Next-Generation Flowsheeting Tools for Green Process Development

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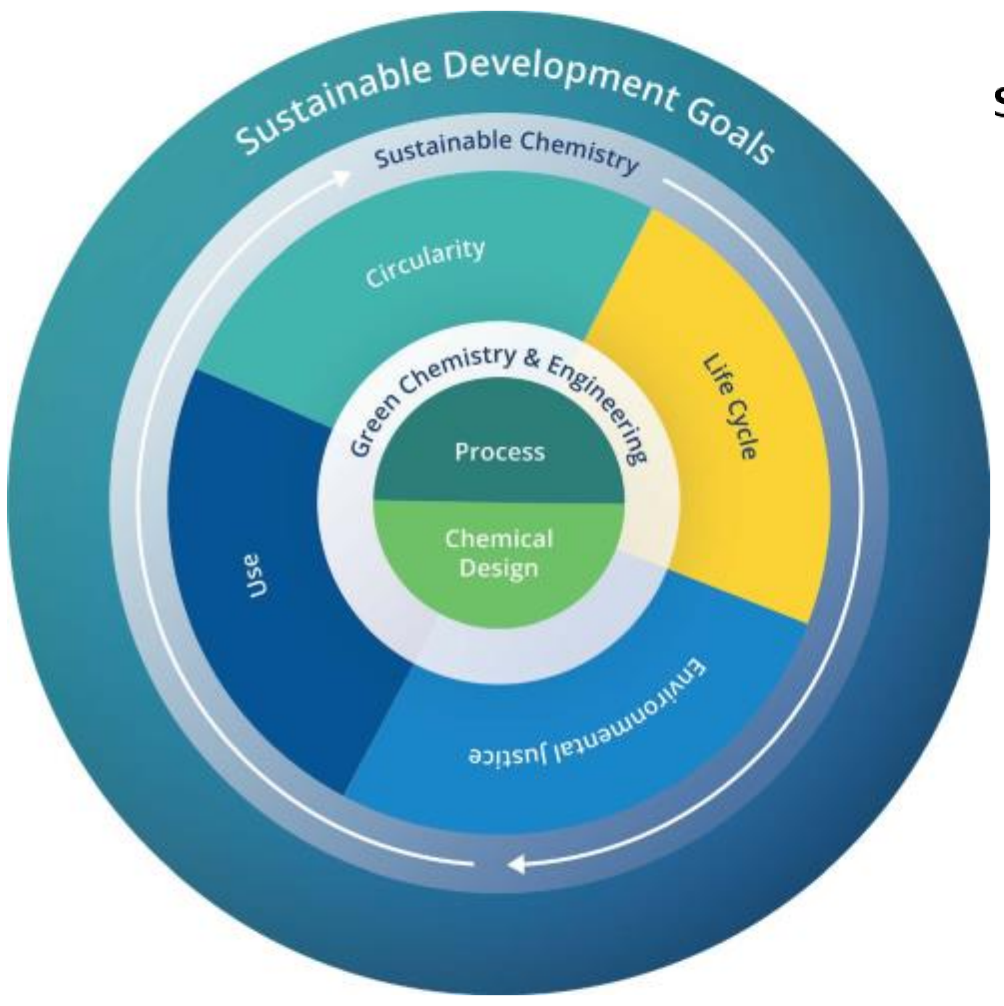
Introduction and Motivation

To incorporate sustainable development goals within chemical engineering processes during the design stage, we need to add these as **objective functions** and **constraints** during the problem formulation. However, by doing so, it makes the design problem even **harder** to solve.

