Single Shooting Method for Semicontinuous distillation design

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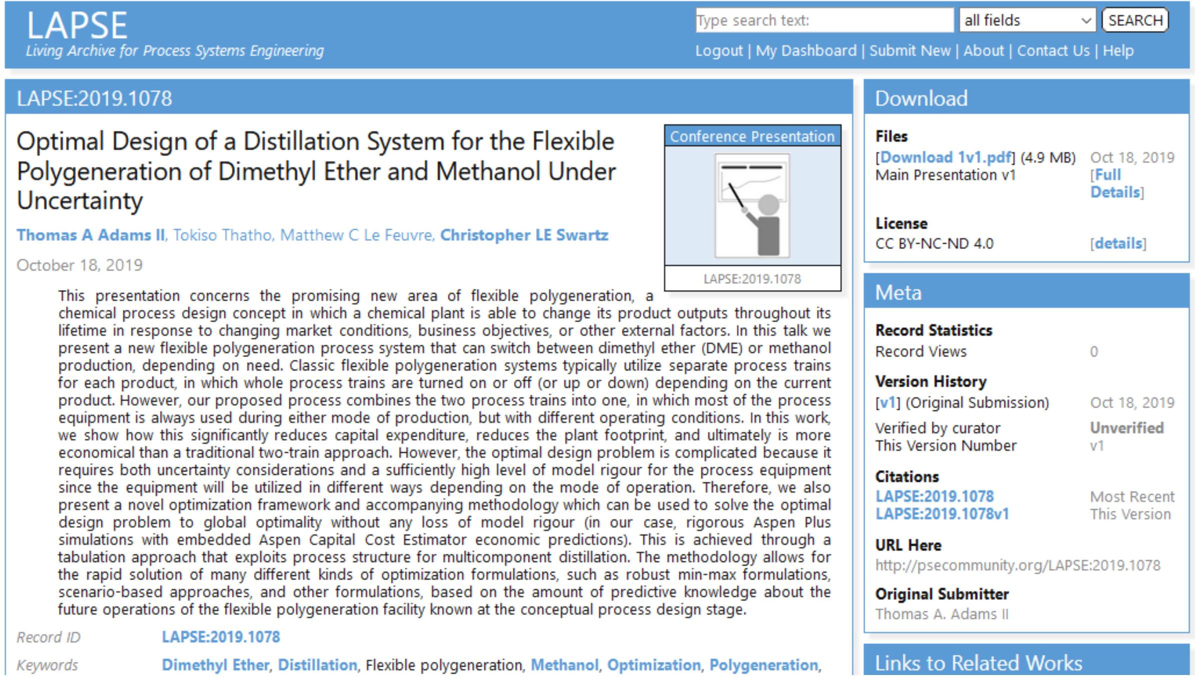

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Optimal Design of a Distillation System for the Flexible Polygeneration of Dimethyl Ether and Methanol Under Uncertainty

Thomas A Adams II, Tokiso Thatho, Matthew C Le Feuvre, **Christopher LE Swartz**

October 18, 2019

This presentation concerns the promising new area of flexible polygeneration, a chemical process design concept in which a chemical plant is able to change its product outputs throughout its lifetime in response to changing market conditions, business objectives, or other external factors. In this talk we present a new flexible polygeneration process system that can switch between dimethyl ether (DME) or methanol production, depending on need. Classic flexible polygeneration systems typically utilize separate process trains for each product, in which whole process trains are turned on or off (or up or down) depending on the current product. However, our proposed process combines the two process trains into one, in which most of the process equipment is always used during either mode of production, but with different operating conditions. In this work, we show how this significantly reduces capital expenditure, reduces the plant footprint, and ultimately is more economical than a traditional two-train approach. However, the optimal design problem is complicated because it requires both uncertainty considerations and a sufficiently high level of model rigour for the process equipment since the equipment will be utilized in different ways depending on the mode of operation. Therefore, we also present a novel optimization framework and accompanying methodology which can be used to solve the optimal design problem to global optimality without any loss of model rigour (in our case, rigorous Aspen Plus simulations with embedded Aspen Capital Cost Estimator economic predictions). This is achieved through a tabulation approach that exploits process structure for multicomponent distillation. The methodology allows for the rapid solution of many different kinds of optimization formulations, such as robust min-max formulations, scenario-based approaches, and other formulations, based on the amount of predictive knowledge about the future operations of the flexible polygeneration facility known at the conceptual process design stage.

Record ID **LAPSE:2019.1078**
Keywords **Dimethyl Ether**, **Distillation**, Flexible polygeneration, **Methanol**, **Optimization**, **Polygeneration**,

