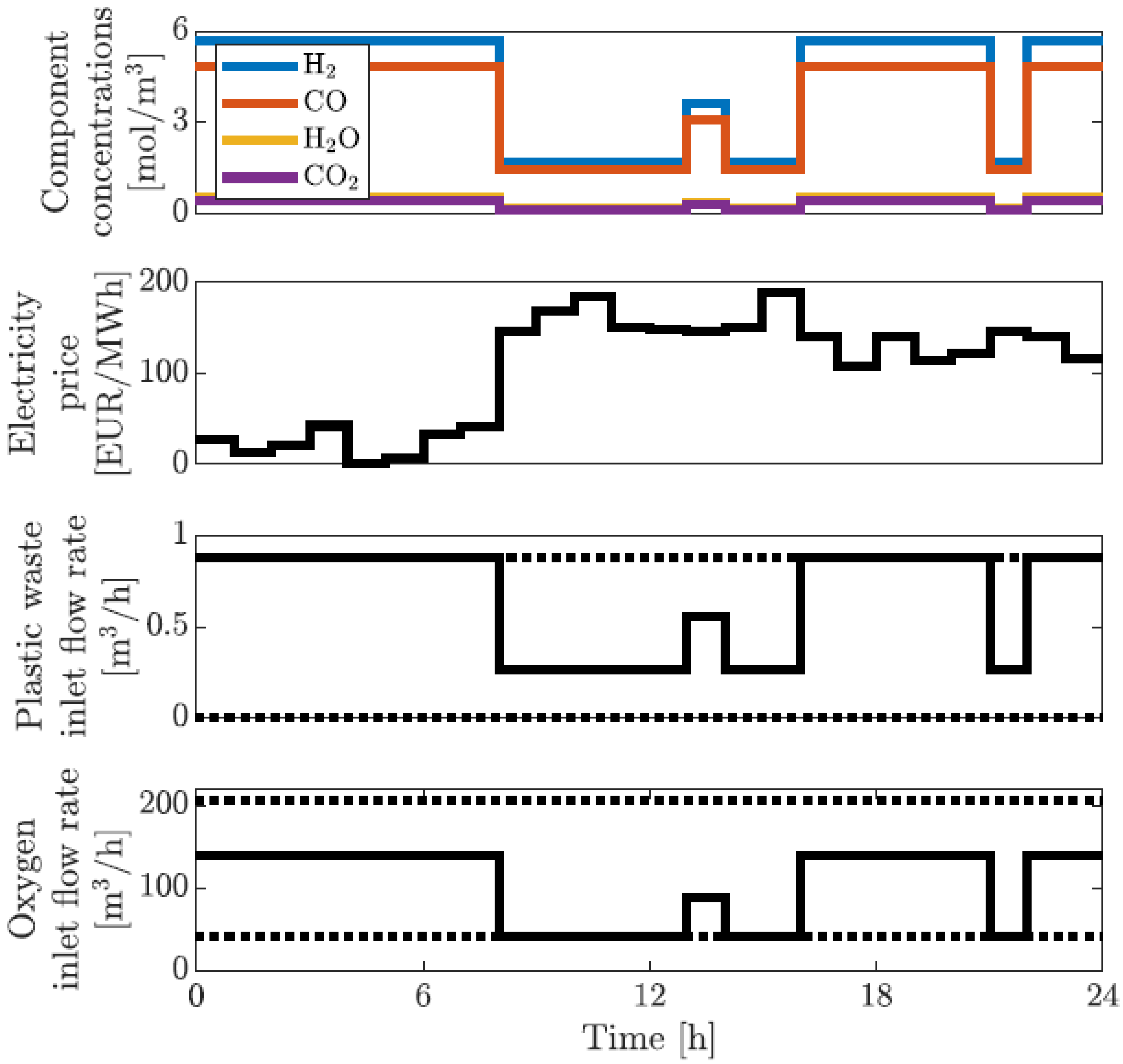
Constant electrolyzer efficiency



Reduced electricity price



Previous work (simpler model)



