Working Fluid Selection for Organic Rankine Cycles based on Continuous-Molecular Targets

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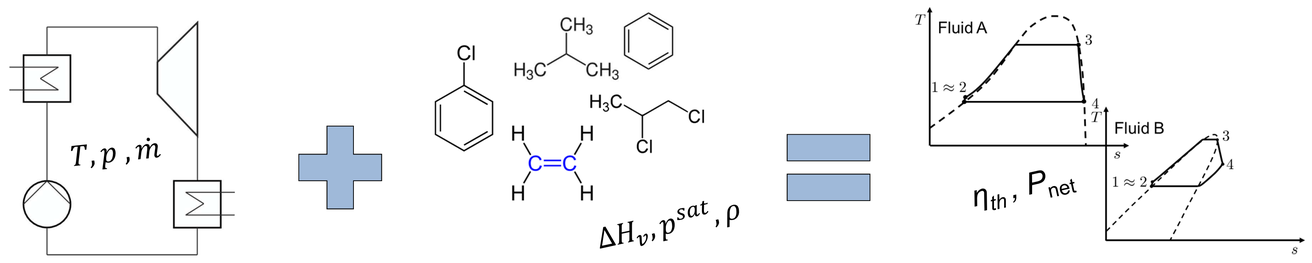
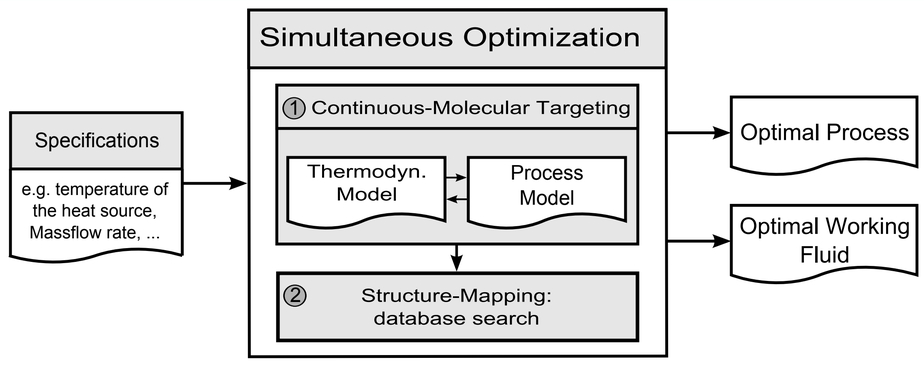
Motivation



optimal process parameters | **optimal working fluid** | **optimal performance**

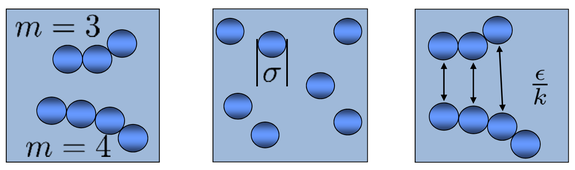
Our approach



Simultaneous Optimization by Continuous-Molecular Targeting (CoMT) + Structure-Mapping[1,2]

Modelling

- **Process:** any process model based on equilibrium properties
- **Working fluid:** PC-SAFT[4] with discrete pure component parameters y



CoMT: Relax working fluid

$$\max_{x,y} f(x,y) \qquad \text{(objective, e.g., } P_{net})$$

$$s.t. \quad g(x,y) \leq 0 \qquad \text{(inequality constraints)}$$

$$h(x,y) = 0 \qquad \text{(equality constraints)}$$

$$x \in \mathrm{R}^{\mathrm{n}} \qquad \text{(process variables)}$$

$$y \in \mathrm{R}^{\mathrm{m}} \qquad \text{(relaxed pure component parameters)}$$

