Integrated Scheduling and Dynamic Optimization of Batch Processes

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Presentation Outline

- Introduction
- Motivating example
- Integrated formulation
- Case study
- Conclusions

Introduction

Batch chemical process

Long History

Before the Industry Revolution

Wide Practice

Pharmaceutical industry
Specialty chemicals
Polymer processes

Complex Characterization

Flexible unit connection
Inherent time-varying dynamics

Process Scheduling

Time Representation

Discrete-time
Continuous-time

Process Sequencing

Operational philosophies
Changeovers
Order fullfillment

Resource Handling

Materials
Equipment
Operators

Operations Optimization

Dynamic Modeling

Data-driven model
First-principle model

Problem Formulation

Direct formulation
Pontryagin's Maximum Principle
Hamiltonian-Jacobi-Bellman optimality

Numerical Solution

Control Vector Parametrization
Simultaneous methods

These two problems are nested in nature
An integrated decision-making approach merits attention

Introduction

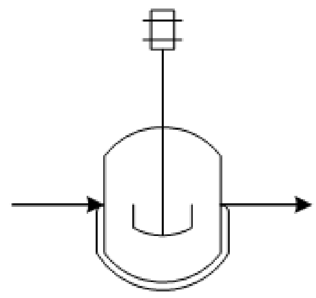
How do we model dynamics?

$A \xrightarrow{k_1} B \xrightarrow{k_2} C$

First-principle model

Reaction kinetics

Mass balance



Differential Algebraic Equations

$$\frac{dc_A(t)}{dt} = -u(t)c_A^2(t)$$

$$\frac{dc_B(t)}{dt} = -\frac{dc_A(t)}{dt} - \frac{dc_C(t)}{dt}$$

$$\frac{dc_C(t)}{dt} = \beta u^2(t)c_B(t)$$

- *Energy cost* $$F = b \cdot C_p \int_0^{t_f} u(t)dt$$
- *Material production* $$R_i^p = b \cdot c_i(t_f) \qquad i = B, C$$
- *Material consumption* $$R_A^c = b \cdot c_A(0)$$
- *Material purity* $$\phi = c_B(t_f)$$

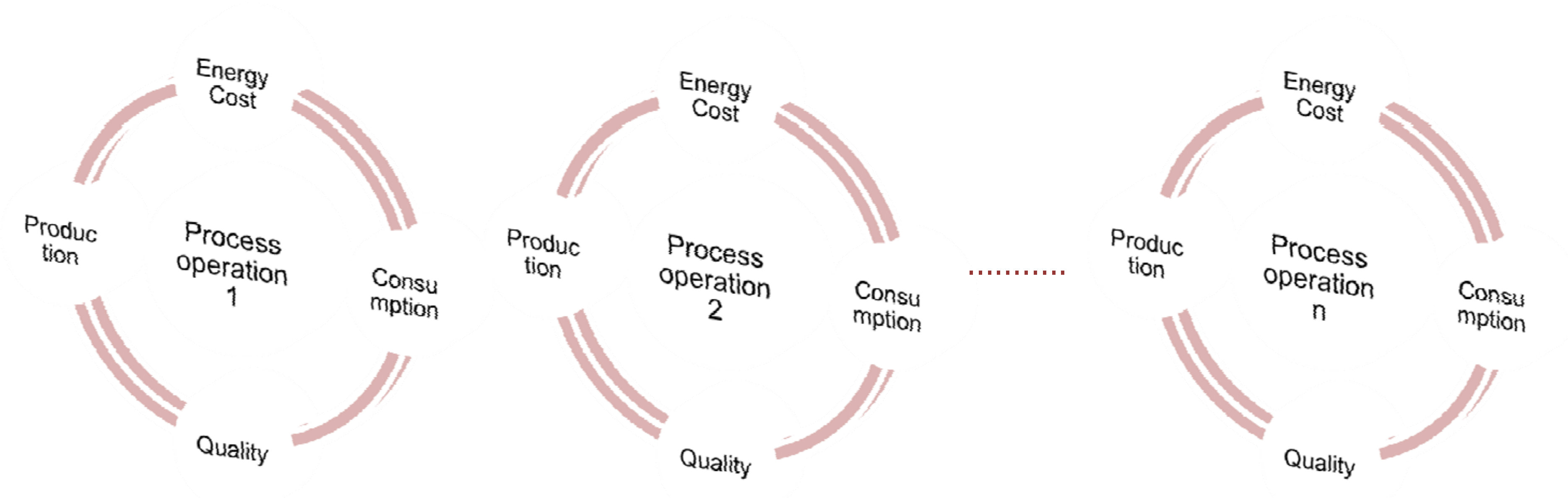
Variables

b	batch size
c	constituent concentration
u	scaled temperature
t	time
t_f	terminal time
C_P	unit energy price
β	model parameter

