IMPERIAL

Sargent Centre for Process Systems Engineering

Extending Superstructure Formulations to Enable Non-Isobaric Flowsheet Alternatives

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Why Superstructures?

Allows for the fast and systematic exploration of the process design space

Permits the otherwise difficult consideration of multiple decisions at once

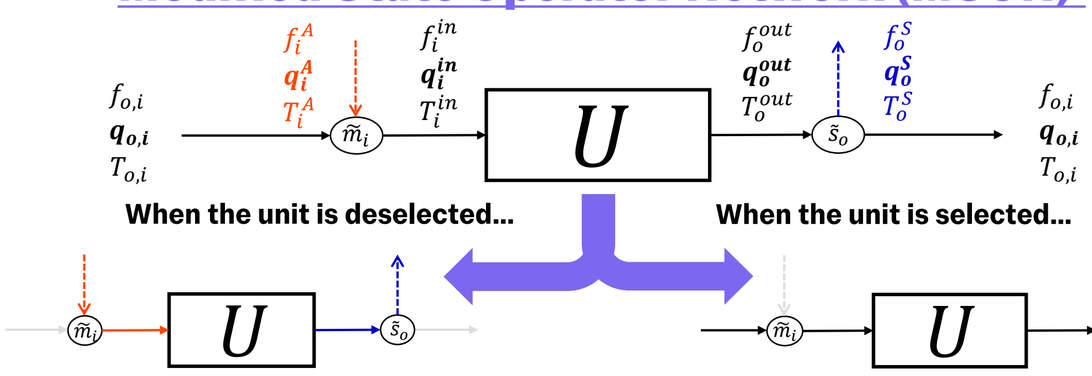
Why Pressure?

Important variable in many reaction and separation processes

Facilitate the modelling of membrane-based processes

Account for impacts of compression & expansion

Modified State Operator Network (MSON)[1]



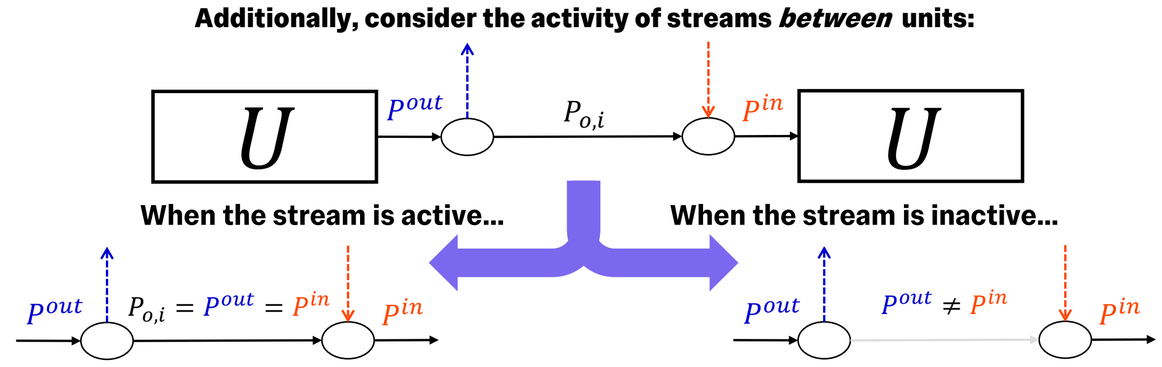
- Fictitious streams flow into units
- Ensures successful convergence to a meaningful solution

- Fictitious streams are disabled, and the unit participates in the flowsheet normally

Avoids numerical instability!

Extended MSON (E-MSON)

Additionally, consider the activity of streams *between* units:



- Inlet and outlet pressures are connected via $P_{o,i}$
- This occurs across multiple connections, ensuring correct flow directions

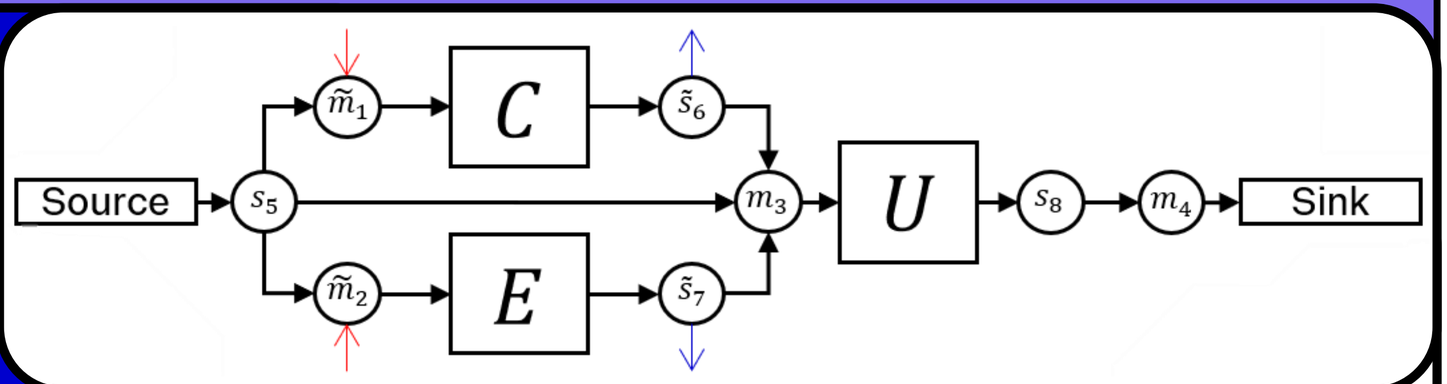
- Inlet and outlet pressures are disconnected and free to vary.

