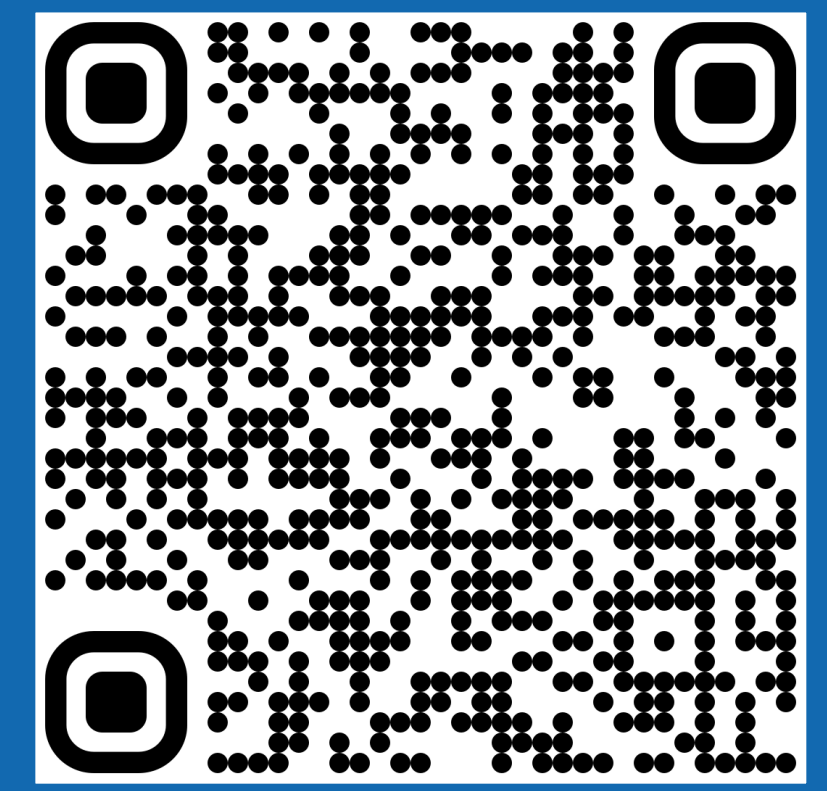


Computer-Aided Mixture Design Using Molecule Superstructures

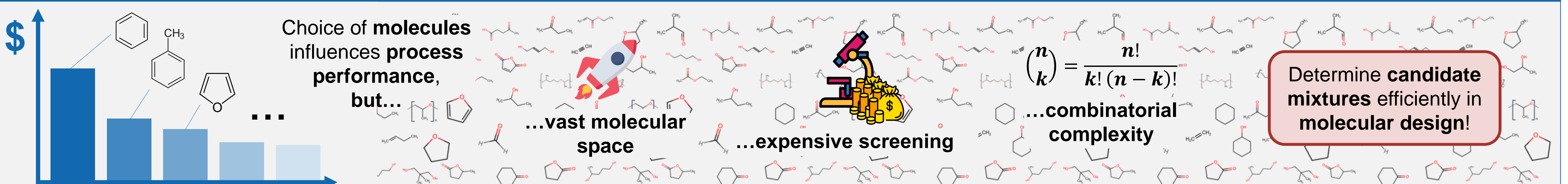
Philipp Rehner, Johannes Schilling, André Bardow

Energy & Process Systems Engineering, ETH Zurich, Switzerland

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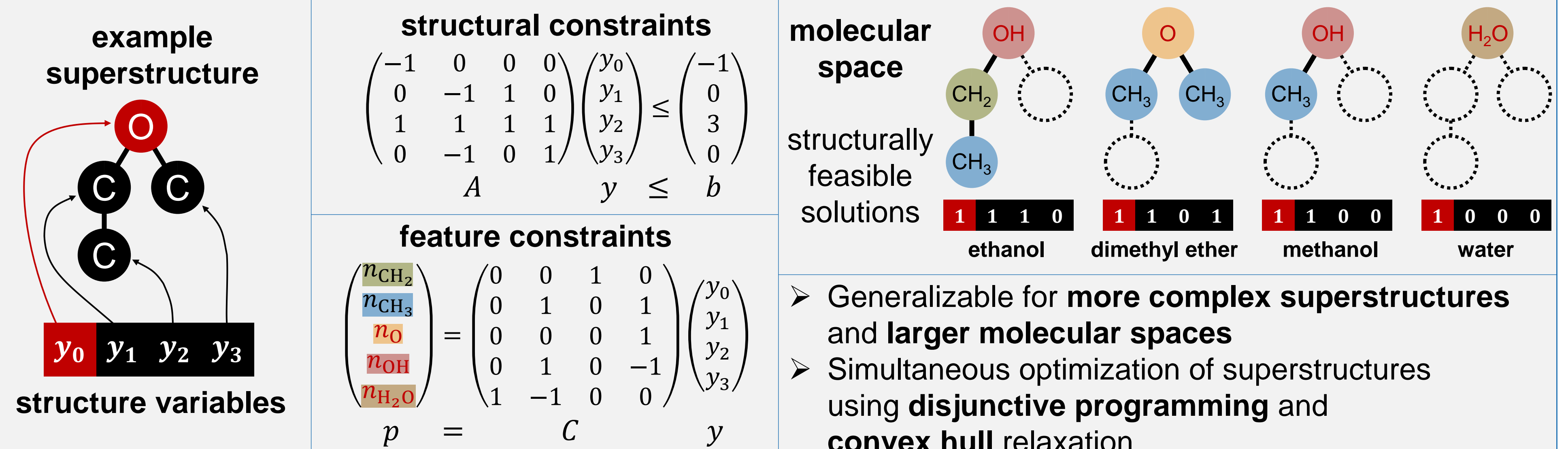
Motivation



