



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

Complex chemical process optimization and its industrial applications

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Content

1 Introduction

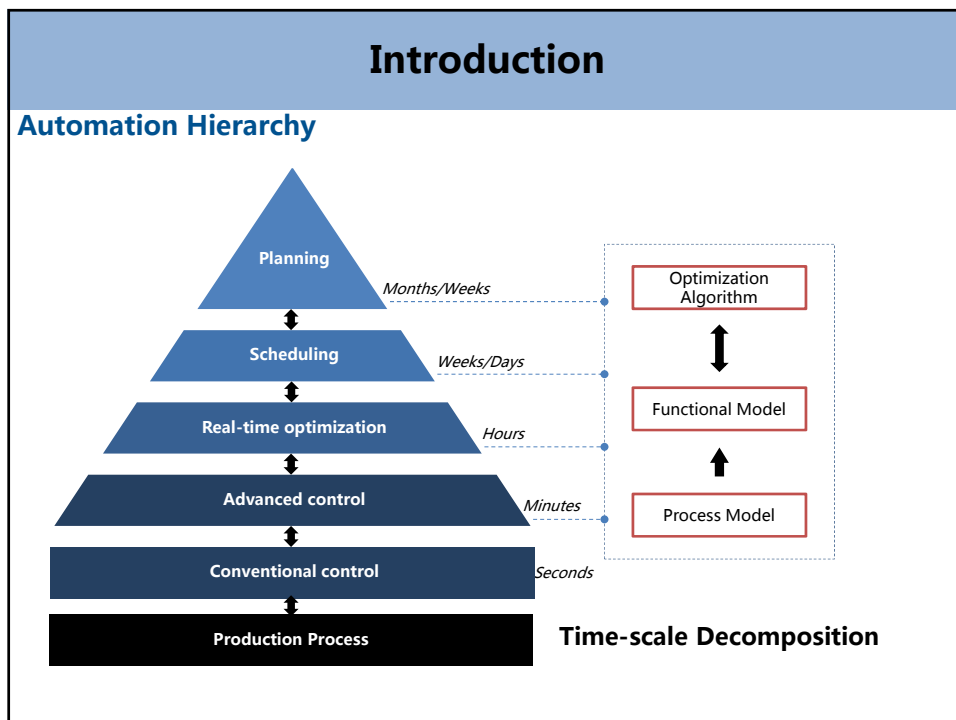
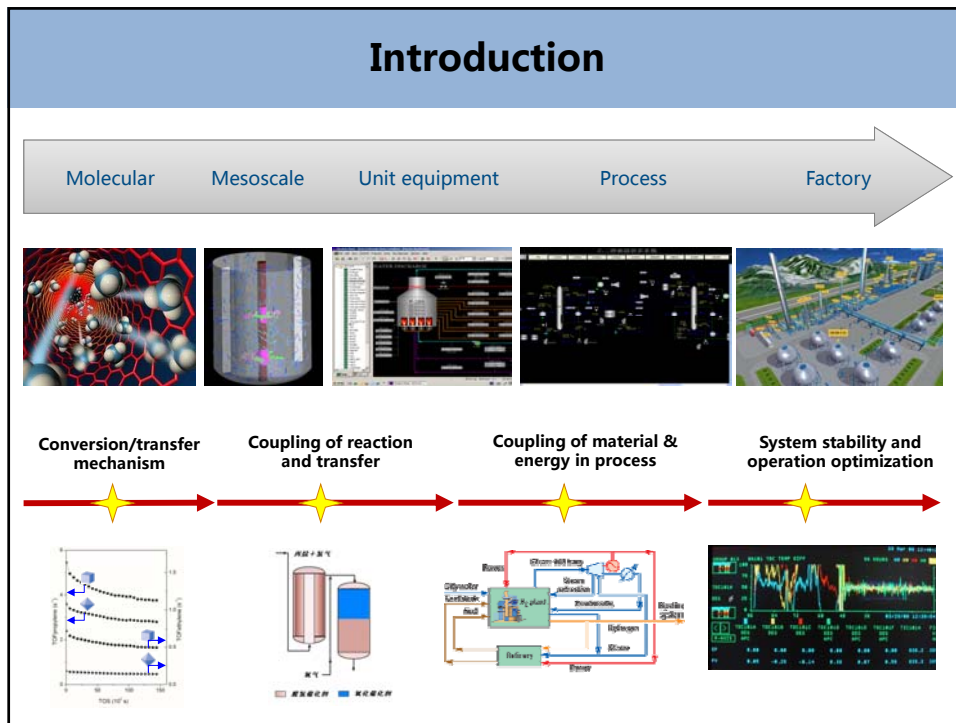
2 Integrated Optimization of Process Automation

