The 5th IFAC Workshop on Mining, Mineral and Metal Processing

Complex chemical process optimization and its industrial applications

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Introduction

Complexity of chemical process and product

- Interconnected, interactive multiscale structure (complexity in structure)
- Diverse performance or property (complexity in behavior)
- System behavior cannot be deduced directly from analyzing the behavior of individual components

Approaches to complex chemical process system

- Creating proper degree of complexity, avoiding unnecessary or “redundant” complexity
- Concentrating on dominant level(s), ignoring undesired details

Flowsheet of Refinery Plant
Introduction

Automation Hierarchy

Planning
- Months/Weeks

Scheduling
- Weeks/Days

Real-time optimization
- Hours

Advanced control
- Minutes

Conventional control
- Seconds

Production Process

Commercial Software
- PIMS/RPMS
- Aspen ORION
- Profit Optimizer
- DMC/RMPCT

Production Process

Introduction

Automation Hierarchy

Planning
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Production Process

Commercial Software
- PIMS/ORION
- Raw Material Acquisition / Run Plan Optimization/Scheduling scheme
  - Plant-wide optimization
  - Based on simplified models, considering balance of material and tanks
  - Linear Programing is used

• What products to make
• When to make them
• What equipment to use
Introduction

Automation Hierarchy

Planning

Scheduling

Real-time optimization

Advanced control

Conventional control

Production Process

Current - Real Time - Operations Optimization

• Unit-scale optimization
• Based on rigorous models, considering balance of material and tanks
• Maximizing profits, considering current states, production constraints and constraints from scheduler - hours

Profit Optimizer/GAMS

Advanced Control Systems

• Unit-scale control
• Based on identified linear dynamic model
• Multi-variable, constrained control
• Predefined constraints with different priorities

RMPCT/DMC
Introduction

Complexity of Chemical Process \rightleftharpoons \text{Hierarchical Automation Structure}

Problems in practical application:

- **Process design**: how to integrated the factors as safety, controllability and flexibility? e.g. Energy coupled process integration VS inadequate freedom
- **Process optimization**: open loop, model mismatch with MPC etc. ...
- **Process scheduling**: only for material balance, lack optimization
- **Process Planning**: fixed DB parameters, hard to match actual situation

Introduction

**Growing trend for integrated optimization**

Published papers in SCIE
(key words: integrated optimization & Process)
Integrated Optimization of Process Automation
Integrated Optimization of Process Automation

- Integration of RTO and MPC in Styrene Plant
- Dynamic Scheduling and Optimization in Olefin Plant
- Integration of Planning and Scheduling in Gasoline Blending

Integration of RTO & APC

Major Problem
- Different execution frequencies
- Different models

One-layered Approach
- Real-Time Optimization
- Model Predictive Controller
- Economically-Oriented MPC

Two-layered Approach
- Real-Time Optimization
- Target / Trajectory Correction
- Model Predictive Controller

Integration of RTO & APC

Methodologies

A: LEMPC
Integrate nonlinear steady-state optimization into linear MPC.
- Economic functions added as additional term of the controller
- Nonlinear steady-state model included as additional constraints (Zanin, 2002), (Glauce, 2010), (Teodoro, 2014)

B: NEMPC
Incorporate a general cost function or performance index in NMPC, EMPC.
- Used for feedback control directly
- Respond to changes in the operating conditions faster (Ellis, 2014), (Tran, 2014), (Biegler, 2015)

C: Insert Steady-State Target Optimization (SSTO) layer between RTO and MPC
- Calculate best admissible target for the MPC using SSTO
- SSTO predicts based on steady-state version of linear model in MPC (Rao, 1999), (Marchetti, 2014)

D: Integrate Dynamic Real-Time Optimization (D-RTO) and Model Predictive Control (MPC)
- Re-optimization trigger strategy
- Fast updates of the trajectories based on NLP sensitivities (Kadam, 2003), (Wolf, 2014)

Integration of RTO & APC

Ethylbenzene dehydrogenation process

Objective & Challenges

\[
\begin{align*}
\text{max} & \quad -y_{pp} - 0.02 \times (y_{pp} - 0.02) + 0.02 \times (y_{cc} - 0.02) + 0.02 \times (y_{cc} - 0.02) \\
\text{s.t.} & \quad y = s(y, u) \\
& \quad y_{cc} + T_{cc} + y_{pp} + T_{pp} + y_{cc} \leq T_{pp} + y_{pp} \\
& \quad 1.3 \leq u_{pp} / (T_{pp} + y_{pp}) \leq 1.8
\end{align*}
\]