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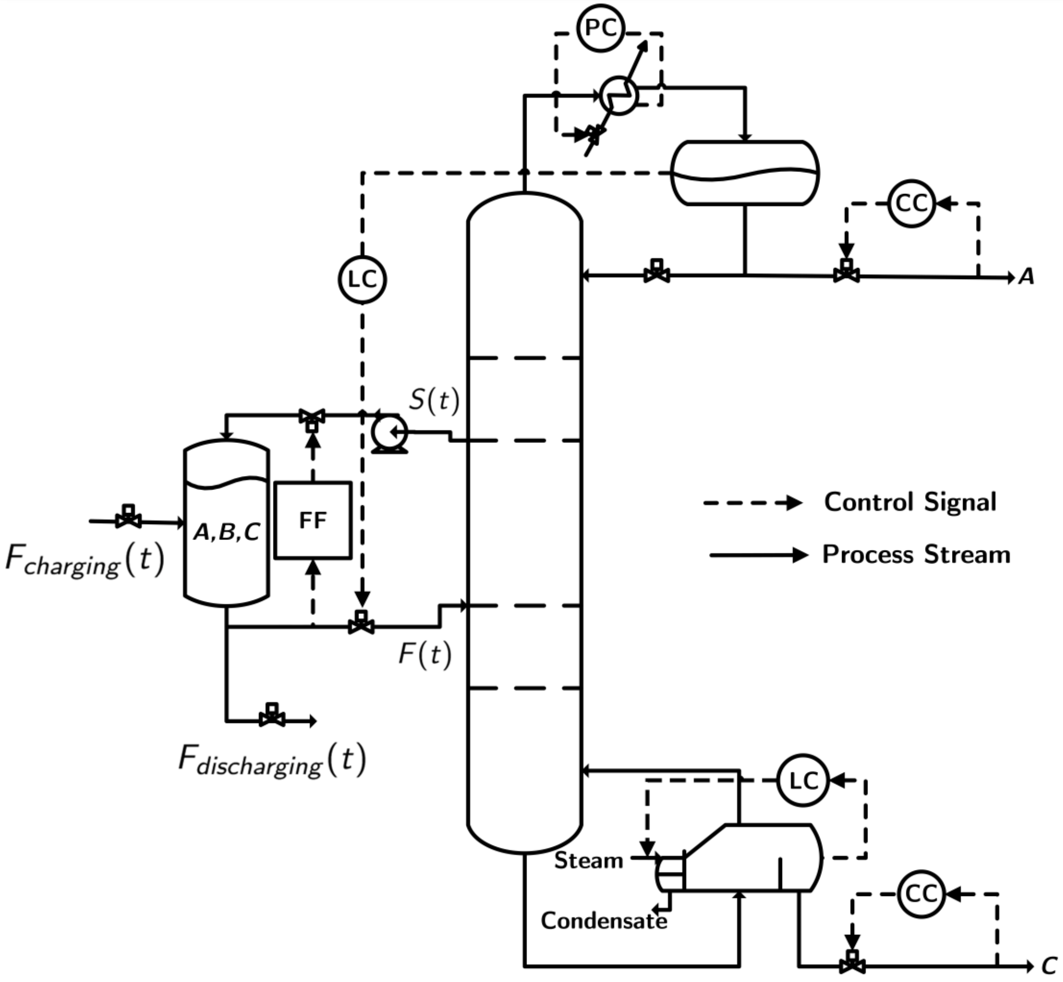
Semicontinuous Distillation Process



PC: Pressure controller | CC: Concentration controller | LC: Level Controller
FF: Feedforward control

Process Equipment:

- Process Vessel [Middle Vessel].
- Distillation column.

Control System:

- Pressure Control
- Distillate Concentration Control
- Bottoms Concentration Control
- Reflux Drum level Control
- Sump level Control
- Side stream flow control

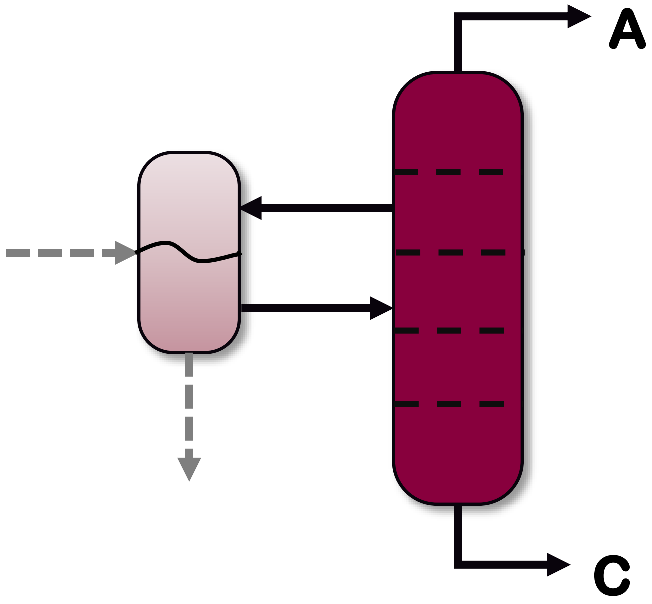
Characteristics of the process:

- Economic at intermediate production rates.
- Flexible operation and modular.

Adams, T.A. and Pascall, A., 2012. Semicontinuous thermal separation systems. *Chemical Engineering & Technology*, *35*(7), pp.1153-1170.

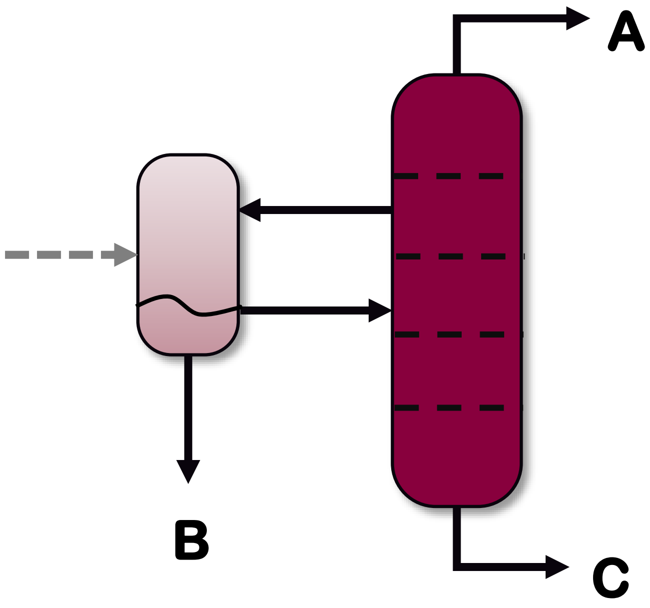
Semicontinuous Distillation Process

Separating Mode



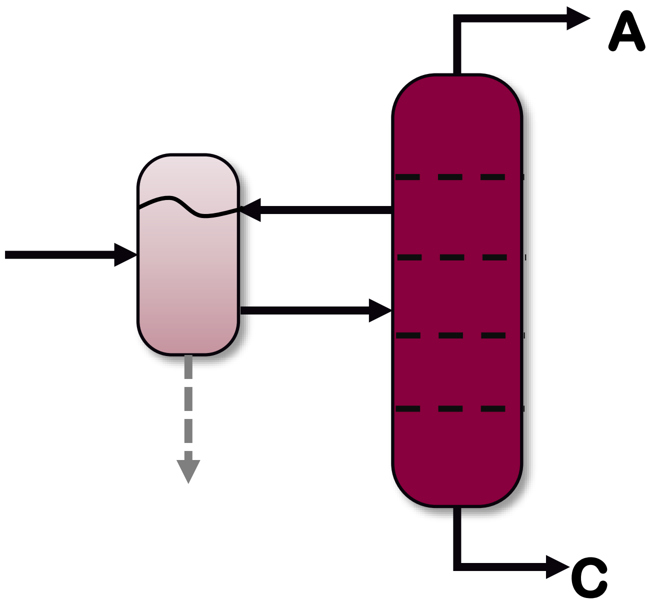
End when desired B product purity is met

