

PhD Open Days



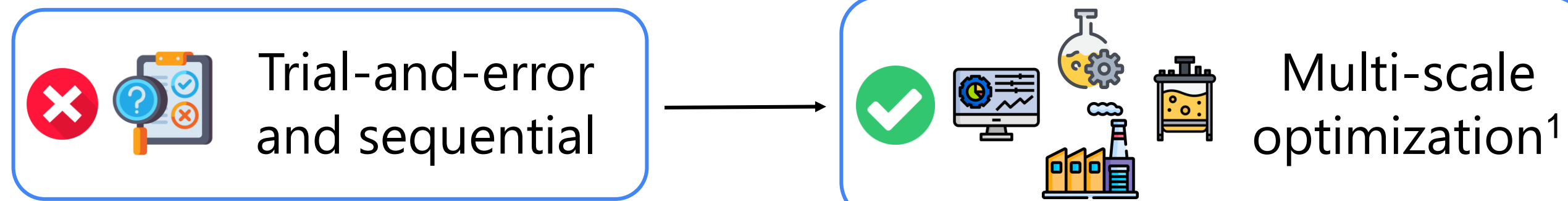
Sustainable catalysts by design: a multi-scale and multi-data approach for informed optimization

PhD in Chemical Engineering

Thomas Hietala (thomas.hietala@tecnico.ulisboa.pt)

Context

Design of novel sustainable catalysts includes objectives at a **catalytic** scale, **reactor** scale, and **process** scale. The current design process **needs improvement**.



Goal

Develop a computational multi-scale methodology for the design of sustainable catalysts.

Catalyst scale

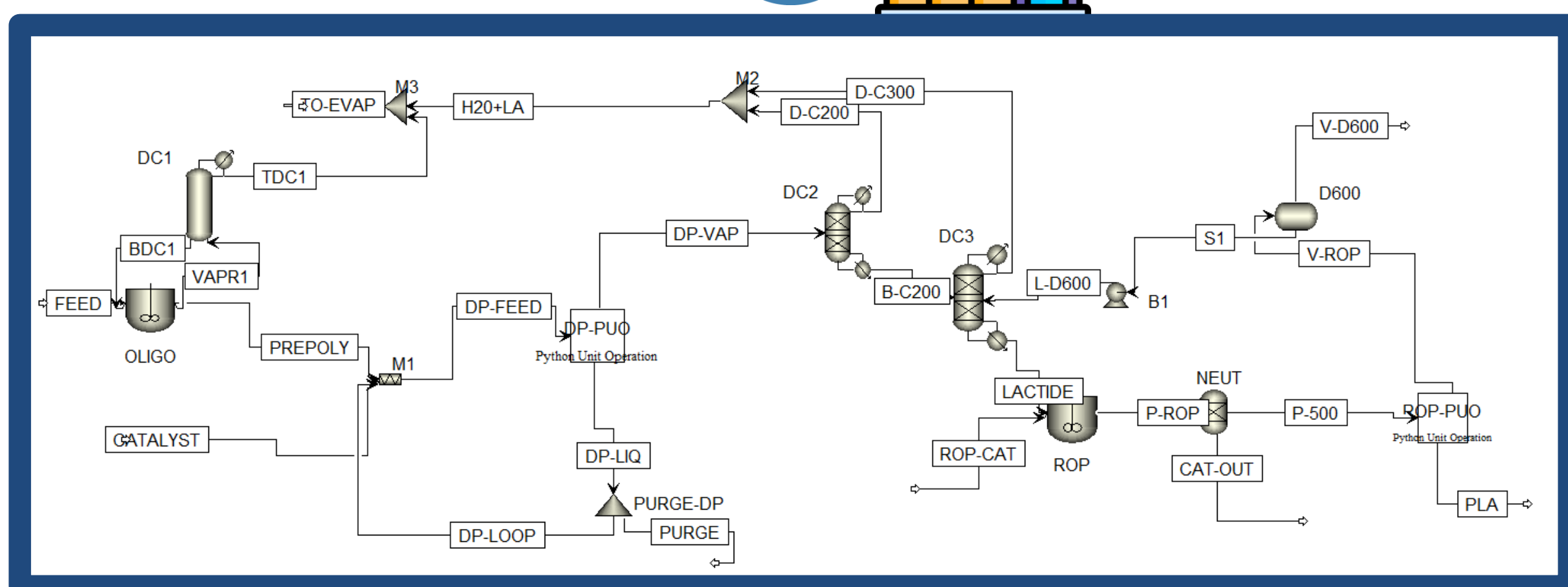
- Scope: **Ring-Opening-Polymerization (ROP)**.
- Goal: compute catalyst's **kinetic descriptors** from its **synthesis variables** using **Machine Learning** techniques.



