

um
2026

**Accelerated Chemical Process Design and Optimization
Using Surrogate Modeling in modeFRONTIER:
Application to CO₂ Capture, Utilization, and Storage**

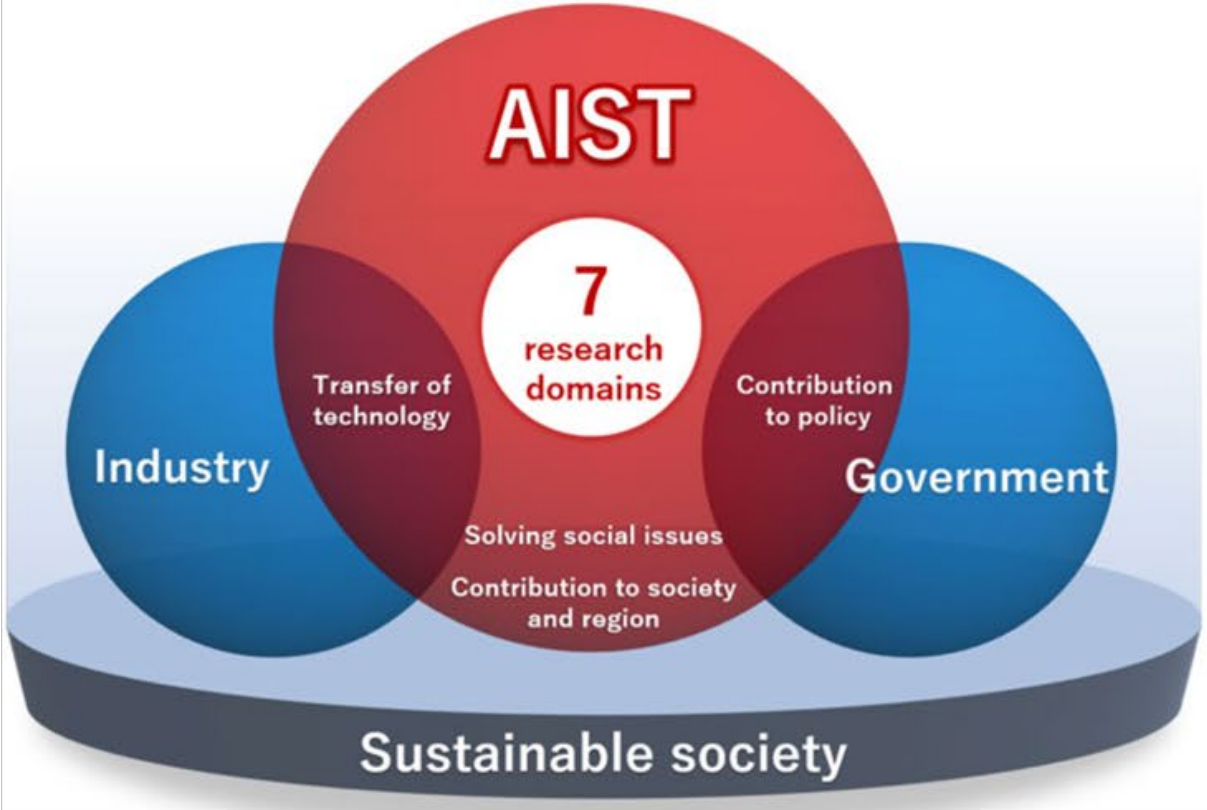
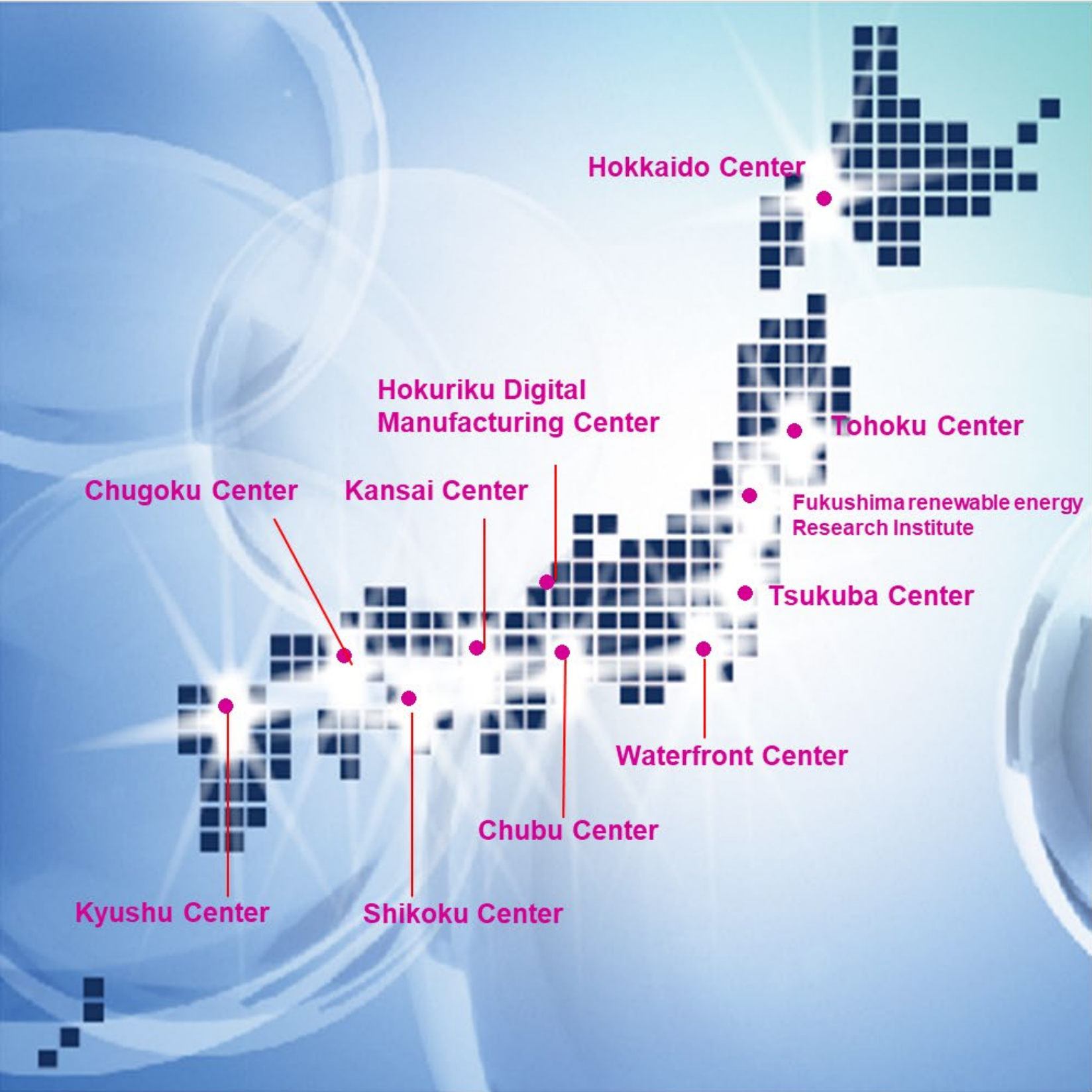
Nguyen Thuy

Senior Research Scientist

National Institute of Advanced Industrial Science and Technology (AIST)



Overview of AIST



- Energy & environment
- Life science & biotechnology
- Information technology
- **Materials & chemistry**
- Electronics & manufacturing
- Geological survey
- National metrology

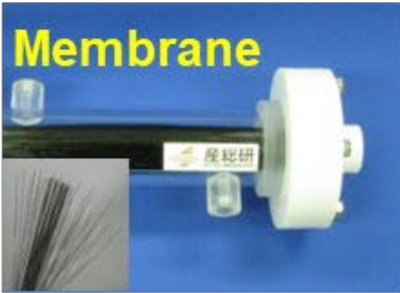
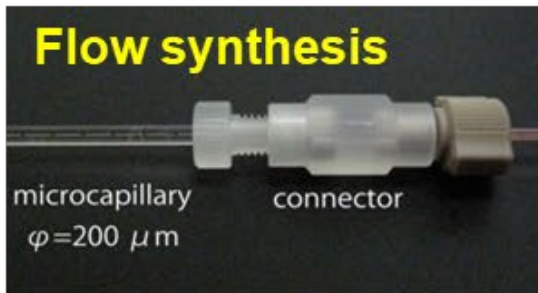
Employees:

| | |
|---|--------|
| Researchers | ~2,300 |
| Administrative employees | ~700 |
| Postdoctoral researchers | ~2,000 |
| Collaborators from universities/companies, etc. | ~5,400 |

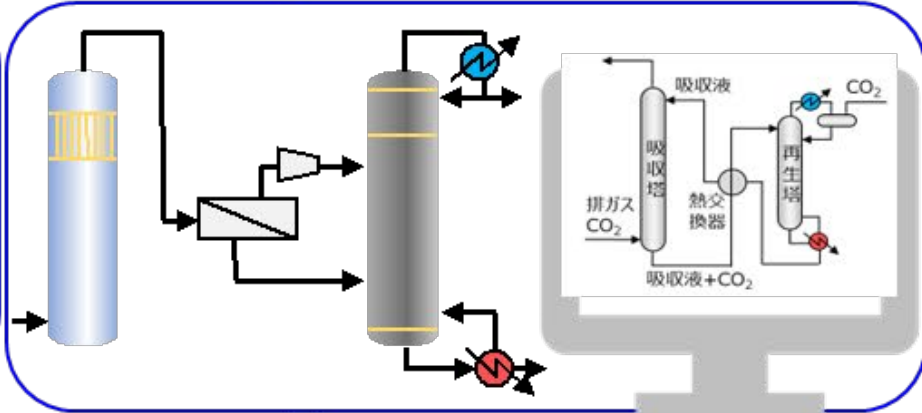
Our Group's Research Activities

Evaluating and optimizing new technologies at early stages of development

Experimental data in AIST



Modeling / Process Simulation



(ASPEN, Pro/II etc.)

- Reaction rate
- LCA data
- Materials data



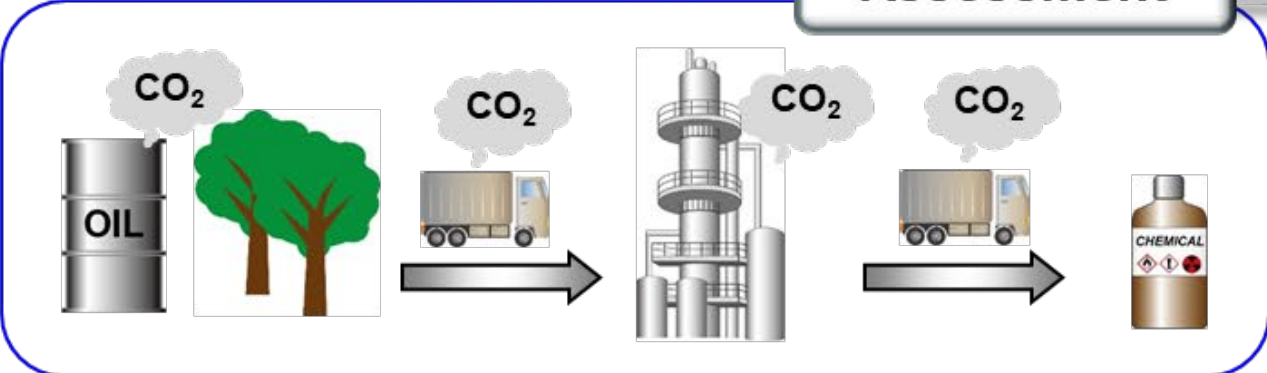
Database

Process design



- Material balance
- Energy balance
- Equipment size etc.

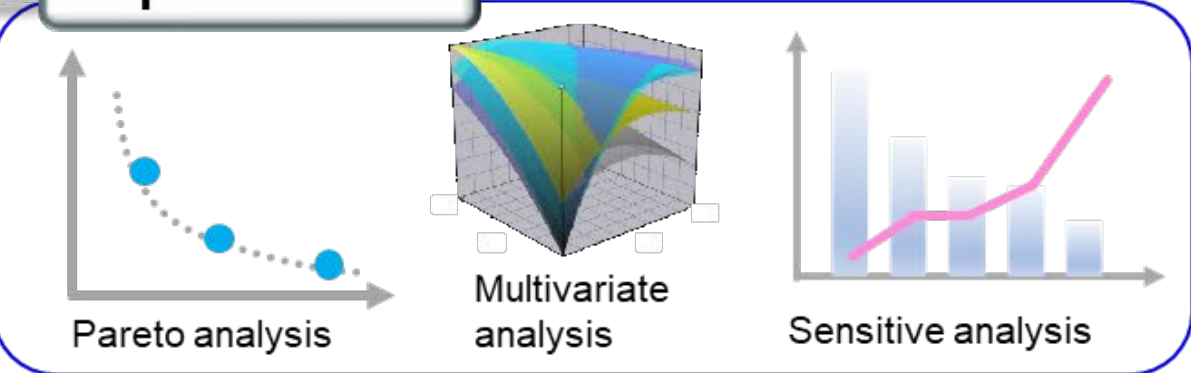
Life cycle assessment (LCA)