Problem Formulation

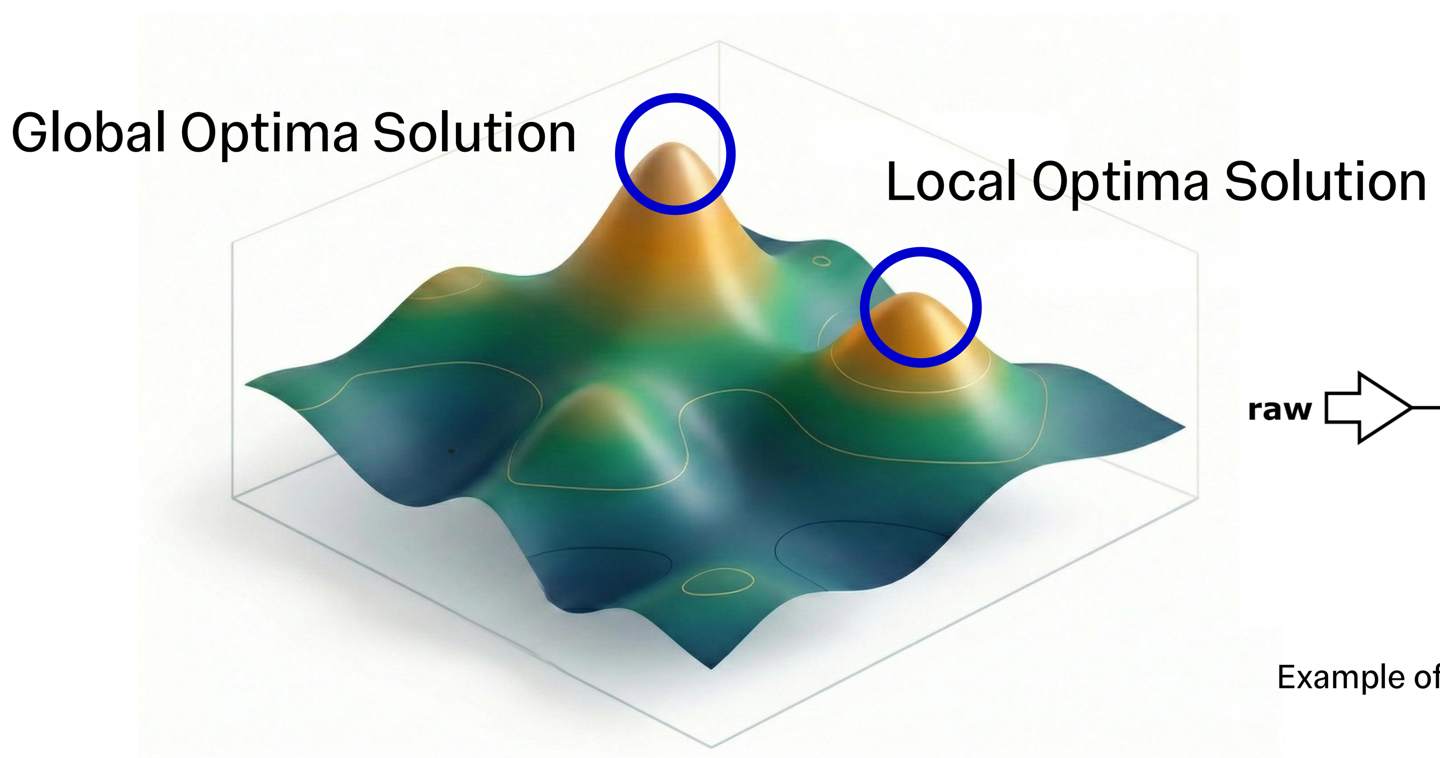


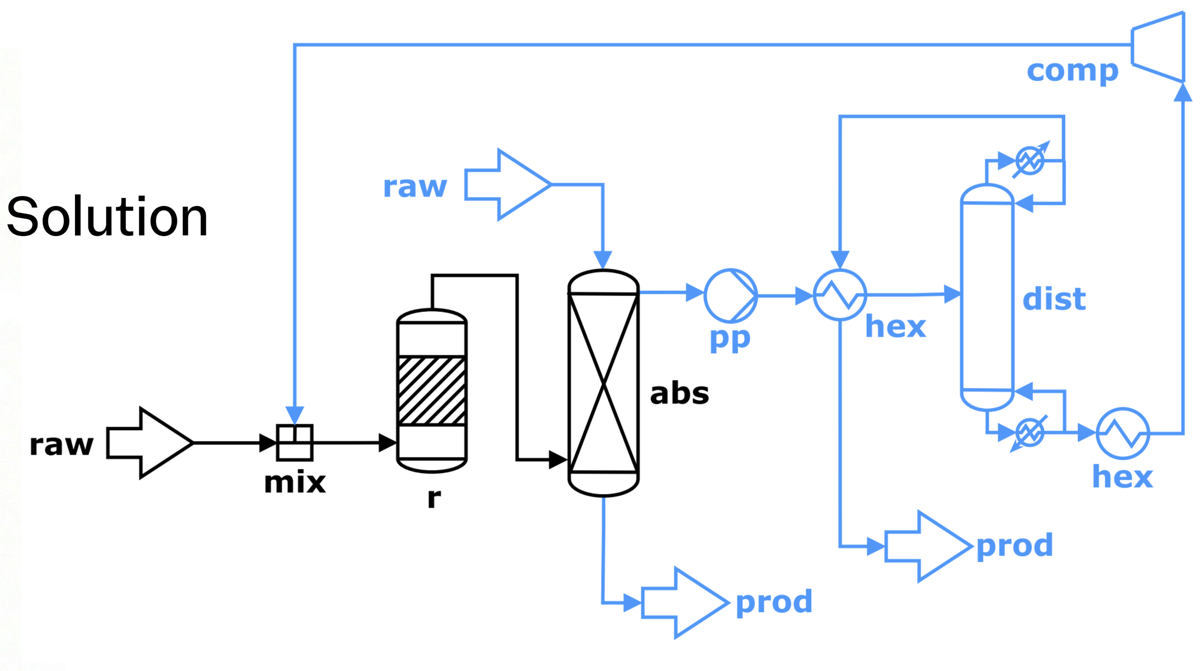
$$\min_{x,y} \left[\phi_{\text{cost}}(x,y), \phi_{\text{energy}}(x,y), \phi_{\text{waste}}(x,y), \phi_{CO_2}(x,y)\right]$$

$$\text{s.t. } g(x,y) = 0 \quad \text{(mass / energy balances, unit models)}$$