Reactor/Kinetics scale

- Scope: **Ring-Opening-Polymerization (ROP)**.
- Goal: develop **first principles** model of a **continuous extrusion reactor** using **kinetic model** which uses **kinetic descriptors** from **catalyst model**.

Process scale



Python interface

LCA and TEA



Life-Cycle-Analysis for socio-environmental KPI's calculation, e.g. CO₂/kg PLA.

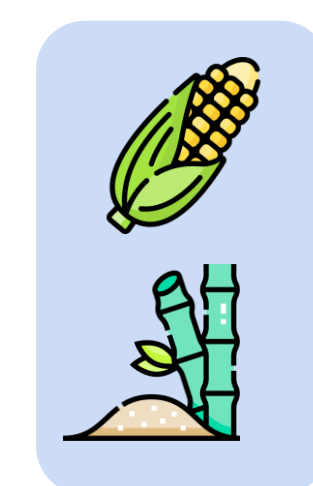


Techno-Economic Analysis for economic KPI's calculation, e.g. OPEX.

Case-study



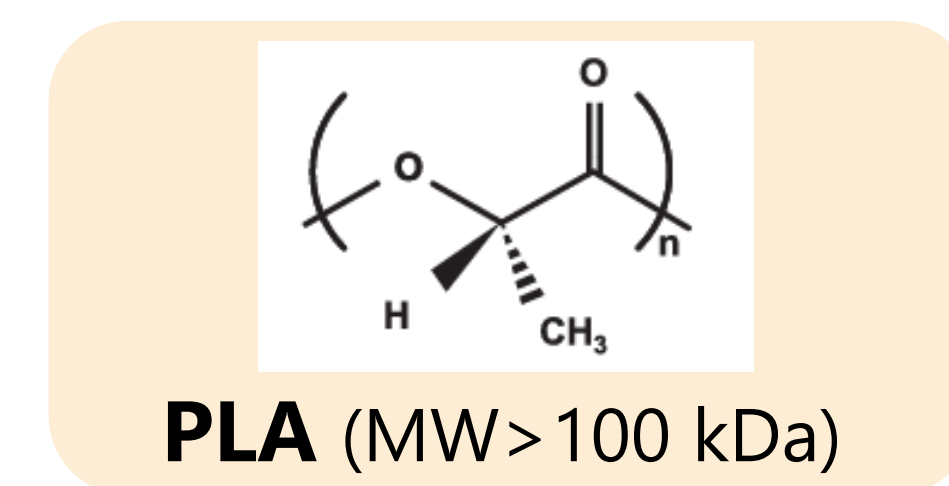
Poly lactid acid (PLA), the most produced bioplastic (31% of global production – 0.68 MT/y²)