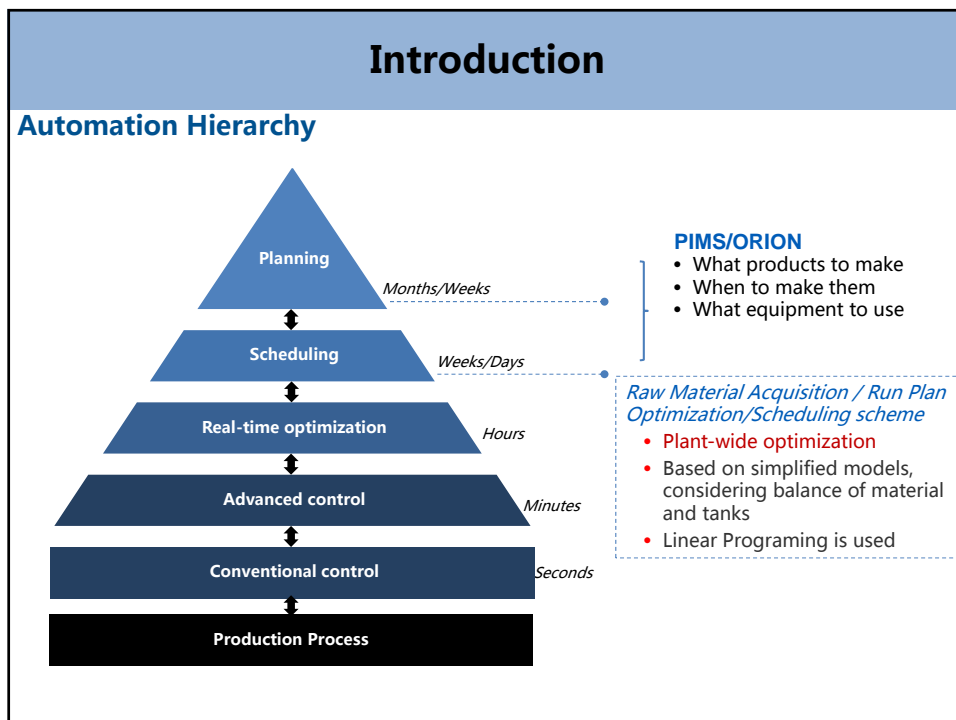
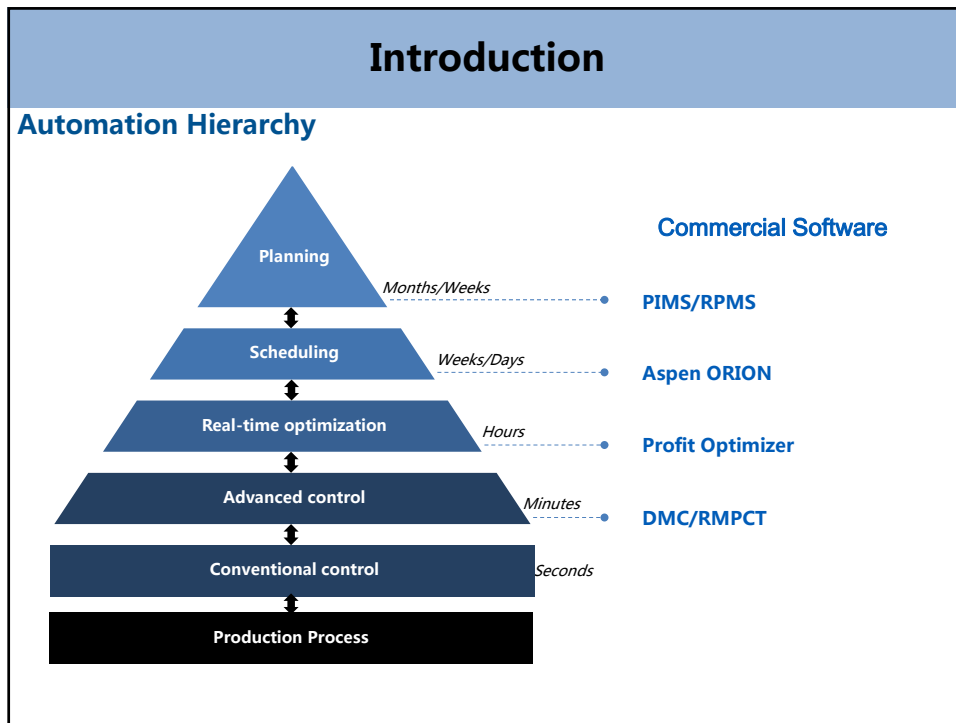
2.1 Integrated RTO & APC

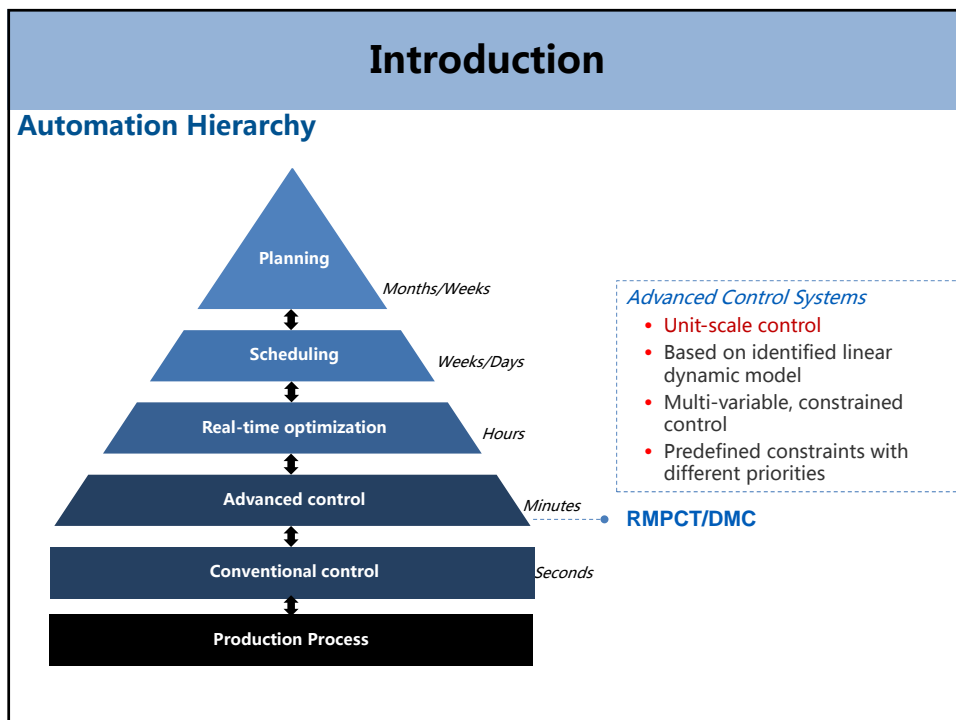
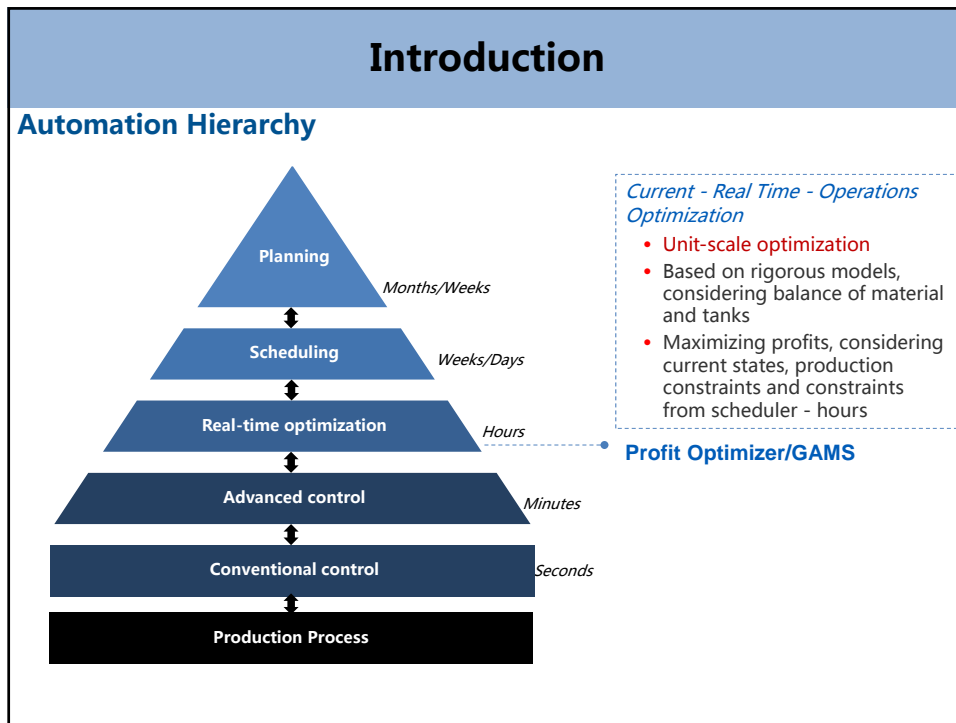
2.2 Integrated Scheduling & RTO

