Sargent Centre for Process Systems Engineering

Life Science and Process Systems Engineering

Digital innovation for sustainable, accelerated development in an era of uncertainty

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Tomorrow is another day

Advanced clinical understanding

Patient specificity

(un)Availability of raw materials

How hard is it to be prepared?

Disease X

Complex supply chains

Sustainability

Evolving strategic objectives

Quality ✓ | Cost ↓ | Product Availability ↑ | Environmental Footprint ↓

AstraZeneca's 'Ambition Zero Carbon' strategy to eliminate emissions by 2025 and be carbon negative across the entire value chain by 2030

WHO calls for transformative action towards a greener future in pharmaceutical manufacturing and distribution

23 December 2024 | Departmental

AUGUST 21, 2024

Sustainability: A key differentiator as biopharma faces momentum challenges, global survey by Cytiva reports

By Cytiva Communications

Classification: Official

NHS England

Delivering a 'Net Zero' National Health Service

Manufacturing | Transport | Storage | Transport | Administration

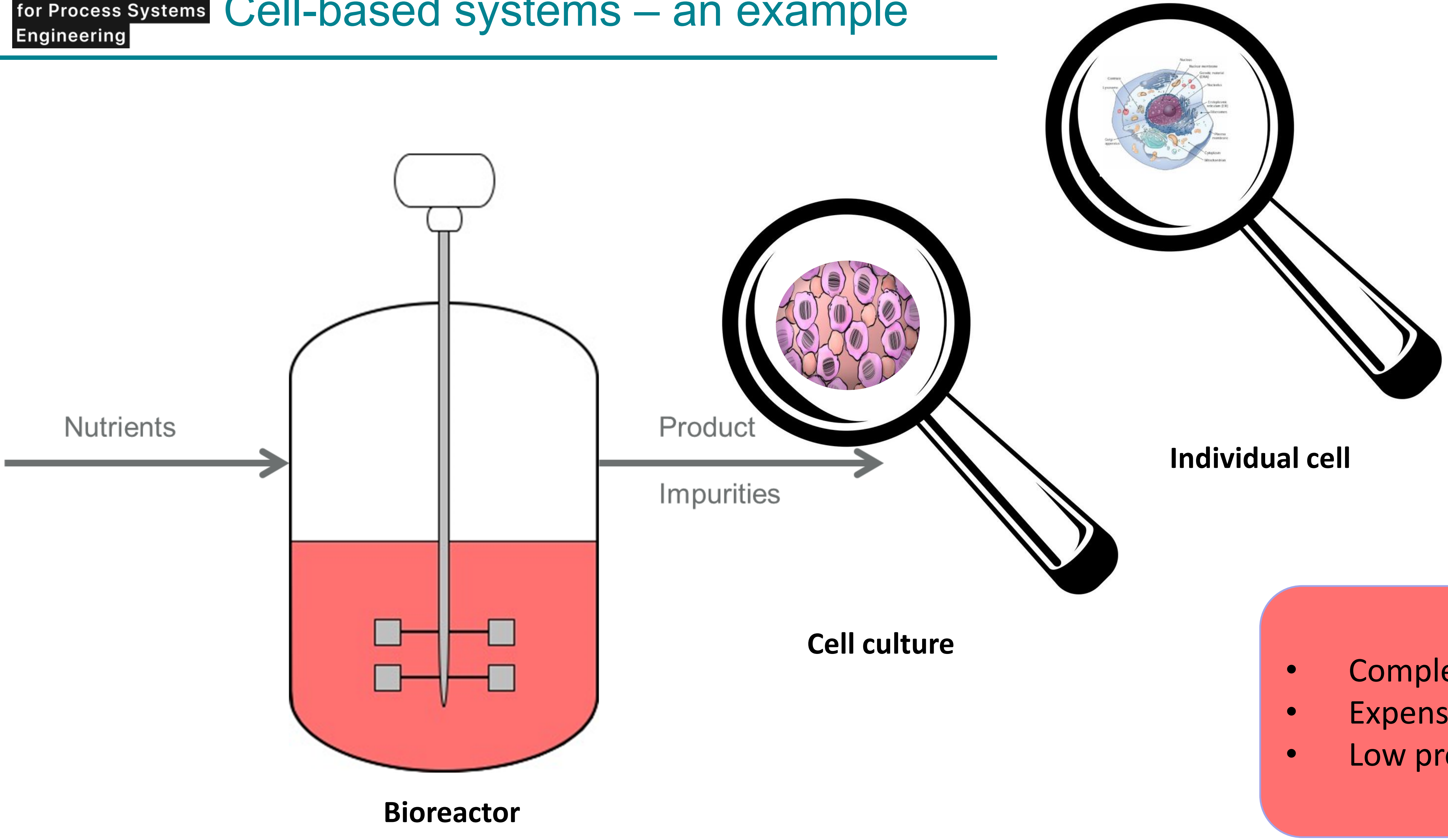
New UKRI funding aims to enhance UK sustainable biomanufacturing

GSK

Our pathway to reach **net zero** carbon by 2030

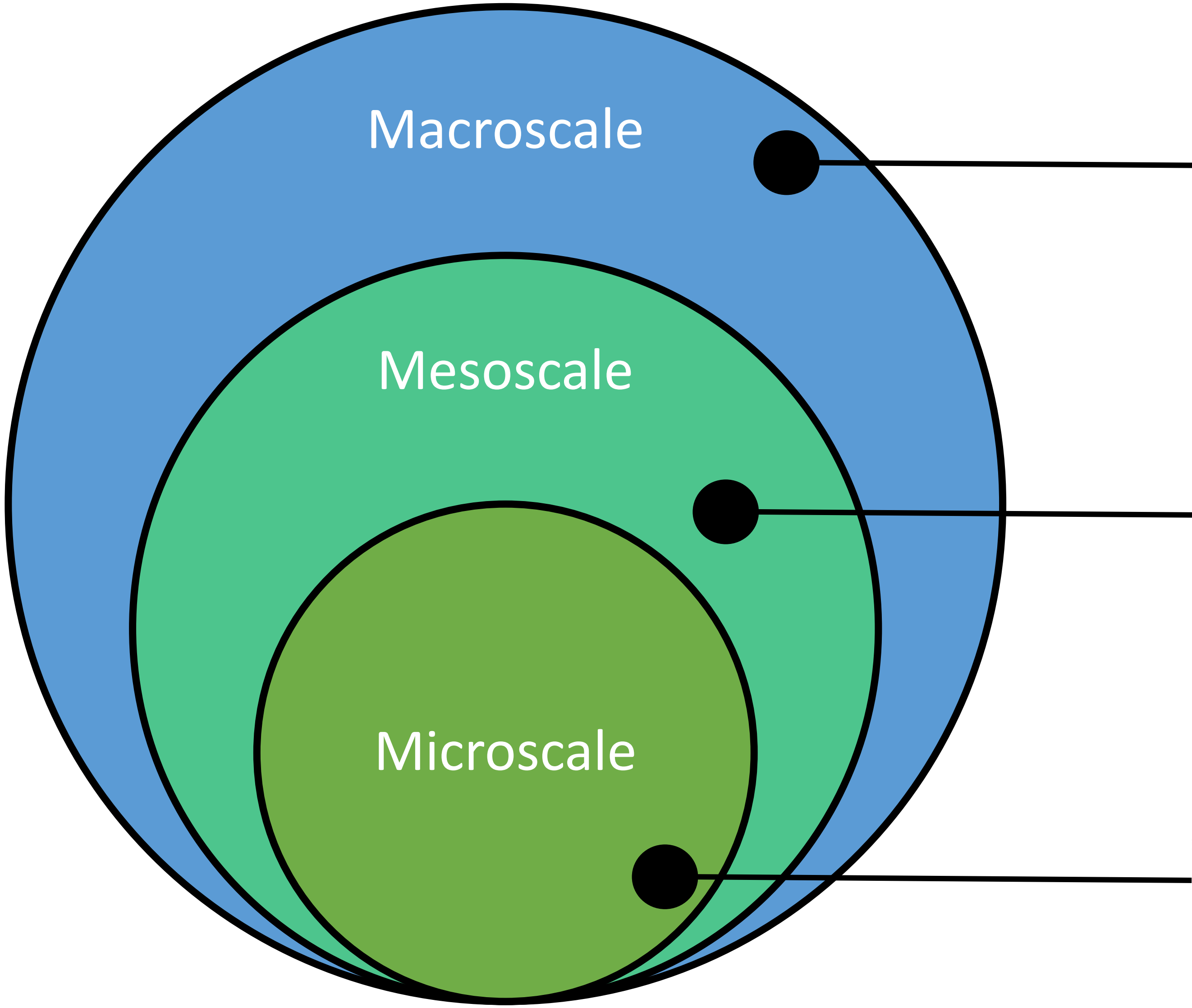
COP26: Biopharmaceutical Industry Actions to Tackle Climate Change