Assessment

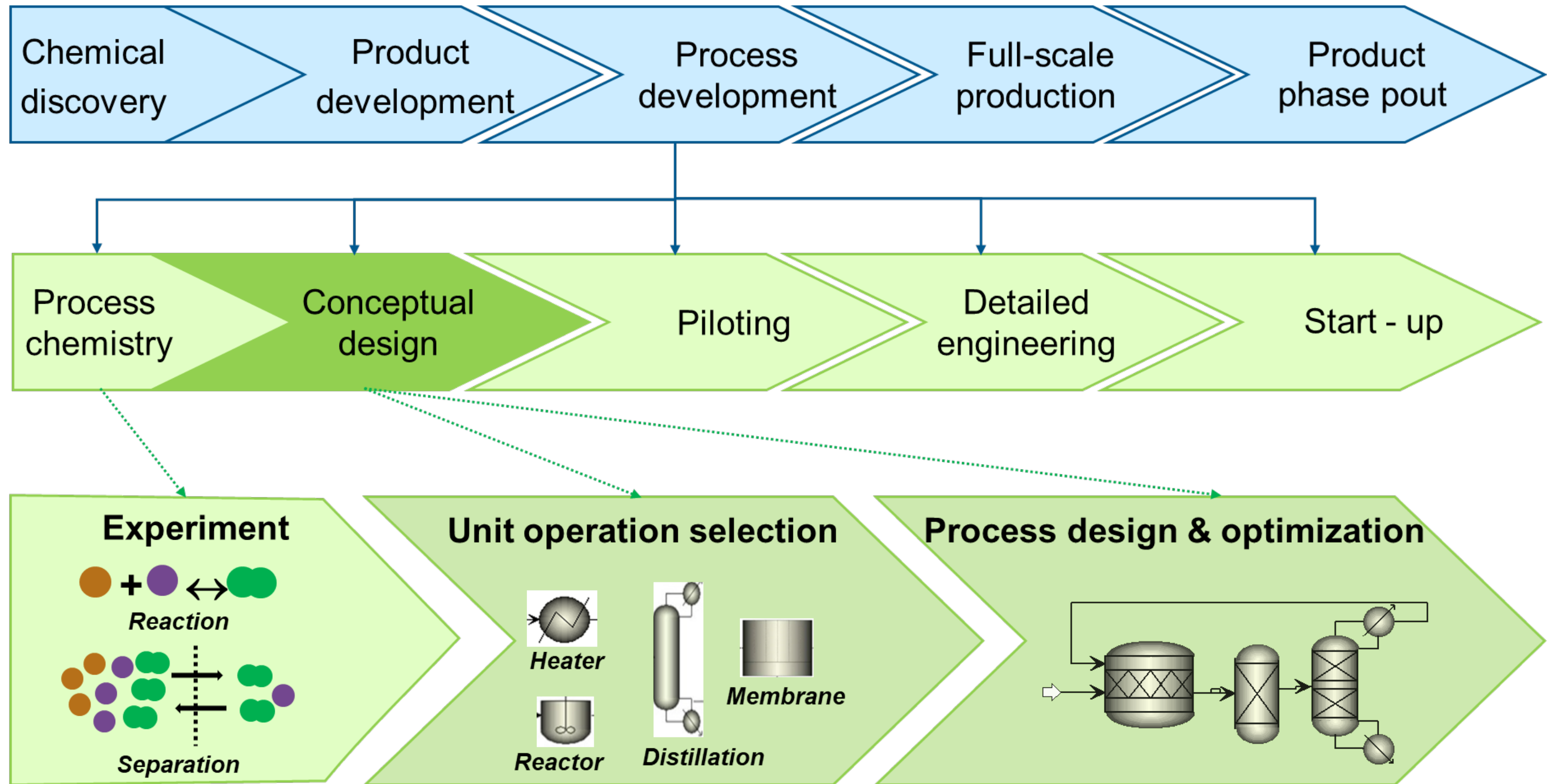
Optimization

Multi-objective optimization



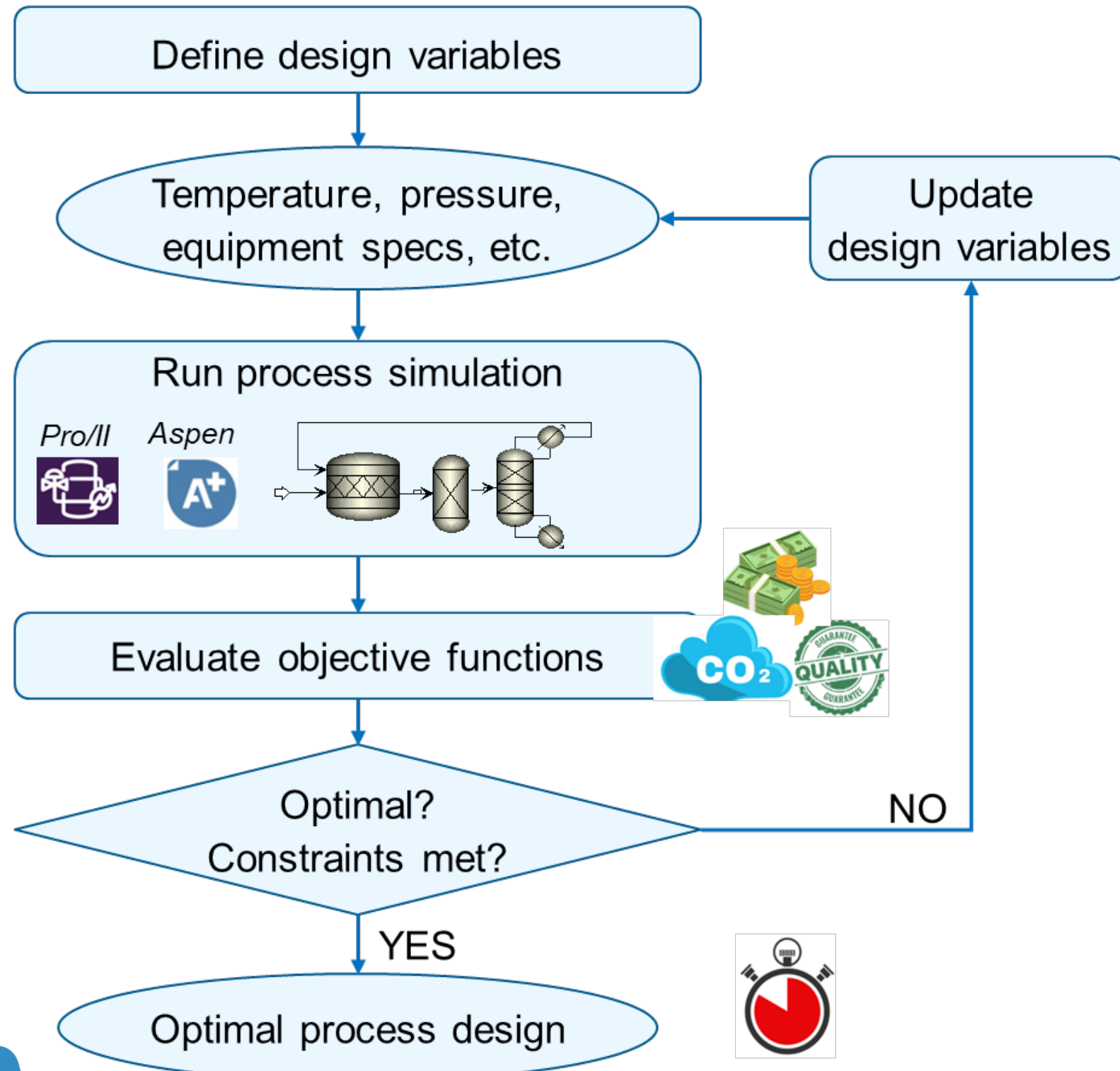
Contributing to the development of innovative process technologies, resource recycling, energy security, and solutions to environmental pollution and global warming

Stages of Chemical Process Development

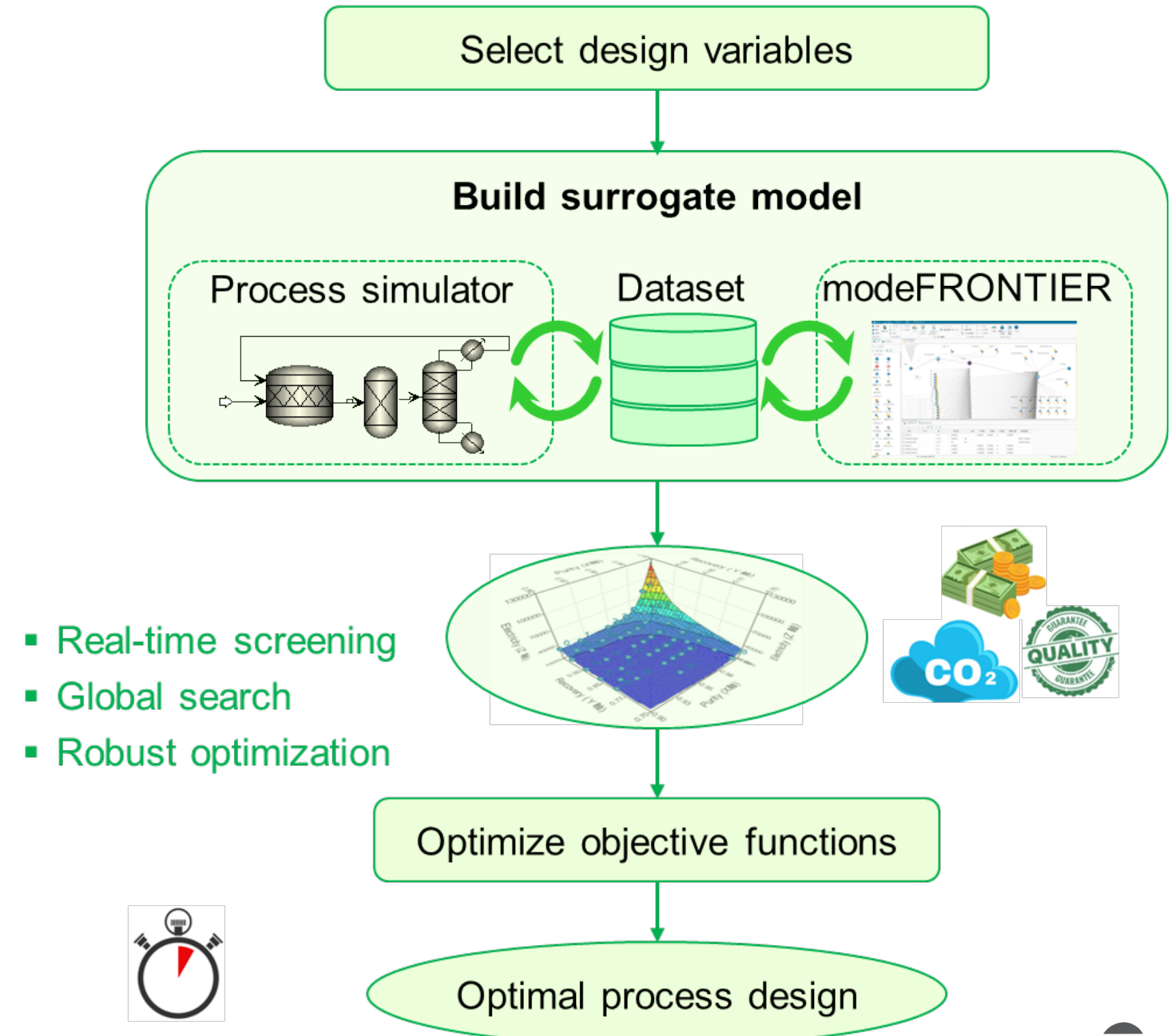


Use of Surrogate Model in Process Design & Optimization

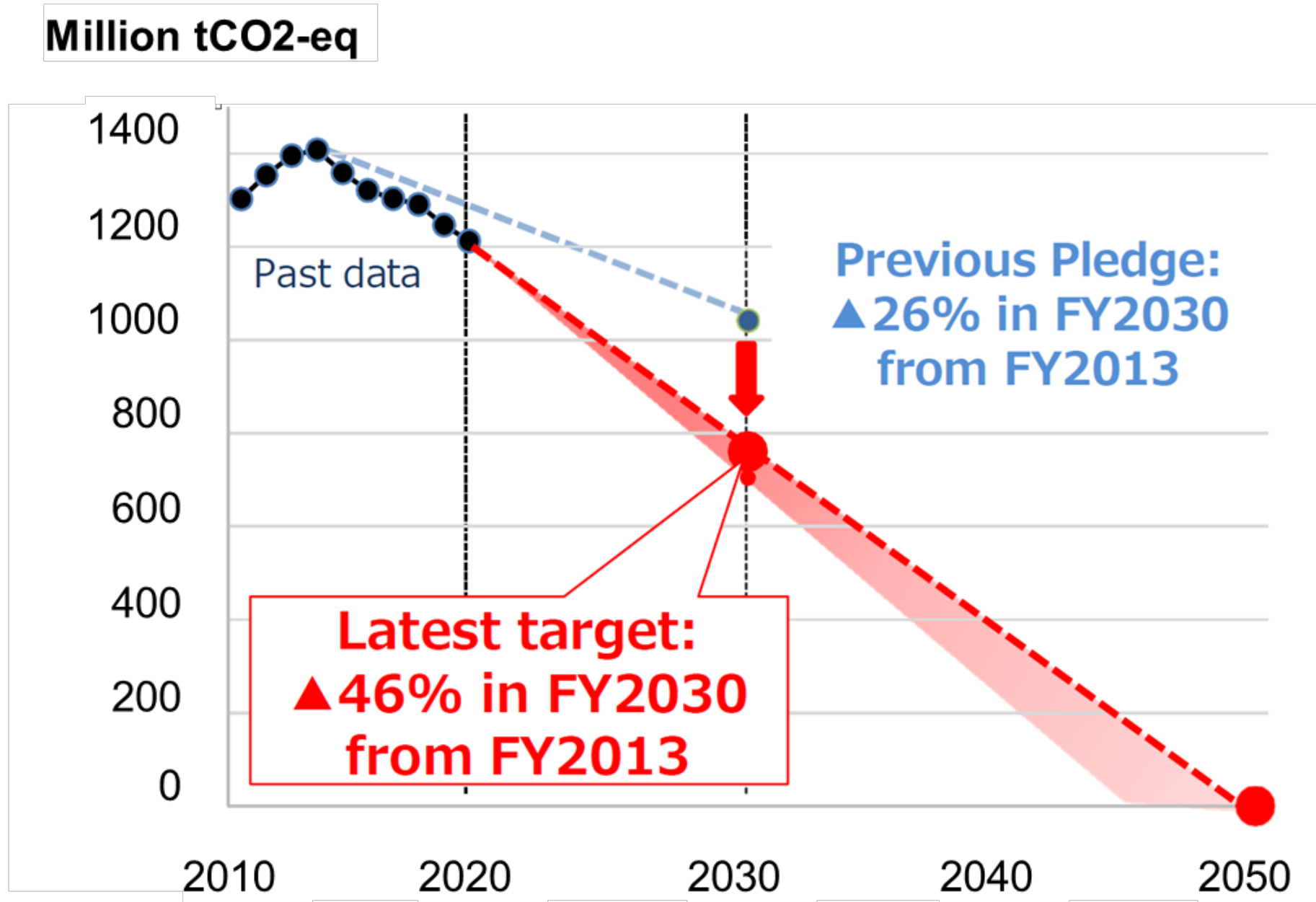
Using process simulator (Conventional approach)