2.3 Integrated Planning & Scheduling

3 Summary & considerations







Introduction

Complexity of
Chemical Process



Hierarchical Automation
Structure

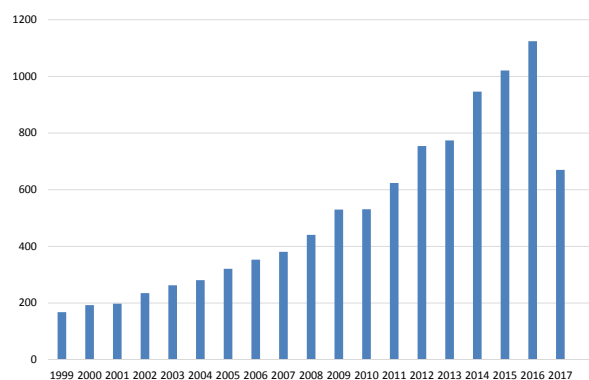
Problems in practical application:


- **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

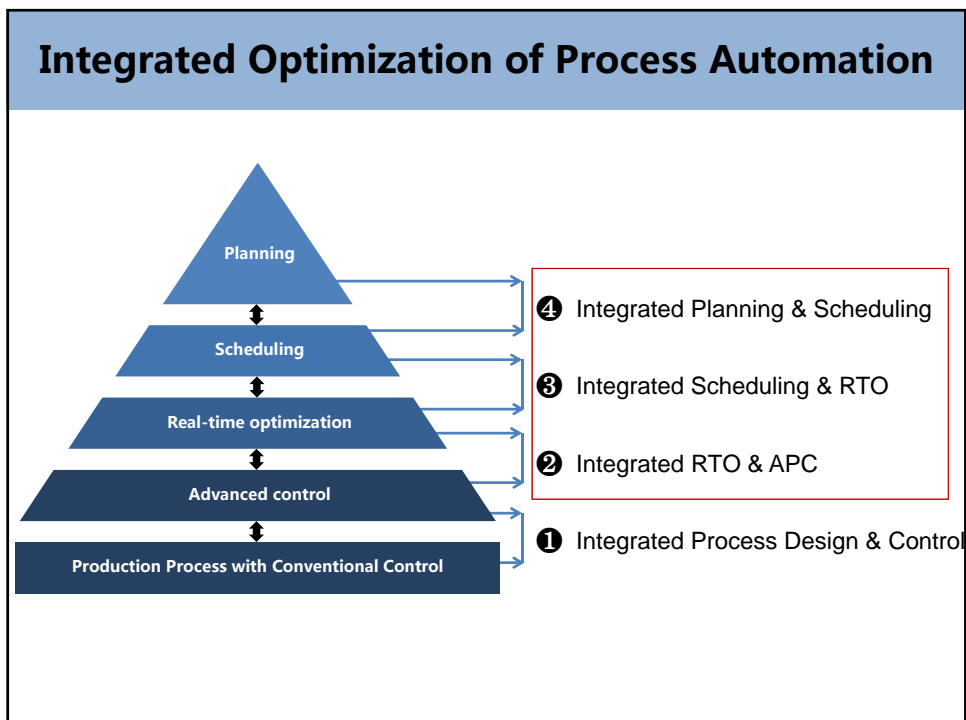
Growing trend for integrated optimization

Published papers in SCIE
(key words: integrated optimization & Process)



 EAST CHINA UNIVERSITY OF SCIENCE & TECHNOLOGY

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

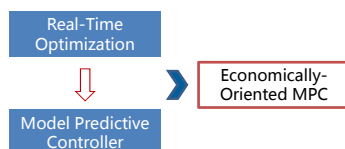
Major Problem

- Different execution frequencies
- Different models



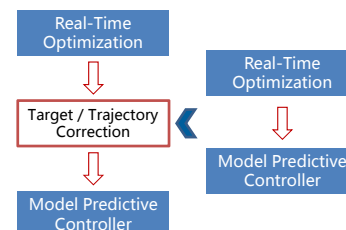
- Conflicts in decisions
- Infeasible for MPC
- Non-optimal conditions

One-layered Approach



Classification

Two-layered Approach



Lynn Würth, Ralf Hannemann, Wolfgang Marquardt . A two-layer architecture for economically optimal process control and operation. Journal of Process Control. 2011, 21(3): 311-321

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

(Zamin, 2002), (Glauce, 2010), (Teodoro, 2014)

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)

Steady-state Optimization

Dynamic Optimization

A

B

One-Layered

ed

$$\min_{u(k+j|k), j=0, \dots, m-1} \sum_{j=1}^p \|W_1(y(k+j|k) - r)\|_2^2 \quad \mathbf{A}$$

$$+ \sum_{j=0}^{m-1} \|W_2 \Delta u(k+j|k)\|_2^2 + W_3 f_{eco}(u(k+m|k), y(k+\infty|k)) \quad \mathbf{C, D}$$

$$\min_{\Delta z} \frac{1}{2} \Delta z^T \frac{\partial^2 L}{\partial z^2} \Delta z + \Delta p^T \frac{\partial L}{\partial p} (p_0) \Delta z + \frac{\partial \varphi}{\partial z} (p_0) \Delta z \quad \mathbf{B}$$

subject to $\frac{\partial g}{\partial z} (p_0) \Delta z + \frac{\partial g}{\partial p} (p_0) \Delta p \geq 0$