Target

Hypothetical Optimum

$$y^* = \begin{pmatrix} m^* \\ \sigma^* \\ \left(\frac{\epsilon}{k}\right)^* \end{pmatrix}$$

$$J(y^*) = \nabla \tilde{f}(y)|_{y=y^*}$$

$$H(y^*) = \left(\frac{\partial^2 \tilde{f}(y)}{\partial y_i \partial y_j}\right)\Big|_{y=y^*}$$

with

$$\tilde{f}(y) = \max_x f(x,y)$$

Structure-Mapping

1. Taylor Approximation around hypothetical Optimum

$$T(y) = \tilde{f}(y^*) + J(y^*)(y-y^*) + \frac{1}{2}(y-y^*)^{\mathrm{T}} H(y^*)(y-y^*)$$

2. Estimate the objective function value f of real fluids from a database

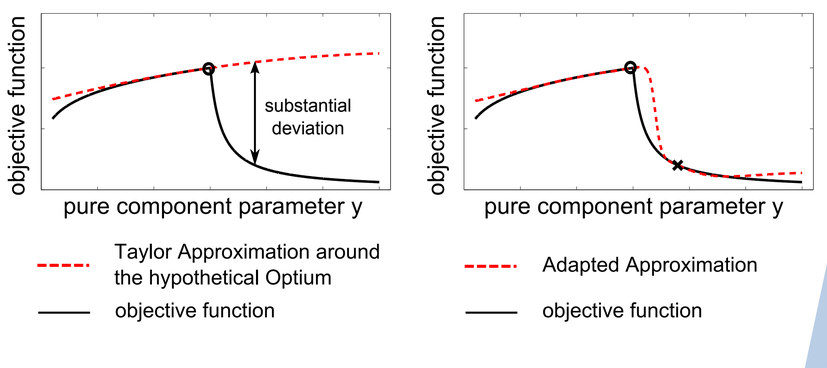
→ Ranking of potential working fluids

Adaptive Structure-Mapping (ASM)

Problem of the Structure Mapping

Taylor approximation does not account for changes in the active set of constraints

Idea: Learn from additional sampling points by combining Taylor Approximations



Adapted Approximation

Sum of weighted Taylor Approximations:

$$A(y) = \sum_{\mathrm{i}=1}^{S} w_{\mathrm{i}}^*(y) \cdot T_{\mathrm{i}}(y)$$

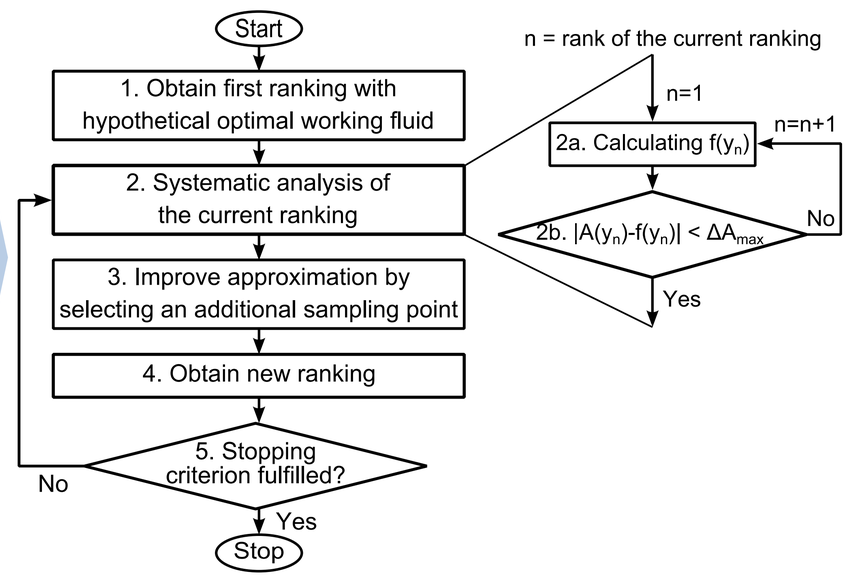
Weighting factors $w_i^*(y)$ based on the Inverse Distance Weighting:

$$d_{\mathrm{i}}^p(y) = \frac{1}{\|y_{\mathrm{n}} - y_{\mathrm{n,i}}\|^p}.$$

and normalized to 1:

$$w_{\mathrm{i}}^*(y) = \frac{d_{\mathrm{i}}^p(y)}{\sum_{\mathrm{u}=1}^{S} d_{\mathrm{u}}^p(y)}.$$