Discharging Mode



End when liquid level falls below a limit

Charging Mode



End when liquid level is above a limit

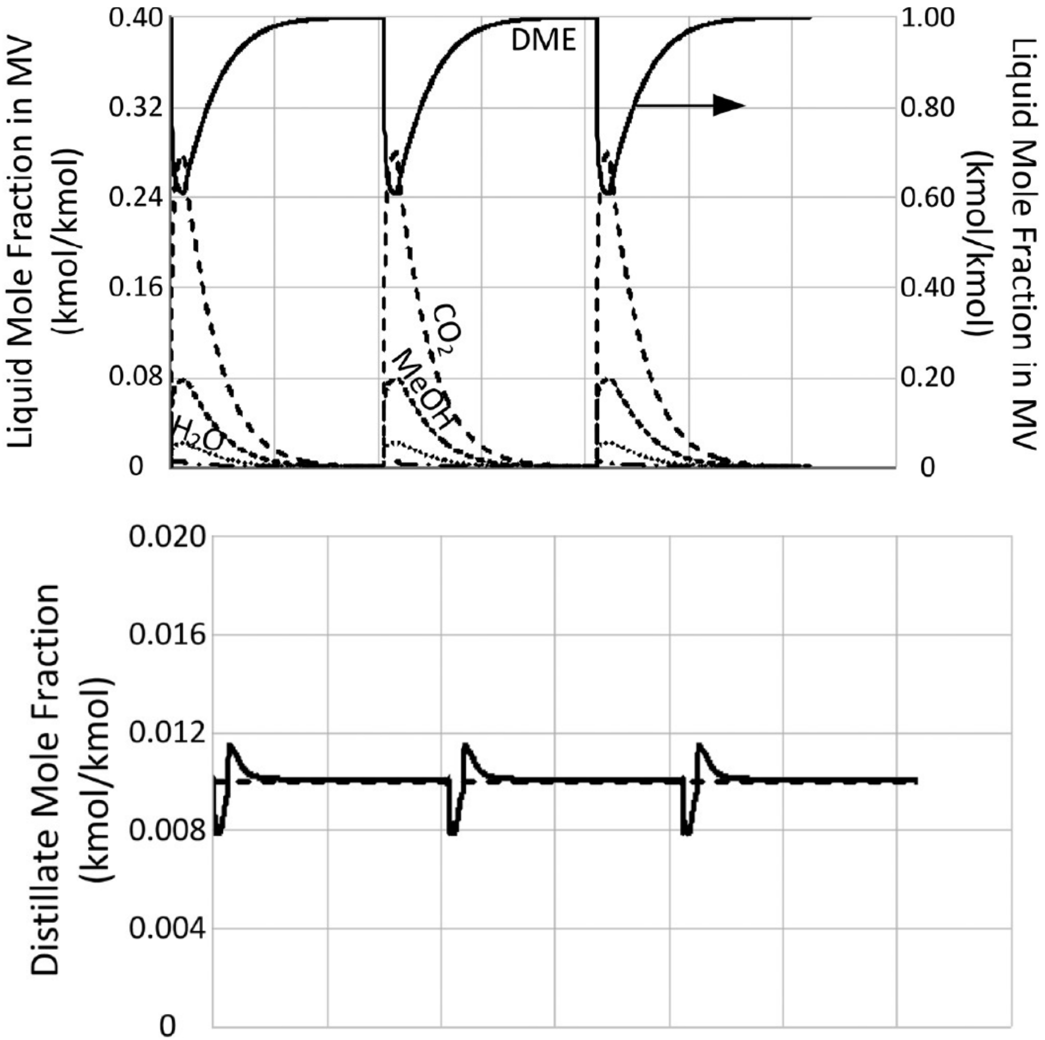
→ **Material Flow**

⇢ **No Material Flow**

Adams, T.A. and Pascall, A., 2012. Semicontinuous thermal separation systems. *Chemical Engineering & Technology*, *35*(7), pp.1153-1170.