$$h(x,y) \leq 0 \quad \text{(product specs, safety, operability, sustainability)}$$

$$x \in \mathcal{X},\ y \in \mathcal{Y} \ \text{(bounds, allowable units / links)}$$

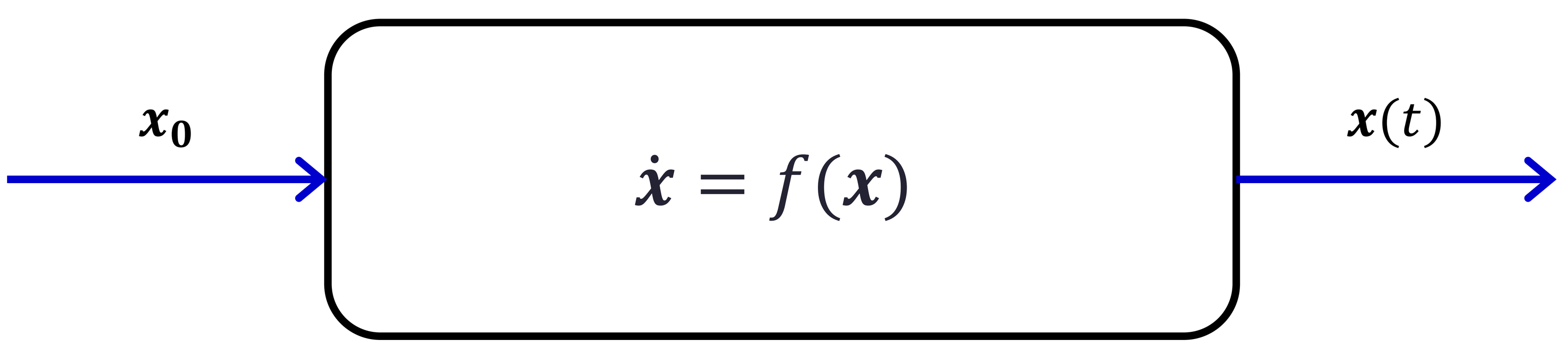




Example of one possible designs from automatic flowsheet completion.[2]