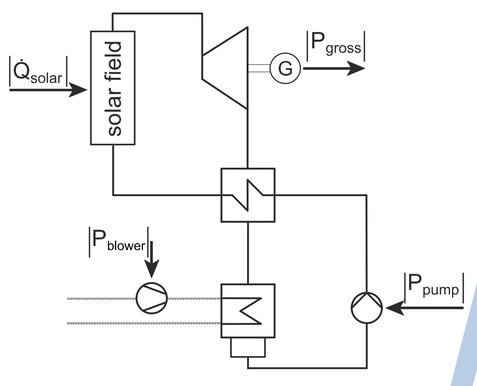
Flow chart for choosing sampling points



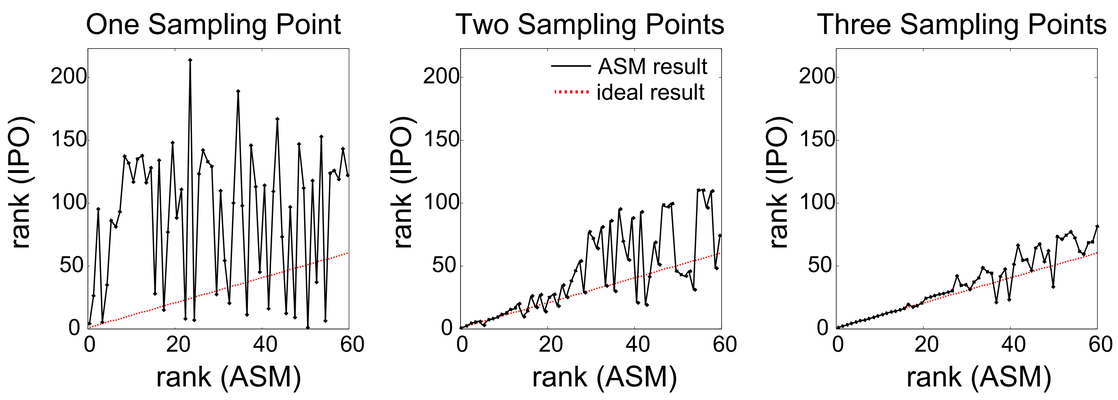
Case Study: Solarthermal ORC

Application

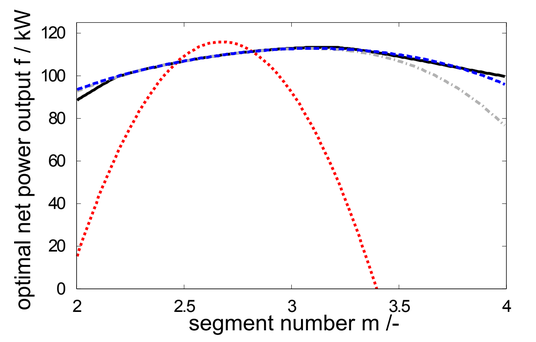
Optimize a solarthermal ORC



Adaptive Structure-Mapping (ASM) vs. Individual Process Optimization (IPO)



Adapted Approximation



optimal net power output f(y)
approximation A(y) with one sampling point
approximation A(y) with two sampling points
approximation A(y) with three sampling points

Results

Rank	Name	P_{net} [kW]
1	1,3,5,7-Cyclooctatetraene	115.0
2	Cyclooctane	113.4
3	p-XYlene	113.2
4	1-trans-3,5-Trimethylcyclohexane	112.7
5	Cycloheptane	112.3

Conclusions

Adaptive Structure-Mapping

- Iterative adaption of Structure-Mapping for CoMT
- Efficient identification of the best working fluids

Case Study

- Identifying all working fluids in the top 10
- In comparison to individual optimization: Reducing the function evaluations by 84.4 %

Further Information

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3. J. Gross, G. Sadowski, 2001. Perturbed-chain SAFT: An equation of state based on a perturbation theory for chain molecules, *Ind Eng Chem Res*, 40, 4, 1244-1260.