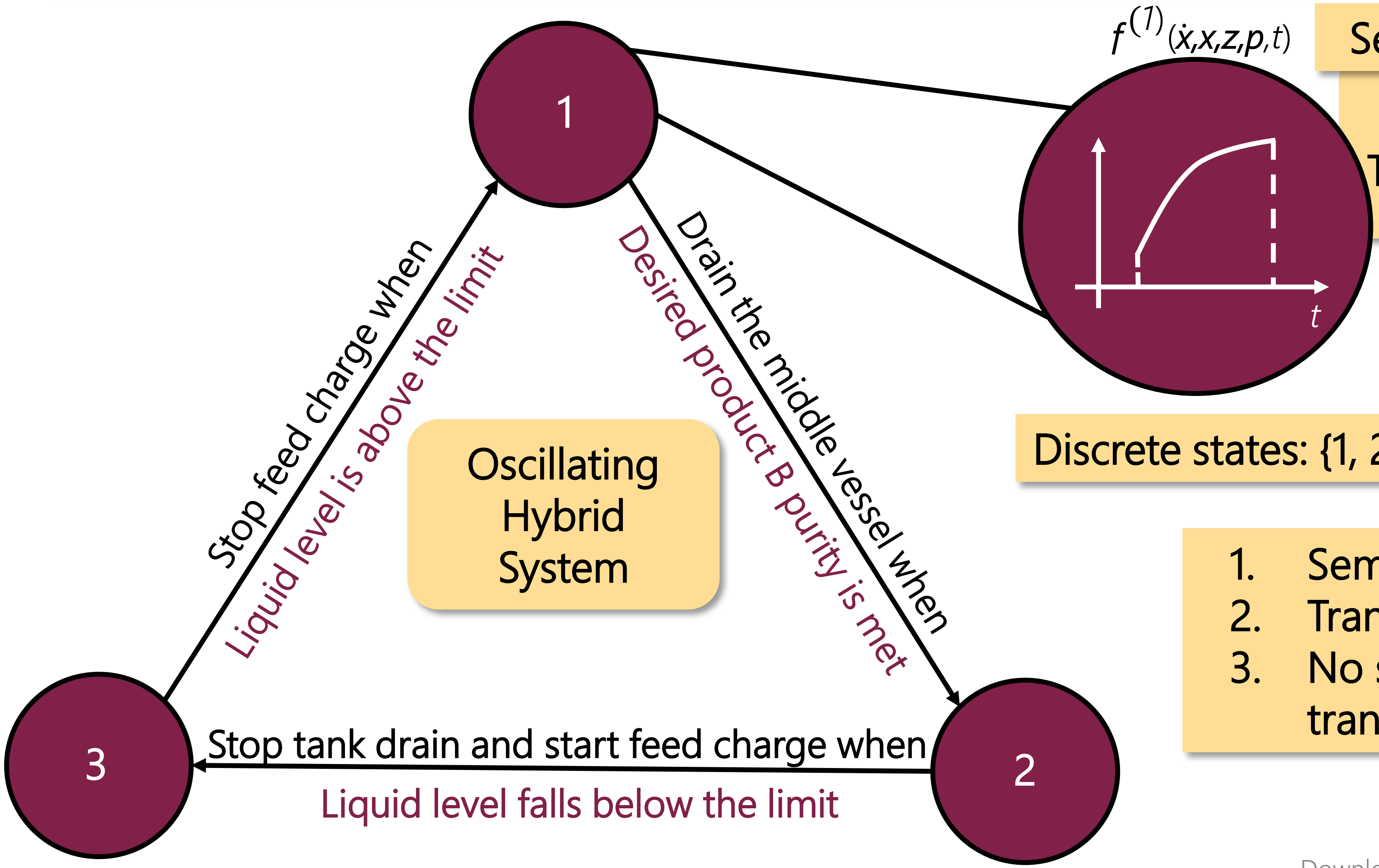
Example Trajectories

This is for:
- Dimethyl Ether
- CO2
- Methanol / Water



*Pascall, A. and Adams, T.A., 2013. Semicontinuous separation of dimethyl ether (DME) produced from biomass. *The Canadian Journal of Chemical Engineering*, *91*(6), pp.1001-1021..

Mathematical description of the process dynamics



$f^{(1)}(\dot{x},x,z,p,t)$

Drain the middle vessel when
Desired product B purity is met

Stop tank drain and start feed charge when
Liquid level falls below the limit

Stop feed charge when
Liquid level is above the limit

Oscillating Hybrid System

Semi-explicit DAEs

Continuous states: x, z
Time invariant parameters: p

Discrete states: {1, 2, 3}

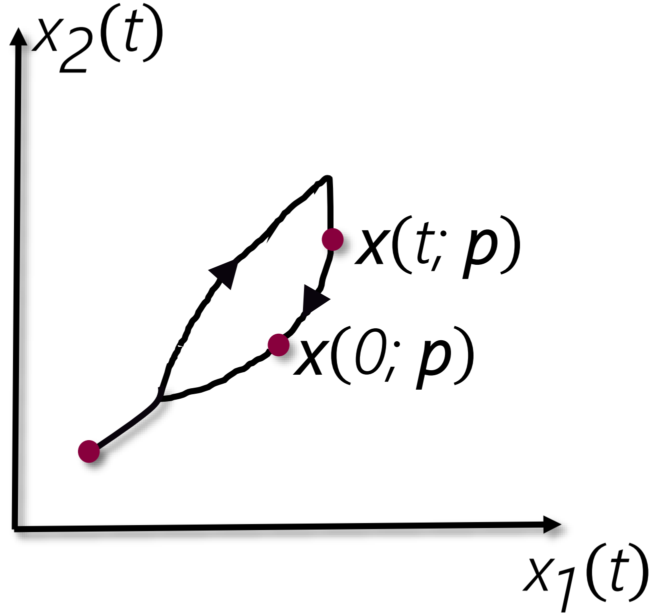
1. Semi-explicit DAE systems: 3
2. Transition Conditions: 3
3. No state variable jumps during transition.

Madabhushi, P.B., and Adams, T.A., 2019. Finding Better Limit Cycles of Semicontinuous Distillation. 1. Back Stepping Design Methodology *Ind. Eng. Chem. Res.* 2019, 58, 36 pp.16654-16666.

Semicontinuous Distillation Process Dynamics

System Characteristics:

1. The system operates in a *limit cycle*, which is its steady-state.
2. A limit cycle is a closed and isolated state trajectory that is uniquely determined by *p* (design variables).
3. The cycle has a period of oscillation *T*(*p*) (an implicit function of *p*).



$$\mathbf{x}(t) := \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix}$$

Madabhushi, P.B., and Adams, T.A., 2019. Finding Better Limit Cycles of Semicontinuous Distillation. 1. Back Stepping Design Methodology *Ind. Eng. Chem. Res.* 2019, 58, 36 pp.16654-16666.

Methods for finding limit cycle

Simple Method

Brute Force Method

i. Guaranteed convergence
ii. Speed of convergence is dependent on the system's parameters.
iii. Difficult to tell if a steady-state is reached.

Sophisticated Methods

Shooting Methods
Collocation Methods

i. Fast convergence.
ii. Can impose quantitative convergence criteria to terminate the algorithm.

Parker, T.S., and Chua, L.O., 1989. Locating Limit Sets. In: Practical Numerical Algorithms for Chaotic Systems. Springer, New York, NY.

Semicontinuous Distillation Process Design

Design Objective

"Meet product quality requirements at the end of the cycle, while maintaining feasible operation during the cycle"

Continuous Design Variables:

- Reflux rate.
- Side stream flowrate.
- Controller tuning parameters.