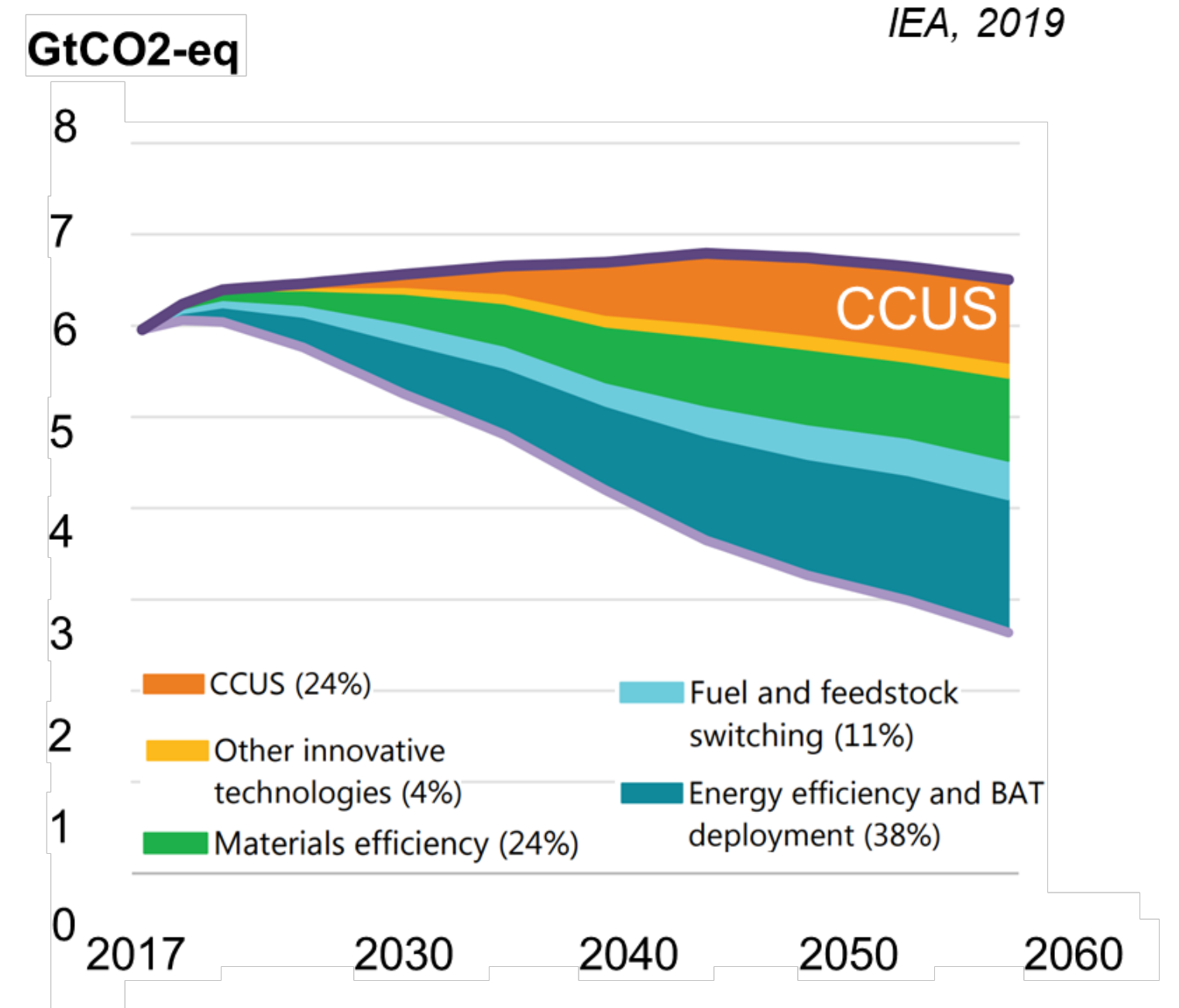
Using surrogate model built with modeFrontier



CO₂ Capture and Utilization/Storage (CCUS) for Global Warming Mitigation



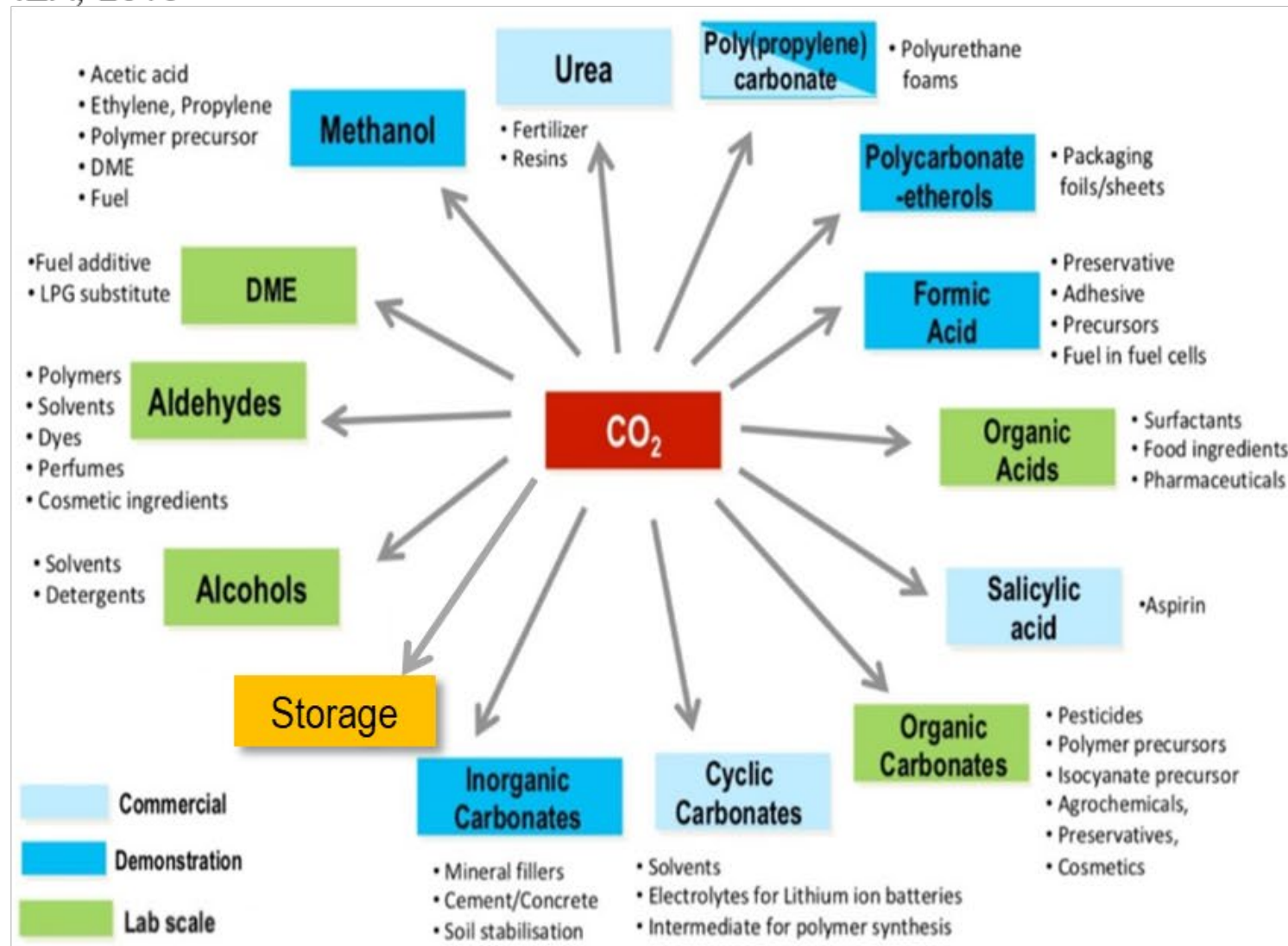
Japan's ambitious goal of achieving carbon neutrality by 2050



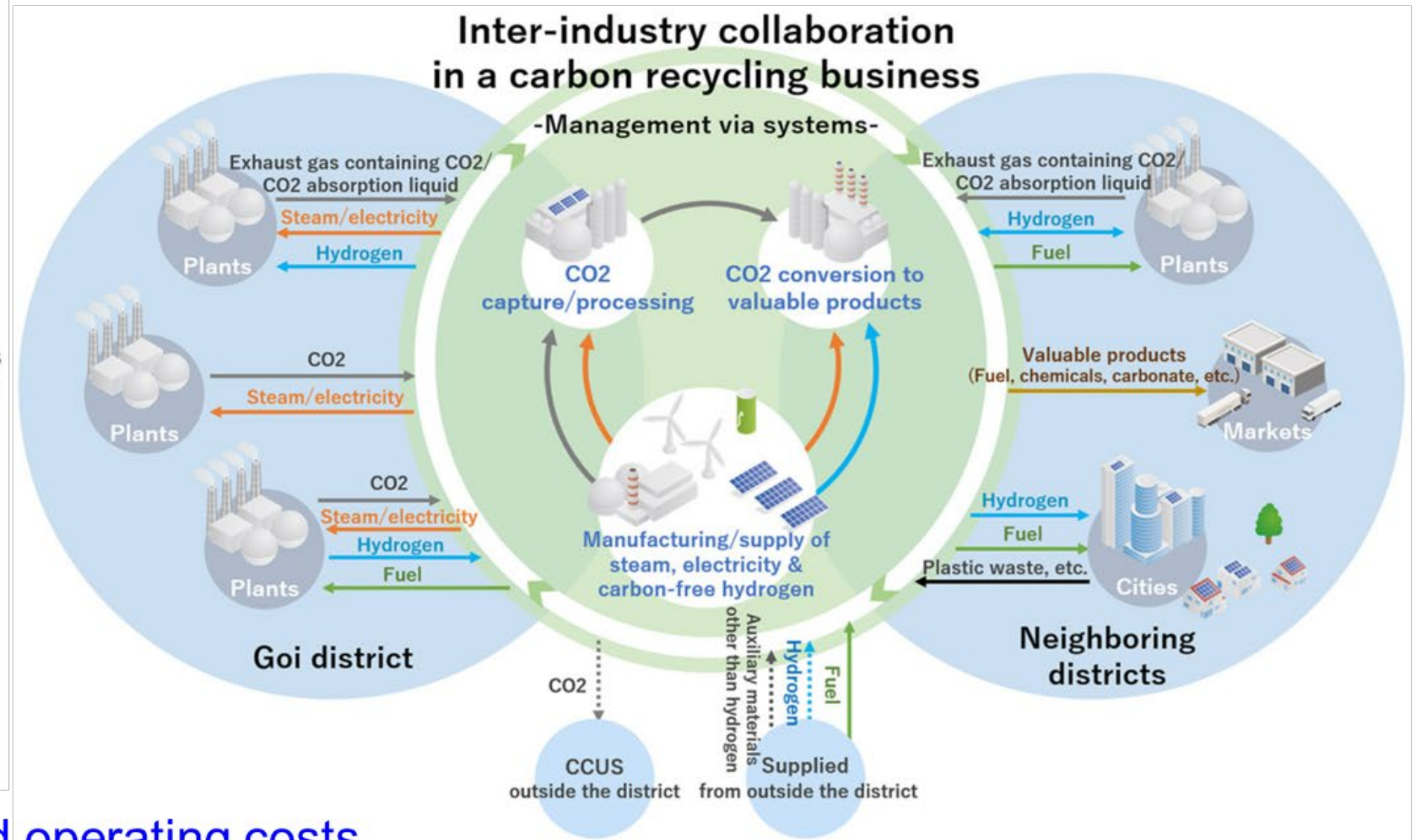
CO₂ Capture and Utilization/Storage (CCU/S)
are key technologies to achieving carbon neutrality

Barriers to Large-scale CCU/S Implementation

IEA, 2019



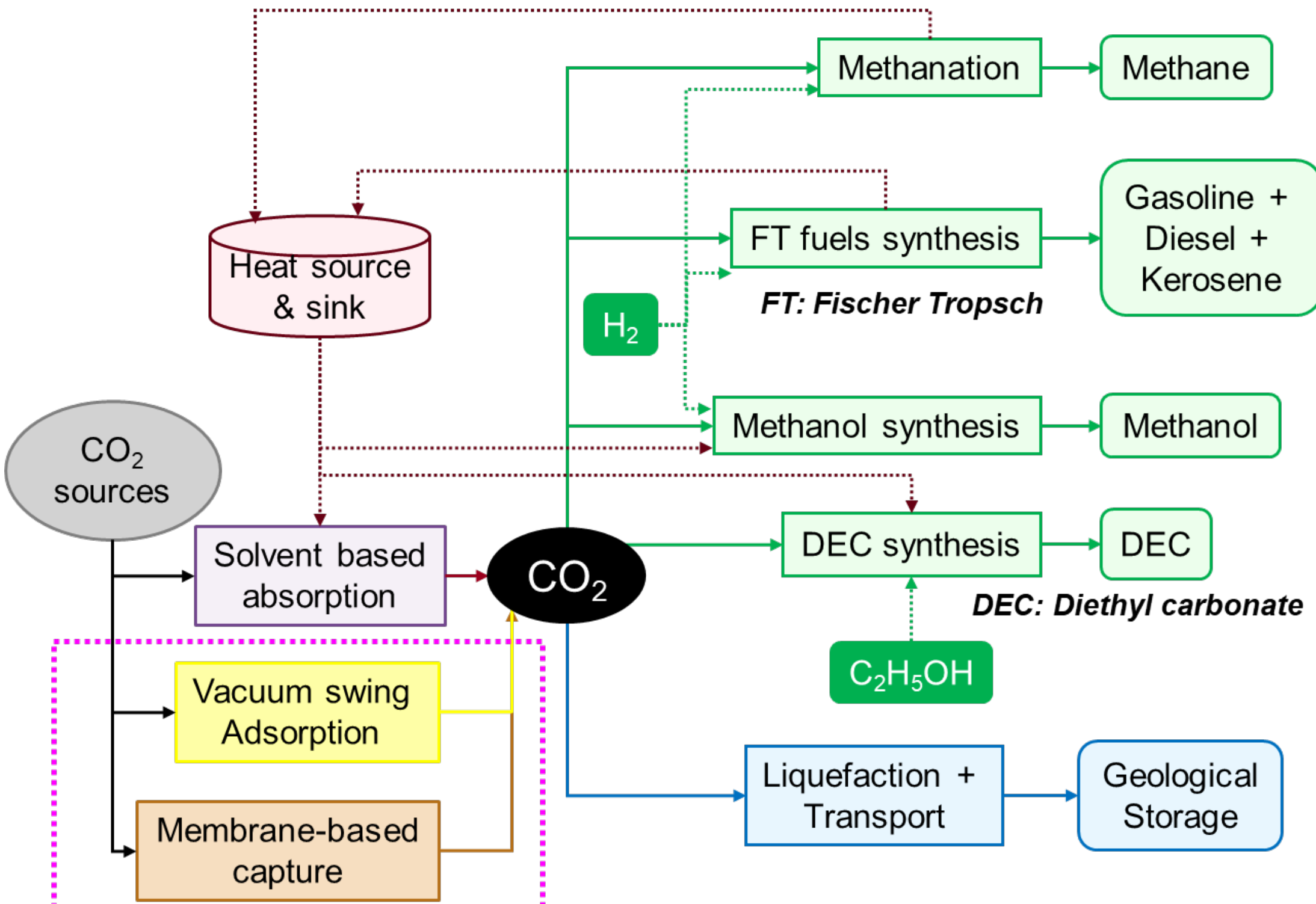
<https://www.yokogawa.com/news/press-releases/2021/2021-07-26/>



- High investment and operating costs
- Limited market demand for CO₂-derived products
- CO₂ supply far exceeds CO₂ use/storage

➔ A need to develop CO₂-based industrial complexes by integrating multiple CCUS pathways to achieve effective and cost-effective CO₂ reduction.

