Integrated Scheduling and Dynamic Optimization of Batch Processes

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Current industrial practice for batch production

- Development of a batch process

$$\text{Product recipe} \xrightarrow{\text{scale-up}} \text{Process recipe} \xrightarrow{\text{scheduling}} \text{Production process}$$

  - Lost productivity and lowered performance in unit operations
  - Schedules sensitive to uncertainties in manufacturing
  - Opportunities for process optimization

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Optimizing the performance of a batch process in real-time

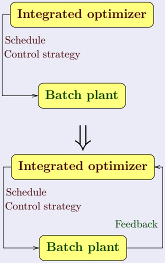
Approach An optimization-based framework with integrated

- Scheduling: assignment of batch operations
- Optimal control: execution of batch operations

Benefit

+ Adding value to existing assets
+ Improving plant profitability and reliability

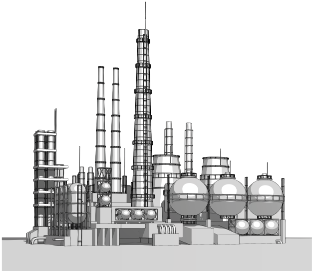
Steps Off-line ⇒ On-line



Problem Description

Integrated scheduling and dynamic optimization of batch plants

- Given
  - A batch plant with existing equipment
  - A time horizon to make products
  - Knowledge of process dynamics



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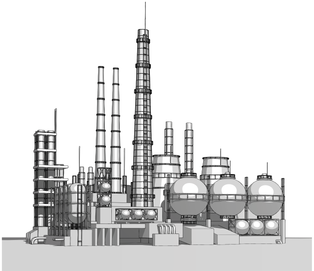

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Carnegie Mellon DOW

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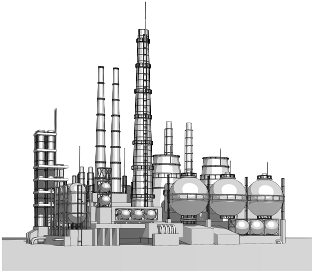
- Via
  1. Process representation using the state equipment network (SEN)
  2. Mathematical optimization formulation



Problem Solving Methodology

Integrated optimization based on the SEN

- The SEN represents the process system as a directed graph connecting two kinds of nodes

Material	Feed, intermediate and final products
Equipment	Process units carrying out operations

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- The integrated formulation

Objective function Max Profit = Product sales - Material cost - Operating cost

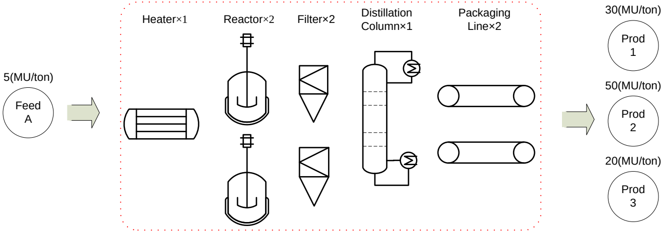
Constraints

- Scheduling considerations
  Assignment constraints, material balance, capacity constraints, timing constraints
- Unit operation
  Dynamic first-principle models, limits on controls and states
- Material quality measurement
  Material blending, quality requirements
- Auxiliary tightening constraints
  Tightening timing constraints, mass balance of process units

Case Study

A jobshop batch plant

- Equipment units and products manufactured in the plant



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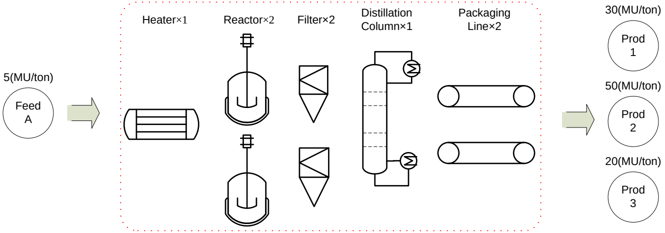

- Maximizing the net profit within a 10-hour time horizon

Model	Type
Recipe-based	MILP
Integrated	MINLP

Model	Profit(MU)
Recipe-based	1374
Integrated	1935

MILP solved by CPLEX, MINLP solved by SBB(CONOPT)

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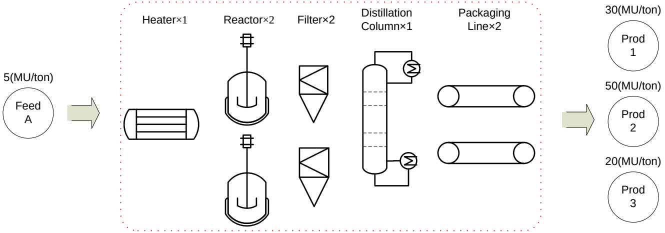

- Maximizing the net profit within a 10-hour time horizon

Model	Statistics			
	Type	Var.(Discrete) #	Nonlinear Var. #	Cons. #
Recipe-based	MILP	676(90)	0	1079
Integrated	MINLP	4978(90)	2292	12507

Model	Solution			
	Profit(MU)	CPU time (s)	Node(Best) #	Gap(%)
Recipe-based	1374	0.366	288(199)	0.0
Integrated	1935	9564	5000(1602)	67.9