Discrete Design Variables:

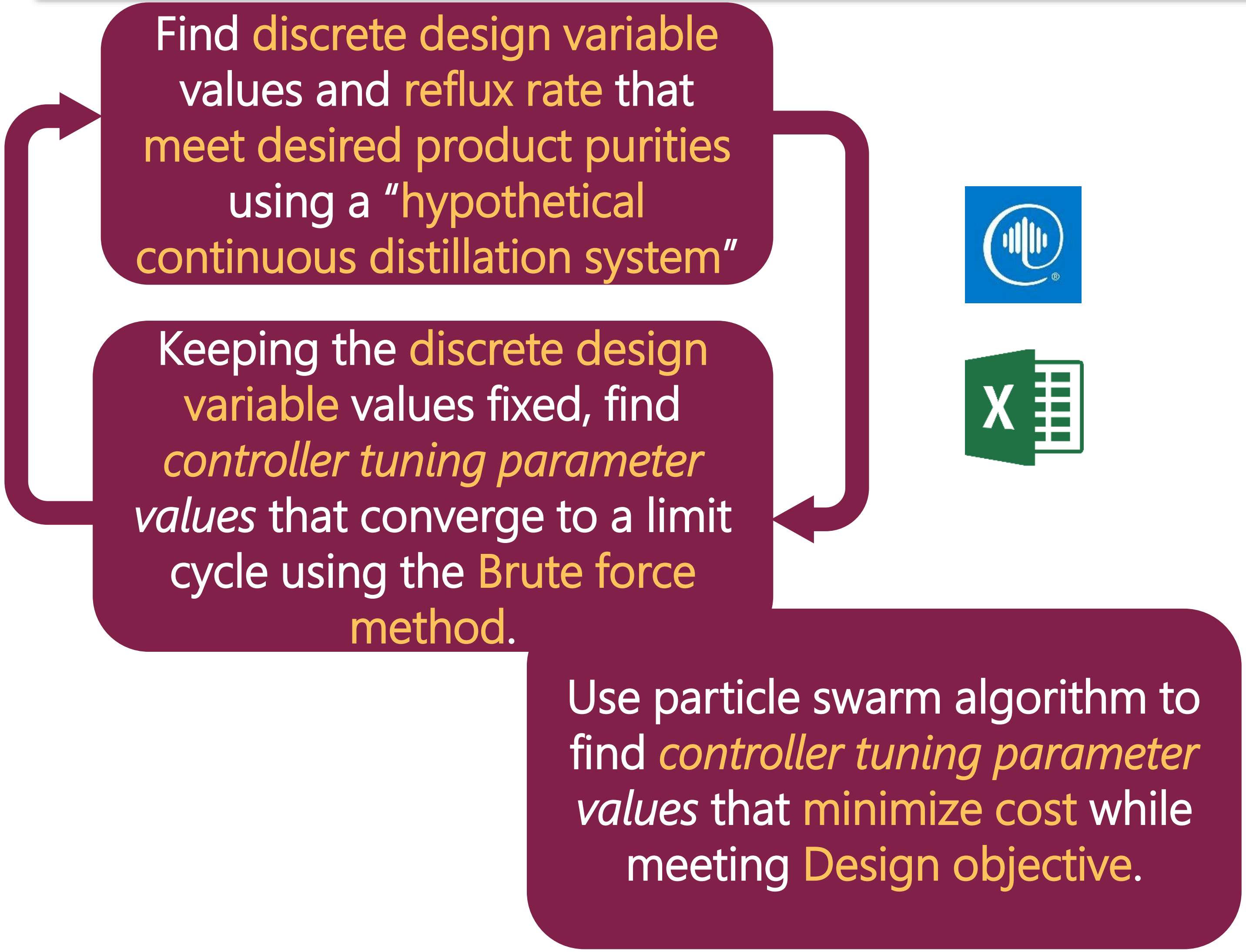
- Number of stages
- Feed stage location
- Side stream stage location
- Equipment sizes

What makes semicontinuous distillation design so complex?

1. The total processing time is unknown ($T(p)$).
2. Time spent in each mode is also unknown ($\Delta t^{(k)}(p)$).
3. The initial state of the system is also unknown ($x(0; p)$).

Adams, T.A. and Pascall, A., 2012. Semicontinuous thermal separation systems. *Chemical Engineering & Technology*, *35*(7), pp.1153-1170.

Sequential Design Methodology



Find discrete design variable values and reflux rate that meet desired product purities using a "hypothetical continuous distillation system"

Keeping the discrete design variable values fixed, find *controller tuning parameter values* that converge to a limit cycle using the Brute force method.