Removes isobaric assumption!

Test Problem Results

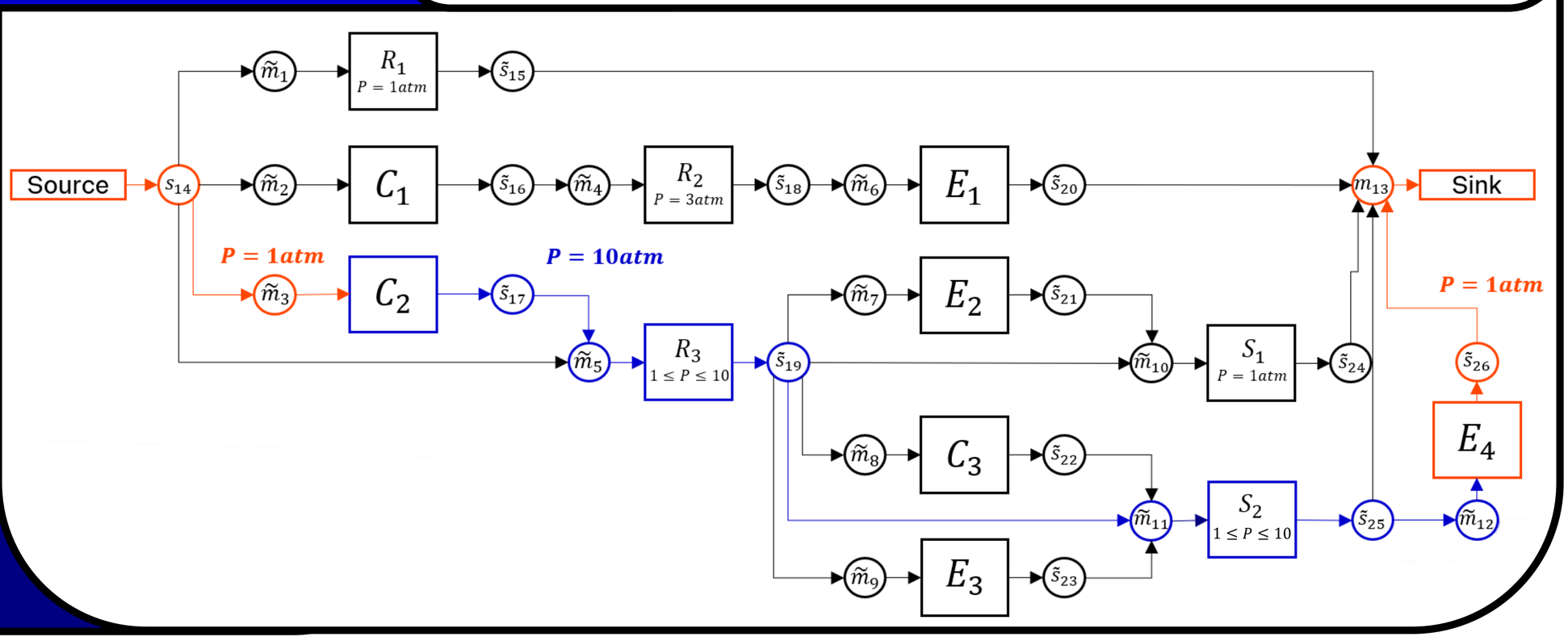
Toy Problem

- Successfully finds all 3 alternatives, with the compressor (C), expander (E), and bypass active, in < 0.4s.
- Shows the amenability of the E-MSON to non-isobaric problems, albeit for a simple case.



Reactor-Separator Synthesis Problem

- Obtained the top 10 solutions out of 27 possible alternatives.
- Successfully identified the optimal operating pressures of high-performing flowsheet **(highlighted)** and other alternatives.
  - Shows that considering a wider range of flowsheet alternatives does not significantly impede the formulation.



Outlook

Automated Problem Generation Tool

- An easy-to-use Python interface allowing the user to implement superstructure diagrams in gPROMS and automatically generate optimisation problems.
- Facilitates greater control over solver execution, allowing alternative algorithms to be used.

Pharmaceutical Applications

- Propose a superstructure with interconnected crystallisation work-up processes, including membrane-based and evaporative solvent swap, evaporative concentration, and liquid-liquid extraction.

Flowsheet and Molecular Design

- In addition to finding optimal process alternatives, integrating computer-aided molecular design techniques allows the interdependence of molecules on process performance to be considered

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1. *Gopinath, S.; Adjiman, C. S. Superstructure Optimization with Rigorous Models via an Exact Reformulation. Computers & Chemical Engineering 2024, 194, 108972. https://doi.org/10.1016/j.compchemeng.2024.108972.*