Introduction

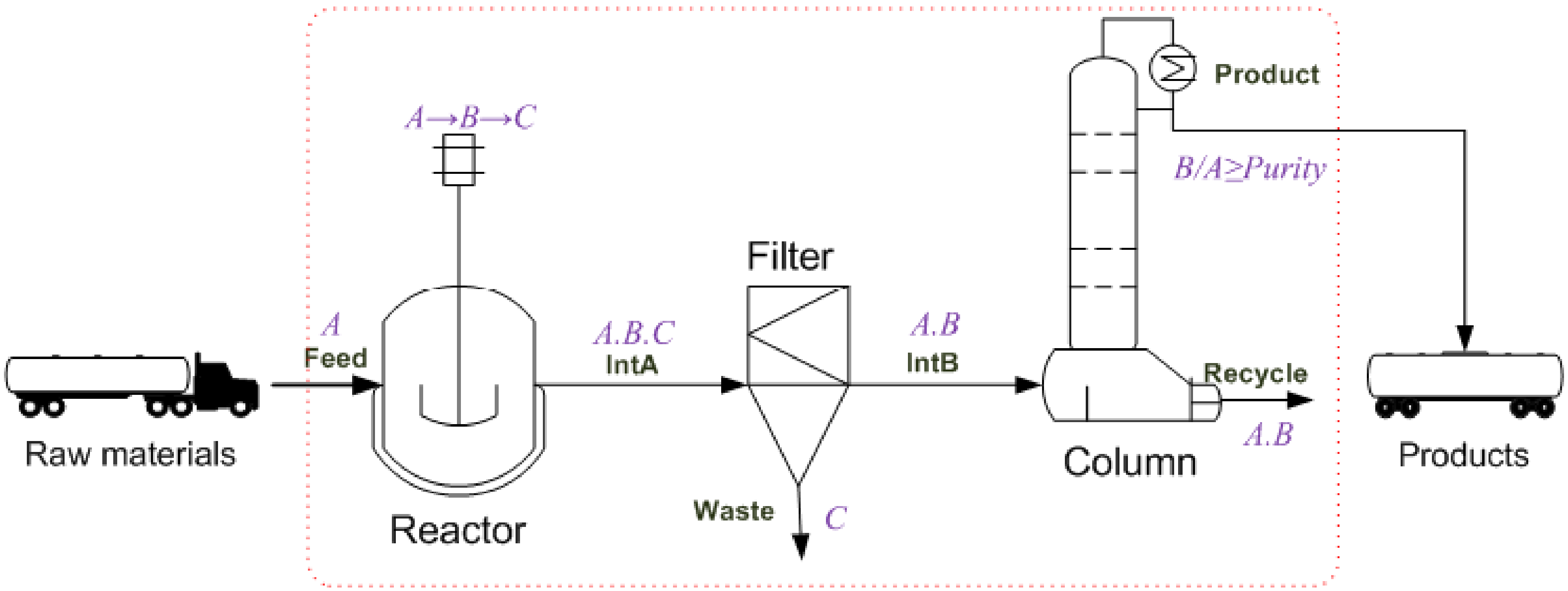
What advantages do dynamic optimization offer?

- Improvement on economic performance of individual operations
- A door to optimal production schedule of overall process



