Integrated Scheduling and Dynamic Optimization of Batch Processes

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Introduction
Background and motivation

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

Optimizing the performance of a batch process in real-time

Approach

An optimization-based framework with integrated scheduling: assignment of batch operations and optimal control: execution of batch operations.

Steps

- Off-line
- On-line

Integrated optimizer

Batch plant
Schedule
Control strategy

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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 $\Rightarrow$ 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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- **Determine**
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  - The optimal equipment control strategy

- **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

The integrated formulation includes:
- Objective function: Maximize Profit = Product sales - Material cost - Operating cost
- Constraints:
  - Scheduling considerations, assignment constraints, material balance, capacity constraints, timing constraints
  - Unit operation limitations: 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
Problem Solving Methodology
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  Equipment Process units carrying out operations

- The integrated formulation

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Case Study
A jobshop batch plant

- Equipment units and products manufactured in the plant

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

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

Yisu Nie (Carnegie Mellon University)
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A jobshop batch plant

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<table>
<thead>
<tr>
<th>Model</th>
<th>Type</th>
<th>Profit (MU)</th>
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<tbody>
<tr>
<td>Recipe-based</td>
<td>MILP</td>
<td>1374</td>
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<td>1935</td>
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A jobshop batch plant

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<tr>
<th>Model</th>
<th>Type</th>
<th>Var.(Discrete) #</th>
<th>Nonlinear Var. #</th>
<th>Cons. #</th>
</tr>
</thead>
<tbody>
<tr>
<td>Recipe-based</td>
<td>MILP</td>
<td>676(90)</td>
<td>0</td>
<td>1079</td>
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<tr>
<td>Integrated</td>
<td>MINLP</td>
<td>4978(90)</td>
<td>2292</td>
<td>12507</td>
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</table>

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<tr>
<th>Model</th>
<th>Solution</th>
<th>Profit (MU)</th>
<th>CPU time (s)</th>
<th>Node(Best) #</th>
<th>Gap(%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Recipe-based</td>
<td></td>
<td>1374</td>
<td>0.366</td>
<td>288(199)</td>
<td>0.0</td>
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<tr>
<td>Integrated</td>
<td></td>
<td>1935</td>
<td>9564</td>
<td>5000(1602)</td>
<td>67.9</td>
</tr>
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MILP solved by CPLEX, MINLP solved by SBB(CONOPT)
Case Study

Optimal production schedules in Gantt charts

Recipe-based approach

Integrated approach

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

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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

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<td><strong>Main results</strong></td>
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### 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

### 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))
    - ![Epoxide Structures]
  - Molecules containing active hydrogen atoms (alcohols, amines)
    - ![Alcohol and Amine Structures]
  - 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

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*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
    \[
    \text{HOCH}_2\text{CH}_2\text{O}^-\text{K}^+ + \text{EO} \rightarrow \text{HOCH}_2\text{CH}_2\text{OEO}^-\text{K}^+
    \]
  - Propagation
    \[
    \text{HOCH}_2\text{CH}_2\text{O}(\text{EO})_i^-\text{K}^+ + \text{EO} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}(\text{EO})_{i+1}^-\text{K}^+
    \]
  - Exchange
    \[
    \text{P}_i\text{O}^-\text{K}^+ \quad \text{growing chain} \quad + \quad \text{P}_j\text{OH} \quad \text{dormant chain} \quad \leftrightarrow \quad \text{P}_i\text{OH} \quad \text{dormant chain} \quad + \quad \text{P}_j\text{O}^-\text{K}^+ \quad \text{growing chain}
    \]

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
**Industrial Application at Dow**

**Proposed future developments**

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- 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?