NLP Sensitivity (QP)

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)

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

$$\min_{u, \theta} -(p_1 \times y_3 - ((p_2 + 0.02 \times (u_3 - T_{ref1}) + 0.02 \times (u_4 - T_{ref2})) \times u_1 + p_2 \times u_2) / 1000 - \rho \times d_{ex})$$

s.t. $y = S(u, \theta)$
 $y_1 + \epsilon_1 \leq T_{max}, y_2 + \epsilon_2 \leq T_{max}, y_3 + \epsilon_3 \leq F_{max}$
 $1.3 \leq (u_1 + u_2) / (\rho \times d_{ex}) \leq 1.8$

Process description

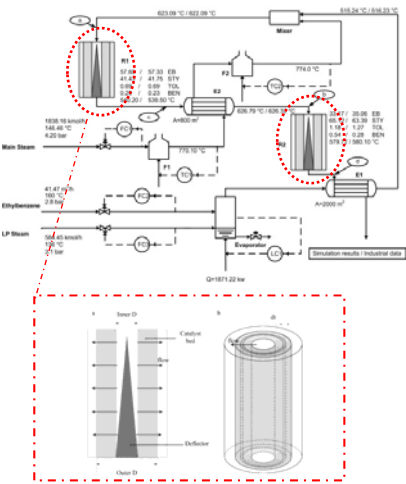
- Radial-flow reactor with strong endothermic reversible reaction
- Reaction Temperature
- Low Temp. → Low yields; High Temp. → thermal cracking
- Ratio of steam to ethylbenzene
- Low Ratio: carbon decomposition; High R. → energy waste

Control difficulties

- Plant-model mismatch
- dynamic change of Constraints related to catalyst deactivation
- Various and frequent disturbances

Integration of RTO & APC

Ethylbenzene dehydrogenation process



The diagram shows a complex industrial process involving ethylbenzene, main steam, and LP steam. It includes two furnaces (F1 and F2), two reactors (R1 and R2), and various heat exchangers and control loops. A detailed view of a reactor is shown below the main diagram, illustrating its internal structure with a catalyst bed and a defluidizer.

Objective & Challenges

$$\min_{u, y} -(p_1 \times y_3 - (p_2 + 0.02 \times (u_3 - T_{ref1}) + 0.02 \times (u_4 - T_{ref2})) \times u_1 + p_2 \times u_2) / 1000 - \rho \times d_{ab}$$

s.t. $y = S(u, \theta)$
 $y_1 + \varepsilon_1 \leq T_{max}, y_2 + \varepsilon_2 \leq T_{max}, y_3 + \varepsilon_3 \leq F_{max}$
 $1.3 \leq (u_1 + u_2) / (\rho \times d_{ab}) \leq 1.8$

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 : flowrate of main steam FC1
- u_2 : flowrate 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 flowrate of styrene

Fat system

Integration of RTO & APC

Integration Structure

Motivation:

- Same model origination
- Model adaptation on a lower level (MPC-NSL)

RTO Layer

- Constraint-adaptation strategy
$$\min_{u, y} \Phi(u, y)$$

s.t.

$$y = S(u, \theta)$$

$$y^l \leq y + \varepsilon \leq y^u$$

$$u^l \leq u \leq u^u$$

$$\varepsilon_i = (1 - K)\varepsilon_{i-1} + K(y'_i - y^i)$$

SSTO Layer

- Approximation of RTO
$$\min_{u, y} \frac{\partial \Phi}{\partial u} (u, -u') + \frac{1}{2} \|u, -u'\|_m^2$$

s.t.

$$y_i = G_i u + y_0(k) + d(k)$$

$$y^l \leq y_i \leq y^u$$

$$u^l \leq u \leq u^u$$

MPC Layer

- MPC with nonlinear successive linearization
$$A_i = \frac{\partial f}{\partial x} (x_i, u_i, \theta) \quad B_i = \frac{\partial f}{\partial u} (x_i, u_i, \theta)$$

$$C_i = \frac{\partial h}{\partial x} (x_i, u_i, \theta) \quad D_i = \frac{\partial h}{\partial u} (x_i, u_i, \theta)$$

Constraint-adaptation strategy

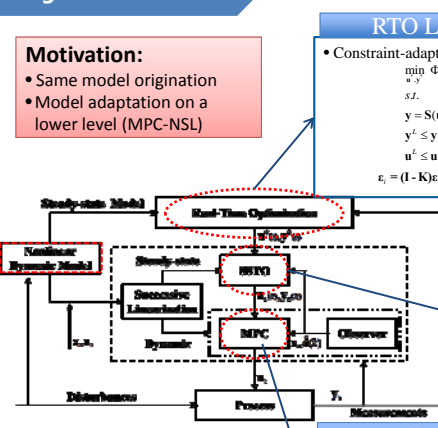
- Easy for model update
- Better for handling the plant-model mismatch

SSTO (Steady State Target Optimization)

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

MPC-NSL

- An approximation/simplification of nonlinear MPC
- Low computational burdens



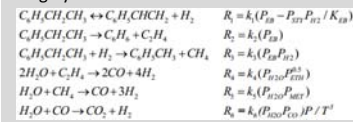
The diagram illustrates the integration structure. It shows a central 'Process' block that receives 'Disturbances' and 'Manipulations' and outputs 'Measurements'. The 'RTO Layer' provides 'Set-Point' to 'Hard-Then Optimization', which in turn provides 'Set-Point' to 'SSTO'. The 'SSTO Layer' provides 'Set-Point' to 'MPC'. The 'MPC Layer' provides 'Manipulation' to the 'Process'. The 'Process' also provides 'Measurements' to an 'Observer', which provides 'State' to the 'MPC'. The 'MPC' also provides 'Manipulation' to the 'Process'. The 'MPC' also provides 'Manipulation' to the 'SSTO'. The 'SSTO' also provides 'Manipulation' to the 'Process'. The 'RTO' also provides 'Manipulation' to the 'Process'.