Trade-offs in an operation *Trade-offs between a group of operations*

Motivating Example

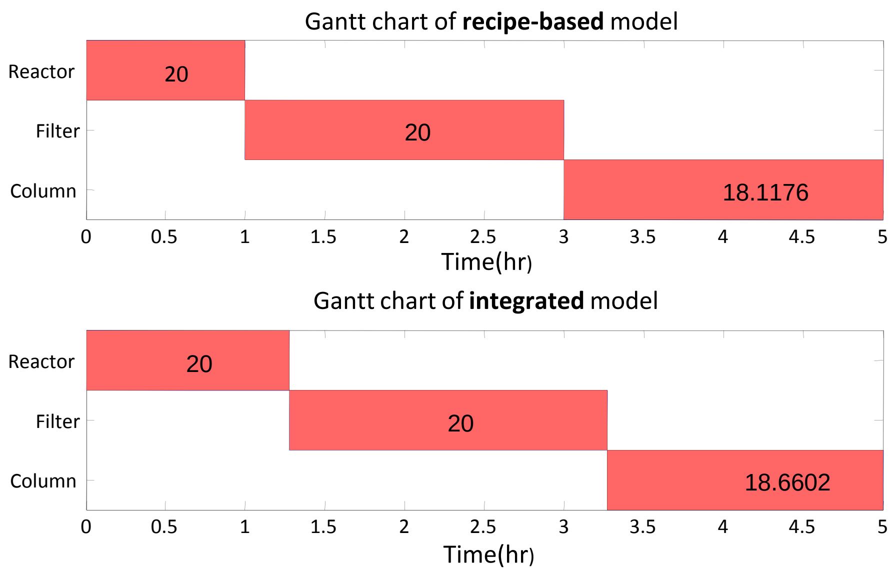


Flowsheet of a typical batch process

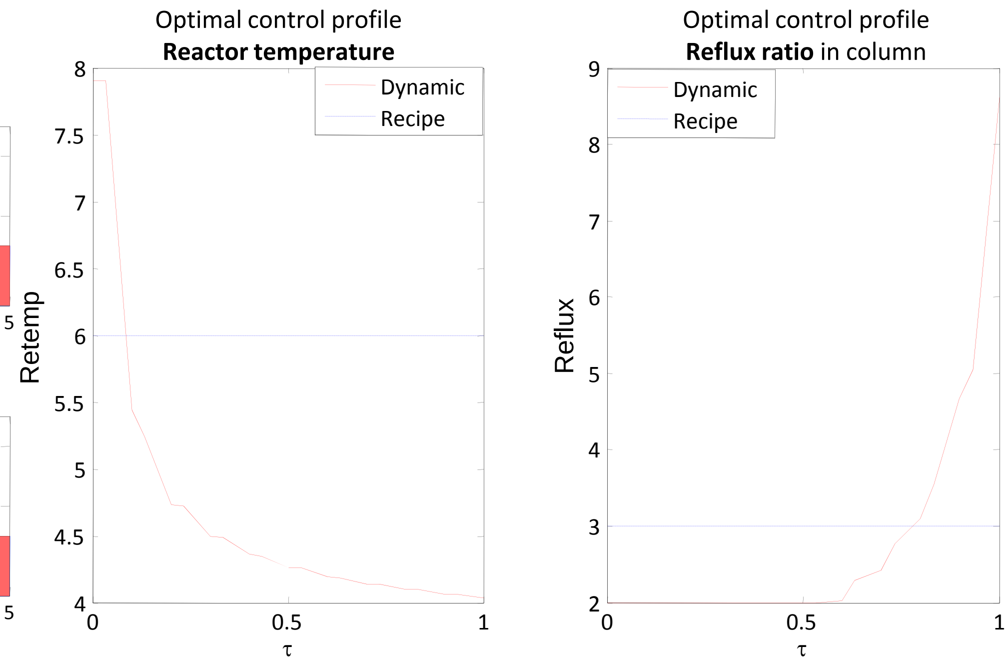
Recipe

1) React feed material in the batch reactor for 1 hour at constant temperature 385 K
2) Remove the waste component generated by side reaction in the filter for 2 hours
3) Purify the intermediate in the distillation column for 2 hours with reflux ratio = 3

Motivating Example



Gantt charts



Optimal control profiles

Example	Profit	$F_{reactor}$	F_{filter}	F_{column}	Prod.	Feed cons.	Purity
Recipe-based	871	180	220	236	15.0	20	0.98
Integrated	983	178	213	212	15.5	20	0.98

Scheduling Formulation

Network-based representation of batch processes

- State Task Network (STN) (E. Kondili et al. 93)

State	Feed,intermediate and final products
Task	Processing operations which transform one or more input states to one or more output states

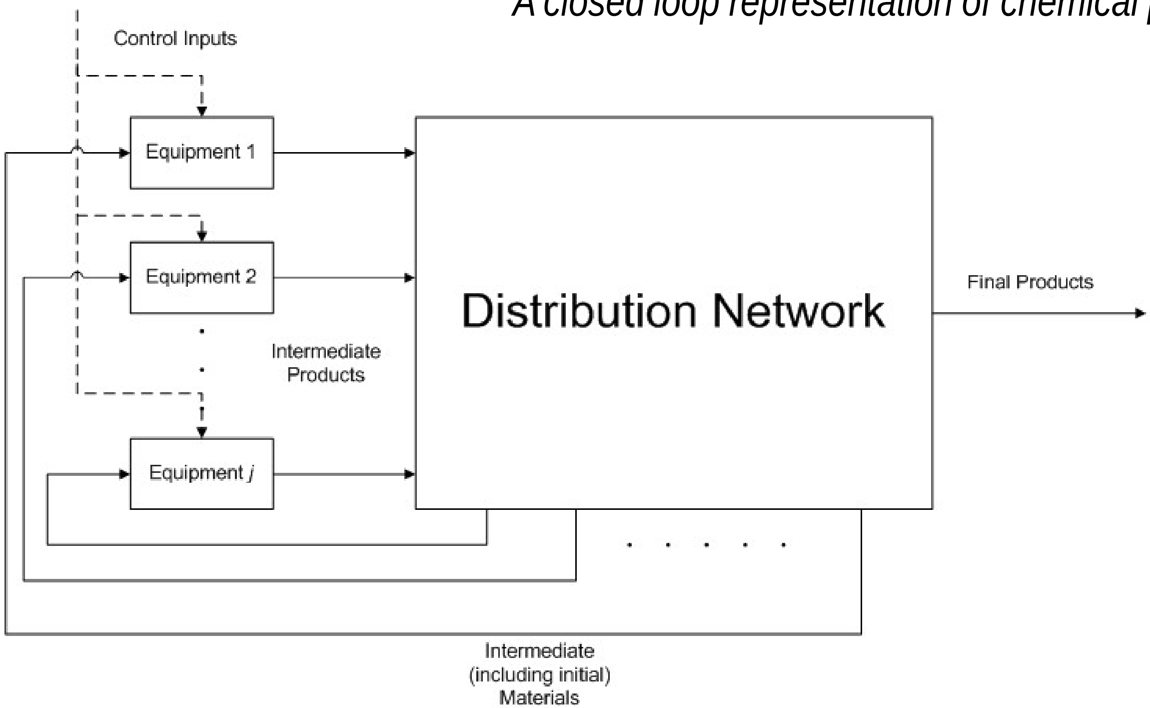
- Resource Task Network (RTN) (C.C. Pantelides 94)