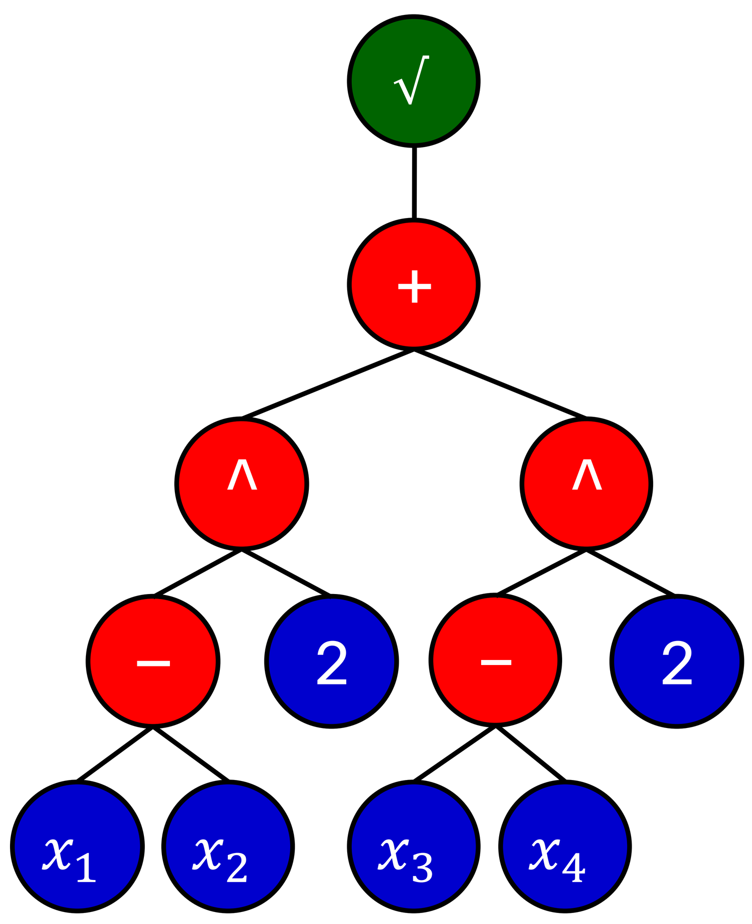
Research Approach

Ultimately, we are trying to solve a combinatorial problem. However, unlike simple combinatorial problems, every unit is a **nonlinear dynamic system** which requires careful implementation.

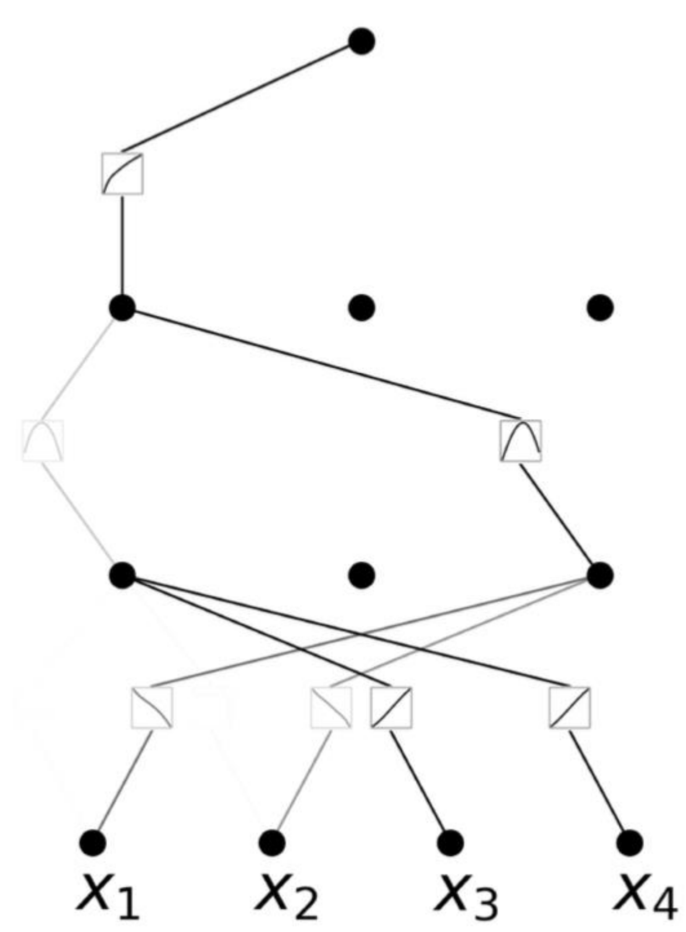


The focus is on utilising **interpretable** surrogate models, which can either be a **symbolic representation** or a **structural representation** of the process unit.