Challenges in Design and Optimization of Integrated CCUS Systems



- Optimal capture method?
- Optimal CCUS pathways?
- Optimal CO₂ amount utilized?
- Optimal CO₂ amount stored?

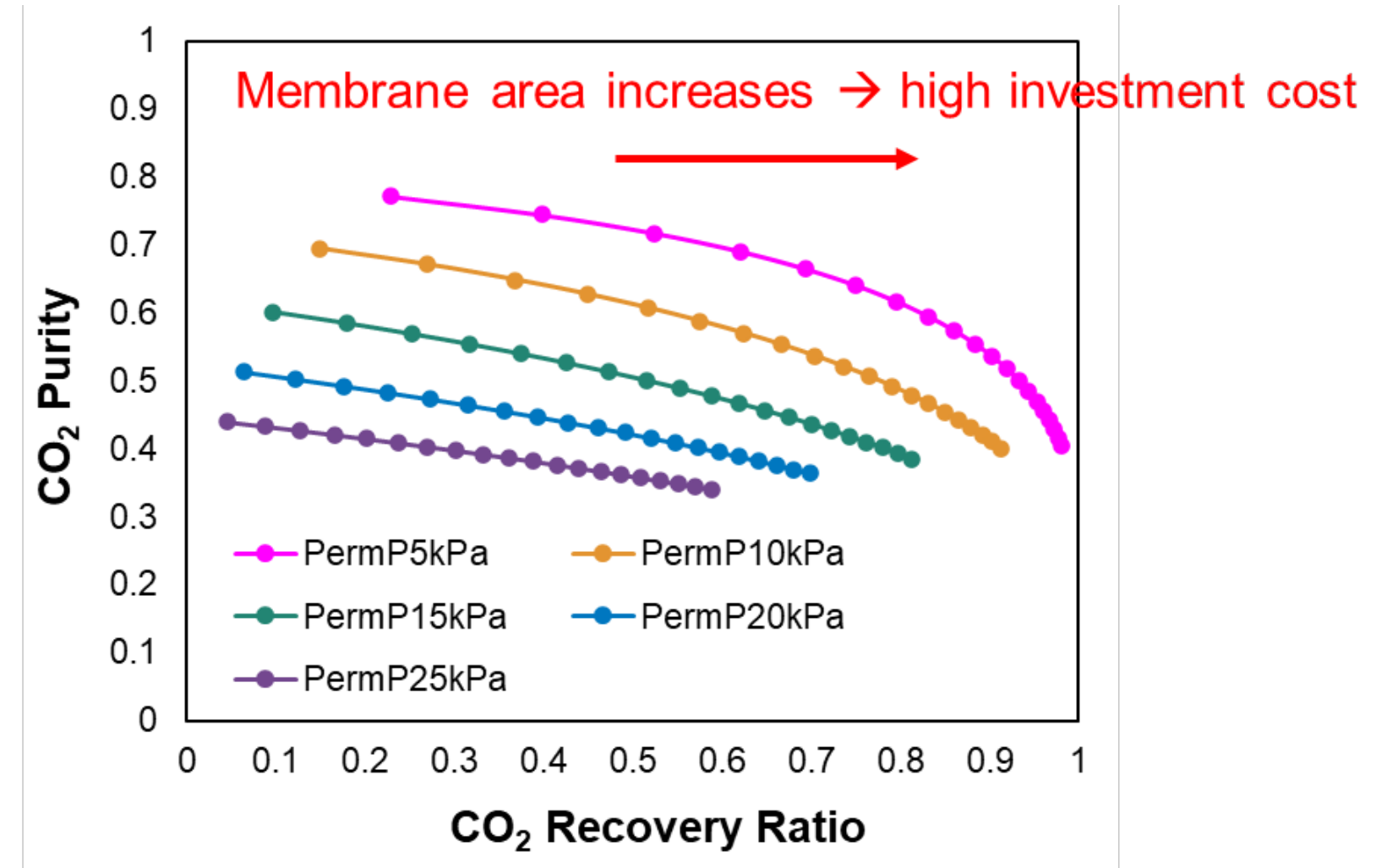
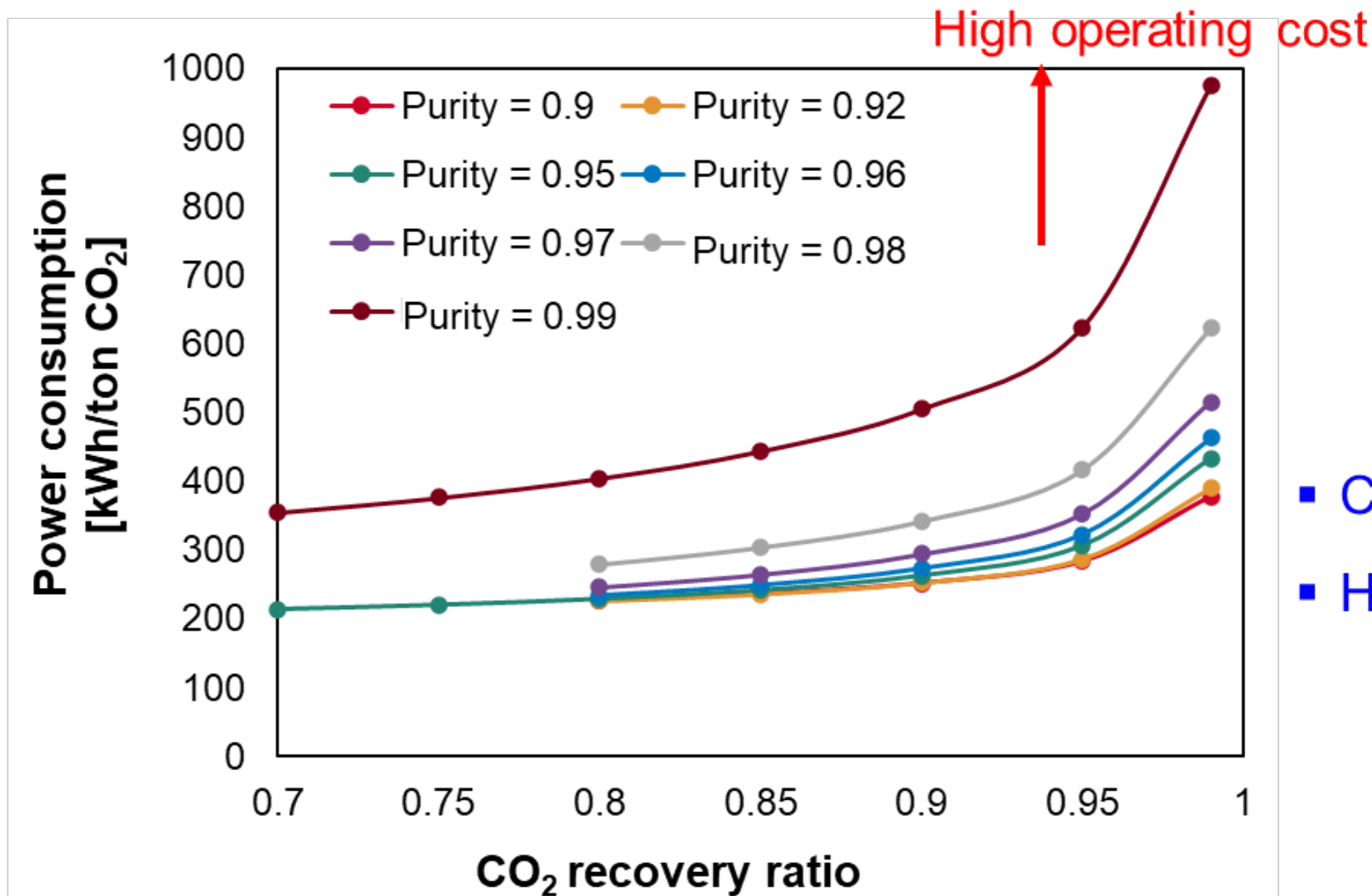
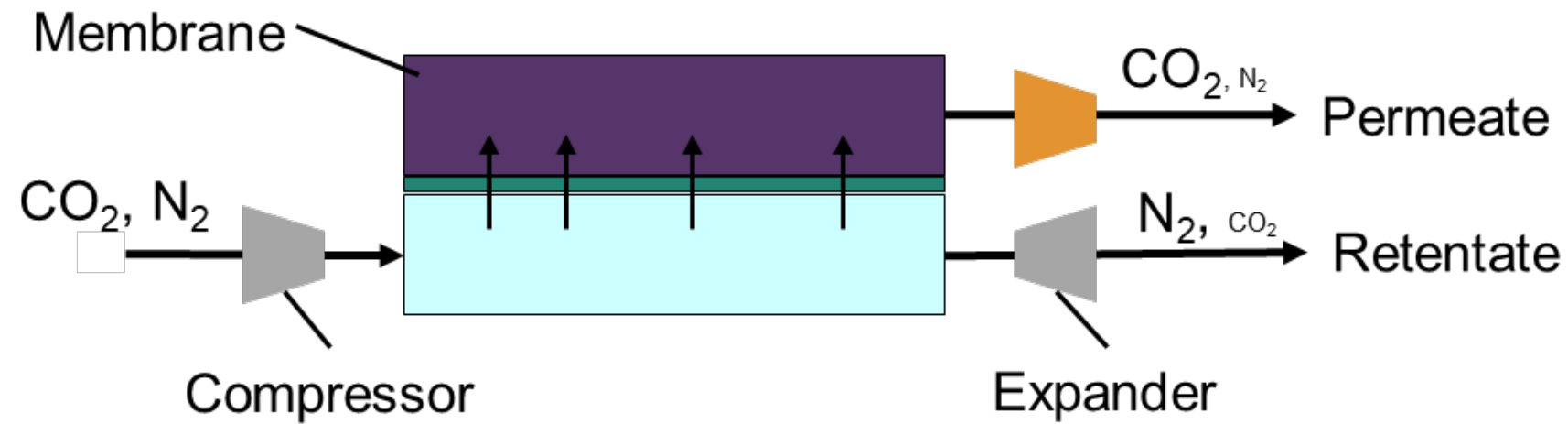


Strong impacts from external factors:

- Market demands and values
- Raw material's availability & price
- Carbon price

Developing a CCUS system design & optimization platform that flexibly responds to dynamic changes in external factors