Optimality conditions

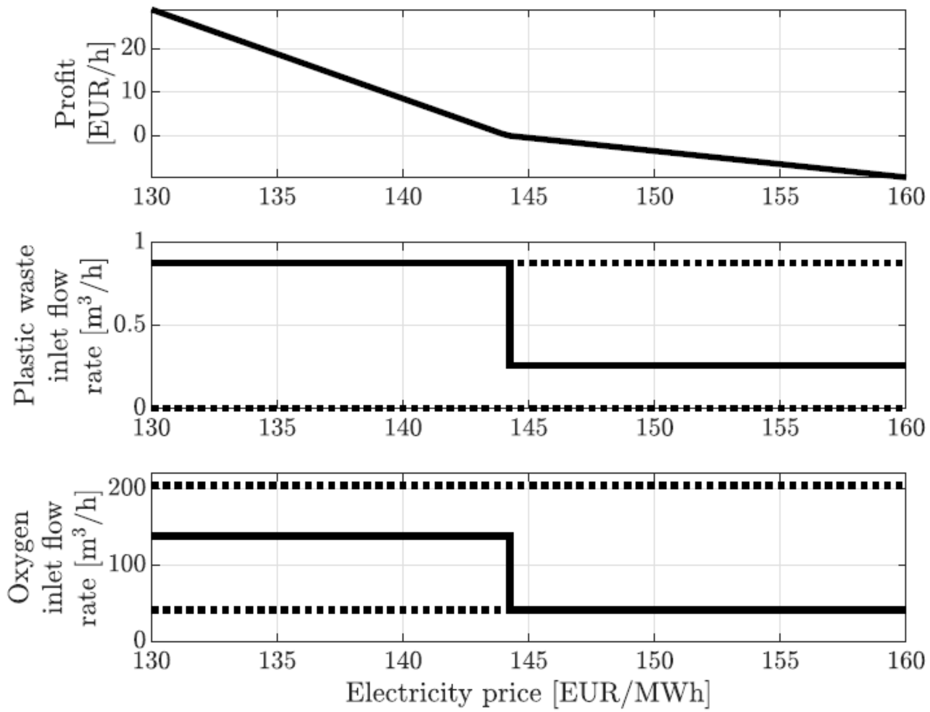
Optimality conditions

$$
\begin{aligned}
-A^T\mu - \nabla_x G(x,y,z)\lambda - \kappa &= 0,\\
\nabla_y \phi(y,u) - \nabla_y G(x,y,z)\lambda - \nu &= 0,\\
-\nabla_z G(x,y,z)\lambda &= 0,\\
\nabla_u \phi(y,u) - B^T\mu - \omega_{\text{min}} + \omega_{\text{max}} &= 0,\\
Ax + Bu + e &= 0,\\
G(x,y,z) &= 0,\\
x - x_{\text{min}} &\perp \kappa,\\
y - y_{\text{min}} &\perp \nu,\\
u - u_{\text{min}} &\perp \omega_{\text{min}},\\
u_{\text{min}} - u &\perp \omega_{\text{max}}
\end{aligned}
$$

Current results

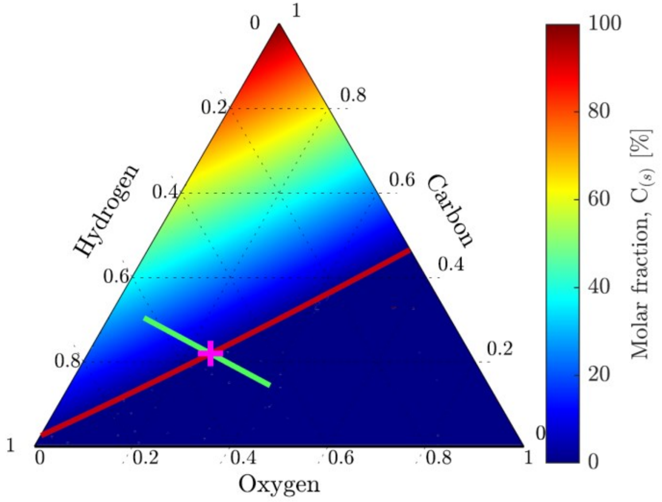
Oxygen and plastic waste flow rates equal to upper bounds?

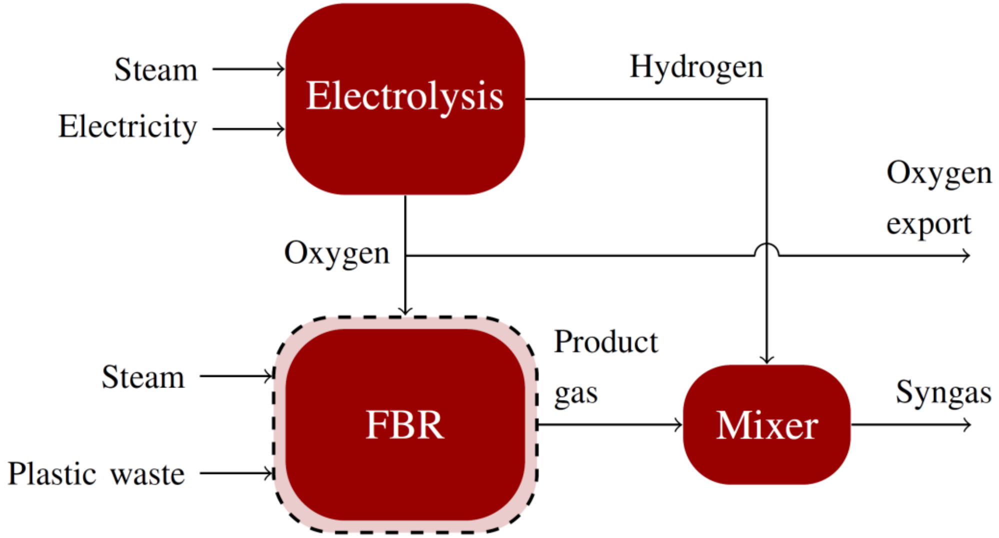
$$B^T\mu > \nabla_u \phi(y,u) \Rightarrow \omega_{\max} > 0 \wedge \omega_{\min} = 0 \Rightarrow u = u_{\max},$$
$$B^T\mu < \nabla_u \phi(y,u) \Rightarrow \omega_{\max} = 0 \wedge \omega_{\min} > 0 \Rightarrow u = u_{\min}$$