Resource	Materials, energy and equipment
Task	Processing steps, cleaning, transportation and other operations

Is there an alternative perspective?

Scheduling Formulation

A closed loop representation of chemical processes



Similar ideas in process synthesis

State Space approach
V. Manousiothakis 92

State Equipment Network
E.M. Smith 96

Material	Feed,intermediate and final products
Equipment	Process units executing process operations under control inputs
Operating state	Specific unit operations

Scheduling Formulation

Mathematical formulation

Unit-specific continuous time representation

- Assignment constraints

$$\sum_{s \in \mathcal{S}_j} w_{j,s,n} \leqslant 1 \qquad \forall j \in \mathcal{J}, n \in \mathcal{N}$$

- Material balance

$$\overbrace{E_{r,n}}^{\text{matl. at } n} = \overbrace{E_{r,n-1}}^{\text{matl. at } n-1} + \overbrace{\sum_{j \in \mathcal{J}_r^p} R^p_{j,r,n-1}}^{\text{production}} + \overbrace{\sum_{j \in \mathcal{J}_r^c} R^c_{j,r,n}}^{\text{consumption}} \qquad \forall r \in \mathcal{R}, n \in \mathcal{N}$$

- Capacity constraints

$$\sum_{s \in \mathcal{S}_j} w_{j,s,n} B_j^{min} \leqslant b_{j,n} \leqslant \sum_{s \in \mathcal{S}_j} w_{j,s,n} B_j^{max} \qquad \forall j \in \mathcal{J}, n \in \mathcal{N}$$

$$E_r^{min} \leqslant E_{r,n} \leqslant E_r^{max} \qquad \forall r \in \mathcal{R}, n \in \mathcal{N}$$

Indices	Sets	
j	$\mathcal{J}$	equipment
s	$\mathcal{S}$	operating states
r	$\mathcal{R}$	materials
n	$\mathcal{N}$	event points

Variables

w	task assigning
E	excess material
b	batch size
R^p	material production
R^c	material consumption

Scheduling Formulation

- Sequencing constraints

Operations in the same unit

$$T_{j,n+1} \geqslant T_{j,n} + Tp_{j,n} \qquad \forall j \in \mathcal{J}, n \in \mathcal{N}$$

Operations in different units

$$\overbrace{T_{j',n'}}^{\text{downstream start}} \geqslant \overbrace{T_{j,n} + Tp_{j,n}}^{\text{upstream end}} - H\Big(2 - \overbrace{\sum_{s \in \mathcal{S}_j, \mathcal{S}_r^p} w_{j,s,n}}^{r \text{ produced}} - \overbrace{\sum_{s' \in \mathcal{S}_{j'}, \mathcal{S}_r^c} w_{j',s',n'}}^{r \text{ consumed}}\Big)$$

$$\forall r \in \mathcal{R}, j \in \mathcal{J}_r^p, j' \in \mathcal{J}_r^c, j \neq j', n, n' \in \mathcal{N}, n < n' \leqslant N$$

- Material quality measurement

Mixture composition

$$\eta_{r,c,n} = \overbrace{\Big(E_{r,n-1} \cdot \eta_{r,c,n-1} + \sum_{j \in \mathcal{J}_r^p} R_{j,r,n-1}^p \cdot \phi_{j,r,c,n-1}\Big)}^{\text{amount of componment } c} \Big/ \overbrace{\Big(E_{r,n-1} + \sum_{j \in \mathcal{J}_r^p} R_{j,r,n-1}^p\Big)}^{\text{amount of material } r} \qquad \forall r \in \mathcal{R}, c \in \mathcal{C}_r, n \in \mathcal{N}$$

Purity requirements

$$\mathcal{H}(\eta_{r,c,n}, \overline{\eta}_{r,c,n}) \geqslant 0 \qquad \forall r \in \mathcal{R}, c \in \mathcal{C}_r, n \in \mathcal{N}$$

Supersripts

p	prodction
c	consumption

Indices	Sets	
j	$\mathcal{J}$	equipment
s	$\mathcal{S}$	operating states
c	$\mathcal{C}$	components
r	$\mathcal{R}$	materials
n	$\mathcal{N}$	event points

Variables

w	task assigning
T	beginning time
Tp	processing time
H	scheduling horizon
η	inventory concentration
ϕ	product concentration

Scheduling Formulation

- Unit operation

Operating state

Idle state

Dynamic model

...