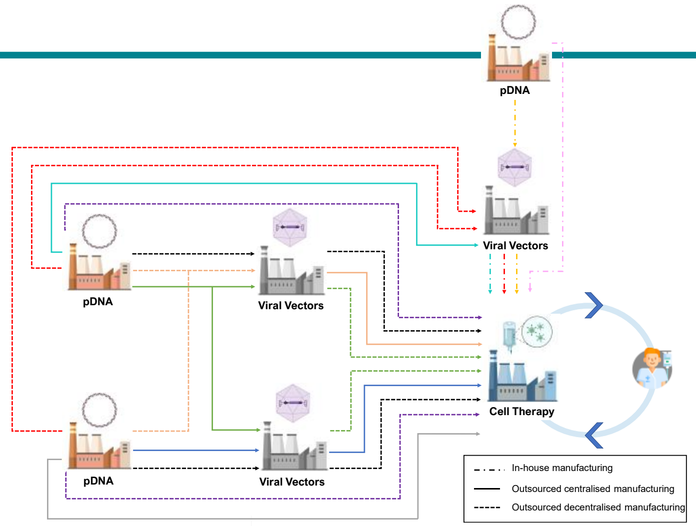
Cell-based systems – an example



- Complex
- Expensive
- Low productivity

Challenge #1: Scal(in)ability





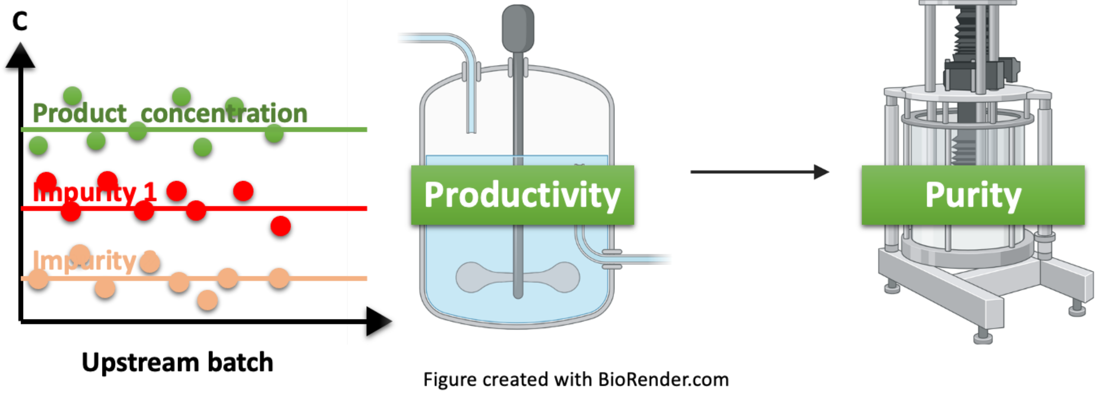
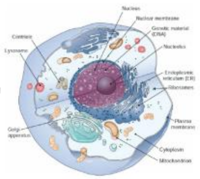
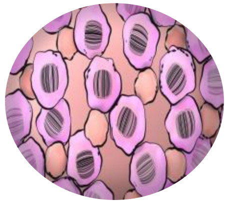


Figure created with BioRender.com





Challenge #2: Sustainability

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To help get ahead of disease and deliver real human health impact we need to look broadly and deeply at the interconnections of climate, nature and health.

We're committed to a net zero, nature positive, healthier planet, with ambitious goals set for 2030 and 2045.

AbbVie's science-based targets to lower emissions

To build a more sustainable future, we've set ambitious emissions reduction targets that are in line with the Paris Climate Agreement. Our targets, which have been validated by the Science Based Targets initiative (SBTi), include:

By 2030

- Reducing absolute scope 1 and 2 CO2 emissions by 42% from a 2021 base year
- Reaching 100% sourcing of electricity from renewable sources

3 Ensure healthy lives and promote well-being for all at all ages

9 Build resilient infrastructure, promote inclusive and sustainable industrialization and foster innovation

12 Ensure sustainable consumption and production patterns

SUSTAINABLE DEVELOPMENT GOALS

Challenge #3: Novel insights, new priorities

Responsiveness and Preparedness

Patient centric approach

In-time, at-point manufacturing

Can we revolutionise the way we design product lifecycle?

From discovery to delivery

Capacity Planning

→ **Sufficient capacity** to meet demand forecasts

Systematic methods

Challenges

Process uncertainty

→ **Prediction of lot sizes** and costs at scales

Investment risk

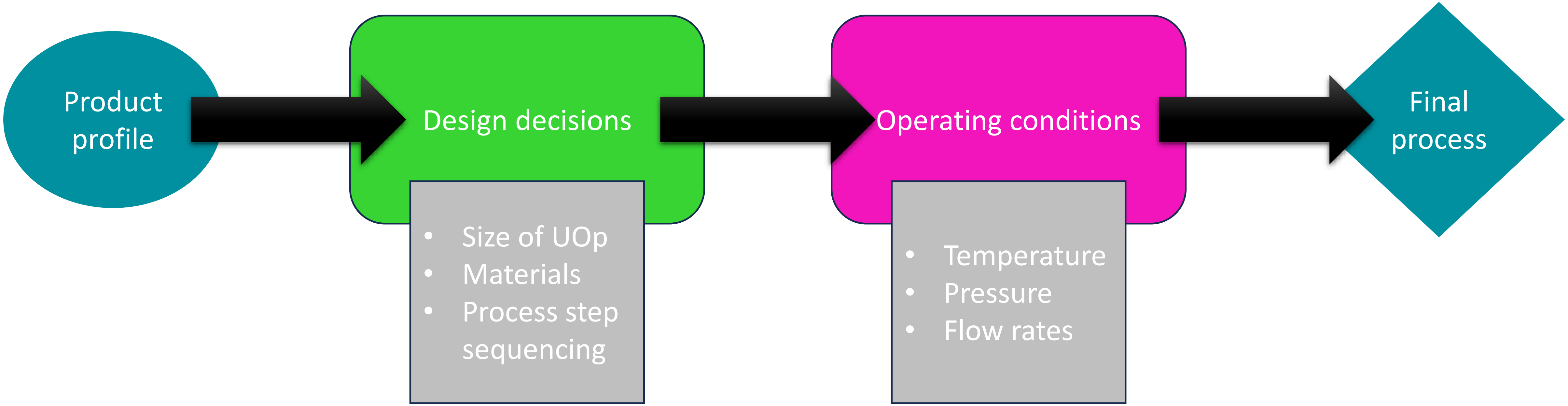
→ **Demand uncertainty:** clinical to commercial

Impact quantification

→ **Awareness and mitigation**

Enough drugs for all, on time.