Process description
- Radial-flow reactor with strong endothermic reversible reaction
- Reaction Temperature
  - Low Temp. → Low yields; High Temp. → thermal cracking
- Ratio of steam to ethylbenzene
  - Low Ratio: carbon decomposition; High R. → energy waste

Control difficulties
- Plant-model mismatch
- Dynamic change of Constraints related to catalyst deactivation
- Various and frequent disturbances
Ethylbenzene dehydrogenation process

**Objective & Challenges**

\[ \begin{align*}
\min & -\Phi(y, y) - ((p + 0.02 \times (u_1 - T_{\text{ref}}) + 0.02 \times (u_2 - T_{\text{ref}})) + u_3 + u_4) / 1000 - \rho \times d_u \\
\text{s.t.} & \quad y = x_{\text{in}}, 0 \\
& \quad x_1 + x_2 + x_3 + x_4 \leq F_{\text{ref}} \\
& \quad 1.3 \times (u_1 + u_2) / (u_3 + d_u) \leq 1.8
\end{align*} \]

**Process description**

- Radial-flow reactor with strong endothermic reversible reaction
- Reaction Temperature
- L: low yields; H: thermal cracking
- ratio of steam to ethylbenzene
- L: carbon decomposition; H: energy waste

**MPC & RTO**

MV(4):
- \( u_1 \): flow rate of main steam FC1
- \( u_2 \): flow rate of LP steam FC3
- \( u_3 \): temperature of furnace 1 TC1
- \( u_4 \): temperature of furnace 2 TC2

CV(3):
- \( y_1 \): inlet temperature of R1
- \( y_2 \): inlet temperature of R2
- \( y_3 \): outlet flow rate of styrene

**Integration Structure**

**RTO Layer**

- Constraint-adaptation strategy
- Easy for model update
- Better for handling the plant-model mismatch

**SSTO Layer**

- Approximation of RTO
- Based on steady-state version of linear dynamic model

**MPC Layer**

- MPC with nonlinear successive linearization

**SSTO (Steady State Target Optimization)**

- Approximate RTO
- Based on nonlinear MPC
- Low computational burdens

**Motivation:**

- Same model origination
- Model adaptation on a lower level (MPC-NSL)
Integration of RTO & APC

Nonlinear dynamic model

- **Reaction mechanism**
  - Highly endothermic reaction:
    - \( C_8H_8 + O_2 \rightarrow CO_2 + H_2O \)
    - \( C_8H_8 + CO \rightarrow 2H_2 + CO_2 \)
    - \( C_8H_8 + CH_4 \rightarrow 2H_2 + CO_2 \)
    - Radial-flow reactor

- **Model validation**
  - Inlet temperature of R1
  - Outlet temperature of R1
  - Inlet temperature of R2
  - Outlet temperature of R2

Integration of RTO & APC

**Implementation**

**Disturbances:**
- Flowrate of ethylbenzene stream
  - 20th hour after the execution of RTO, decreases by 3%
- Composition of ethylbenzene stream
  - 50th hour after the execution of RTO, ethylbenzene mass fraction decreases by 5%

- Open-loop RTO
- Algorithm I
- Algorithm II: our study

**Improved:**
1) Control performance
2) RTO convergence

Integration of RTO & APC

Implementation

Disturbances:

• flowrate of ethylbenzene stream
  20th hour after the execution of RTO, decreases by 3%

• composition of ethylbenzene stream
  50th hour after the execution of RTO, ethylbenzene mass fraction decreases by 5%

Improved

1) Control performance
2) RTO convergence

• Open-loop RTO
• Algorithm I
• Algorithm II: our study


Algorithm II: Real-time optimization and control of an industrial ethylbenzene dehydrogenation process. Chemical Engineering Transaction. 2017 (61) 331-336

Integrated Optimization of Process Automation

• Integration of RTO and MPC in Styrene Plant
• Dynamic Scheduling and Optimization in Olefin Plant
• Integration of Planning and Scheduling in Gasoline Blending
**Integration of Scheduling & Operation Optimization**

**Task of Scheduling:**
- Keep process operation continuously (with reasonable level, inventory etc.), while need smooth transition among process units.
- Pursue the economic profit with less time or the cost.