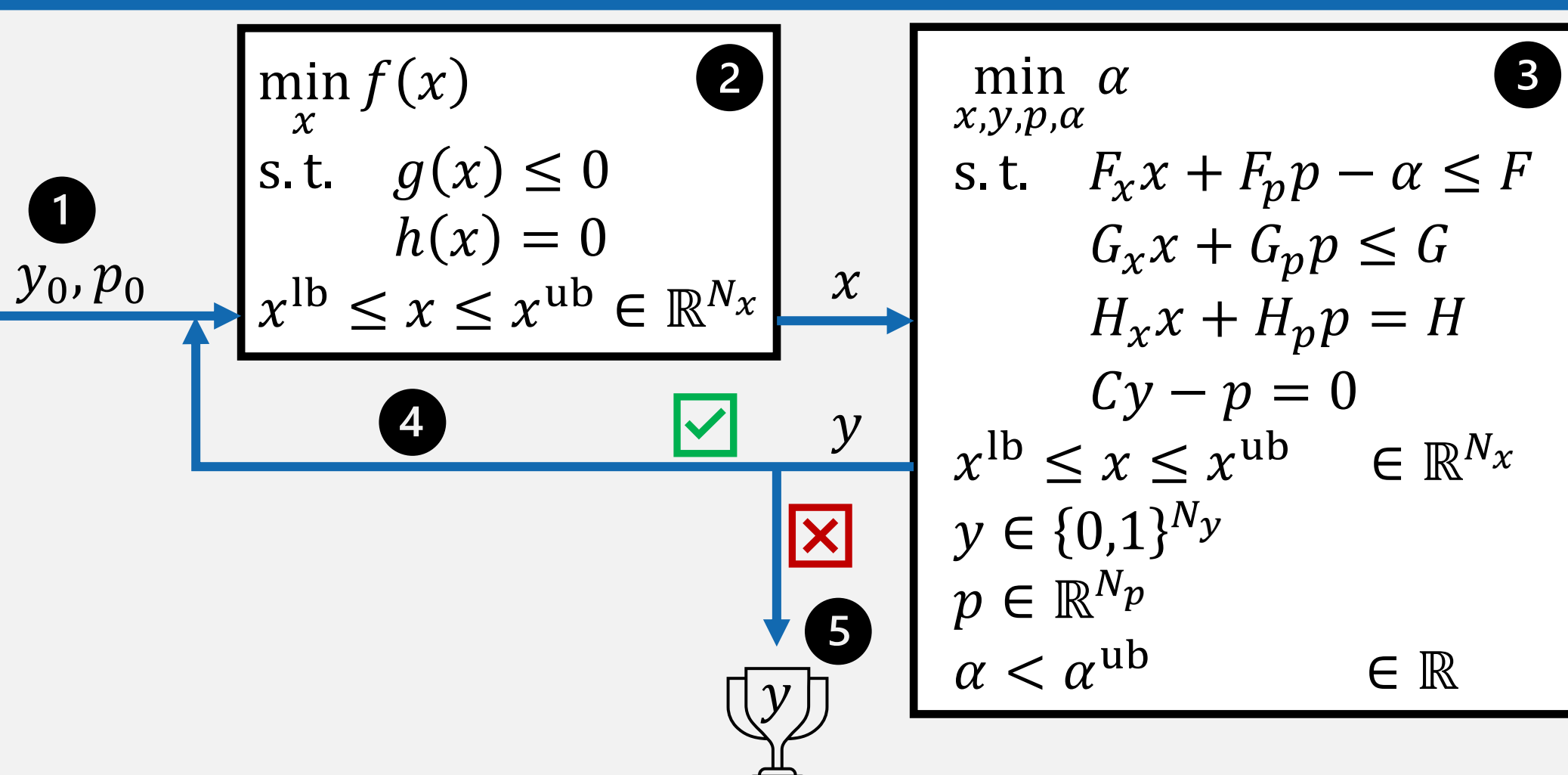
Optimization problem

$$\begin{aligned} \min_{x,y,p} \quad & f(x,p) \quad \text{process target} \\ \text{s.t.} \quad & g(x,p) \leq 0 \quad \text{process model and constraints} \\ & h(x,p) = 0 \\ & Ay \leq b \quad \text{structural constraints} \\ & Cy - p = 0 \quad \text{feature constraints} \\ & x^{\text{lb}} \leq x \leq x^{\text{ub}} \in \mathbb{R}^{N_x} \quad \text{process degrees of freedom} \\ & y \in \{0,1\}^{N_y} \quad \text{structure variables} \\ & p \in \mathbb{R}^{N_p} \quad \text{molecular features} \end{aligned}$$