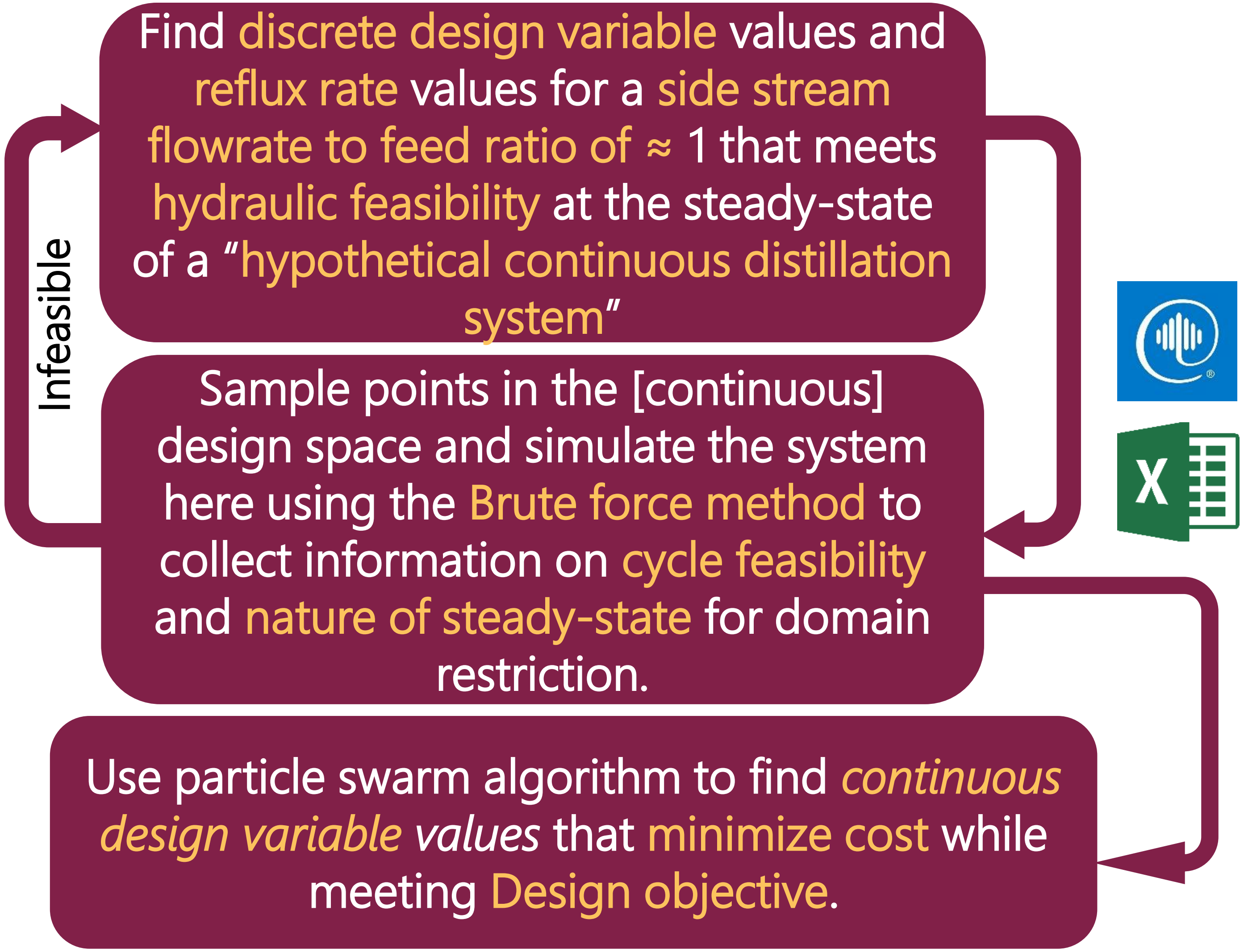
Use particle swarm algorithm to find *controller tuning parameter values* that minimize cost while meeting Design objective.

Disadvantages:

1. Used some state variables to visually ascertain convergence to a limit cycle.
2. Difficult to tell if a steady-state (limit cycle) is reached during optimization phase.
3. Could not exploit problem structure to use better optimization techniques.

Adams, T.A. and Pascall, A., 2012. Semicontinuous thermal separation systems. *Chemical Engineering & Technology*, *35*(7), pp.1153-1170.

Back-stepping Design Methodology



Find discrete design variable values and reflux rate values for a side stream flowrate to feed ratio of ≈ 1 that meets hydraulic feasibility at the steady-state of a "hypothetical continuous distillation system"

Sample points in the [continuous] design space and simulate the system here using the Brute force method to collect information on cycle feasibility and nature of steady-state for domain restriction.

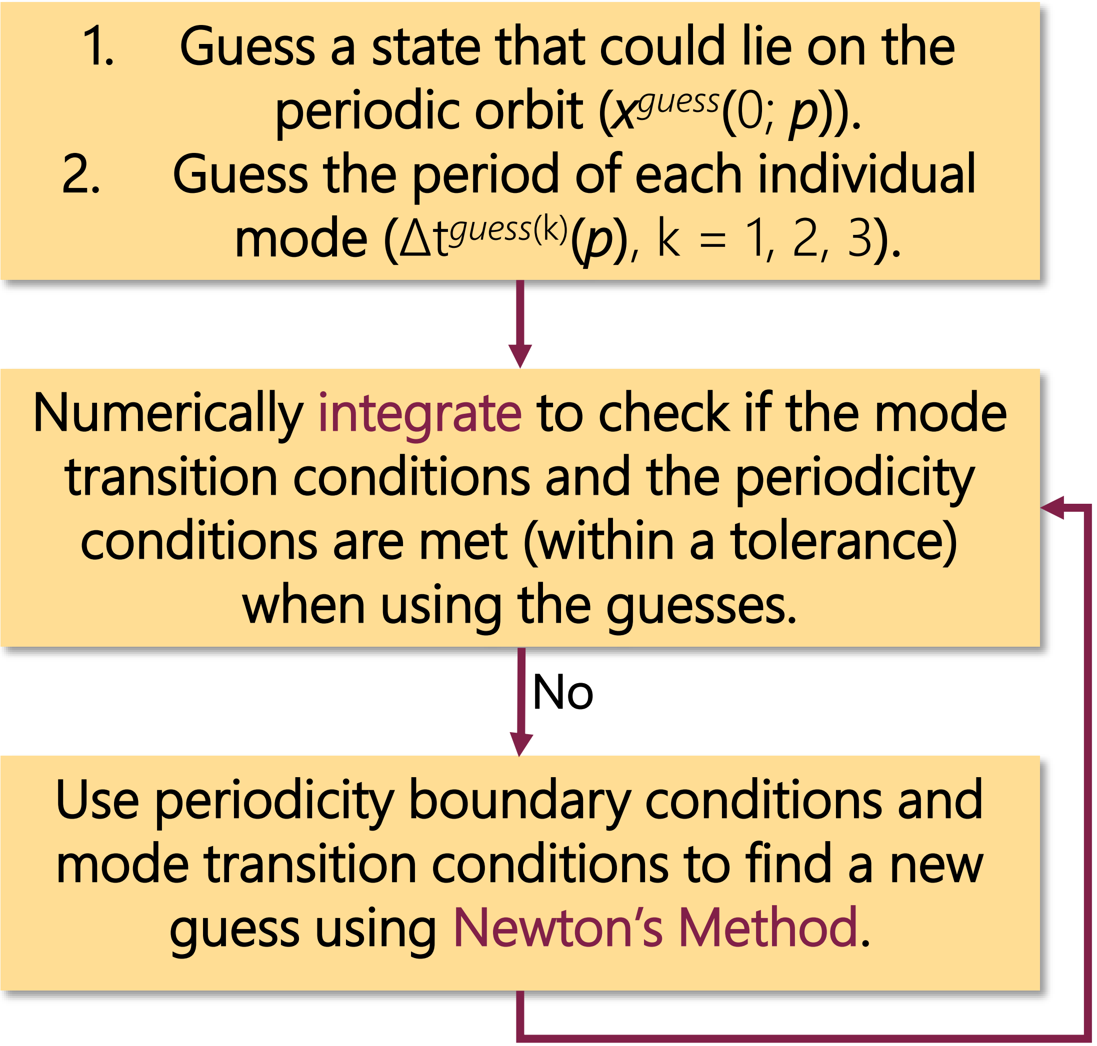
Use particle swarm algorithm to find *continuous design variable values* that minimize cost while meeting Design objective.