$$f(x) = \sqrt{(x_2 - x_1)^2 + (x_4 - x_3)^2}$$



Expression Tree representation of $f(x)$

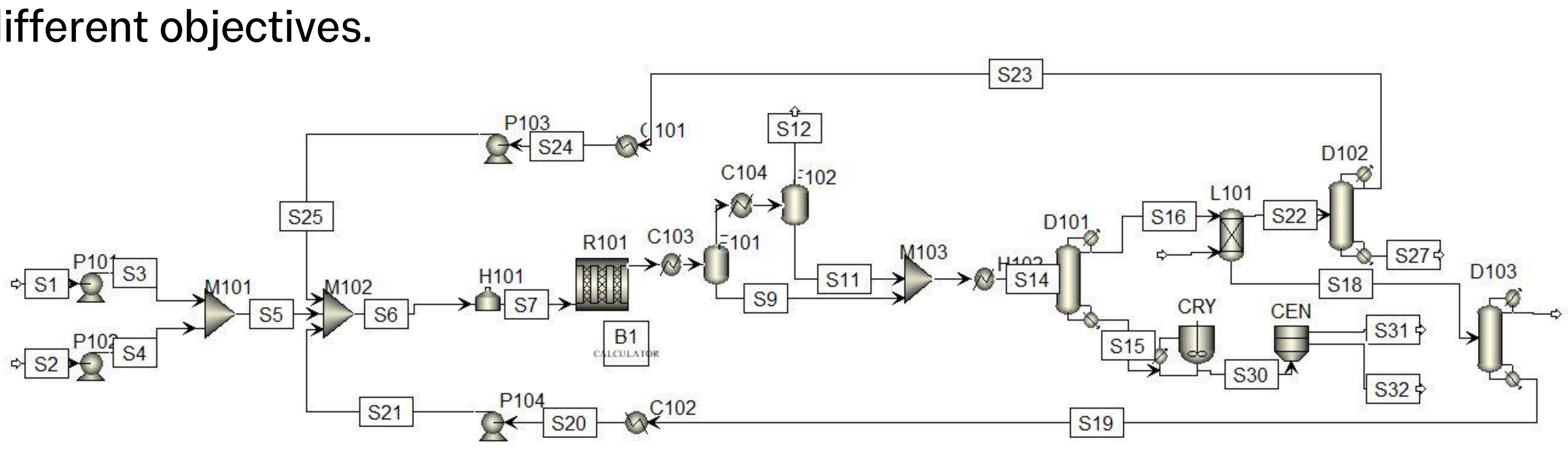


KAN representation of $f(x)$[3]

