# PhD Open Days

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

PhD in Chemical Engineering
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### Context

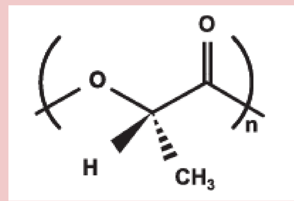
Design of novel sustainable catalysts includes objectives at a **catalytic** scale, **reactor** scale, and **process** scale. The current design process **needs improvement.**

Trial-and-error and sequential → Multi-scale optimization[1]

### Case study

**Polylactid acid (PLA),** the most produced **bioplastic** (31% of global production – 0.68 MT/y[2])

Lactic acid → PLA (MW<5 kDa) → Lactide → Ring-opening-polymerization (**ROP**) → **PLA** (MW>100 kDa)

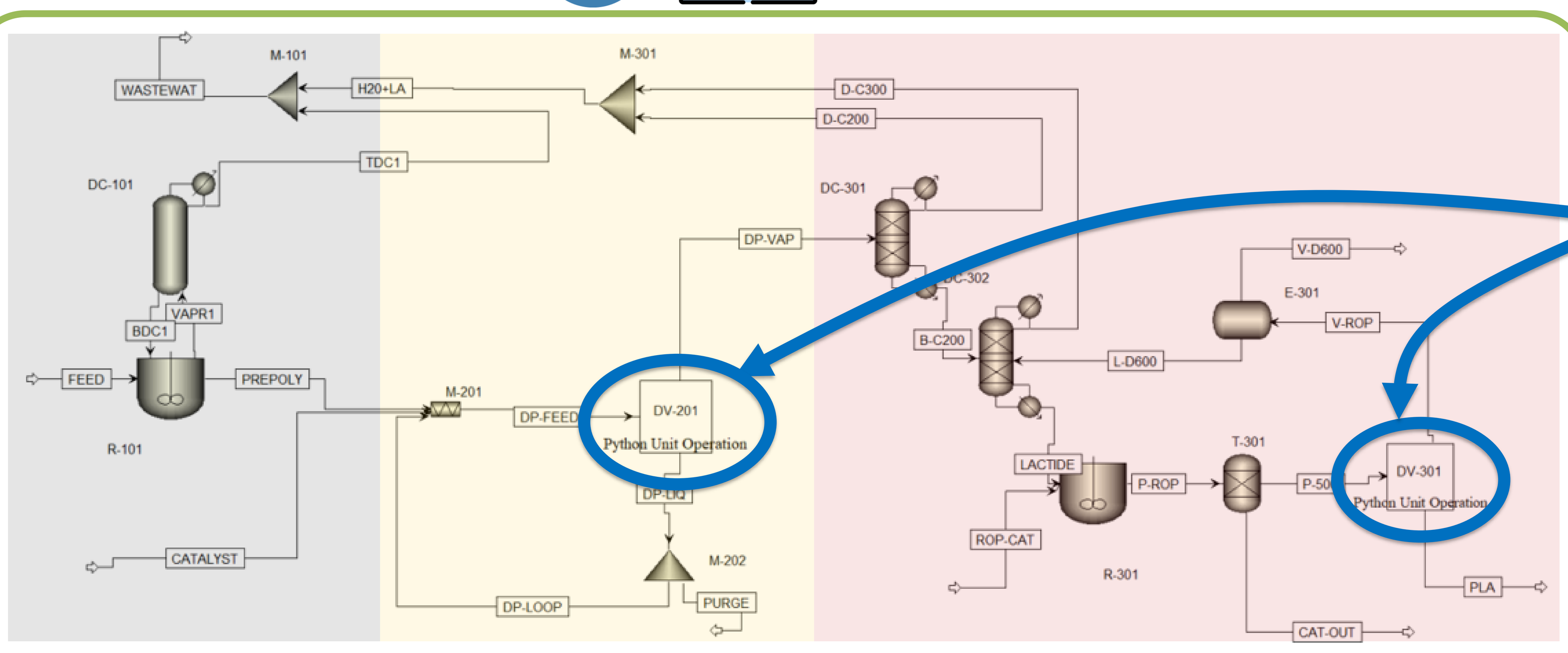


### Goal

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

## Multi-scale model

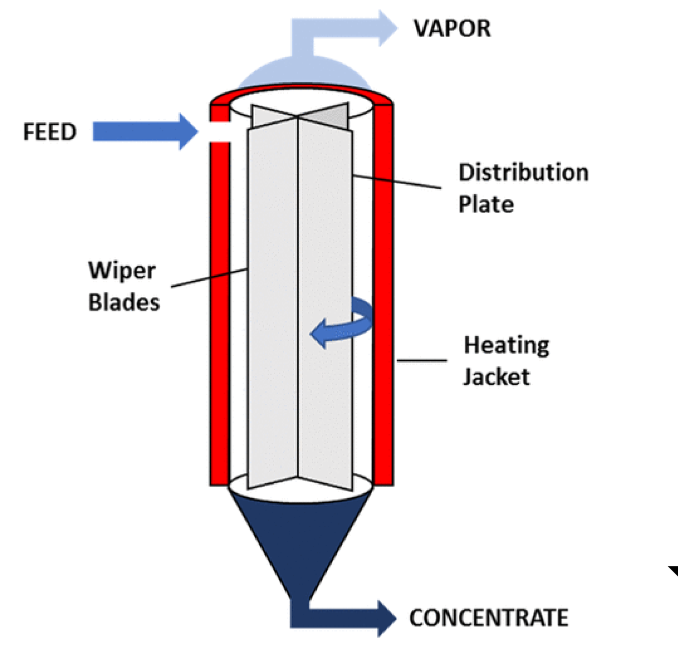
### Process scale



PLA MW: 100 kDa [3] Flowrate: 8 785 kg/hr; Purity: 99.7% wt; PolyNRTL model

### Reactor scale

Devolatilizer [4] :




Pre-polymer ⇌ Lactide

Custom Python model

In each ΔV

Adaptive step size strategy for improved convergence and simulation time

Simultaneous phenomena

Reaction
$r_1, r_2, r_3 \ldots$
Step-growth kinetics

Mass transfer from liquid to interface
$$F_{evap} = k_L \cdot a_{int} \cdot (C_{eq} - C_{liq})$$
$k_L$ and $a_{int}$ depend on liquid film thickness and MW, op. Temp. reactor geometry and blade velocity

Liquid-vapor equilibrium (LVE) at the interface
**LVE** surrogate model
$x_{liq,1}, \ldots, x_{liq,n}$, $T$, $P$ → $x_{eq,1}$, …, $x_{eq,n}$

### Catalyst scale

Goal: compute catalyst's **kinetic descriptors** from its **synthesis variables** using **Machine Learning** techniques.

New design variable values

Python interface

Python interface

Process model outputs

## Multi-objective Optimization

**Optimization algorithm** implemented in the **python interface**.

e.g.: $\min f_1(x) = CO_2 \,/kg\ PLA$
$\min f_2(x) = OPEX + CAPEX$
$x = T_{devolatilizer\ reactor}$

## LCA and TEA

openLCA

**Life-Cycle-Analysis** for environmental impact, e.g. $CO_2$/kg PLA.

**Techno-Economic Analysis,** for economic KPI's, e.g. OPEX+CAPEX.

Environmental and economic KPI values

[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.
[3] Seavey et al., Step-growth polymerization process modeling and product design 2008
[4] Lee et al., Ind. Eng. Chem. Res., August 2020