Disadvantages:

1. Use some state variables to visually ascertain convergence to a limit cycle.
2. Requires sampling of a number of points in the design space to ensure cycle feasibility and ascertain the nature of steady-state.
3. Could not exploit problem structure to use better optimization techniques.

Madabhushi, P.B., and Adams, T.A., 2019. Finding Better Limit Cycles of Semicontinuous Distillation. 1. Back Stepping Design Methodology *Ind. Eng. Chem. Res.* 2019, 58, 36 pp.16654-16666.
Madabhushi, P.B., and Adams, T.A., 2019. Finding Better Limit Cycles of Semicontinuous Distillation. 2. Extended Back Stepping Design Methodology *Ind. Eng. Chem. Res.* 2019, 58, 36 pp.16667-16675.

Algorithm for using the Single Shooting Method for semicontinuous distillation design



1. Guess a state that could lie on the periodic orbit ($x^{guess}(0; p)$).
2. Guess the period of each individual mode ($\Delta t^{guess(k)}(p)$, k = 1, 2, 3).

Numerically integrate to check if the mode transition conditions and the periodicity conditions are met (within a tolerance) when using the guesses.

Use periodicity boundary conditions and mode transition conditions to find a new guess using Newton's Method.

Repeat until desired tolerance is met

What is a good initial state?

Choose the state of previously described continuous distillation system as an initial guess. (Obtained by solving a system of nonlinear algebraic equations.)

How is time period of each mode guessed?

1. Use Newton's method to better estimate the time periods of individual modes.
2. Use these estimates as initial guess in the algorithm.

Some Implementation Details

1. Modeled semicontinuous distillation system in python using the CasADi modeling language.

   CasADi

2. *Distillation modeling details*: Fixed pressure drop, fixed top stage pressure, constant molar overflow, no vapour holdup, theoretical trays, perfect mixing on trays, total condensation without sub-cooling, adiabatic operation, partial reboiler.

3. Differential Equations were reformulated to add a dummy time state variable to fix the integration horizon to $t \in [0 \quad 1]$.

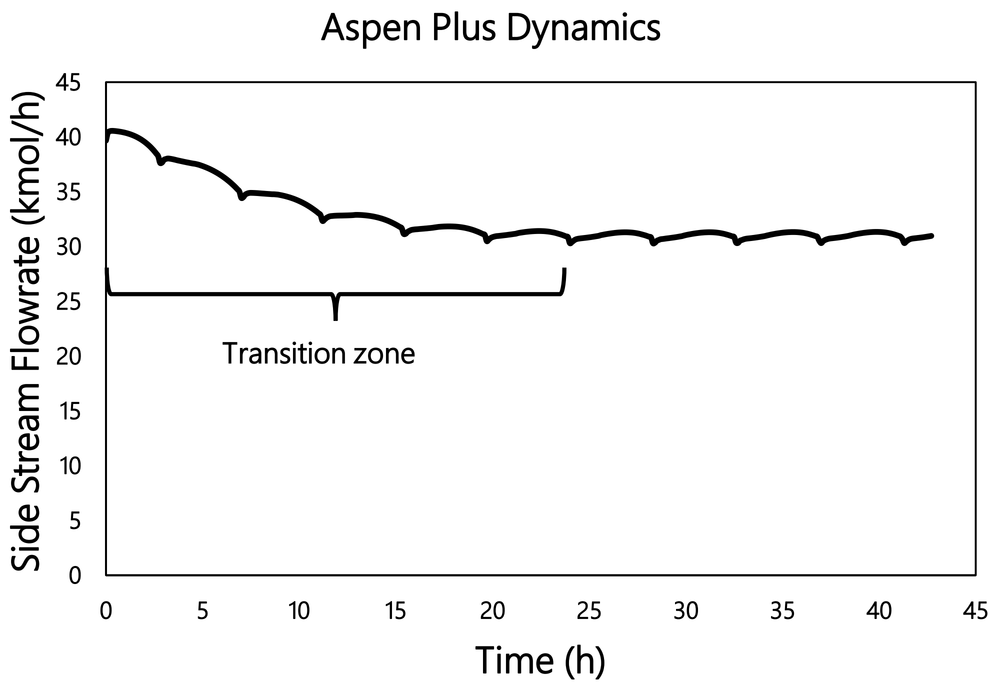
4. Periodicity constraints ($x(t) - x(t+T) = 0$) were imposed on the differential state variables and not on the algebraic state variables for well-posedness (avoiding over specification).