Bioprocess design: from tradition to the future

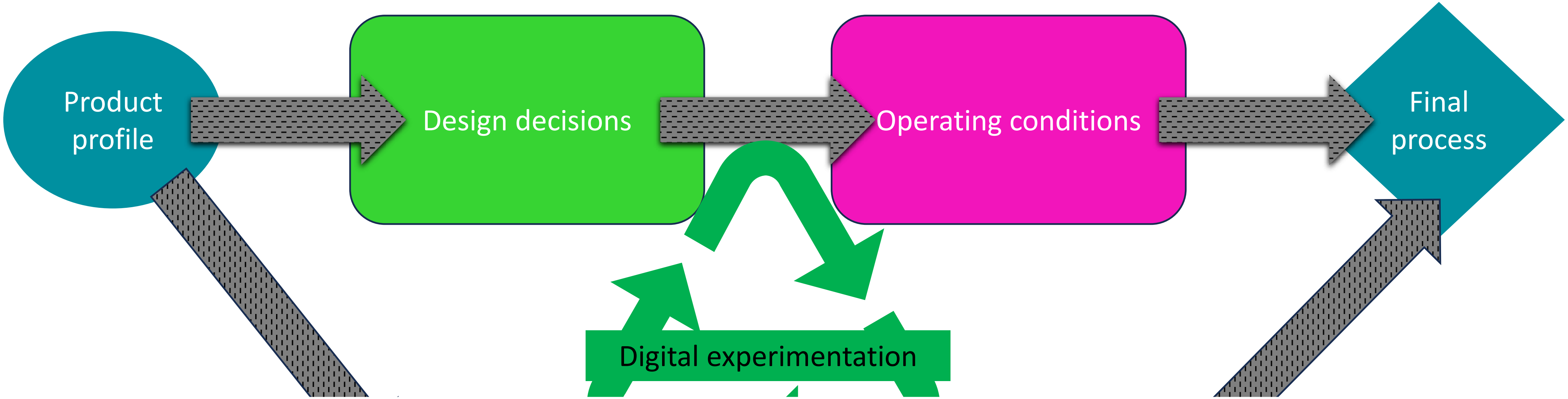


- ✓ It works!
- ✓ It meets the specs

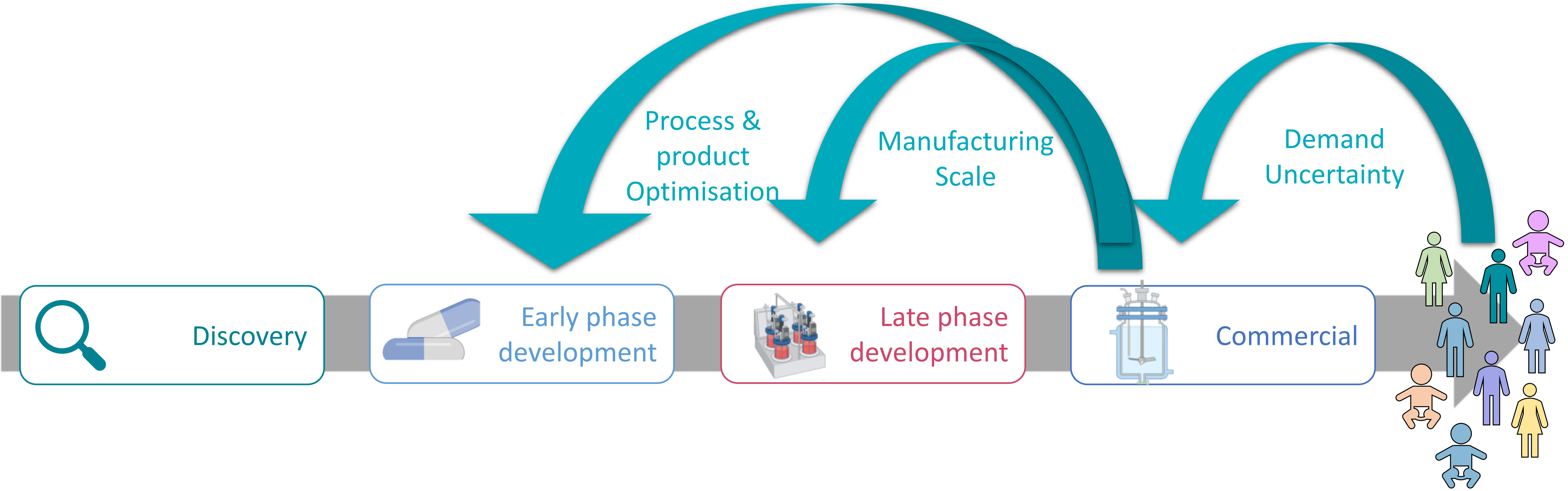
- ✗ It's inflexible
- ✗ It costs
- ✗ Isolates process steps

?

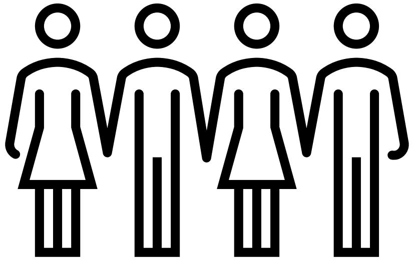
Bioprocess design: from tradition to the future



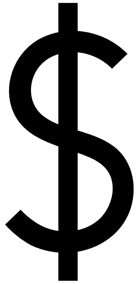
Come with the end in the mind first



Sustainability 3 ways



Enough



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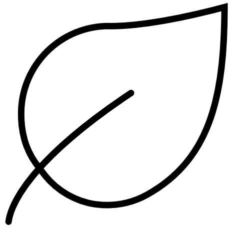


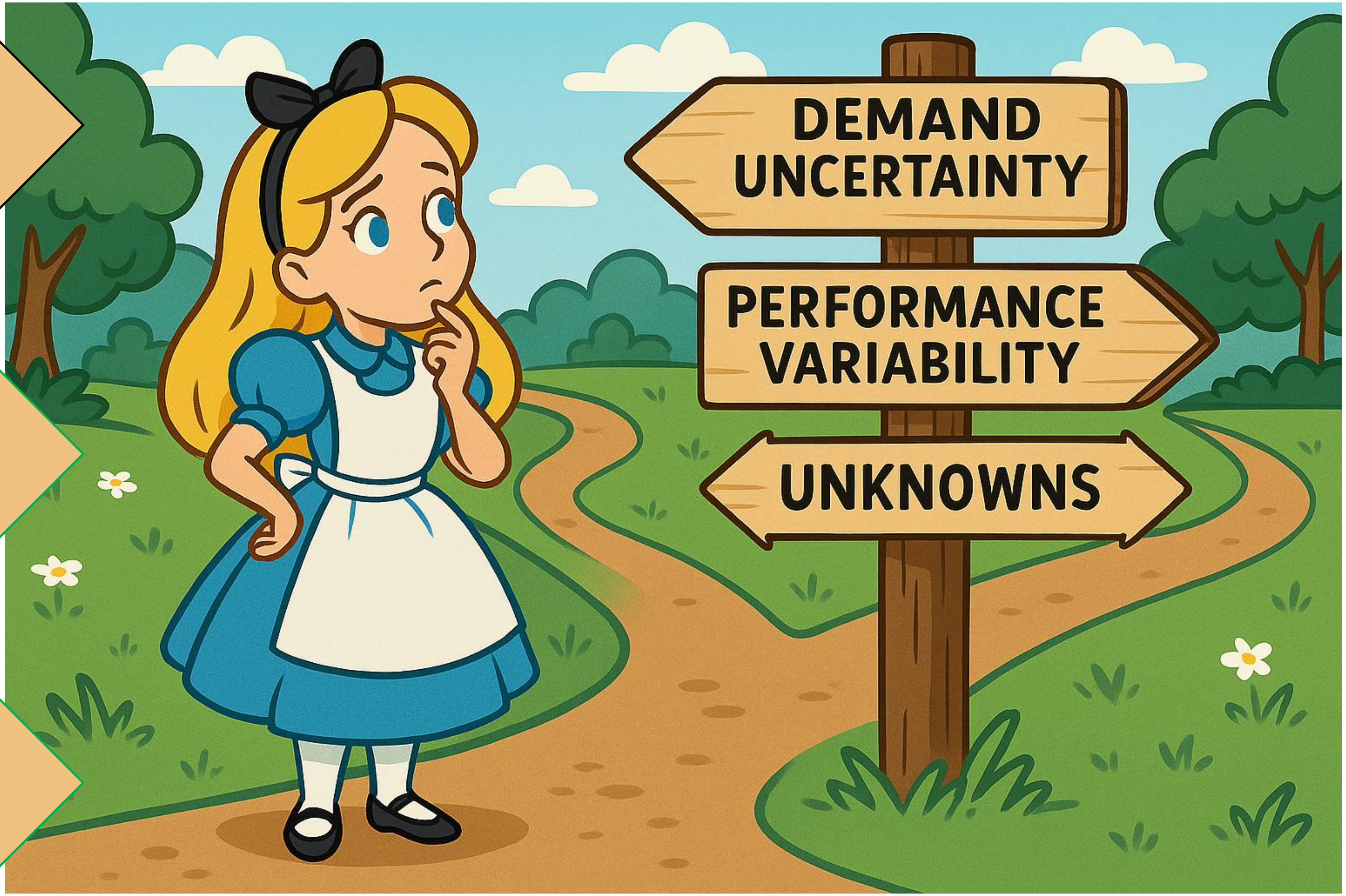
Greener

Options, is all we need!