**Problems:**
- Simulation driven scheduling policy (**NO optimization**)
- Difficult to define a general problem or solved by general algorithm, especially for large scale process with uncertainties.

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**Integration of Scheduling & Operation Optimization**

**Cracking furnaces system in ethylene plant**

- Various feedstocks with different yields
  - NAP, LNAP, LPG, HVGO...
- Multiple cracking furnaces with different characteristics
- Thermal cracking reaction & coking inside coils

**Goal:**
- $\text{Max.}$ Yields of high added-value products
- $\text{Max.}$ Run-length of furnaces

**By**
- Feedstock selection
- Load dispatching
- Operating condition optimization
Integration of Scheduling & Operation Optimization

Reaction Kinetics / Reactor Model

Free-radical mechanism

\[ \ldots \]

1-D reactor model

\[ \ldots \]

Process Conditions
- Feedstock composition
- Reactor & Furnace
- Operating conditions

Integration of Scheduling & Operation Optimization

Reaction Kinetics / Reactor Model
Integration of Scheduling & Operation Optimization

Thermal condition simulation in the furnace

- Convection section model
- Radiant box model

Run length Simulation


Integration of Scheduling & Operation Optimization

Coupled modeling of furnace and reactor

- Reaction tube
- Radical reaction
- Geometry
- heat flux
- Couple model
- Prediction results

Coupled simulation of convection section with dual stage steam feed mixing of an industrial ethylene cracking furnace. Chemical Engineering Journal. 2016, 286: 436-446
Integration of Scheduling & Operation Optimization

Feedstock molecular reconstruction (NAP)

Yields of C₂H₄, H₂, C₃H₆, benzene etc. products (NAP)

Full composition analysis of industrial data
(Analyzed by Beijing Research Institute of Chemical Industries)

Coupled modeling of furnace and reactor

Sinopec Zhenhai Refining & Chemical Company
BA105 furnace (HCR), BA109 furnace (NAP)

Integration of Scheduling & Operation Optimization

Surrogate model of cracking furnace

Prediction of change rate of coke thickness

Feedforward Neural Networks – State Space Model (FNN-SSM)

\[
\begin{align*}
\frac{dx(t)}{dt} &= f_{\text{feed}}(x(t), y(t), T(t)) \\
y(t) &= f_{\text{out}}(x(t), y(t), T(t)) \\
x_{\text{out}}(t) &= x(t) + k_x(t) \cdot T(t) \\
x_{\text{out}}(t) &= x_{\text{out}}(t)
\end{align*}
\]

Comparison with traditional surrogate model

Prediction of product yield and KPI
Integration of Scheduling & Operation Optimization

Integration of cyclic scheduling & operation optimization

\[
\max_{\mathbf{x}} \sum_{i} \left[ \sum_{j} \left( x_{ij}^{0} f_{ij}(\mathbf{y}) - C_{ij} \right) \right] d \sum_{t} w_{it} \]

- DCFE is used for discretization on time
- MIDO is transformed into MINLP solved by sBB
- Decision variables of scheduling and operation are determined simultaneously

\[
\sum_{j} x_{ij}^{0} \leq \sum_{j} x_{ij} ; \forall i \in \mathbb{N}
\]

Day mean profit increases by 13.5%

Implementation results

Applied in Shanghai Petrochemical:
- Average yield of ethylene and propylene increased by 0.187%.
- Fuel consumption reduced by 1.806 kg/t (feedstock), i.e. 1.64% under same feedstock load.

Sinopec Shanghai Petrochemical Company Limited
Integrated Optimization of Process Automation

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Integration of Planning & Scheduling

Model mismatch with plant (e.g. feedstock properties fluctuation, device capabilities …) → Temporal aggregation model

Production Planning → Scheduling

Similar model Similar optimizer

Solved by human experience

Production Planning

Short-term Planning
Difficult to get the statistics of the current inventory, product ..., difficult to respond to temporary order

→ Temporal aggregation model

Scheduling

?
Integration of Planning & Scheduling

Hierarchical
- McKay, 1995
- Lin et al., 2002
- Menezes et al., 2016
- Vogel et al., 2017

Iterative
- Papageorgiou and Pantelides, 1996
- Stefanopoulou and Shah, 2006
- Wu and Ierapetritou, 2007

Integrated Formulation
- Joly et al., 2002
- Neiro and Pinto, 2005
- Blanco et al., 2005
- Yan and Zhang, 2007


Integration of Planning & Scheduling

Online gasoline blending process

Target
- Demand driven optimal recipe & blending conditions

Difficulties
- Online measurement of oil properties
- Blending rules or recipe models
- Functional models for Planning and Scheduling optimization
Integration of Planning & Scheduling

Online measurement of oil properties

Wavelength selection is the basis of NIR system. It is directly related to prediction performance and model complexity.