Integration of RTO & APC

Nonlinear dynamic model

Reaction mechanism

Highly endothermic reaction

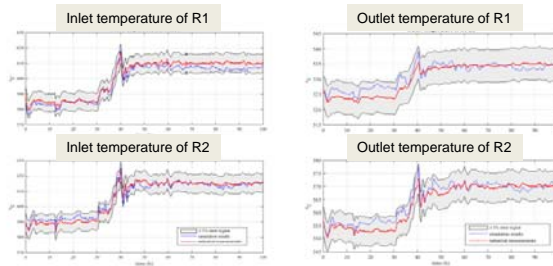


Reactor model

Radial-flow reactor

$$\begin{aligned}
 \varepsilon C_i \frac{\partial C_i}{\partial t} &= - \frac{F_i}{A_c} \frac{\partial C_i}{\partial r} + R_i \rho_b \\
 \varepsilon \frac{\partial T}{\partial t} &= - \frac{F_c}{A_c} \frac{\partial T}{\partial r} + \rho_b \sum_{j=1}^N R_j (-\Delta H_j) \\
 \frac{dP}{dr} &= -1 \times 10^4 \frac{(1-\varepsilon)G}{d_p \varepsilon \rho_g} \left[\frac{150(1-\varepsilon)\mu}{d_p} + 1.75G \right]
 \end{aligned}$$

Model validation

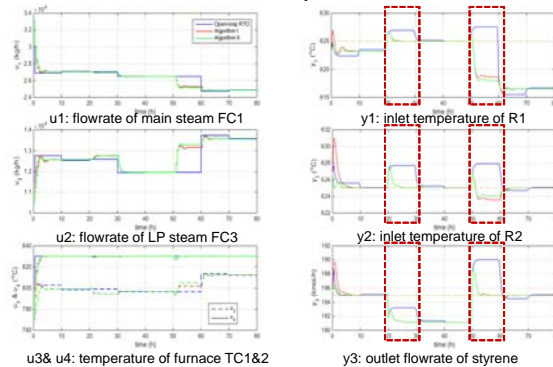


Integration of RTO & APC

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

Algorithm I: Steady-state target optimization designs for integrating real-time optimization and model predictive control. Journal of Process Control, 2014, 24(1):129-145.

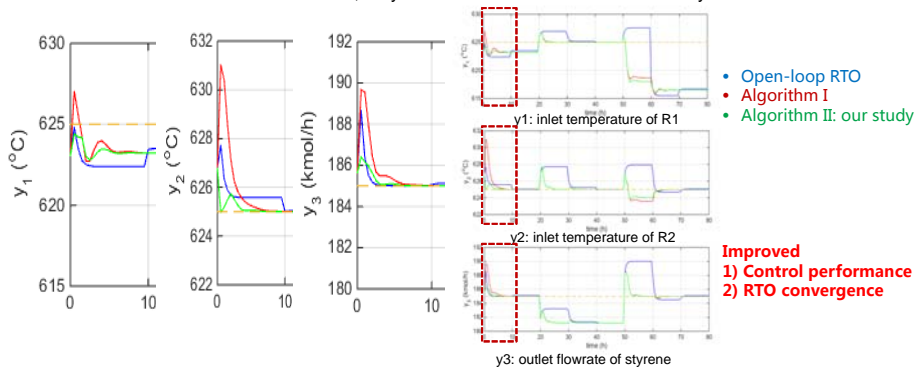
Algorithm II: Real-time optimization and control of an industrial ethylbenzene dehydrogenation process. Chemical Engineering Transaction, 2017 (61) 331-336

Integration of RTO & APC

Implementation

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Integrated Optimization of Process Automation

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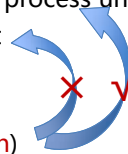
Integration of Scheduling & Operation Optimization

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



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:

Max. Yields of high added-value products

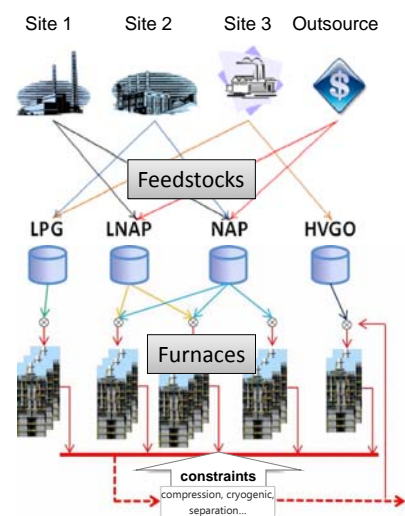
Max. Run-length of furnaces

By

Feedstock selection

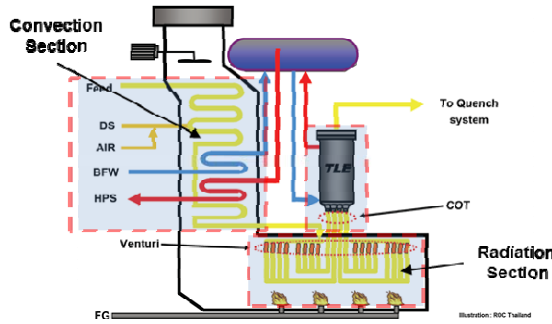
Load dispatching

Operating condition optimization

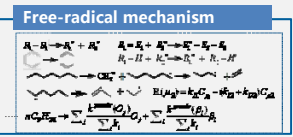


Integration of Scheduling & Operation Optimization

Reaction Kinetics / Reactor Model



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

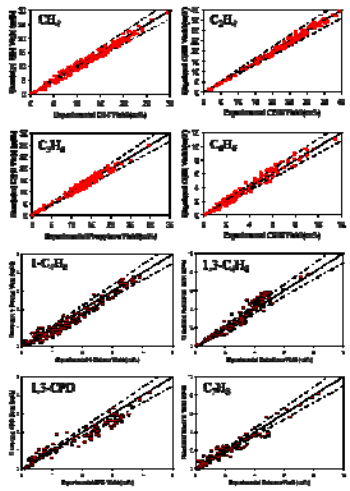
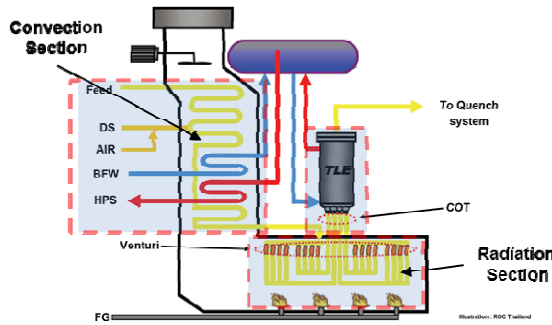