Initial condition

Production

Consumption

Quality

Operating cost

$$\begin{bmatrix} Y_{j,s,n} \\ \frac{dz_{j,n}(\tau)}{d\tau} = f_{j,s}(z_{j,n}(\tau), y_{j,n}(\tau), u_{j,n}(\tau)) Tp_{j,n} \\ g_{j,s}(z_{j,n}(\tau), y_{j,n}(\tau), u_{j,n}(\tau)) = 0 \\ z_{j,s}^{min} \leqslant z_{j,n}(\tau) \leqslant z_{j,s}^{max} \\ y_{j,s}^{min} \leqslant y_{j,n}(\tau) \leqslant y_{j,s}^{max} \\ u_{j,s}^{min} \leqslant u_{j,n}(\tau) \leqslant u_{j,s}^{max} \\ z_{j,n}(0) = \mathcal{Z}(b_{j,n}, \eta_{r,c,n}, w_{j,s,n}) \\ R_{j,r,n}^{p} = \mathcal{R}^{p}(z_{j,n}(\tau), y_{j,n}(\tau), w_{j,s,n}) \\ R_{j,r,n}^{c} = \mathcal{R}^{c}(z_{j,n}(\tau), y_{j,n}(\tau), w_{j,s,n}) \\ \phi_{j,r,c,n} = \phi(z_{j,n}(\tau), y_{j,n}(\tau), w_{j,s,n}) \\ F_{j,n} = \mathcal{F}(u_{j,n}(\tau), Tp_{j,n}, b_{j,n}, w_{j,s,n}) \\ w_{j,s,n} = 1 \end{bmatrix}_{s \in \mathcal{S}_j} \cdots \bigvee \begin{bmatrix} \neg \bigcup_{s \in \mathcal{S}_j} Y_{j,s,n} \\ R_{j,r,n}^{p} = 0 \\ R_{j,r,n}^{c} = 0 \\ Tp_{j,n} = 0 \\ F_{j,n} = 0 \\ \sum_{s \in \mathcal{S}_j} w_{j,s,n} = 0 \end{bmatrix} \quad \forall j \in \mathcal{J}, n \in \mathcal{N}$$

z	differential state variable
y	algebraic state variable
u	control variable
τ	normalized time

Scheduling Formulation

- Overall formulation

Mixed-Logic Dynamic Optimization (MLDO)

$$\max \quad \overbrace{\sum_{r\in\mathcal{R}} P_r\left(E_{r,N} + \sum_{j\in\mathcal{J}_r^p} R^p_{j,r,N}\right)}^{\text{Product sales}} - \overbrace{\sum_{r\in\mathcal{R}} P_r E_{r,0}}^{\text{Material costs}} - \overbrace{\sum_{n\in\mathcal{N}}\sum_{j\in\mathcal{J}} F_{j,n}}^{\text{Operating costs}}$$

$s.t.$
Assignment constraints
Material balance
Capacity constraints
Sequencing constraints
Material quality
Unit operation

- Reformulation strategy

Mixed-Integer Nonlinear Program (MINLP)