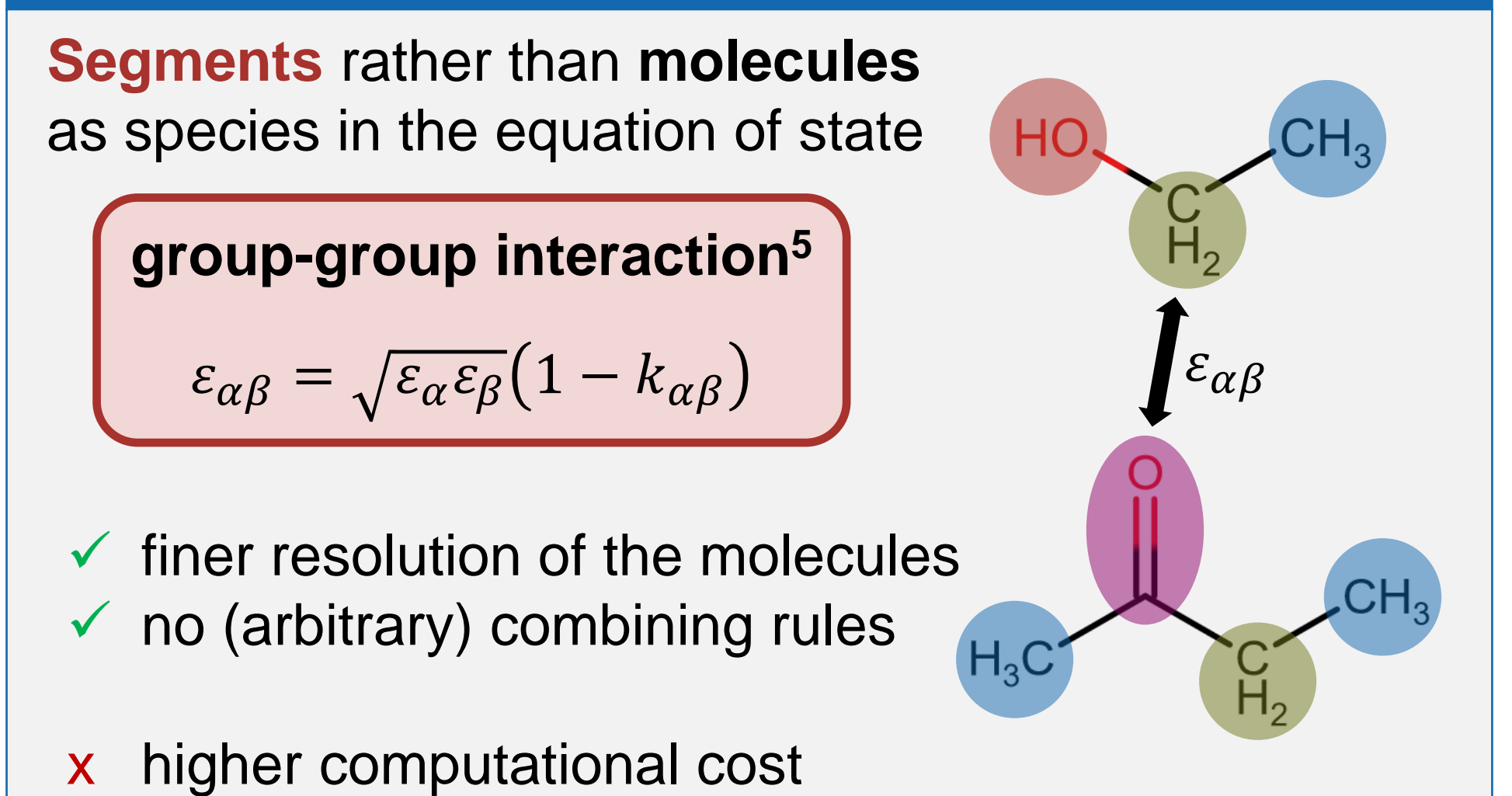
Molecule superstructures¹



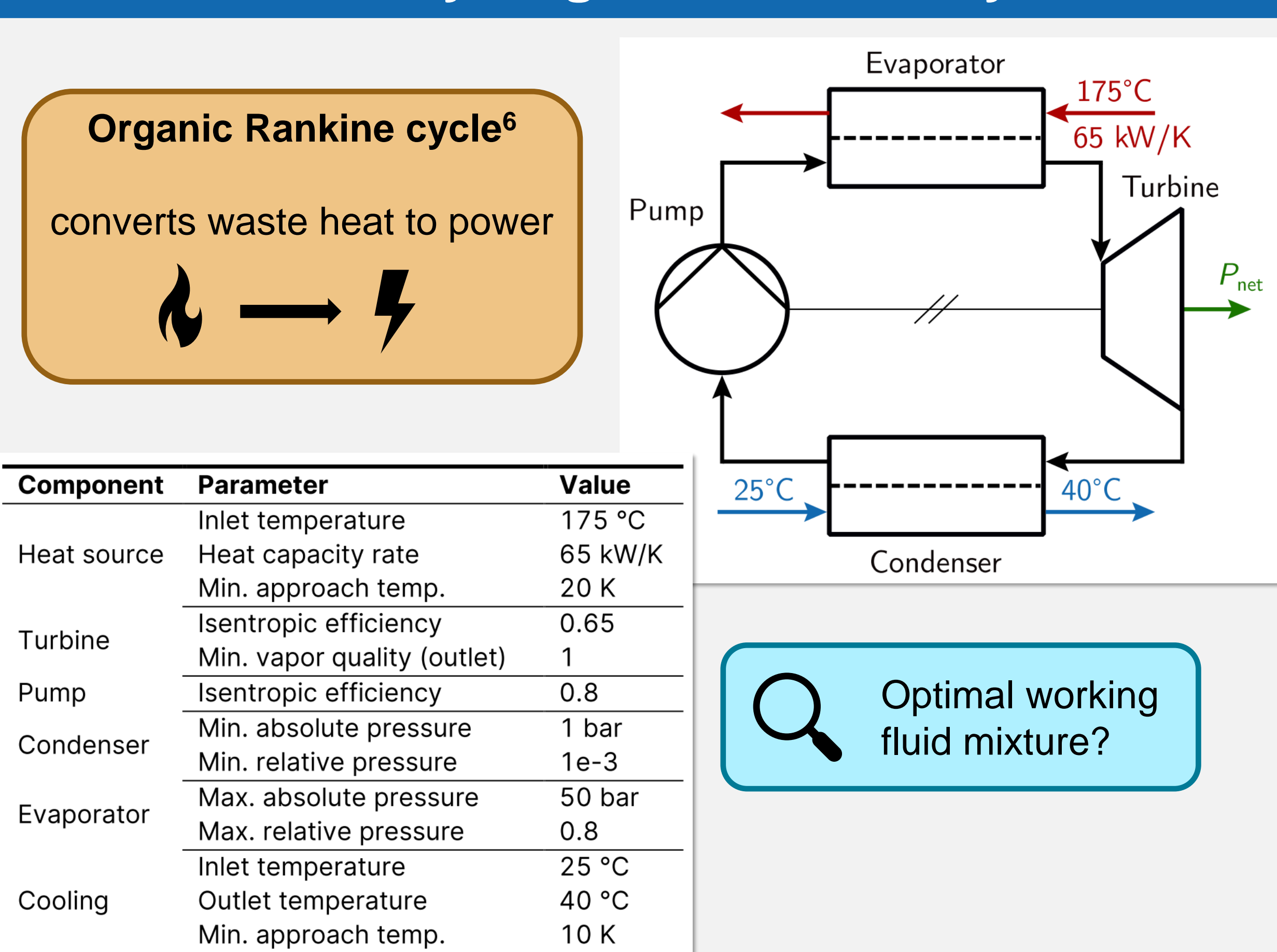
Outer approximation algorithm^{2,3}



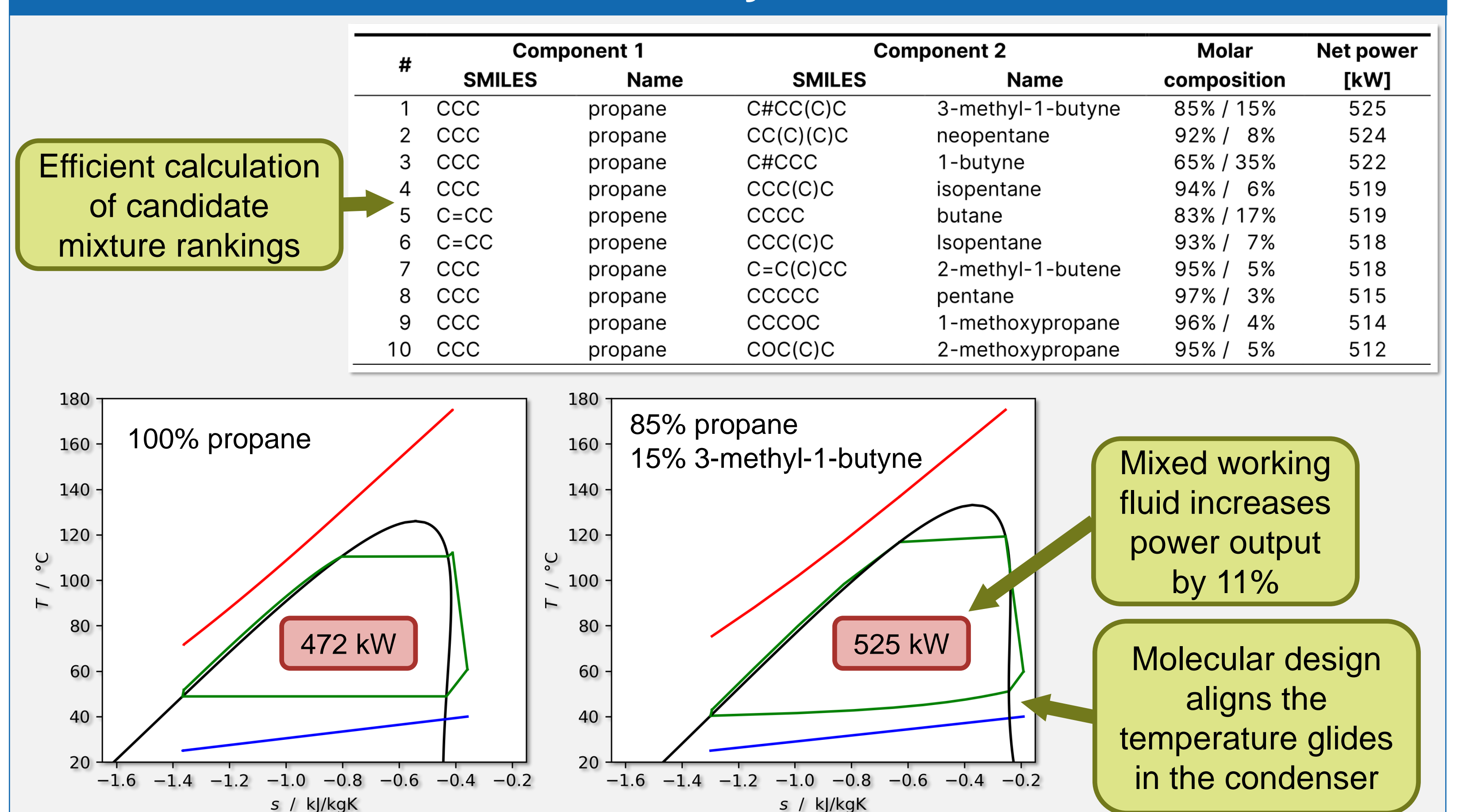
Heterosegmented gc-PC-SAFT⁴



Case study: organic Rankine cycle



Case study results



Conclusion & Outlook

- ✓ Integrated molecular and process design of pure components and mixtures
- ✓ **Process target function** to assess performance beyond molecular heuristics
- ✓ **Molecule superstructures** unlock **high-fidelity property predictions** with gc-PC-SAFT
- ✓ Tailored **outer approximation algorithm** for efficient calculation of **candidate rankings**

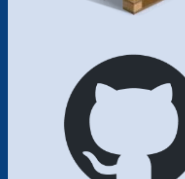


Extend method to include **economic and environmental** performance of working fluid⁷

Code based on FeO_s framework⁸ and published open-source



crates.io/crates/feos-campd



github.com/feos-org/feos-campd



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