1-D reactor model

$$\frac{dF_i}{dz} = \left(\sum_{j=1}^N \nu_{ij} r_j \right) \Omega$$
$$\sum_j F_j c_p \frac{dT}{dz} = \omega q + \Omega \sum_j r_j (-\Delta H_j)$$
$$-\frac{dp_i}{dz} = a \left(\frac{2f}{d_i} + \frac{\zeta}{\pi r_i} \right) \rho_s u^2 + a \rho_s u \frac{du}{dz}$$

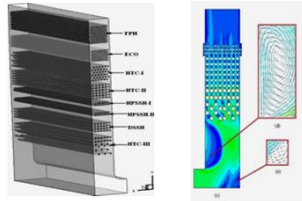
Integration of Scheduling & Operation Optimization

Reaction Kinetics / Reactor Model

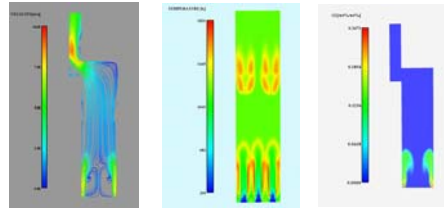


Integration of Scheduling & Operation Optimization

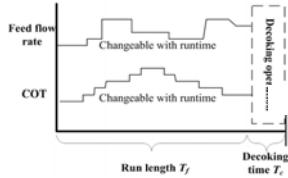
Thermal condition simulation in the furnace



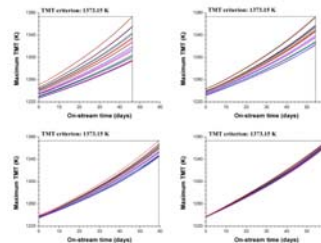
Convection section model



Radiant box model



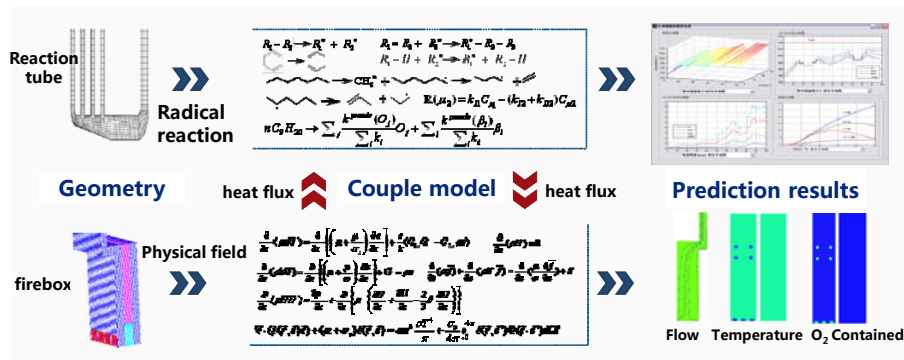
Run length Simulation



Chem. Eng. Sci., 2011, 66(8): 1600-1611; Ind. Eng. Chem. Res. 2013, 52(5): 645-657; AIChE J 2017, 63, (7), 3199-3213

Integration of Scheduling & Operation Optimization

Coupled modeling of furnace and reactor



Coupled simulation of convection section with dual stage steam feed mixing of an industrial ethylene cracking furnace. *Chemical Engineering Journal*, 2016, 286: 436-446
 Impact of flue gas radiative properties and burner geometry in furnace simulations. *AIChE Journal* 2015, 61, (3), 936-954.
 Numerical simulation on flow, combustion and heat transfer of ethylene cracking furnaces. *Chemical Engineering Science*, 2011, 66(8): 1600-1611
Industrial & Engineering Chemistry Research, 2013, 52(2): 645-657

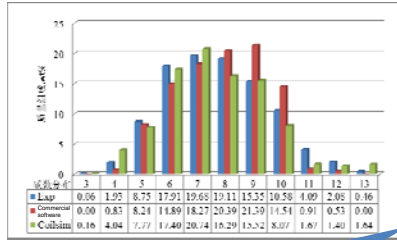
Integration of Scheduling & Operation Optimization

Coupled modeling of furnace and reactor

Sinopec Zhenhai Refining & Chemical Company

BA105 furnace (HCR), BA109 furnace (NAP)

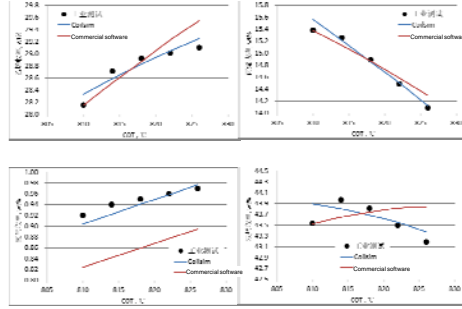
Feedstock molecular reconstruction(NAP)



Full composition analysis of industrial data

(Analyzed by Beijing Research Institute of Chemical Industries)

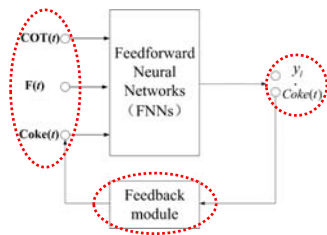
Yields of C₂H₄, H₂, C₃H₆, benzene etc. products (NAP)



Integration of Scheduling & Operation Optimization

Surrogate model of cracking furnace

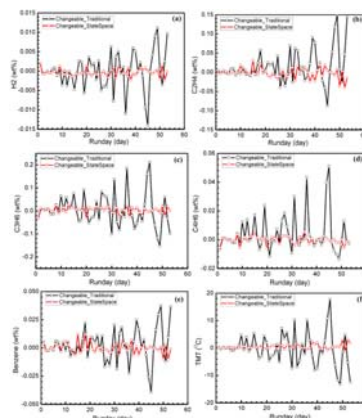
Prediction of change rate of coke thickness



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

$$\begin{cases} \dot{x}_{coke}(t) = f_{ANN}(coke(t), COT(t), F(t)) \\ y_i(t) = g_{ANN}(coke(t), COT(t), F(t)) \\ x_{coke}(t+1) = x_{coke}(t) + \dot{x}_{coke}(t) \cdot T_s(t) \\ x_{coke}(1) = x_{coke,ini} \end{cases}$$