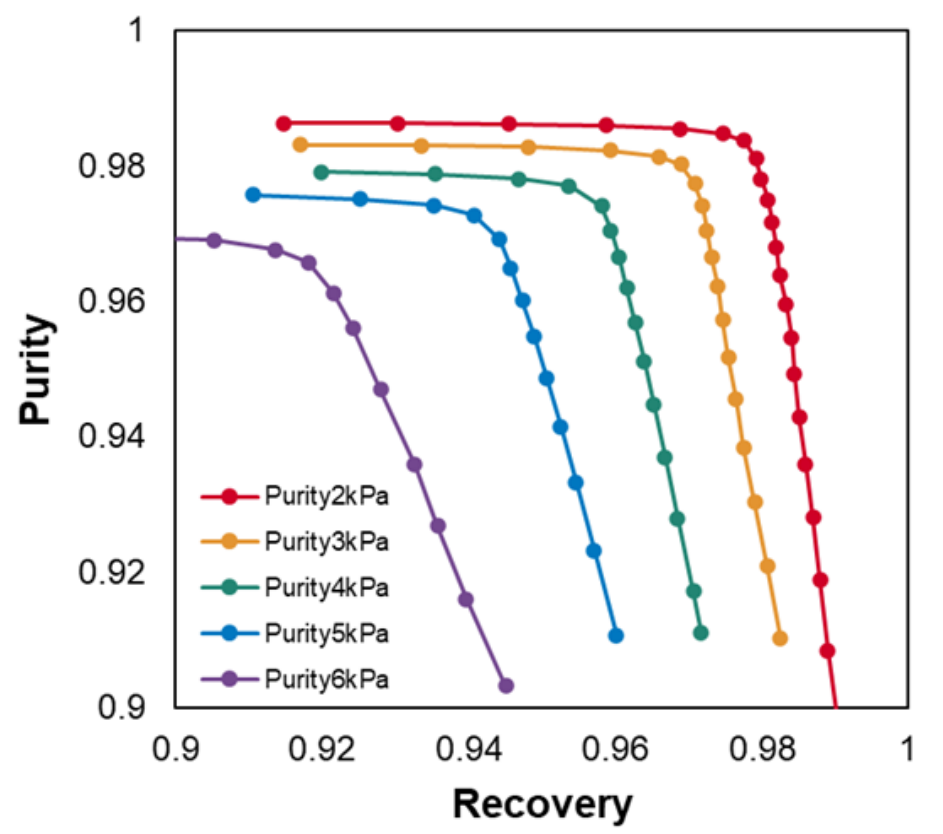
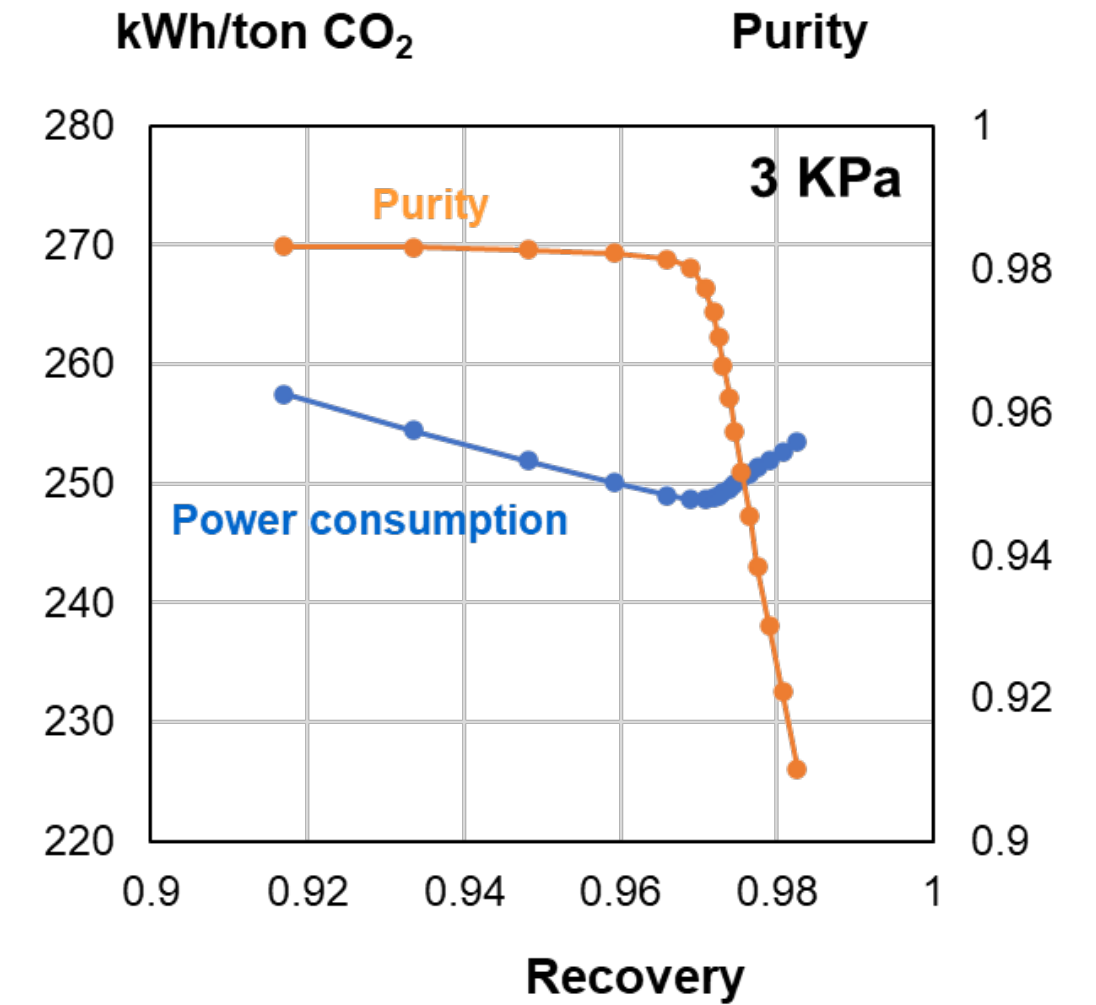
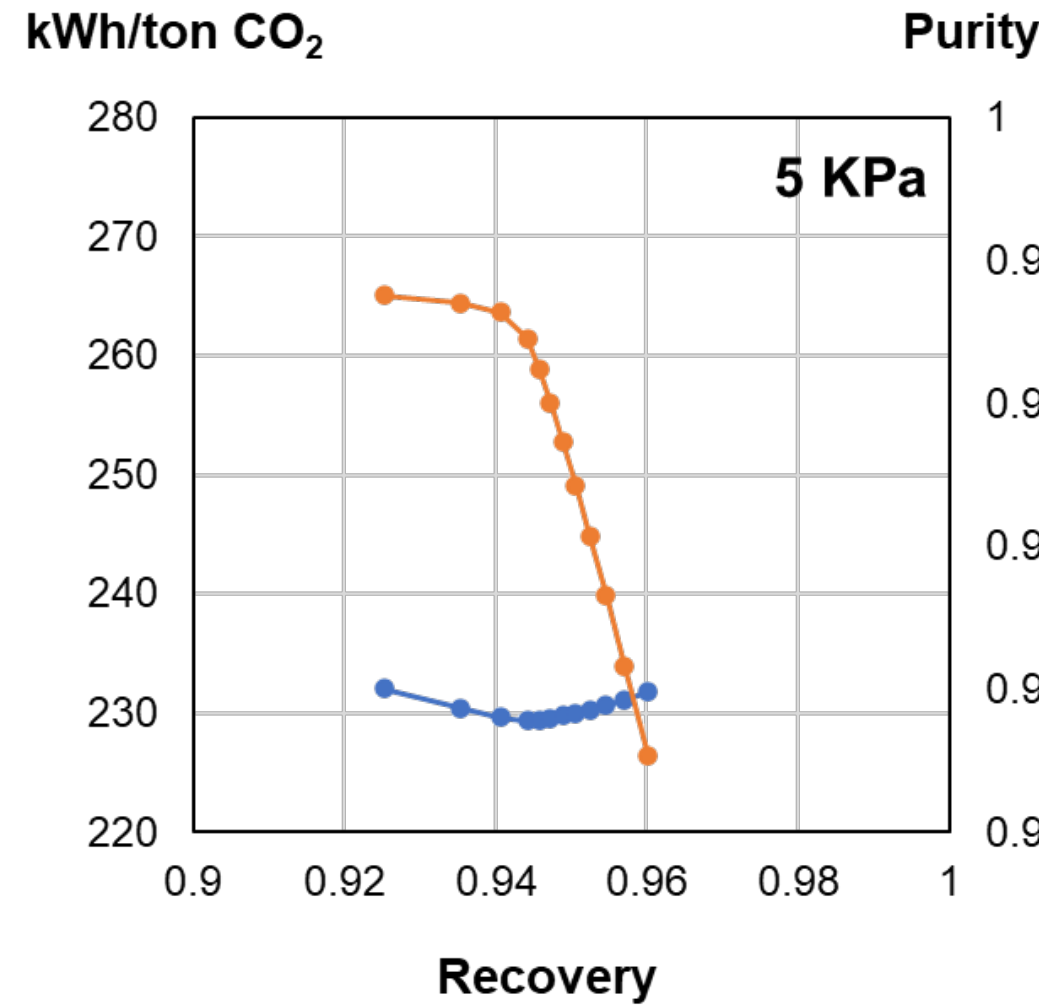
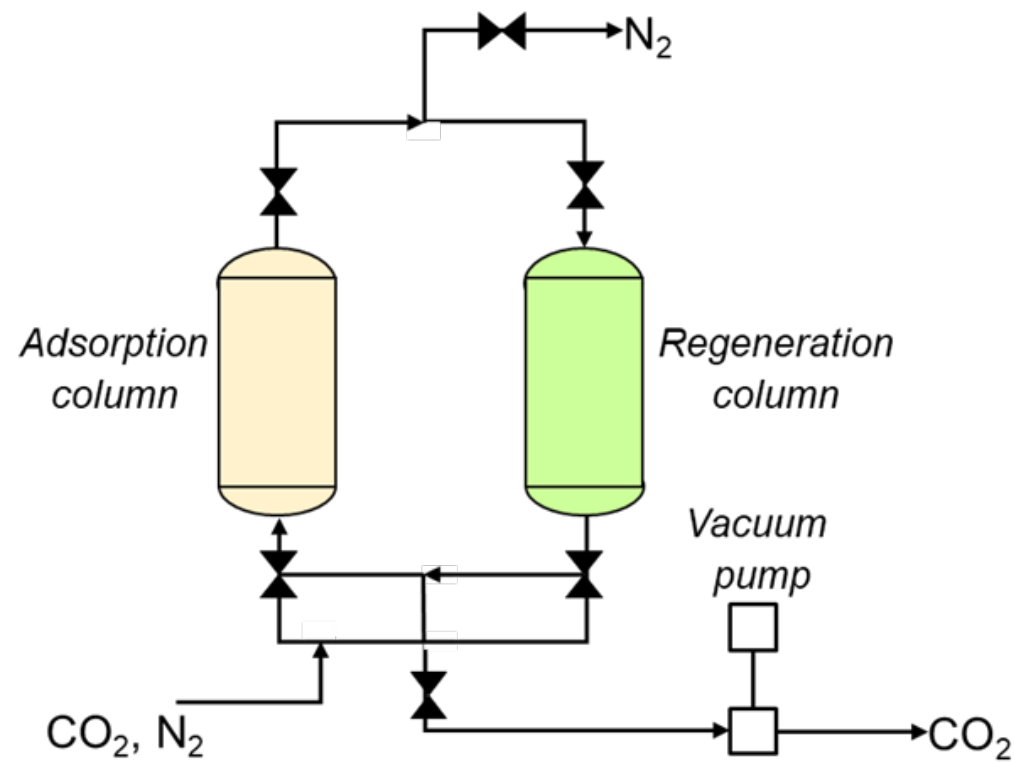
Membrane-based Method for CO₂ Capture and Purification



- Complex trade-off between CO₂ purity & recovery ratio
- Highly nonlinear dependence of costs on CO₂ purity & recovery ratio

Need for surrogate modeling to efficiently predict costs across a wide operating range

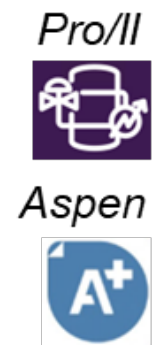
Vacuum Swing Adsorption Method for CO₂ Capture and Purification



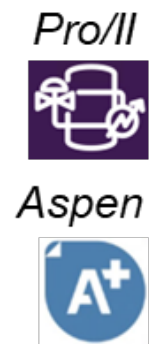
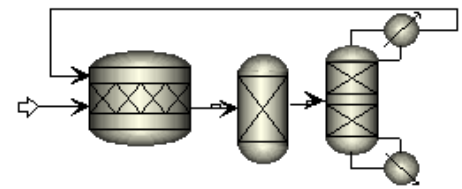
- Complex trade-off between CO₂ purity & recovery ratio
- Strongly nonlinear effects of desorption pressure on power consumption, CO₂ purity & recovery

➔ Need for surrogate models to rapidly predict power consumption over a wide operating pressure range

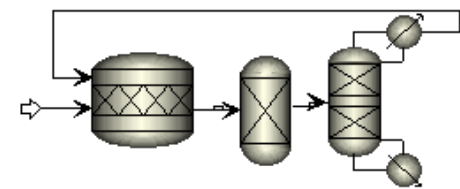
Building Surrogate Models Using modeFRONTIER



Process simulator



Process simulator



Problem definition

- Decision variables: CO₂ purity and recovery ratio
- Objectives: Costs, power consumption

Data generation

- Generate data using a rigorous process simulator
- Collect input-output datasets covering operating range

Surrogate model development

- Select modeling technique
- Train model, validate accuracy and select the best model

Surrogate model analysis

- Perform parameter studies and sensitivity analysis
- Verify solutions using rigorous process simulator

NO

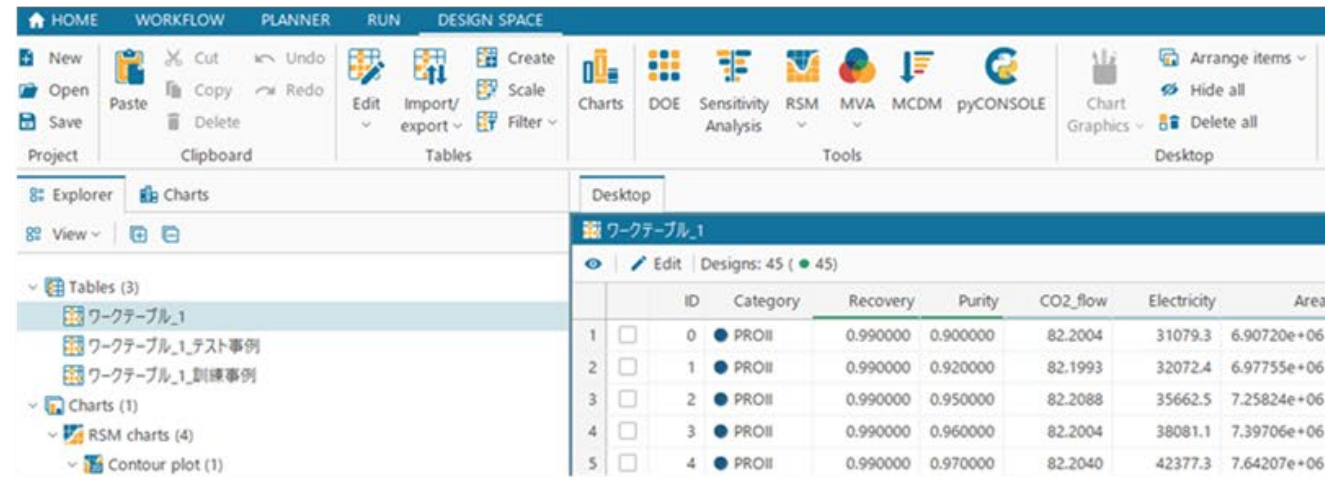
Model accurate?