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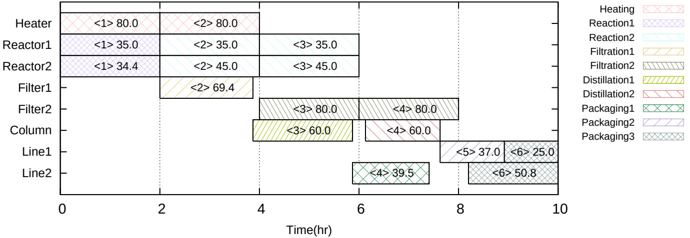
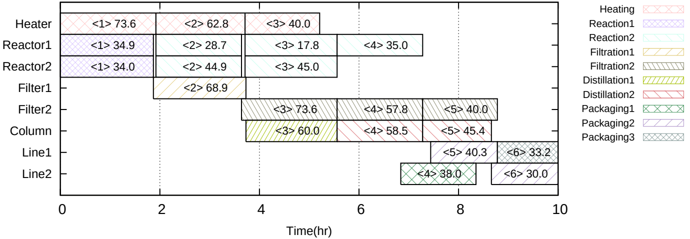
Case Study

Optimal production schedules in Gantt charts

Recipe-based approach



Integrated approach

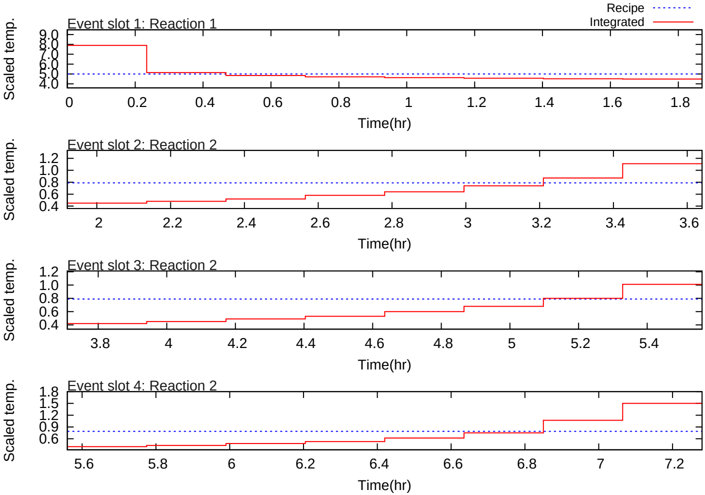


Numbers in a slot: <event pt.> batch size

Case Study

Optimal operating profiles for batch units

- Optimal temperature profiles of *Reactor 1*



Dynamic profiles also obtained for *Reactor 2* and *Distillation Column*

Industrial Application at Dow

Optimizing a real-world process with the integrated method

Methodology development

- Main results
  - An integrated optimization formulation for batch scheduling and dynamic optimization based on the *state equipment network*
  - A proof-of-concept case study: verified benefits of the integration

Industrial Application at Dow

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Application at Dow: an alkoxylation process

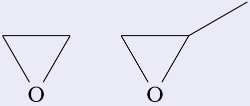
- Process characteristics
  - Polymerization reactions in semi-batch stirred tank reactors
  - Finishing train as a continuous process
  - Multiple products differ in composite monomers, molecular weights, functionality, etc.

Industrial Application at Dow

Alkoxylation process

Process chemistry*

- Key ingredients
  - Epoxides (ethylene oxide (EO), propylene oxide (PO))



  - Molecules containing active hydrogen atoms (alcohols, amines)

  - A basic catalyst (potassium hydroxide (KOH))
- Basic procedures
  - Starters are first mixed with catalyst in the liquid phase
  - Alkylene oxides are fed in controlled rates

** Ionescu, M. Chemistry and Technology of Polyols for Polyurethanes; Rapra Technology: Shawbury, U.K., 2005.*

Industrial Application at Dow

Development of process dynamic models

Modeling reaction kinetics

- Open literature example: Ethoxylation reaction*
  - Initiation

$$HOCH_2CH_2O^-K^+ + EO \rightarrow HOCH_2CH_2OEO^-K^+$$

  - Propagation

$$HOCH_2CH_2O(EO)_i^-K^+ + EO \rightarrow HOCH_2CH_2O(EO)_{i+1}^-K^+$$

  - Exchange

$$\underbrace{P_iO^-K^+}_{\text{growing chain}} + \underbrace{P_jOH}_{\text{dormant chain}} \leftrightarrow \underbrace{P_iOH}_{\text{dormant chain}} + \underbrace{P_jO^-K^+}_{\text{growing chain}}$$

$$P = HOCH_2CH_2(EO)$$

** Di Serio, M. Tesser, R. Dimiccoli, A. Santacesaria, E. Kinetics of Ethoxylation and Propoxylation of Ethylene Glycol Catalyzed by KOH Ind. Eng. Chem. Res. 2002*

Industrial Application at Dow

Proposed future developments

Planned work for the project

- Dynamic model development
  - Alternative monomers, copolymers
  - Vapor-liquid equilibrium
  - Molecular weight distributions
- Scheduling method development
  - Discrete-time resource task network
- Integration and on-line implementation

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Conclusions and acknowledgments

- Integration of scheduling and dynamic optimization using SEN revisited
- Application at Dow
- Thank you and any questions?