Optionality

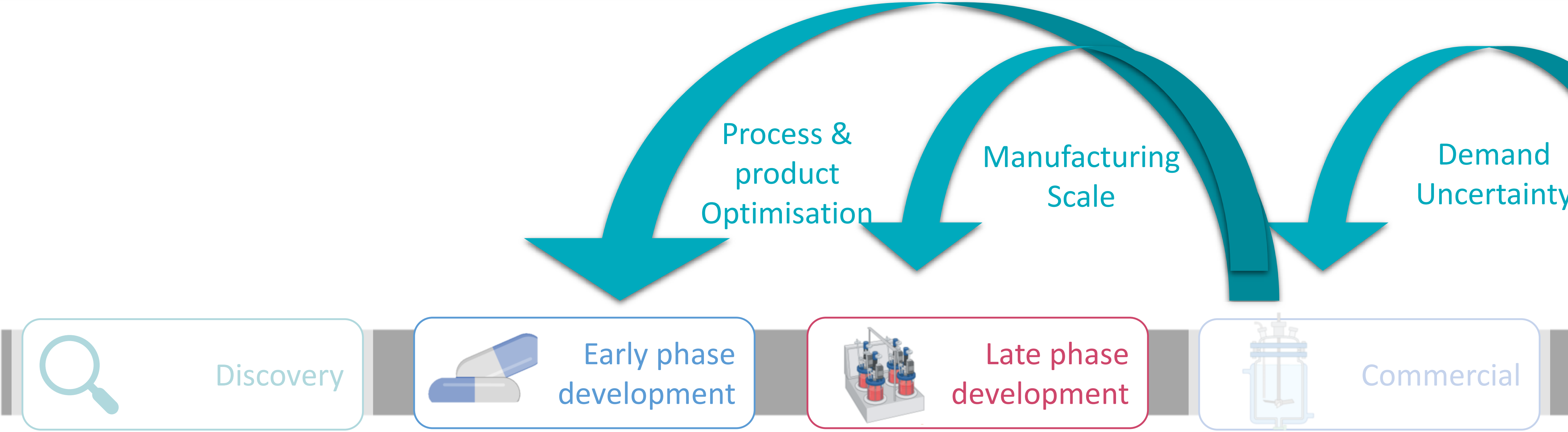
Agility

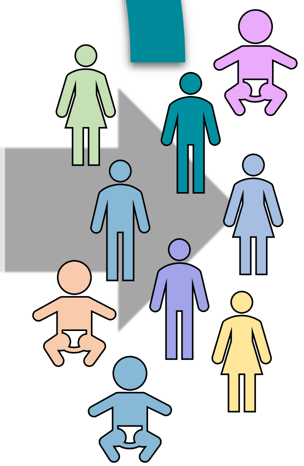
Responsiveness



Digital innovation at the service of biopharma

Accelerated process development



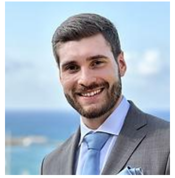


Challenge #1: Performance variability

Challenge #2: Unit operation interdependency

- Sachio *et al.* (2023), *Chem Eng Res Des, 197, 800-820*
- Michalopoulou & Papathanasiou (2025), Dig ChE, 14, p.100215
- Galeazzi et al.(2025), *J Chrom A, 21:46619*
- Pessina et al. (2026), DChE, 1;18:100292
- Chiplunkar et al. (2026)*, Chem Eng* Sci, 16:124255

Dr Ranjith Chiplunkar



Dr Andrea Galeazzi

Dr Steven Sachio

Dr Foteini Michalopoulou

Daniele Pessina

- **Design space identification**
- **Hybrid modelling**
- **Process control**

Smart process design


Early phase development


Late phase development

Dr Steven Sachio

Computer-aided framework for process design

1. Model Development & Problem Formulation

- Process modelling & validation
- Design problem definition

2. Design Space Identification

- Virtual experimentation
- Point cloud classification

Alpha Radius Problem

- a) no prior knowledge: Tolerance based
- b) average prior knowledge: Combinatorial
- c) established prior knowledge: Resolution support

- Alpha shape hull

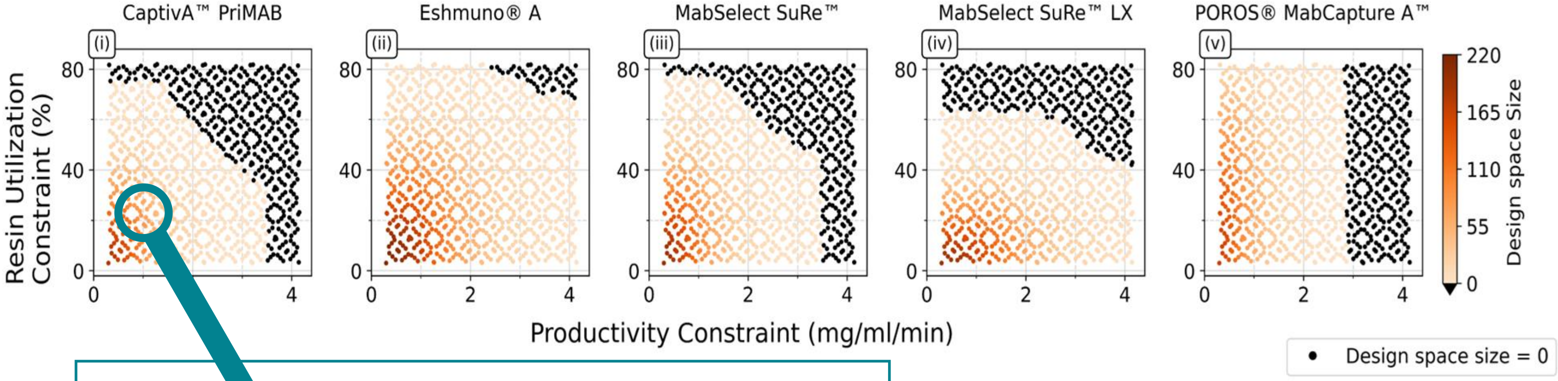
3. Design Space Analysis

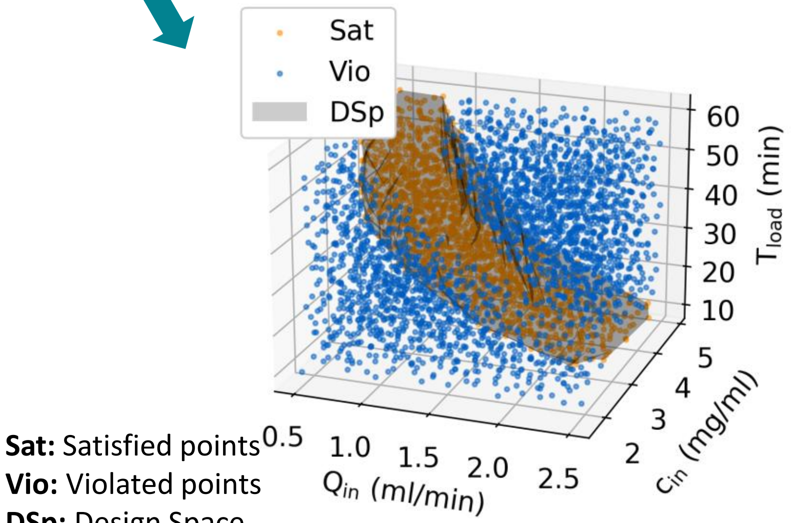
- Acceptable operating region identification
- Acceptable ranges quantification

Python package:
dside.readthedocs.io

Beta software package also available

Material screening in chromatography





Sat: Satisfied points
Vio: Violated points
DSp: Design Space

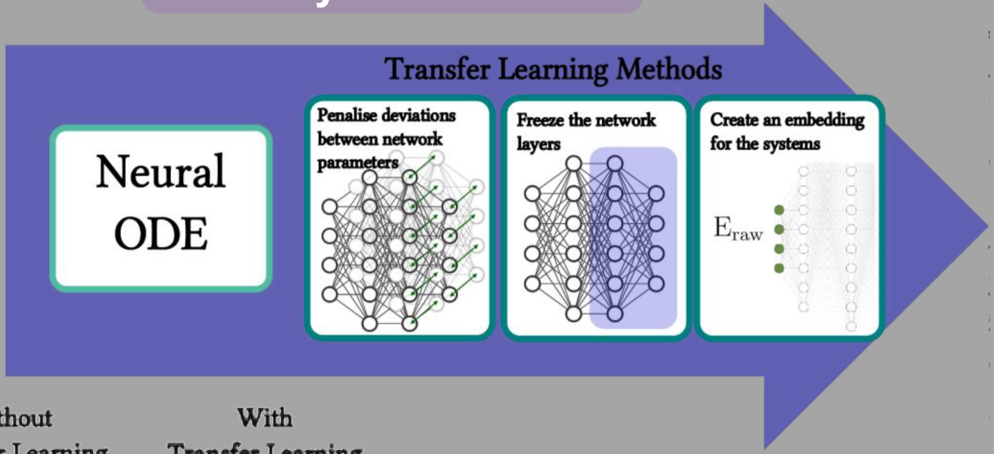
- Over 20k combinations screened and assessed
- 5k design spaces generated
- Trade-off quantification
- Process resilience to variations