Simultaneous collocation

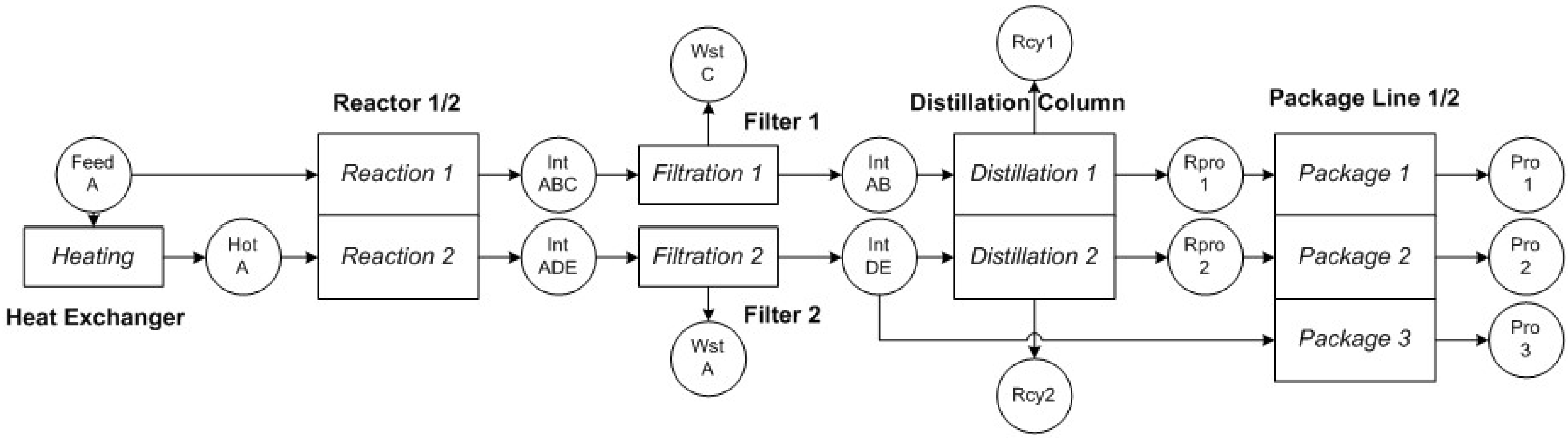
DAE ⟶ Nonlinear algebraic equations

Big-M reformulation

Disjunctions ⟶ Relaxed inequalities

Case Study

A state equipment representation of a multiproduct batch process



Product recipes

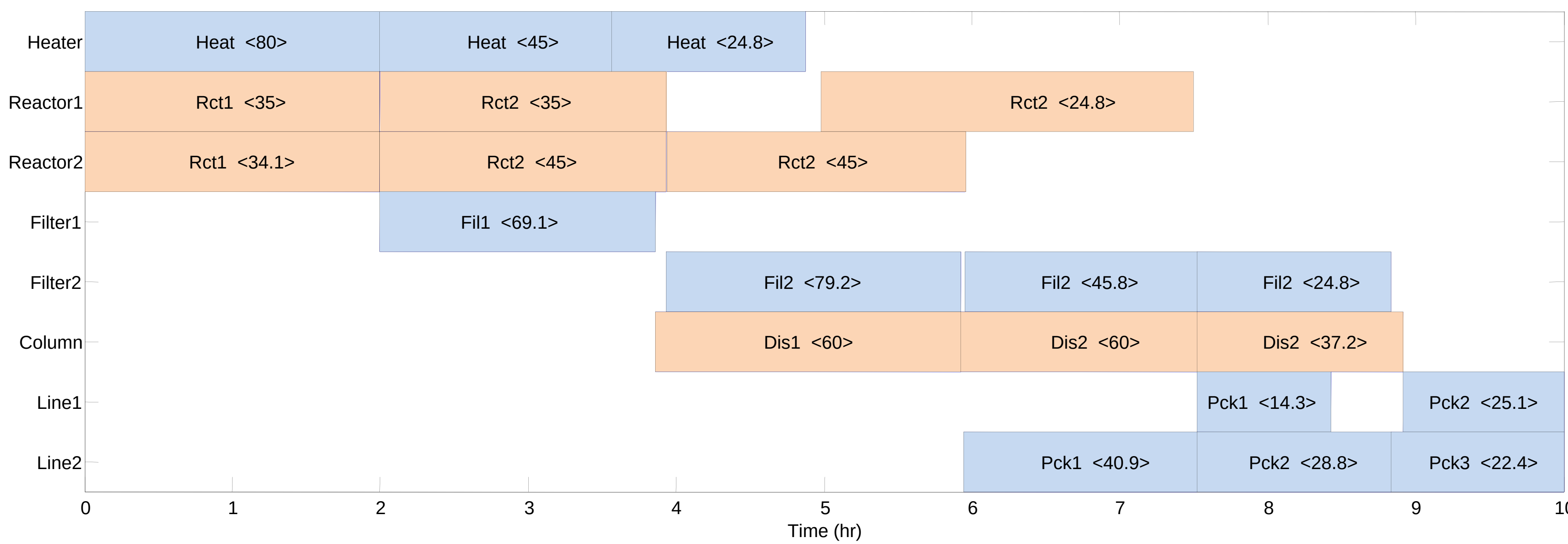
$$FeedA \xrightarrow{Reaction1} IntABC \xrightarrow[\dashrightarrow WasteC]{Filtration1} IntAB \xrightarrow[\dashrightarrow Recycle1]{Distillation} Rpro1 \xrightarrow{Package1} Product1$$

$$FeedA \xrightarrow{Heating} HotA \xrightarrow{Reaction2} IntADE \xrightarrow[\dashrightarrow WasteA]{Filtration2} IntDE \xrightarrow[\dashrightarrow Recycle2]{Distillation2} Rpro2 \xrightarrow{Package2} Product2$$

$$FeedA \xrightarrow{Heating} HotA \xrightarrow{Reaction2} IntADE \xrightarrow[\dashrightarrow WasteA]{Filtration2} IntDE \xrightarrow{Package3} Product3$$