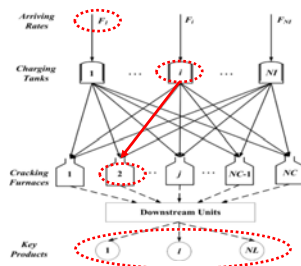
Prediction of product yield and KPI



Comparison with traditional surrogate model

Integration of Scheduling & Operation Optimization

Integration of cyclic scheduling & operation optimization



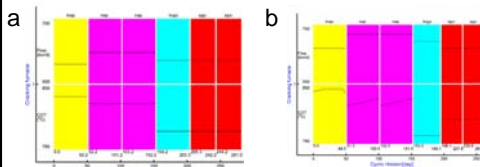
$$\max obj^{NS} = \sum_{i,j} \left[\beta_{ij} \left[\sum_{t=1}^{T_{ij}} \left(\sum_{k=1}^{N_k} u_{F_{ij,k}}(t) \cdot y_{ij}(t) \cdot P_{ij}(t) - C_{S_{ij}} \right) \right] - \delta \cdot \sum_{i,j} SV_i^2 \right]$$

$$\begin{cases} \dot{x}_{c_{take},ij}(t) = f_{ij}(x_{c_{take},ij}(t), u_{COT,ij}(t), H_{F_{ij}}(t)) \\ y_{ij}(t) = g_{ij}(x_{c_{take},ij}(t), u_{COT,ij}(t), H_{F_{ij}}(t)) \\ TMT_{ij}(t) = g_{COT,ij}(x_{c_{take},ij}(t), u_{COT,ij}(t), H_{F_{ij}}(t)) \end{cases}$$

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

$$T_{ij} = n_{ij} \cdot (t_{ij} + t_{ij}^0) \quad \forall i, j \quad \sum T_{ij} \leq H \quad \forall j$$

$$H \geq 0, t_{ij} \geq 0, T_{ij} \geq 0, \varepsilon \leq n_{ij} \leq NK, \quad \forall i, j, w_{ij} \in \{0,1\} \quad \forall i, j, k.$$



- a. Traditional cyclic scheduling
- b. Cyclic scheduling with operation optimization

Day mean profit increases by 13.5%

Industrial & Engineering Chemistry Research, 2015, 54 (15), 3844-3854 ; Chemical Engineering & Technology, 2015, 38 (5), 900-906;
Chinese Journal of Chemical Engineering, 2013 21(5): 537-543 Knowledge-Based Systems, 2016, 96(C):156-170

Integration of Scheduling & Operation Optimization

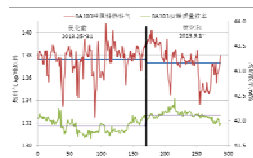
Implementation results

Applied in Shanghai Petrochemical :

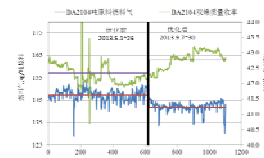
- Average yield of ethylene and propylene increased by 0.187% ;
- Fuel consumption reduced by 1.806kg/t(feedstock), i.e. 1.64% under same feedstock load.



Sinopec Shanghai Petrochemical Company Limited



Comparison of yields and fuel gas consumption of BA103 before and after optimization