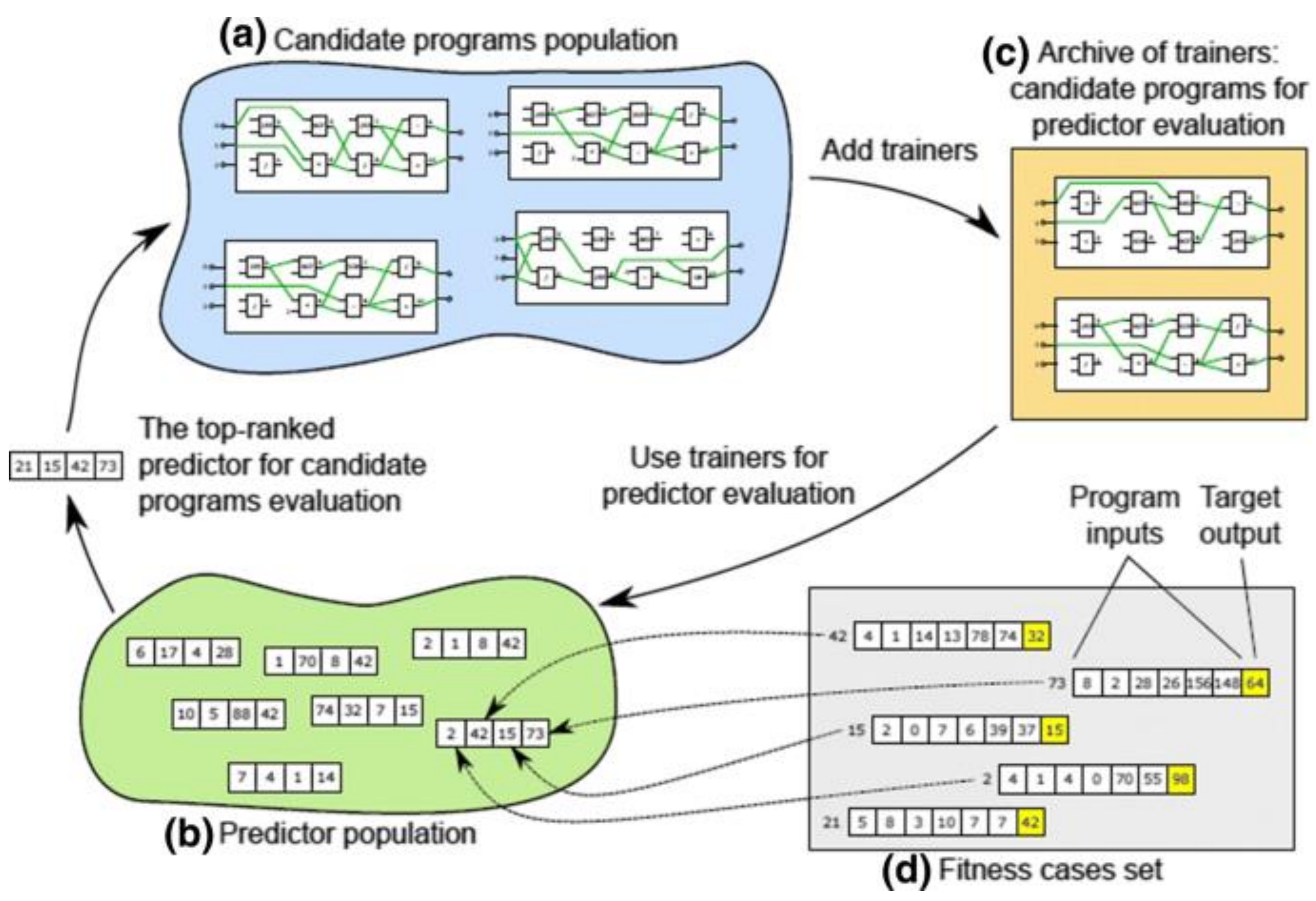
Future Work and Contributions

After choosing the types of surrogate models to use to evaluate the flowsheet, a suitable **encoding** can be to utilise a **genetic program** to obtain the **pareto front** of the multi-objective design problem.

The goal is to produce a tool that can explore new process options efficiently, allowing chemical engineers to be able to compare trade-offs between the different objectives.



Example of a locally optimal separation sequence obtained from ASPEN Plus.



General Cartesian Genetic Programming Algorithm[4]

[1] A. Cannon, S. Edwards, M. Jacobs, J. Moir, M. A. Roy and J. Tickner, *RSC Sustainability*, 2023, **1**, 2092–2106.
[2] G. Vogel, L. Schulze Balhorn and A. M. Schweidtmann, *Computers & Chemical Engineering*, 2023, **171**, 108162.
[3] Z. Liu, Y. Wang, S. Vaidya, F. Ruehle, J. Halverson, M. Soljačić, T. Y. Hou and M. Tegmark, KAN: Kolmogorov-Arnold Networks.
[4] J. F. Miller, *Genetic Programming and Evolvable Machines*, 2019, **21**, 129–168.

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