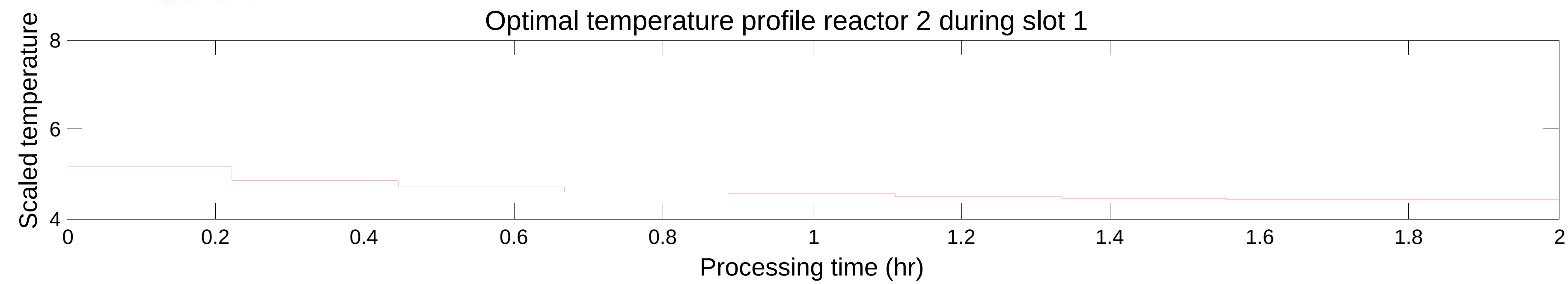
Case Study

Gantt-chart for the case study

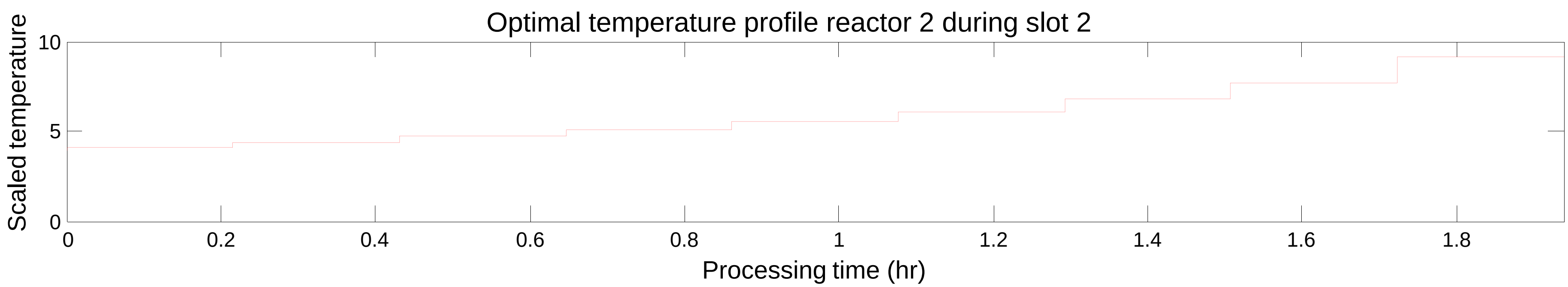


Time horizon	10 hrs
Event points	6

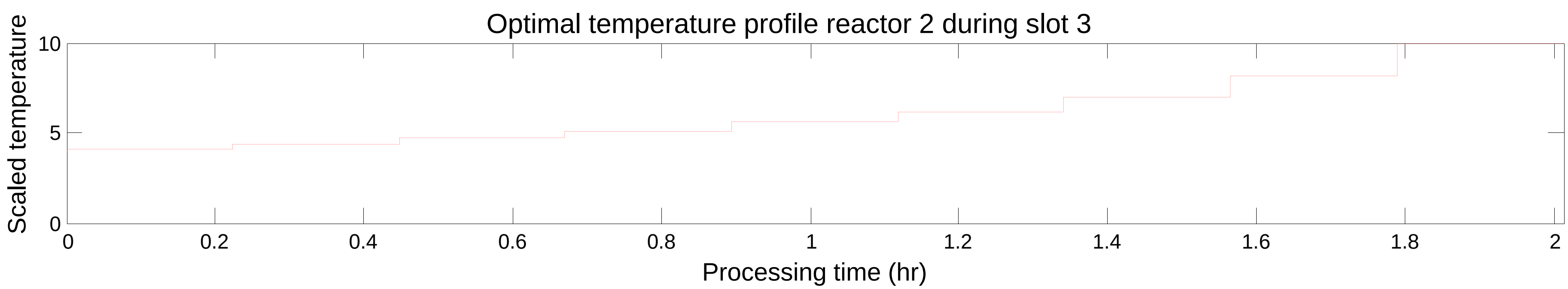
Case Study



Optimal temperature profile reactor 2 during slot 1
Scaled temperature
8
6
4
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
Processing time (hr)