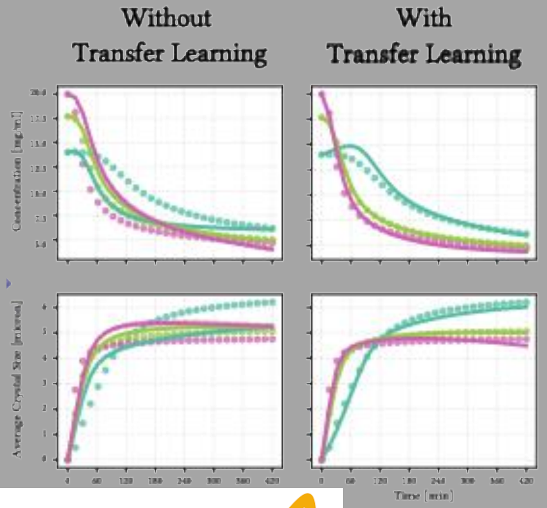
Sachio *et al*. (2023), *Chem Eng Res Des*, *197*, 800-820
Sachio et al (2024), *J. of Chrom. A*, *1722*, p.464890

Increasing adaptability, reducing experimental data

Predictive modelling in crystallisation

Daniele Pessina





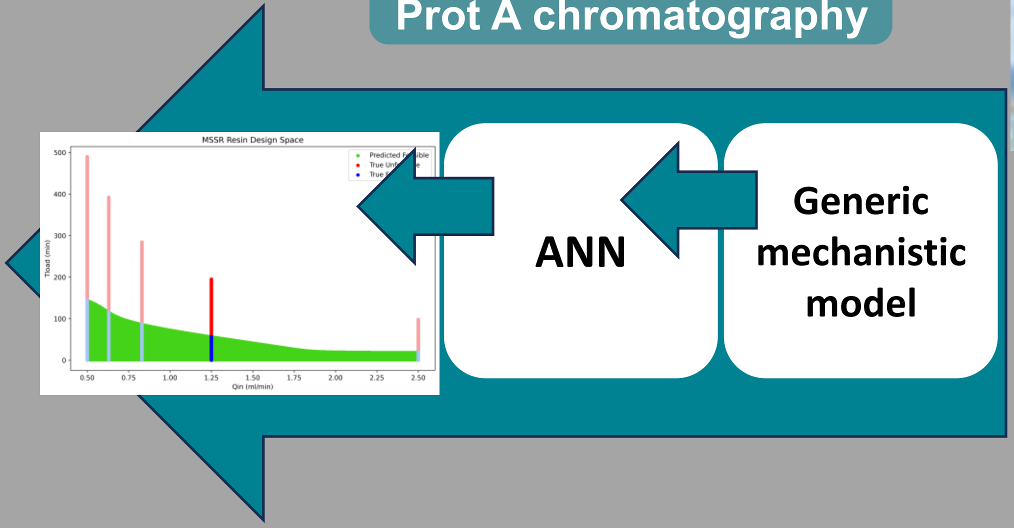
- Transfer learning for crystallisation modelling
- 4 crystallisation systems assessed
- Consumption and growth kinetics captured

AstraZeneca

Pessina et al. (2026), DChE, 1;18:100292

Pessina et al. (2024), Industr & Eng Chem Res, 64 (24), 12025-12035

Design space for Prot A chromatography



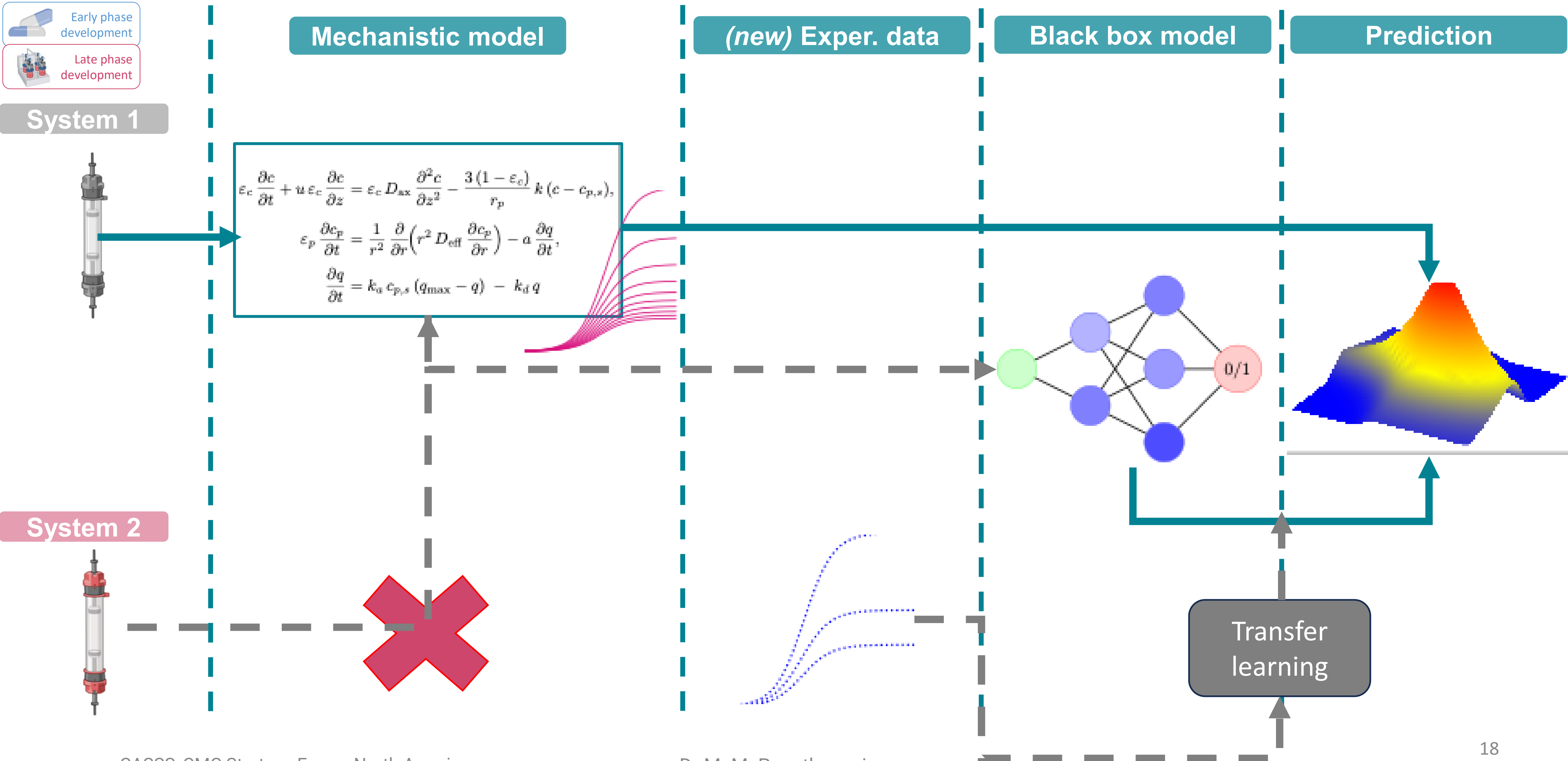
Dr Andrea Galeazzi

- Good predictions with only 9 experimental runs
- Data quality plays a key role (more than quantity)