Miscellaneous

$$\mu = -\frac{1}{a}\lambda_z \qquad \begin{bmatrix} H & 0 & -M^g \\ 0 & 0 & -M^s \\ -(M^g)^T & -(M^s)^T & 0 \end{bmatrix} \begin{bmatrix} \lambda_g \\ \lambda_s \\ \lambda_z \end{bmatrix} = \begin{bmatrix} \nabla_{n^g}\phi(y,u) - \nu_g \\ \nabla_{n^s}\phi(y,u) - \nu_s \\ 0 \end{bmatrix}$$





Fluctuations in the feed composition

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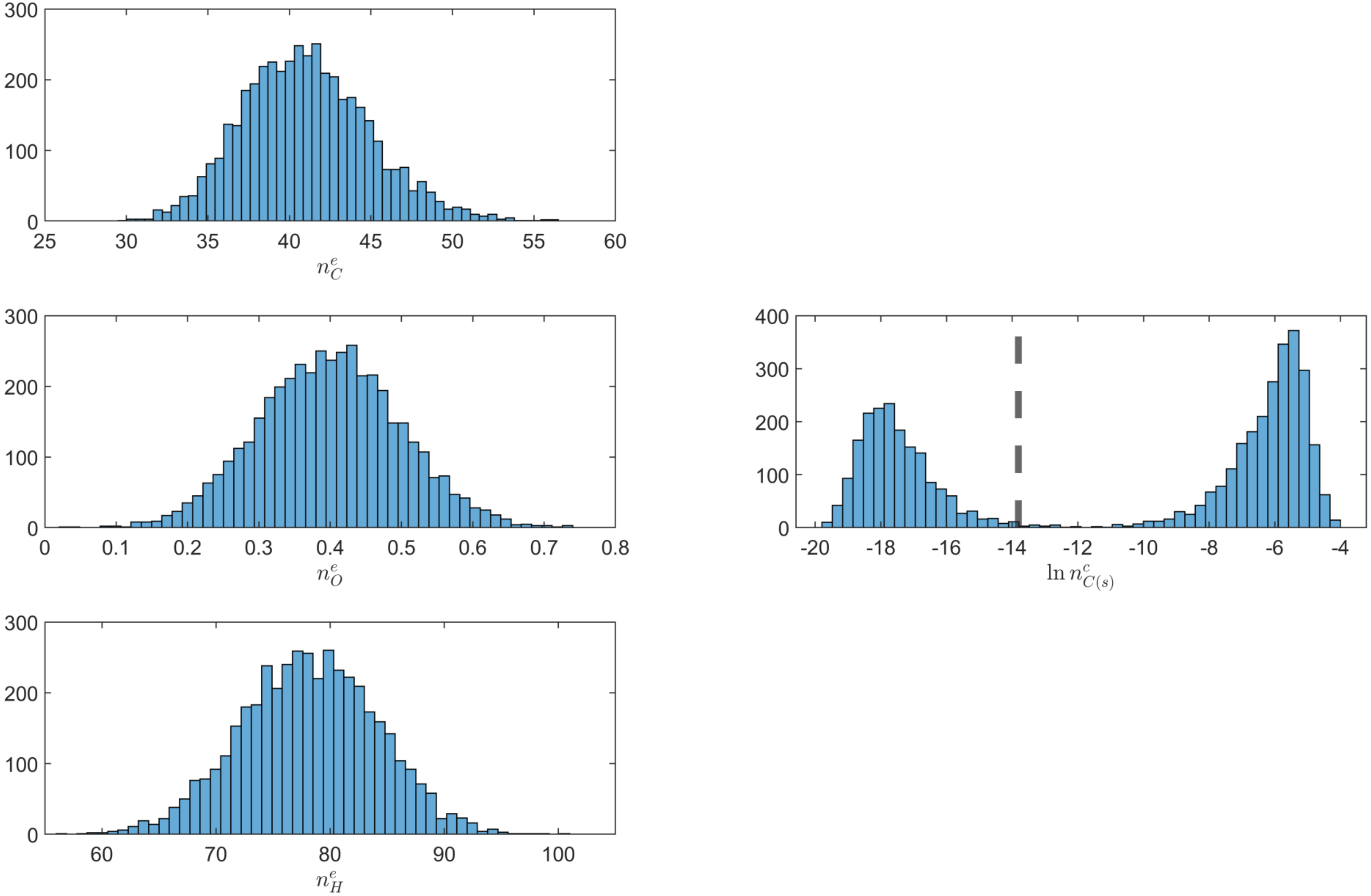