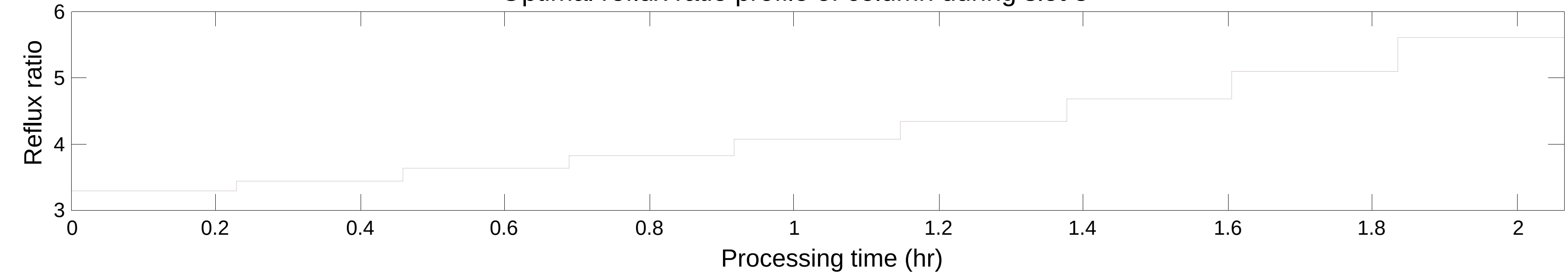
Optimal temperature profile reactor 2 during slot 2
Scaled temperature
10
5
0
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
Processing time (hr)



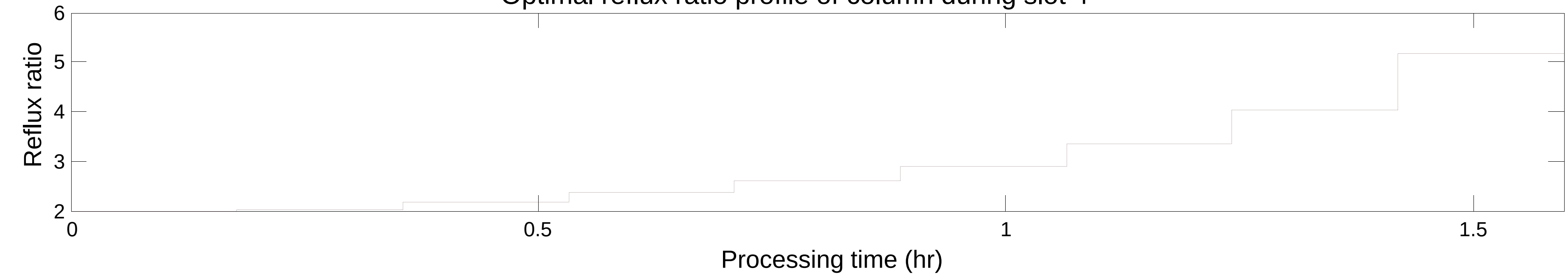
Optimal temperature profile reactor 2 during slot 3
Scaled temperature
10
5
0
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
Processing time (hr)

Case Study

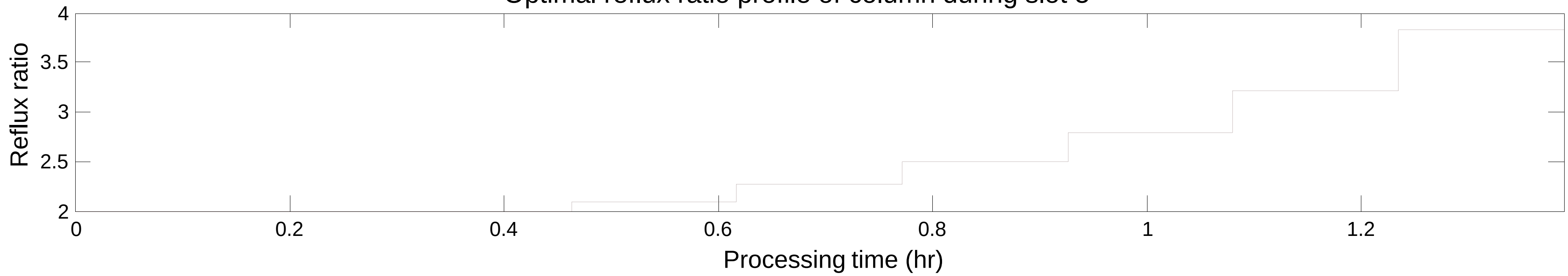
Optimal reflux ratio profile of column during slot 3



Optimal reflux ratio profile of column during slot 4



Optimal reflux ratio profile of column during slot 5



Conclusions

- Concluding remarks
  - An integrated framework for short-term scheduling and dynamic real-time optimization of batch processes
  - A reformulation strategy of mixed-logic dynamic optimization problems

- Future developments
  - Decomposition techniques for practical applications
  - Implementation with fast dynamic models
  - Nonconvex MINLP solution strategies
  - Material transportation and storage, changeovers and order fulfillment in scheduling

Acknowledgements

köszönöm תודה! děkuji

mahalo 고맙습니다

thank you

merci 谢谢 danke

Ευχαριστώ شكرا

どうもありがとう gracias