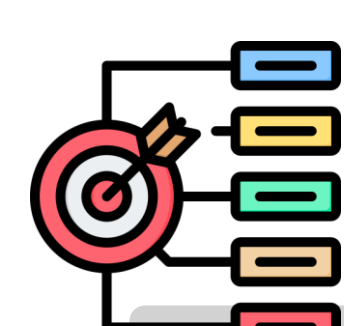
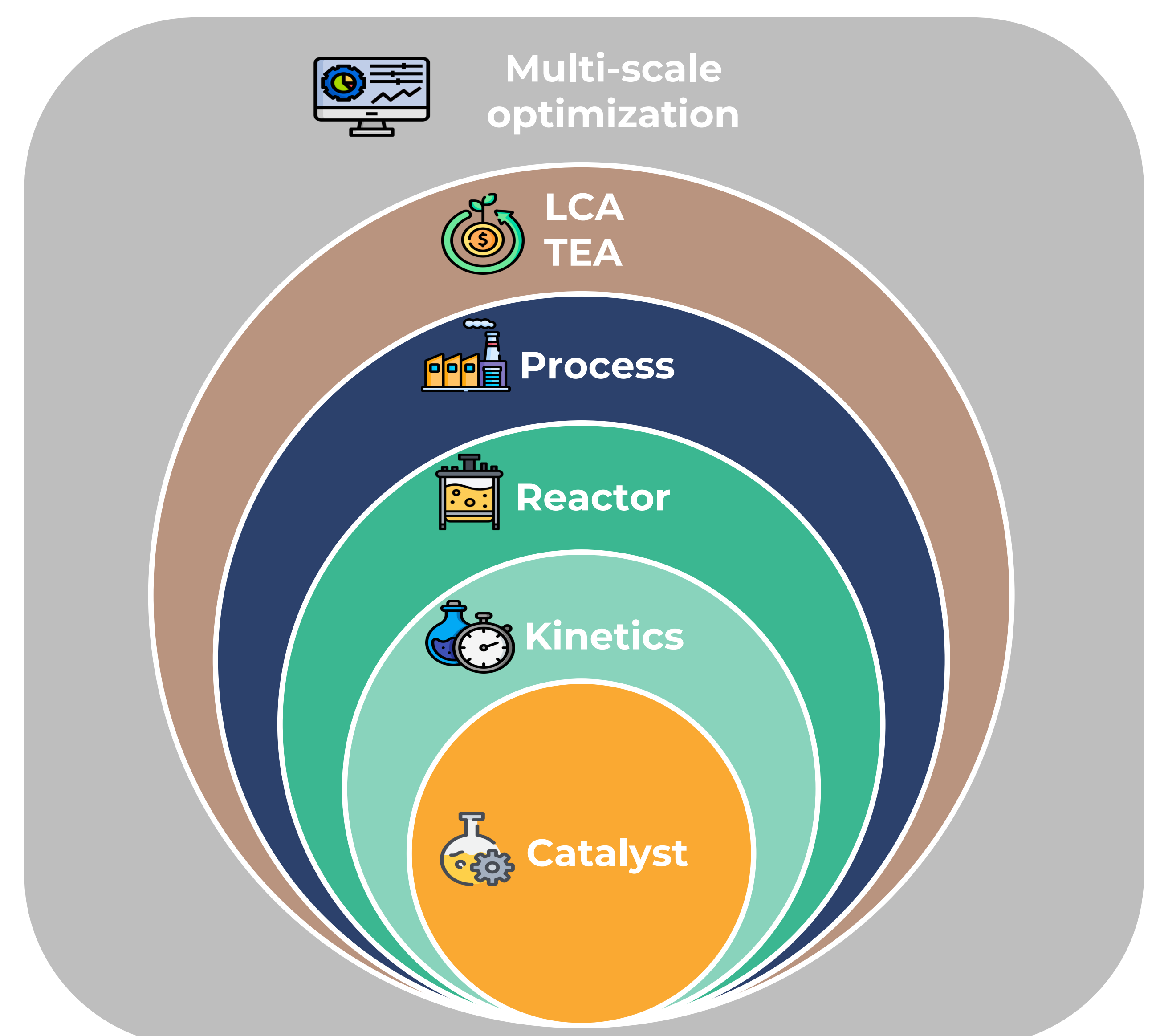
Lactic acid

PLA (MW < 5 kDa)

Lactide



Ring-opening-polymerization (ROP)



Multi-objective Optimization

Optimization algorithm implemented in the python interface.

$$\begin{aligned} \text{e.g.: } \min f_1(x) &= \text{CO}_2 / \text{kg PLA} \\ \min f_2(x) &= \text{OPEX} \\ x &= T_{ROP \text{ reactor}} \end{aligned}$$

[1] Mitchell S et al, Nature Chemical Engineering (2024) vol. 1, pp. 13–15.

[2] European Bioplastics, Bioplastics market data, 2023, <https://www.european-bioplastics.org/news/publications/> accessed 04/03/2024.