YES

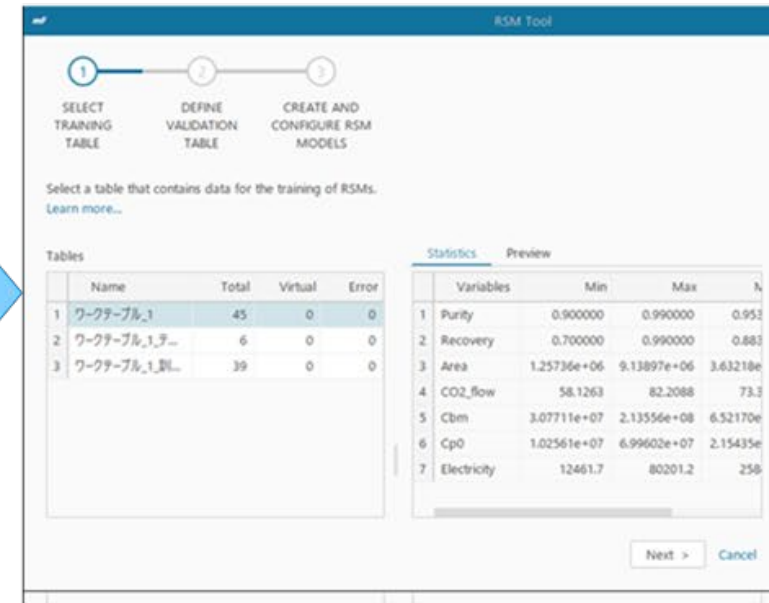
Output and embed surrogate models into the CCUS design and optimization platform

Building Surrogate Models Using modeFRONTIER

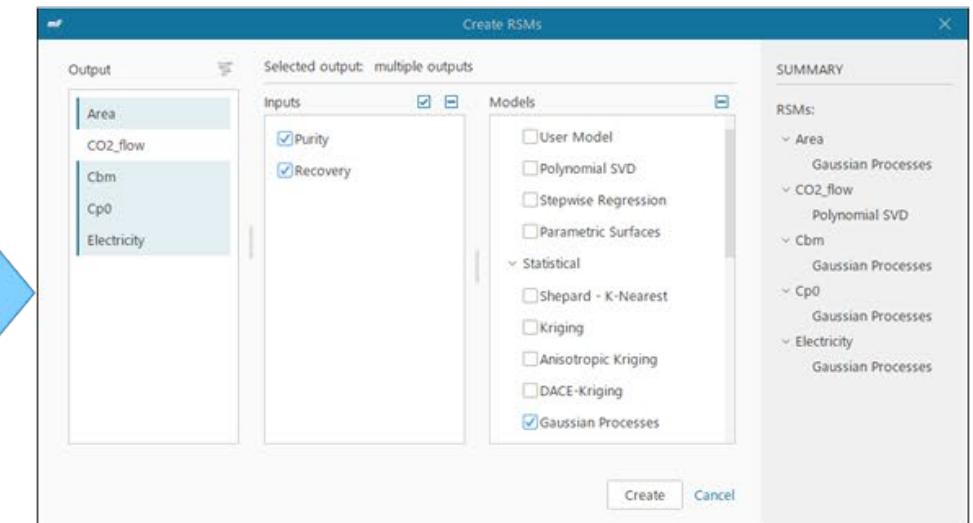
Import dataset



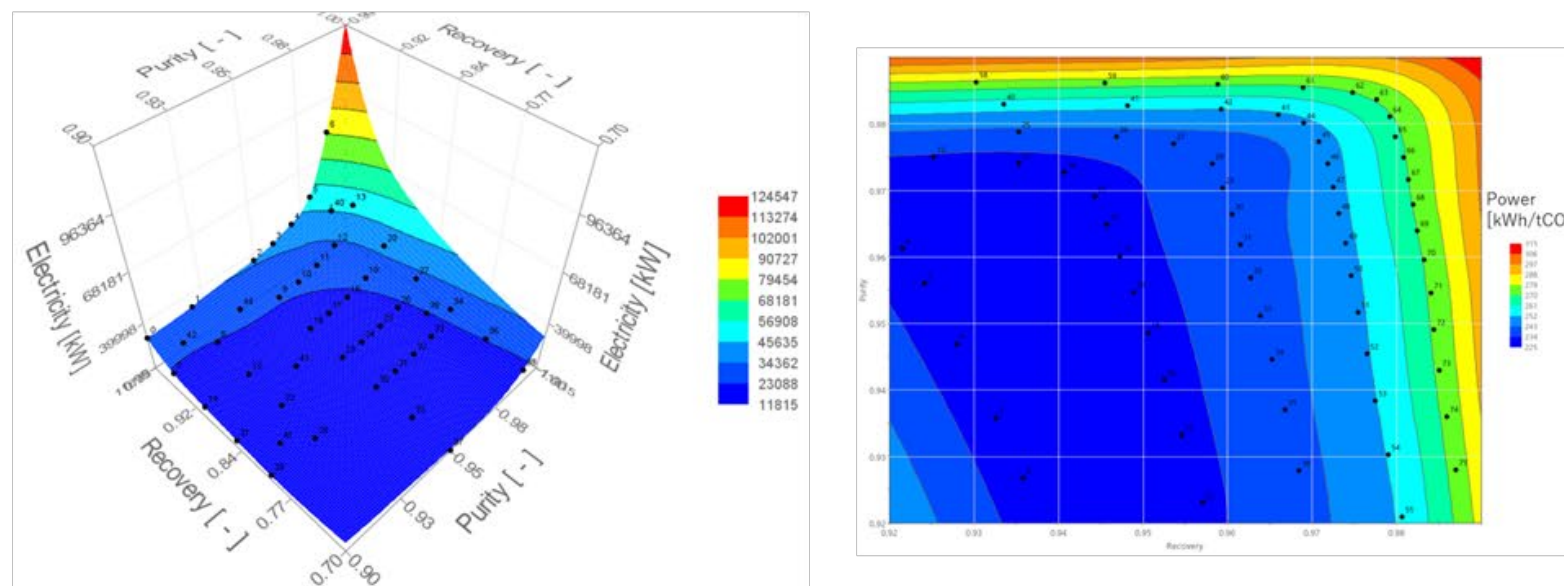
Select training & validation data



Select modeling techniques



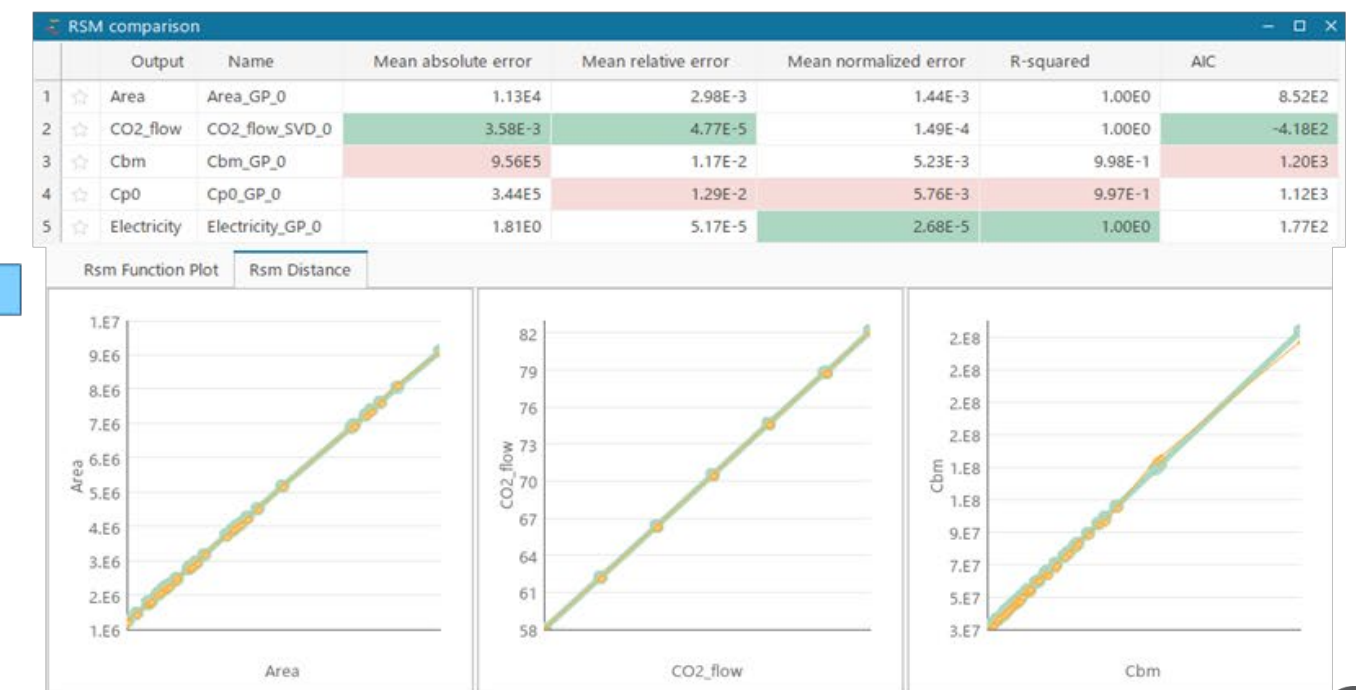
Output Excel-based surrogate models (Macro-enabled workbook)