Response to change of operating conditions

- Intermediate component type
- Intermediate component property
- Oil additives

Proposed framework (AWL-PLS)

1. Sample database and data pre-processing
2. Model parameters initialization
3. Selection of local sample sets from database
4. Wavelength structure update of calibration set
5. Local calibration model and property prediction

Integration of Planning & Scheduling

NIR spectral analysis and modeling

Adaptive strategies for online model update (ORL-PLS)

- Outlier detection
- Locally weighted learning
- Improved recursive strategy

Adaptive algorithm and outlier detection are two key factors for adaptive modeling

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### Table: Model Performance

<table>
<thead>
<tr>
<th>Model</th>
<th>$R^2$</th>
<th>RMSEP</th>
<th>Mean error</th>
<th>Max error</th>
</tr>
</thead>
<tbody>
<tr>
<td>VIP-PLS</td>
<td>0.9134</td>
<td>0.2199</td>
<td>0.1460</td>
<td>0.6998</td>
</tr>
<tr>
<td>RV-PLS</td>
<td>0.8312</td>
<td>0.1939</td>
<td>0.1458</td>
<td>0.7015</td>
</tr>
<tr>
<td>LW-PLS</td>
<td>0.9133</td>
<td>0.2367</td>
<td>0.1467</td>
<td>0.7101</td>
</tr>
<tr>
<td>AWL-PLS</td>
<td>0.8329</td>
<td>0.1774</td>
<td>0.1338</td>
<td>0.5998</td>
</tr>
</tbody>
</table>
Integrated planning and blend recipes optimization

Three-level optimization structure

Proposed scheduling strategy

Top-level
Long-range strategic planning (NLP)

Middle level
Initial blend recipes and scheduling (N time periods)

Lower level
Recipe updating via real-time optimization approach

Plan horizon
Verify the effectiveness of initial planning

Schedule periods
Compute decisional scheduling/batch production, volume, recipes, and inventory for each period

Recipe optimization periods
Optimize blend recipes

Planning
A. Verify the initial planning
B. Maximum capacity

Scheduling
A. Blending batch sequences
B. Initial recipe for each batch & inventory management

Optimization
A. RTO of blending recipe
B. Handle uncertain events
C. Update blending model

Integrated Planning & Scheduling

Integrated planning and blend recipes optimization

The necessity for integration

<table>
<thead>
<tr>
<th>Blend recipe calculated by scheduling level</th>
<th>Blend recipes by Real-time optimization</th>
</tr>
</thead>
<tbody>
<tr>
<td>Period</td>
<td>1</td>
</tr>
<tr>
<td>NORM</td>
<td>0.92</td>
</tr>
<tr>
<td>OCTN</td>
<td>0.98</td>
</tr>
<tr>
<td>REFOR</td>
<td>0.28</td>
</tr>
<tr>
<td>NOAR</td>
<td>0.01</td>
</tr>
<tr>
<td>NORM</td>
<td>0.64</td>
</tr>
<tr>
<td>OCTN</td>
<td>0.96</td>
</tr>
<tr>
<td>REFOR</td>
<td>0.12</td>
</tr>
<tr>
<td>NOAR</td>
<td>0.18</td>
</tr>
</tbody>
</table>

Response to temporary delivery

Optimized recipe for the temporary delivery

Implementation Results:

- The cost of the blending is reduced by 95M ¥/a;
- The blending period is reduced by 6-8hour/tank;
- VOC emission is reduced by 3000t/a;
- The quality giveaway (Octane Number) is decreased from 0.5 to 0.2,
Summary and considerations

Summary

• Traditional hierarchical automation structure
• Cases for integrated optimization method
  • Styrene Plant: RTO & MPC
  • Olefin Plant: Scheduling & RTO
  • Gasoline blending: Planning & Scheduling + RTO
Considerations

Hierarchical solution strategy seems to be currently the only realistic approach to tackle industrial size problems, but needs appropriate cooperative solution.

CPS (Cyber Physical System): ubiquitous perception, interconnection
CAPS (Collaborative Process Automation Systems): infrastructure, interaction with user/human operator, ...

Thanks for your attention