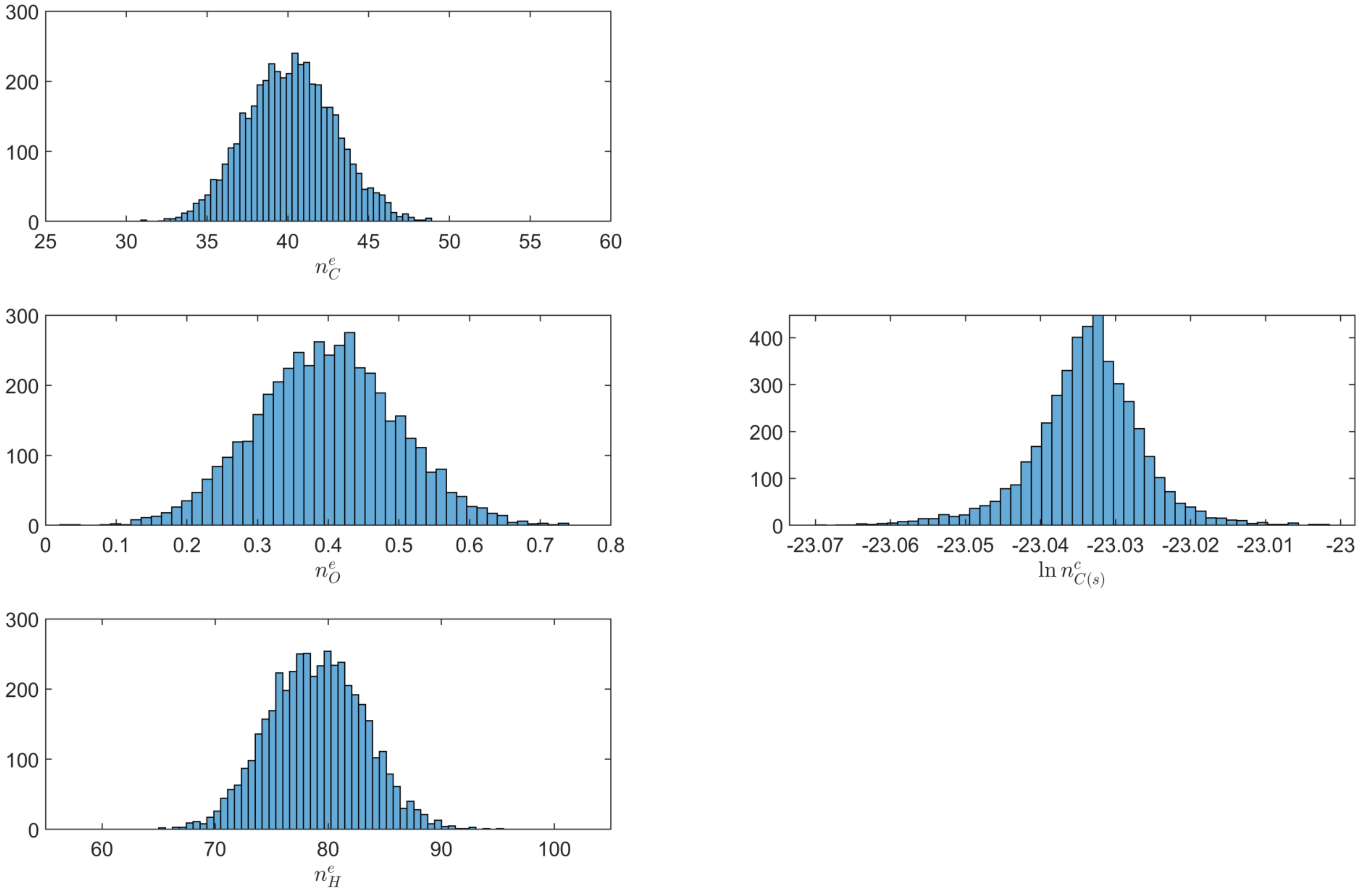


Mitigation of fluctuations in the feed composition



Summary

Water: Important,
but not expensive

Electrolyzer efficiency:
Limited effect on results

Single-stage optimization
for various electricity prices

Multi-stage optimization
for time-varying electricity prices

Mitigating fluctuations
in the feed stream

THANK YOU