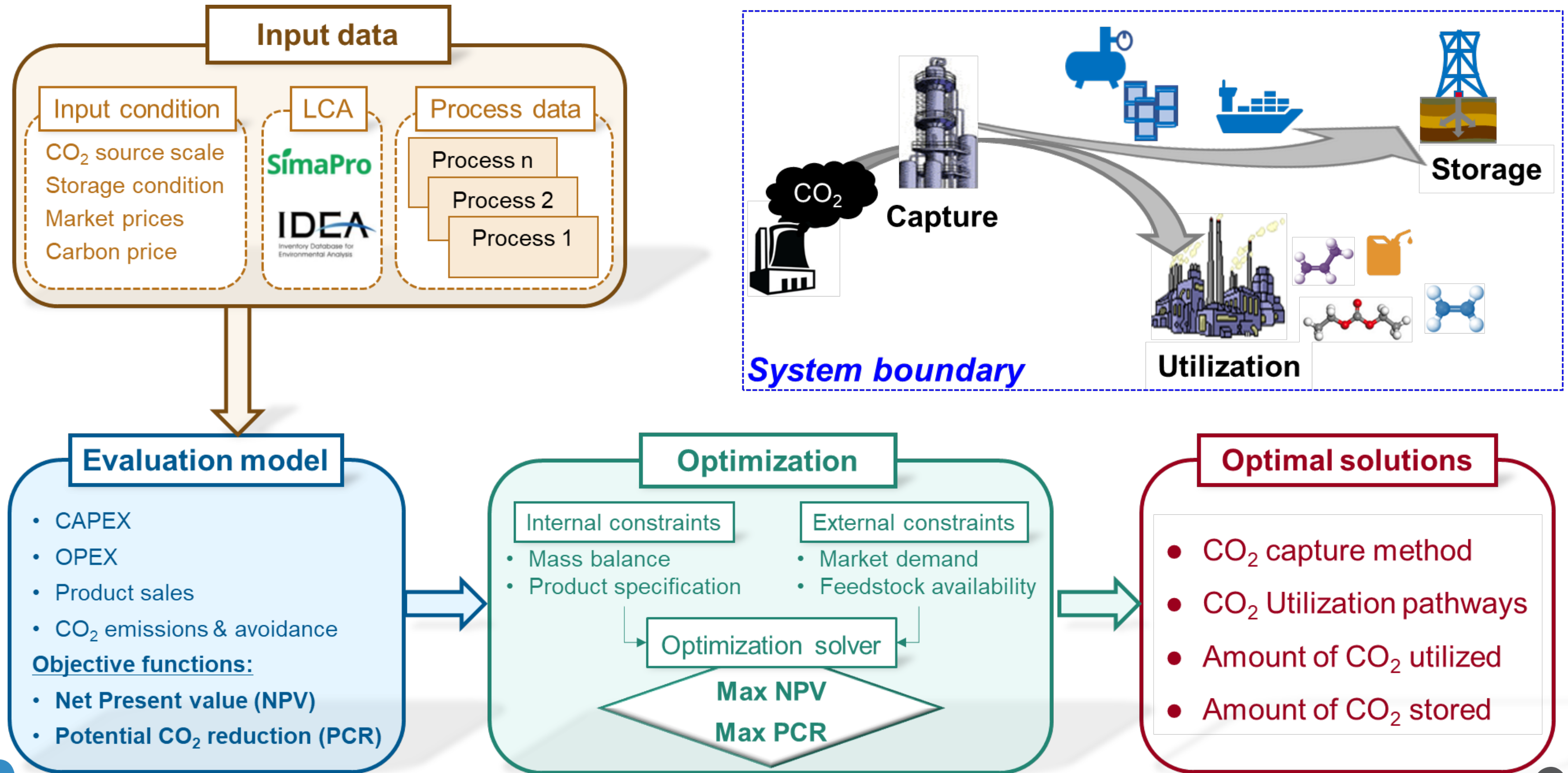
Membrane-based Method

Vacuum Swing Adsorption Method

Validate and select the best modeling technique

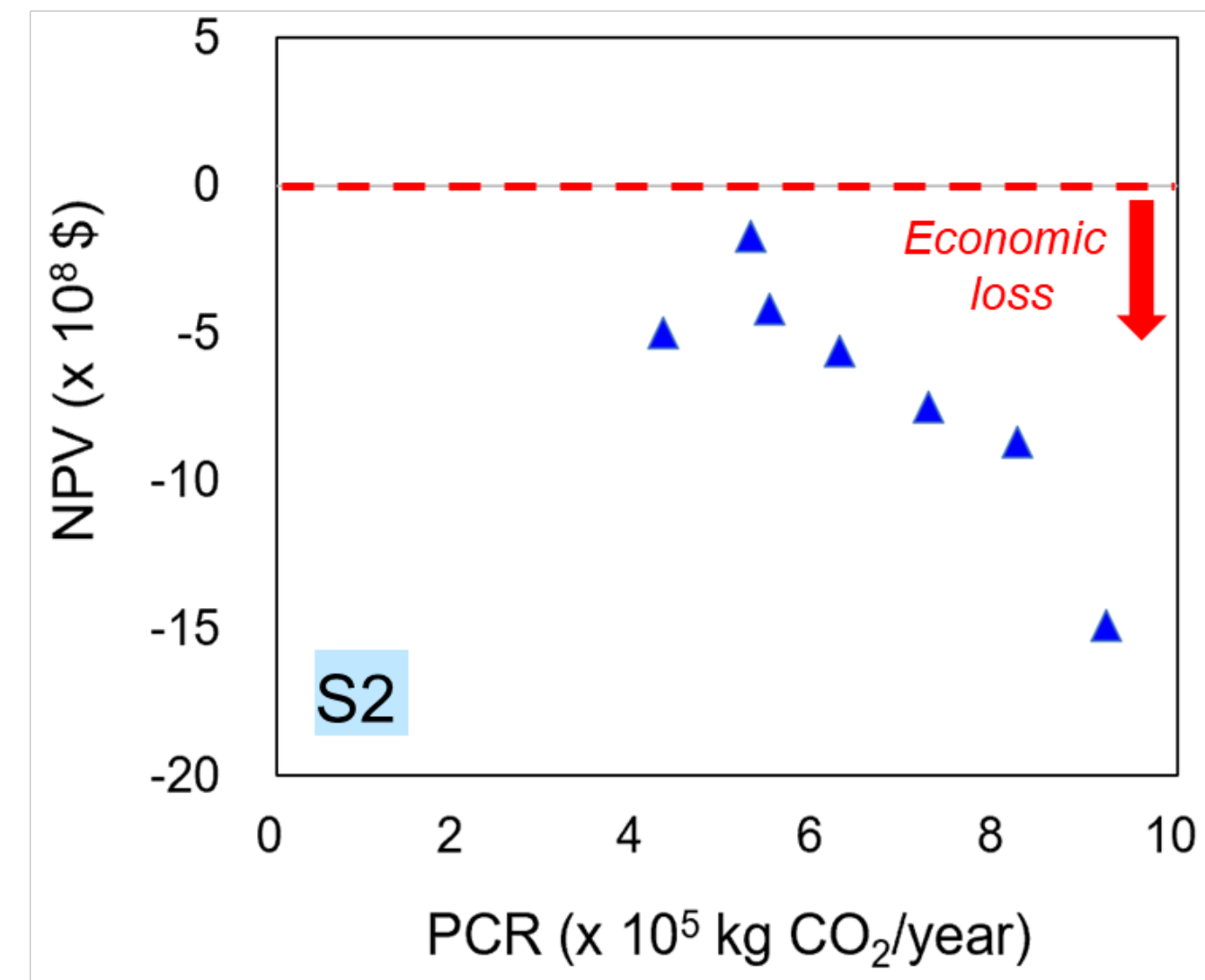
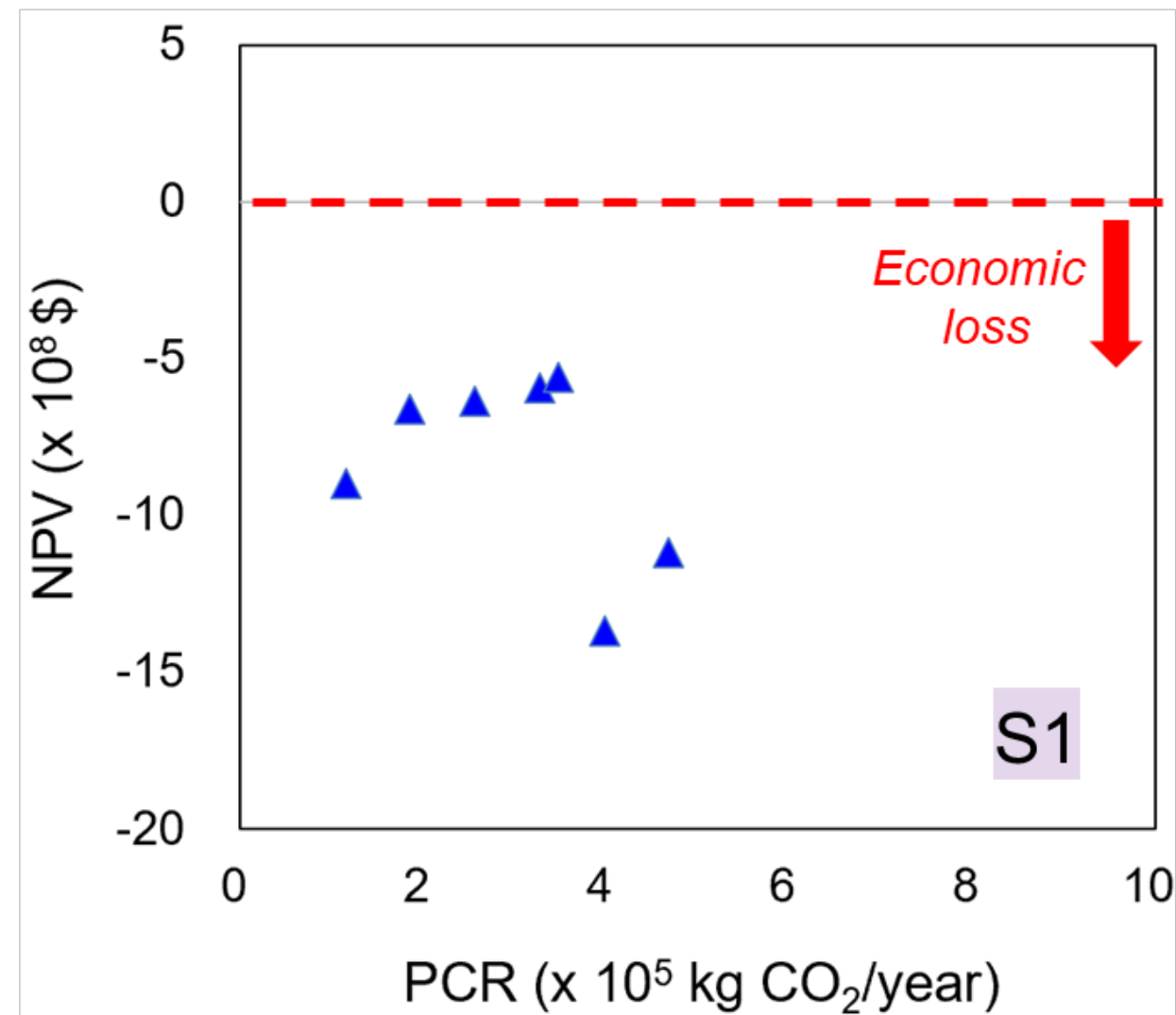


Platform for System-Wide CCUS Design and Optimization Platform



Optimization Results

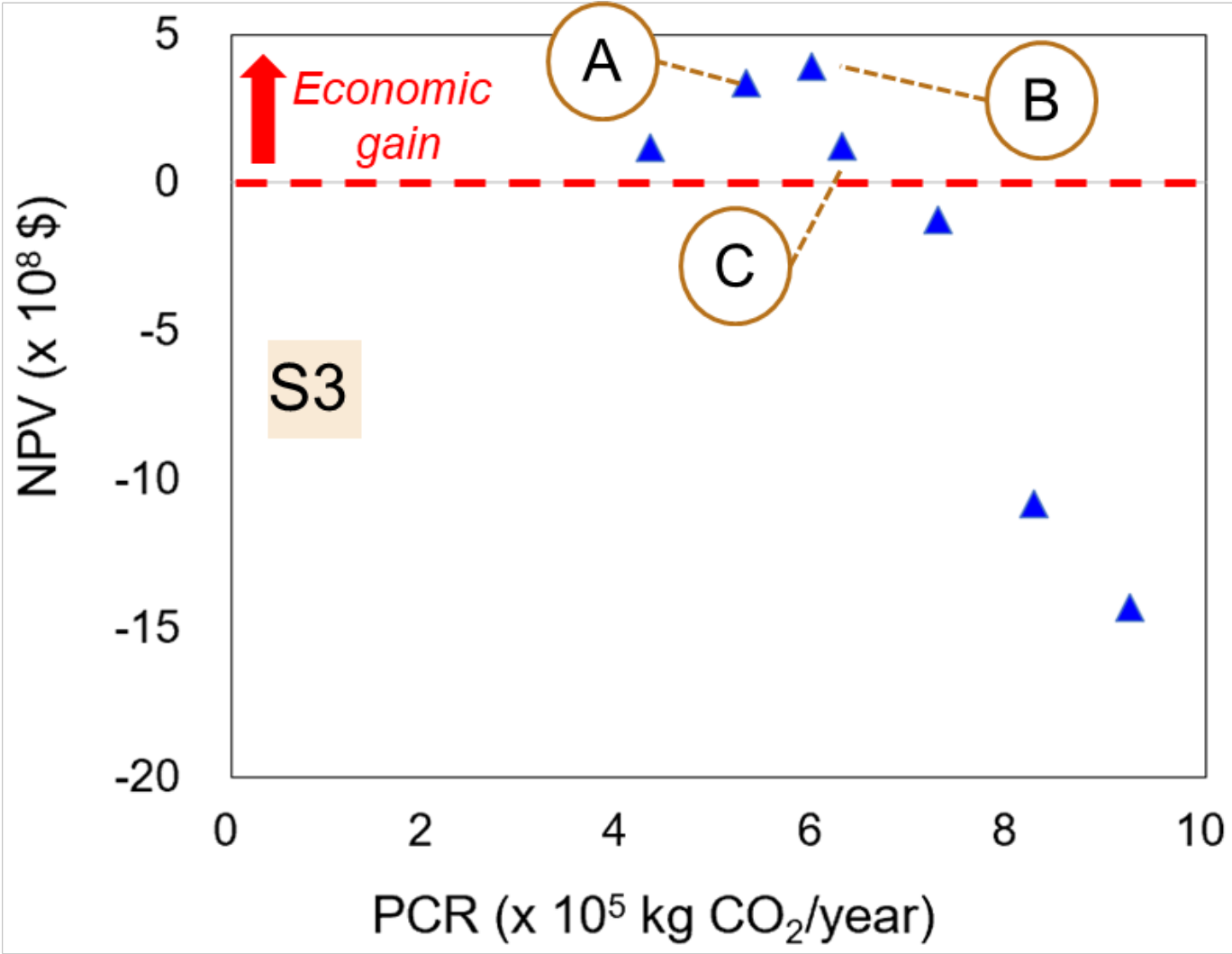
| Scenario ID | S1 | S2 |
|--|----------------------------|---------------------|
| Hydrogen type and price | Blue – 2.0 \$/kg | Green – 1.3 \$/kg |
| Electricity type and price | Conventional – 0.18 \$/kWh | Green – 0.09 \$/kWh |
| Membrane cost (\$/m ²) | 50 | 50 |
| Carbon price (\$/ton CO ₂) | 0 | 0 |



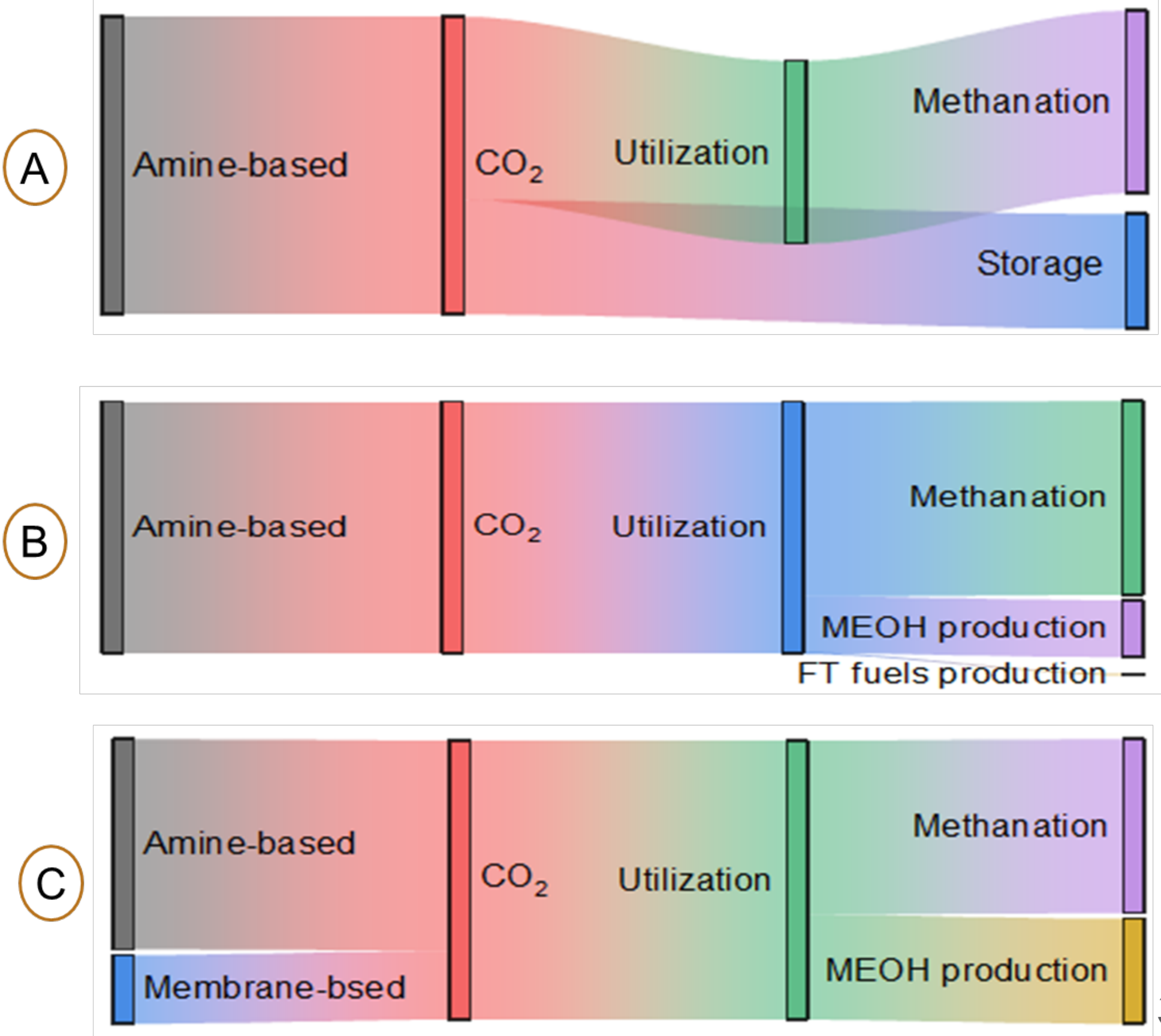
- Using green hydrogen & utilities enables significant CO₂ reduction.
- Even with low hydrogen & utility costs, CCUS system is not profitable without a carbon price.