Galeazzi et al.(2025), J Chrom A, 21:46619

GSK

Transferring system and product knowledge



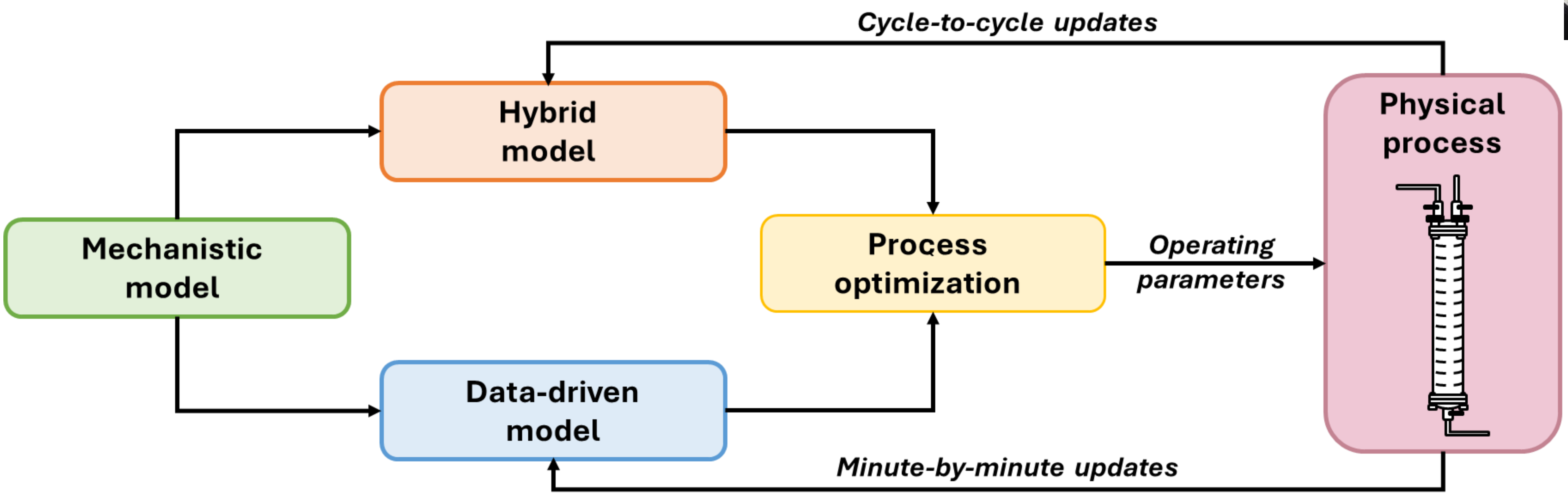
A toolkit from simulation to monitoring


Early phase development


Late phase development

The case of ion-exchange chromatography

Dr Foteini Michalopoulou



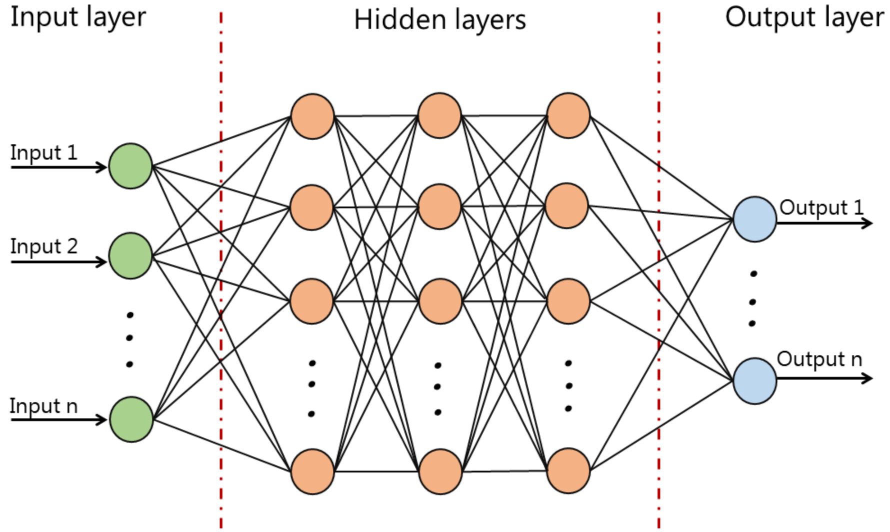
Michalopoulou & Papathanasiou (2024), *AIChe J, e18600*
Michalopoulou & Papathanasiou (2025), Dig ChE, 14, p.100215
Michalopoulou (2025), Incorporating AI Tools Into Downstream Process Optimization, Bioprocess Online

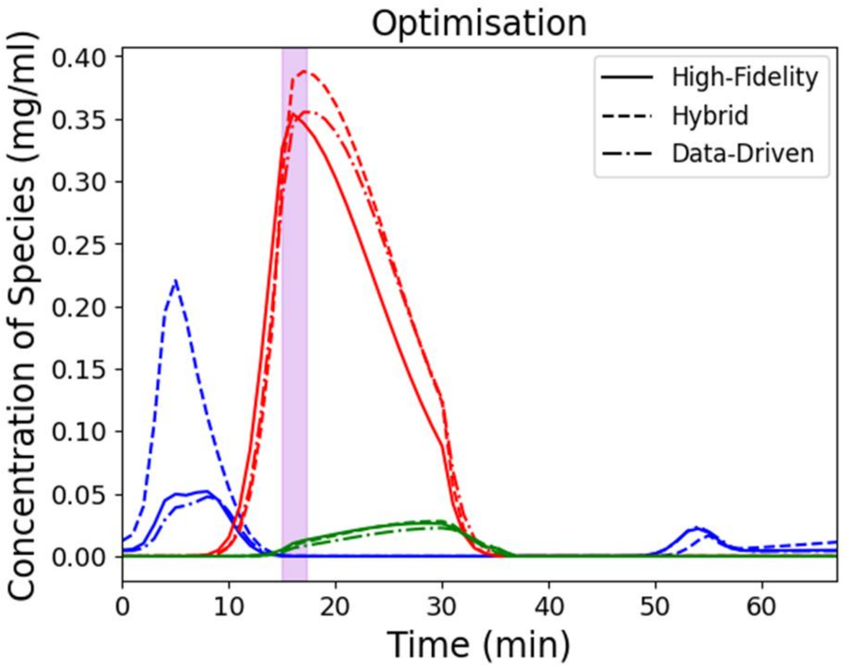
A toolkit from simulation to monitoring (cont'd)

Early phase development

Late phase development

Dr Foteini Michalopoulou





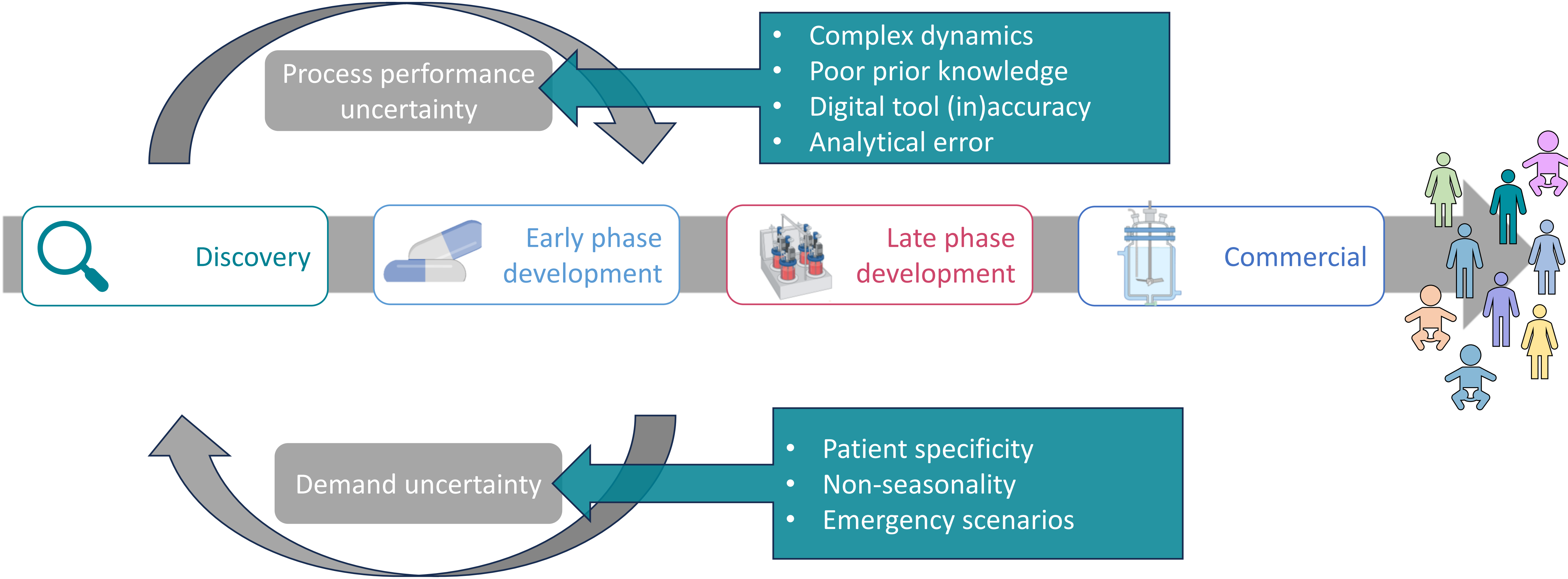
Input Layer:
- All operating conditions → understanding of the process
- Dynamic Inputs → understanding of the time step