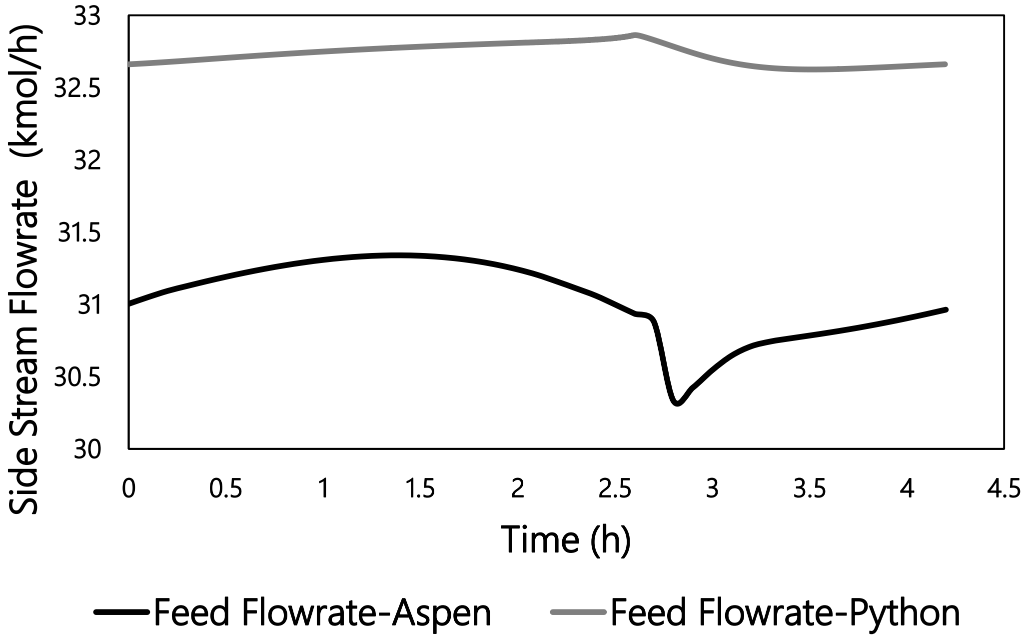
IDAS sundials

IPOPT (COIN-OR)

Case study – Hexane, Heptane, Octane

1. *Total number of stages* : 5, *Side stream stage*: 2, *Feed Stage*: 3 [24 differential variables; 39 algebraic variables];
2. Max error in residual: less than 0.0005; Same design variable values.
3. *Assumptions*: ideal vapour and solution.





Case study – Hexane, Heptane, Octane

$$\min_{x} \quad Cycle\,Time$$

$$x = continuous\ decision\ variables$$

$$s.t.$$

$$Boundary\,Value\,Problem$$

$$Distillation\,Model\,Equations$$

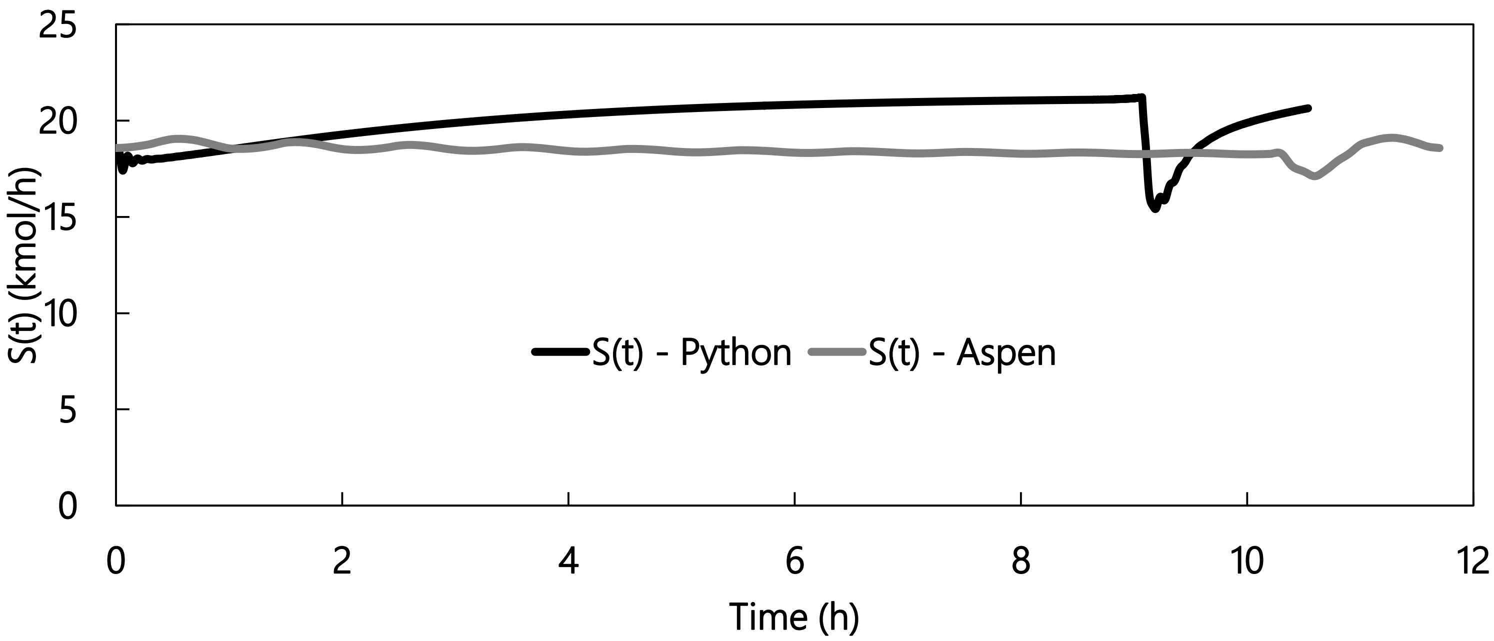
Started from poor initial guess.

Solution time: 40 minutes in CasADi

Optimal found to be close to previously known best from other methods (PSO, by hand, etc.)

Case study – Hexane, Heptane, Octane

1. *Total number of stages* : 40, *Side stream stage*: 14, *Feed Stage*: 25 [129 differential variables; 319 algebraic variables]
2. *Assumptions*: ideal vapour and solution.
3. Max error in residual: less than 0.0005



(*takes approx. 40 wall clock min vs. approx. 1 wall clock day to find a cycle*)

Conclusions and Future work

1. The new design methodology is an automatic way of directly finding the cycle for chosen values of the design variables.
2. A quantitative termination criteria is available.
3. Explore the influence of various design variables on the limit cycle characteristics (such as cycle time).
4. Explore the use of gradient-based optimization techniques for design optimization.

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