Optimization Results

| | |
|--|---------------------|
| Scenario ID | S3 |
| Hydrogen type and price | Green – 1.3 \$/kg |
| Electricity type and price | Green – 0.09 \$/kWh |
| Membrane cost (\$/m ²) | 25 |
| Carbon price (\$/ton CO ₂) | 250 |



High carbon price is required to enhance economic viability

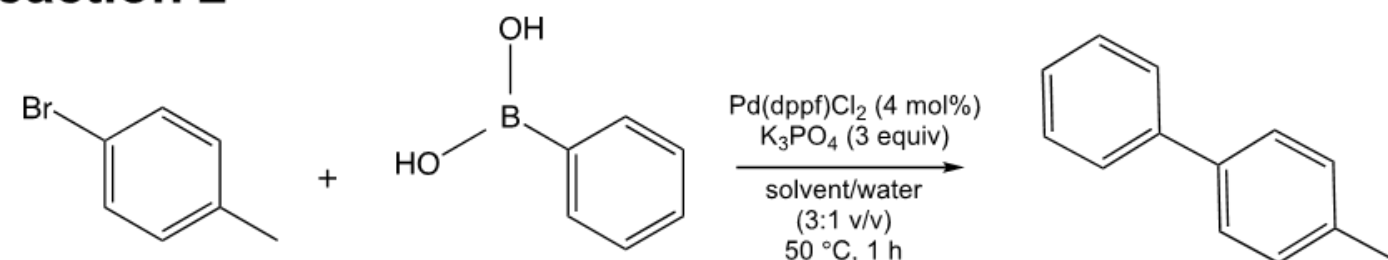


Accelerated Chemical Process Design and Optimization Using Surrogate Modeling in modeFRONTIER: Application to Selection of Solvents for Chemical Reaction

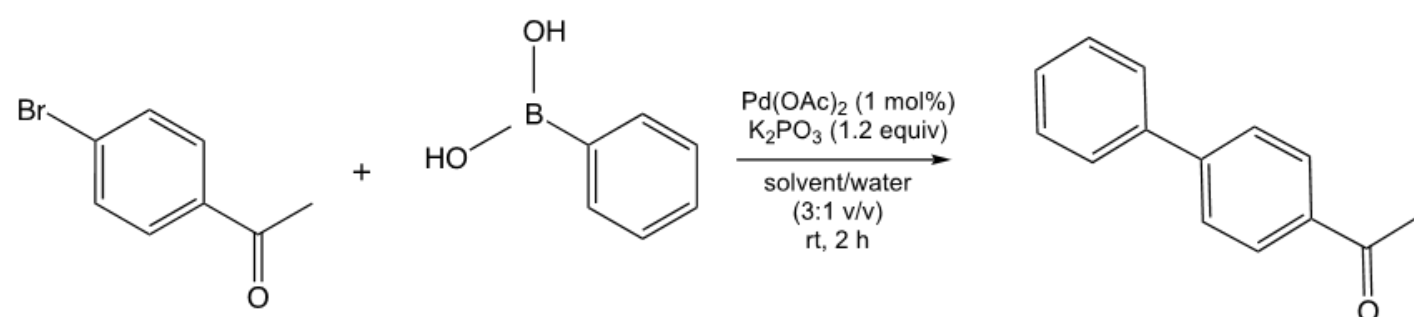
Importance of Solvent Selection for Chemical Reaction

Suzuki-Miyaura coupling reaction

Reaction 1

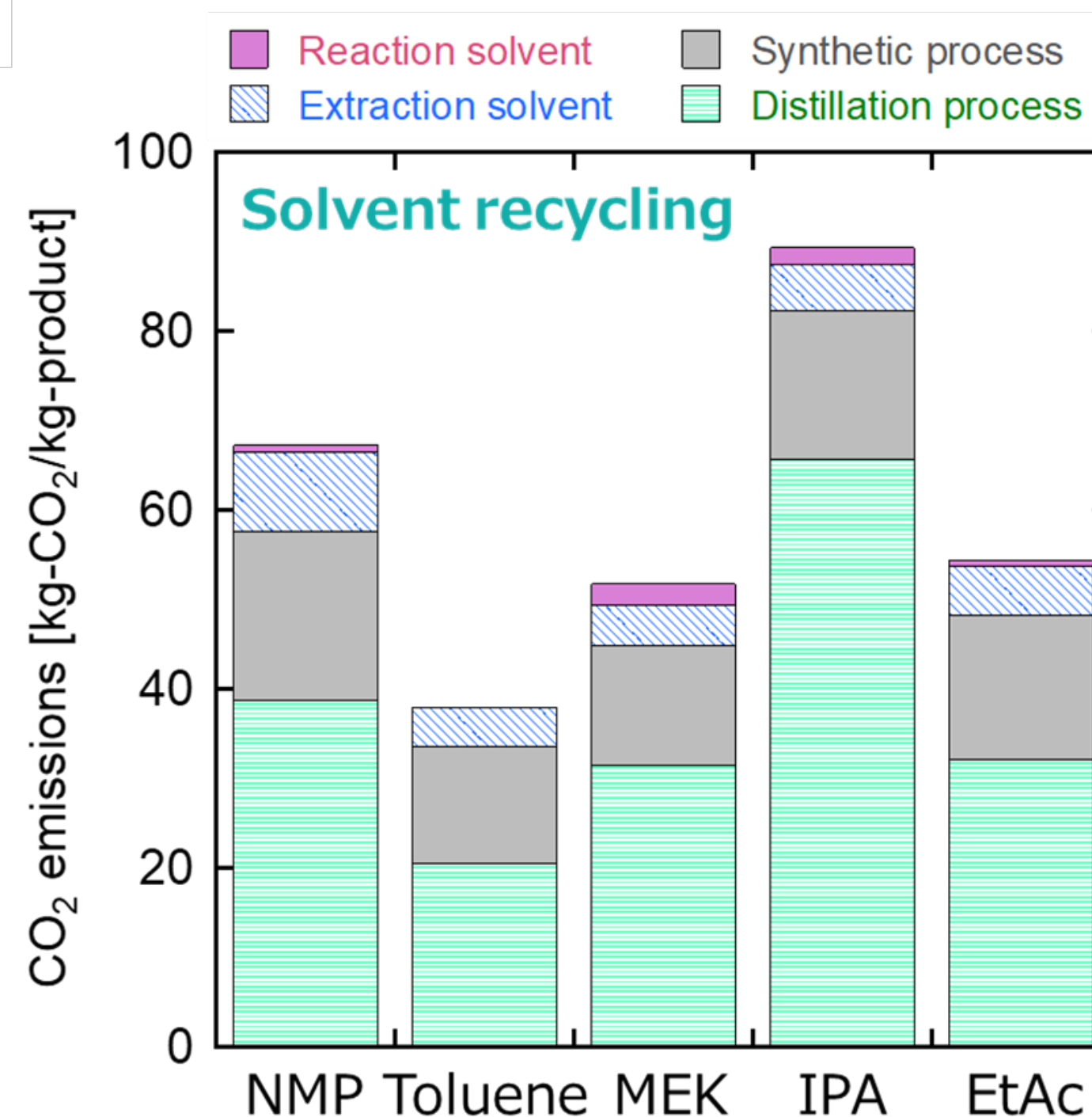


Reaction 2



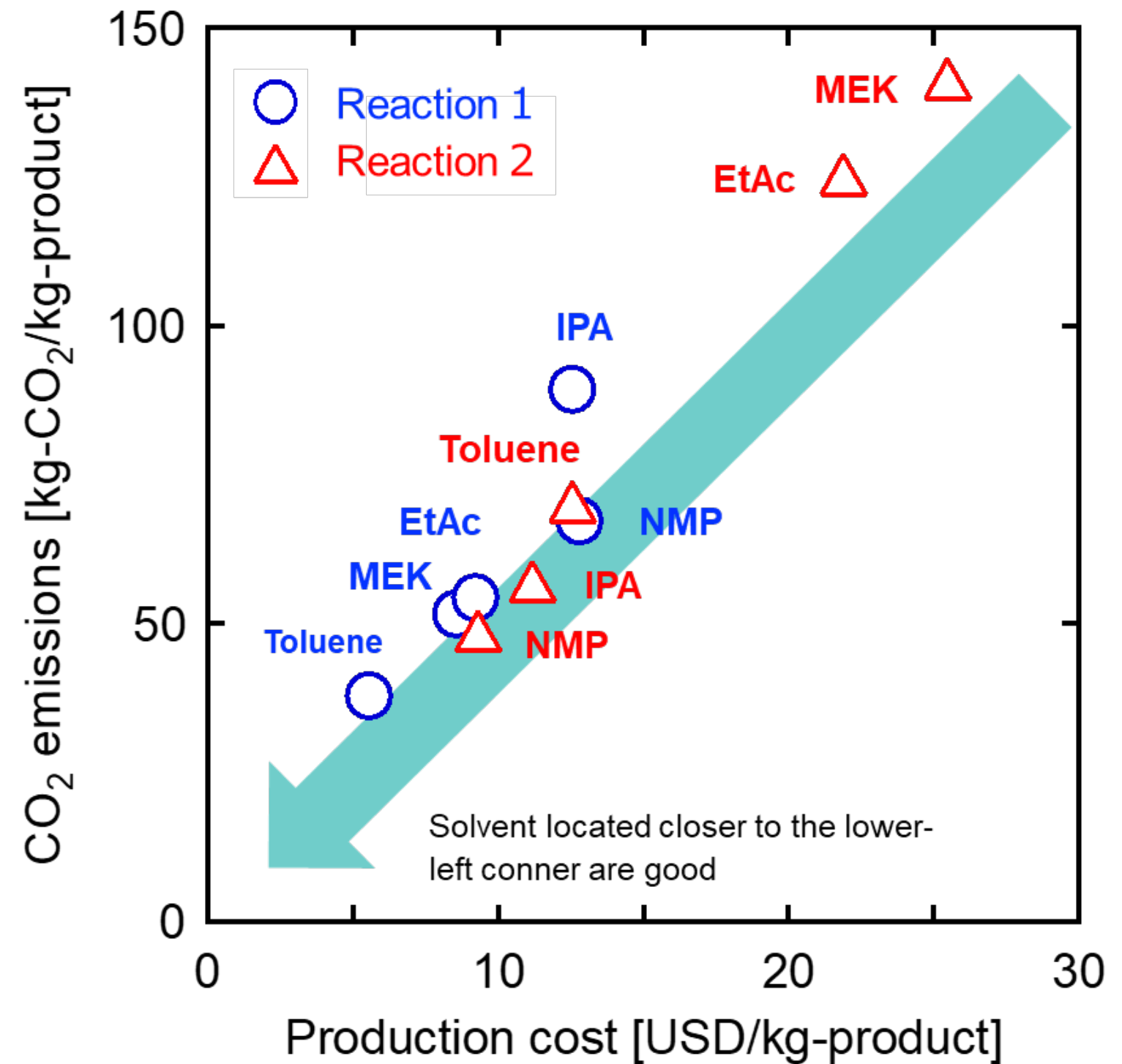
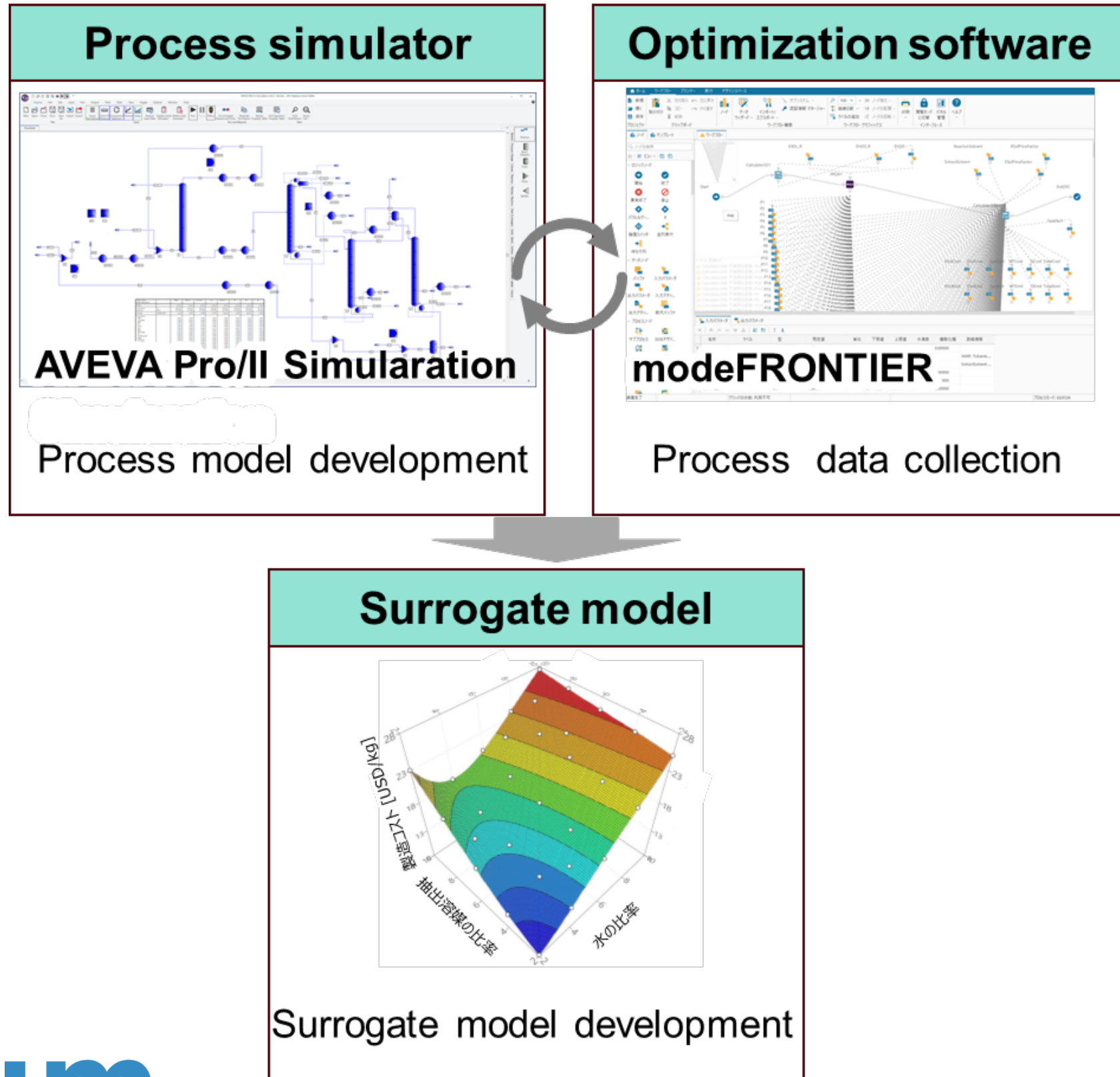
| Solvent | Reaction yields | |
|---------|-----------------|------------|
| | Reaction 1 | Reaction 2 |
| NMP | 0.85 | 1 |
| Toluene | 0.94 | 0.42 |
| MEK | 0.92 | 0.30 |
| IPA | 0.81 | 1 |
| EtAc | 0.76 | 0.28 |

*Beilstein J. Org. Chem. 2020, 16, 1001-1005



Solvent selection affects the overall CO₂ emissions

Surrogate Model Development for Solvent Selection



Selecting suitable solvent for reducing both cost and CO₂ emissions

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2026

Thank you

[esteco.com](https://www.esteco.com)