Hidden Layers:
- 1-4 hidden layers → uniform structure
- 16 – 256 neurons

Output Layer:
- Concentrations at end of column
- Predictions at CSS

Michalopoulou & Papathanasiou (2024), *AIChe J, e18600*
Michalopoulou & Papathanasiou (2025), Dig ChE, 14, p.100215
Michalopoulou (2025), Incorporating AI Tools Into Downstream Process Optimization, Bioprocess Online

Hedging against uncertainty

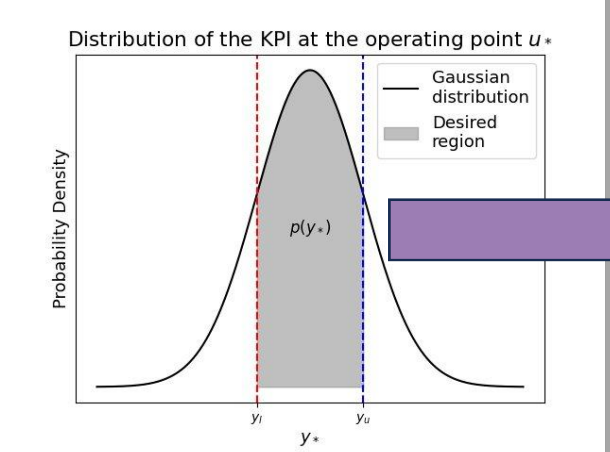


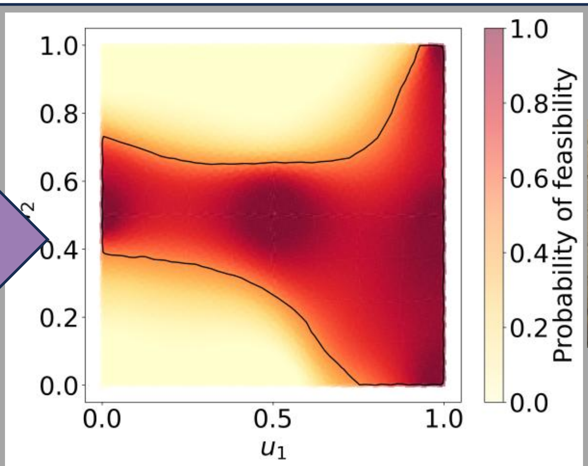
Preparing for the worst case

In design

GSK

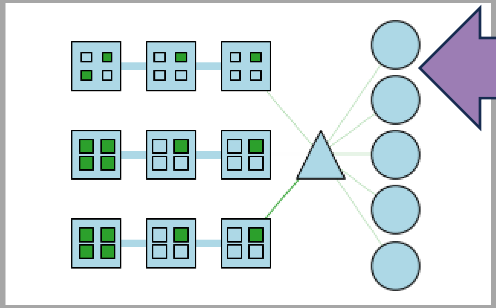
- Data driven design space using GPs
- Guide and minimise experimentation
- Estimation of probability of constraint satisfaction

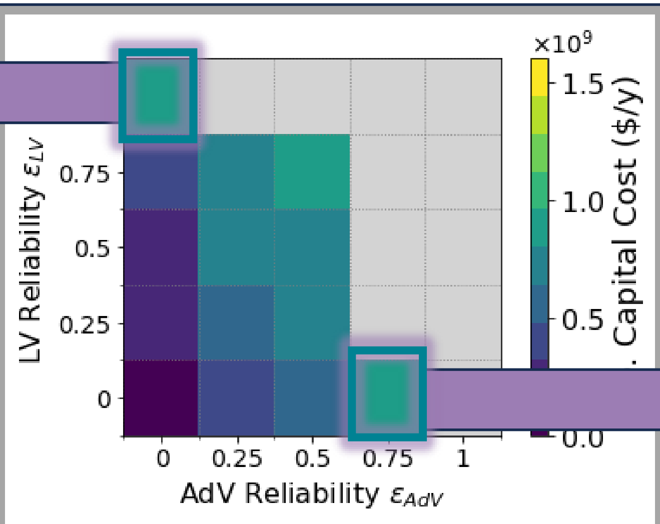


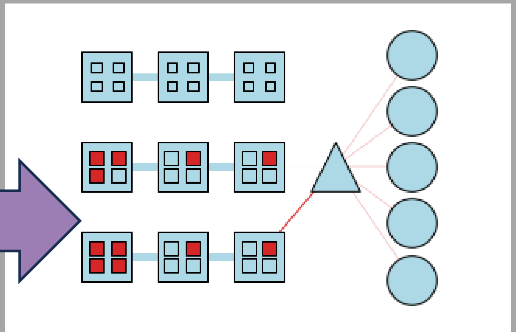


Dr Ranjith Chiplunkar

Chiplunkar et al. (2025), Syst and Contr Trans Proceedings of ESCAPE35







In distribution

Dr Miriam Sarkis

Sarkis et al. (2025), Comp Chem Eng, p.10901

Cross-cutting challenges

- Demand uncertainty
- Personalised routes
- Unexplored scale up effects

- Rapid scale up
- Costly processes
- (lack of) Analytics

- Wet-lab experiments driving
- Scale-out manufacturing
- Ultra-cold chain logistics

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A digital approach to sustainable process design

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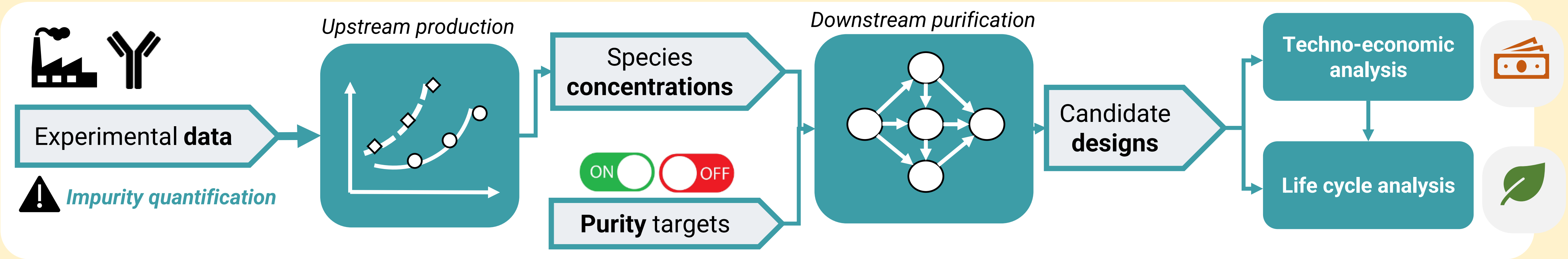
Life Science and Process Systems Engineering

Sarkis et al. *Comp. Chem. Eng.* Decarb. And Circ. Economy SI, 205, 109454

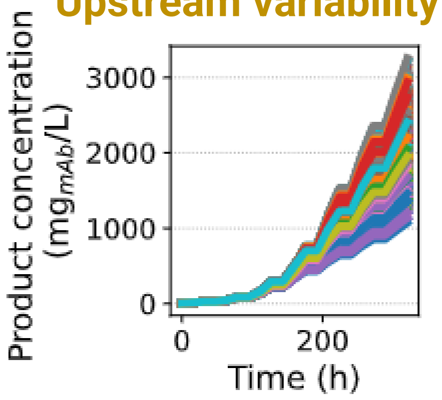
Dr Miriam Sarkis

Methodology

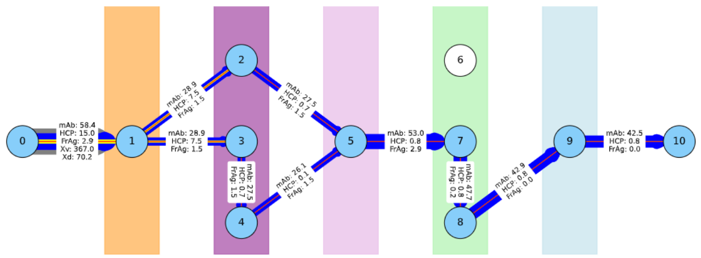


Key results

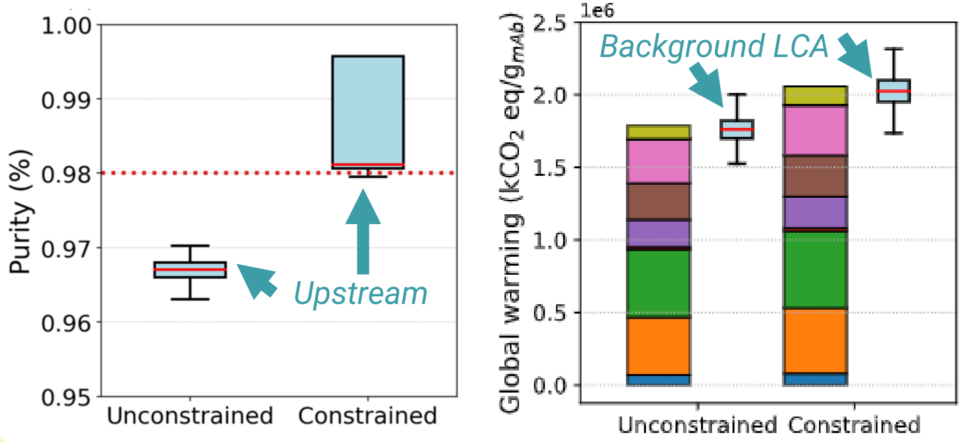
Upstream variability



Nominal design



Robustness vs footprint trade-off



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A digital approach to sustainable responsive supply chains

IMPERIAL | Life Science and Process Systems Engineering

Sarkis et al (2025). *Comp. Chem. Eng. Foundations of Computer Aided Process Design, Special Issue*, 201, 109197

Dr Miriam Sarkis

Methodology

Sampling

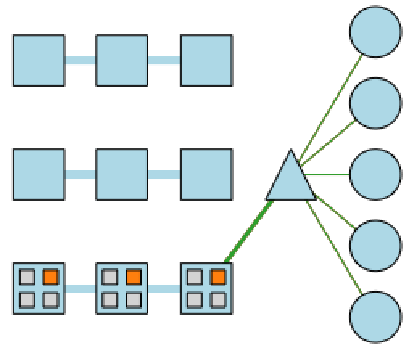
- **Fixed** design to meet demand D_{LV}
- **Unforeseen** demand D_{AdV}
- **Process** scale **manipulation**

Deterministic Optimization → **Feasibility** region → **Space quantification**

MU SU

Key results

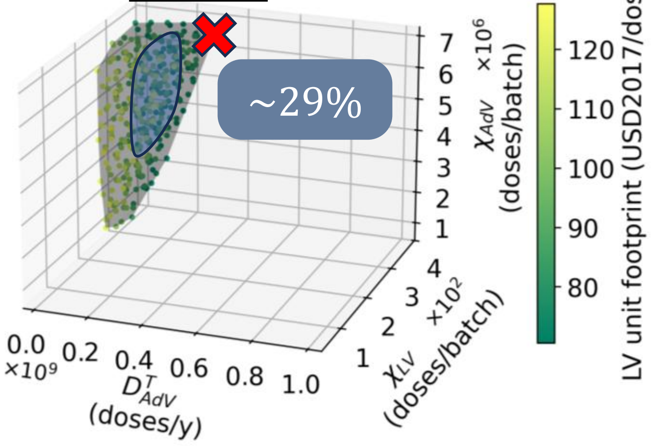
Nominal design



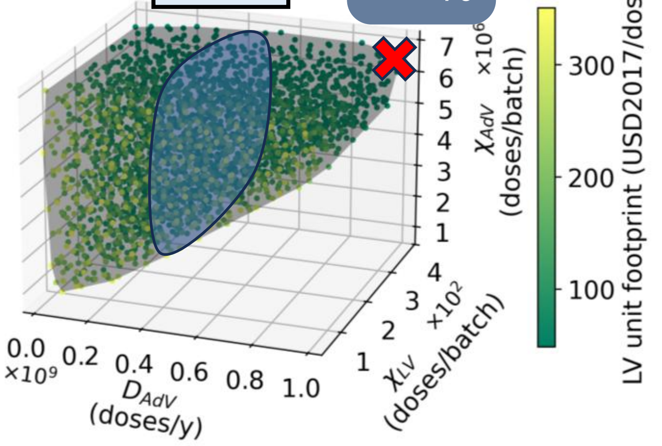
Process
Scale-out

Present
Demand

MU

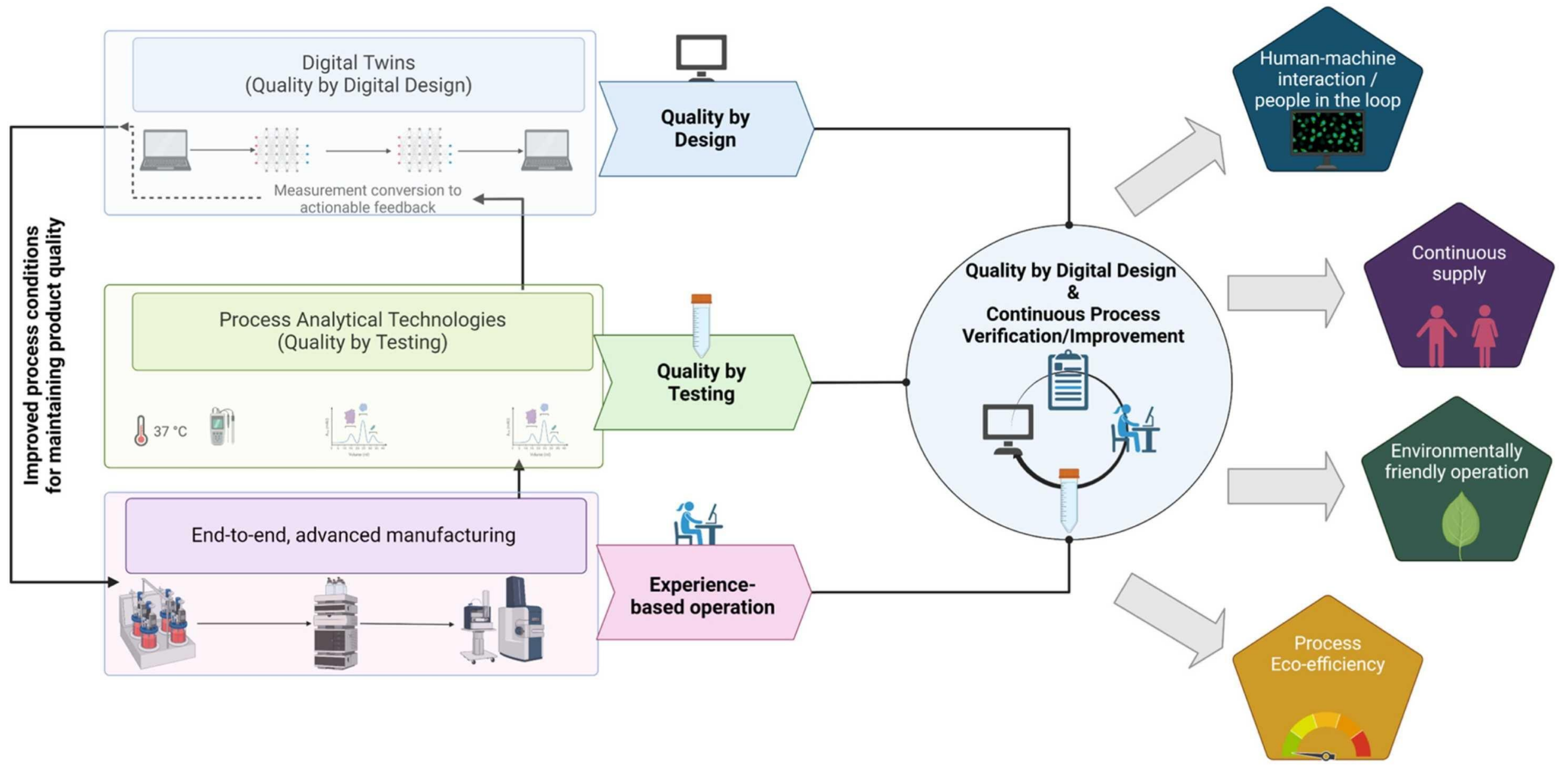


SU



Quantification of **manufacturing trade-offs** between Cost | Sustainability | Scalability | Flexibility

Future directions



Sarkis et al. *Curr Op Chem Eng* 44:101027

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