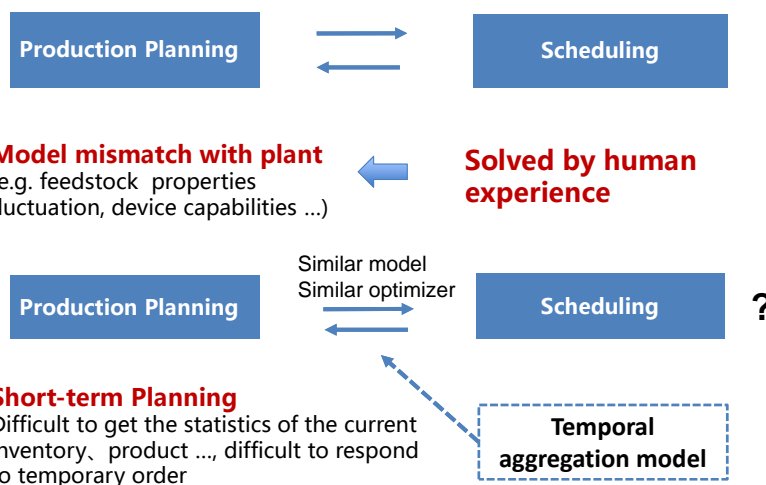


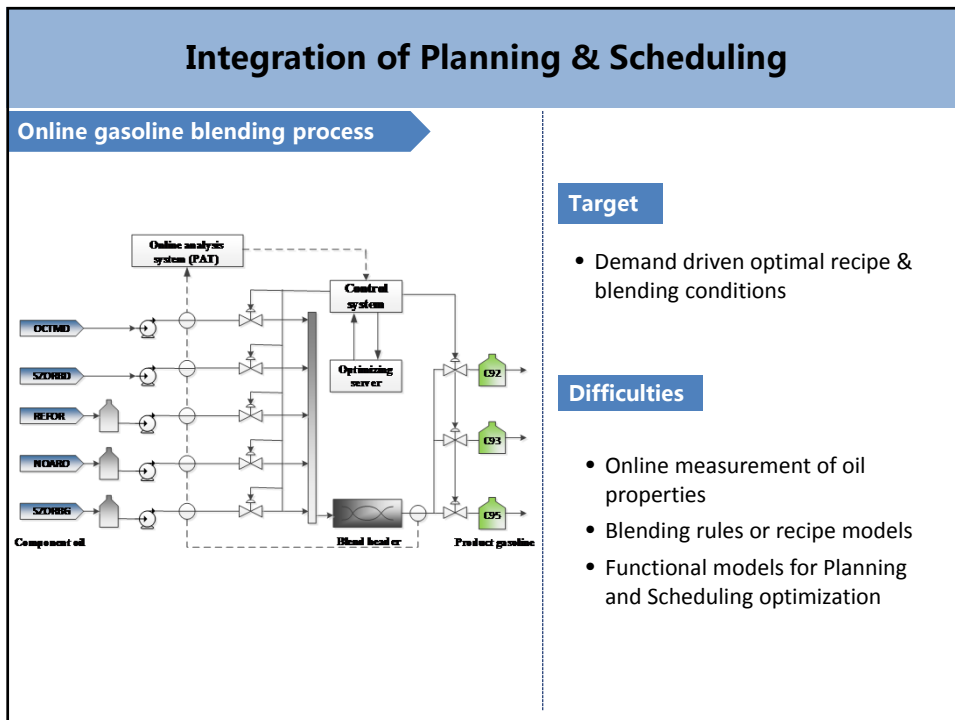
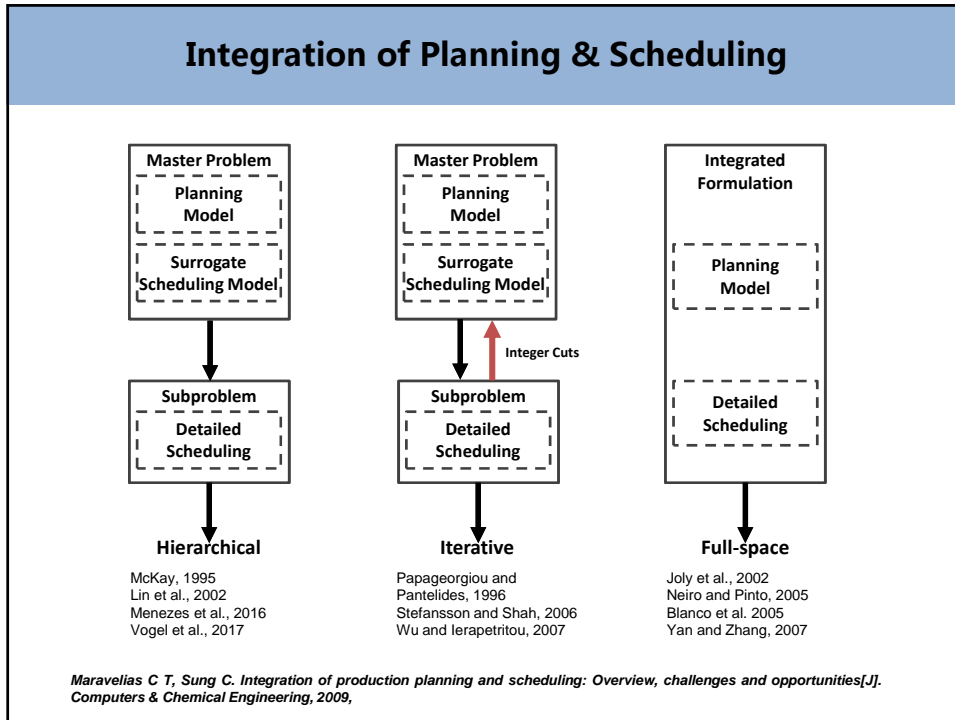
Comparison of yields and fuel gas consumption of BA2104 before and after optimization

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 Planning & Scheduling





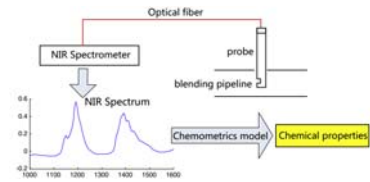
Integration of Planning & Scheduling

Online measurement of oil properties

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

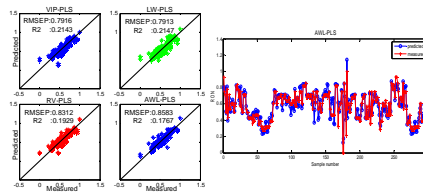
Response to change of operating conditions

- 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



Model	R ²	RMSEP
VIP-PLS	0.7916	0.2143
RV-PLS	0.8312	0.1929
LW-PLS	0.7913	0.2147
AWL-PLS	0.8583	0.1767

Integration of Planning & Scheduling

NIR spectral analysis and modeling

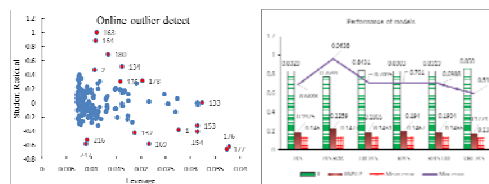
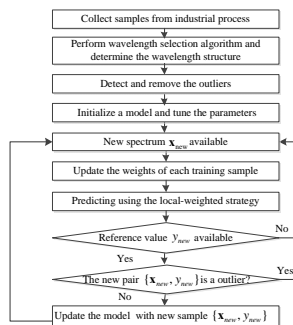
Adaptive strategies for online model update (ORL-PLS)

Outlier detection

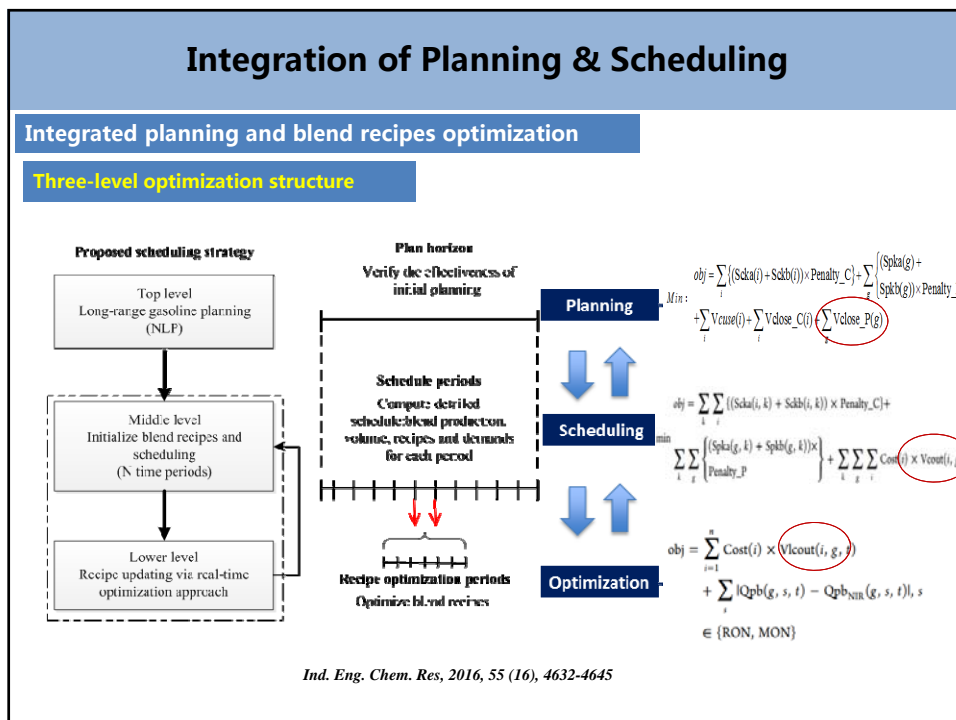
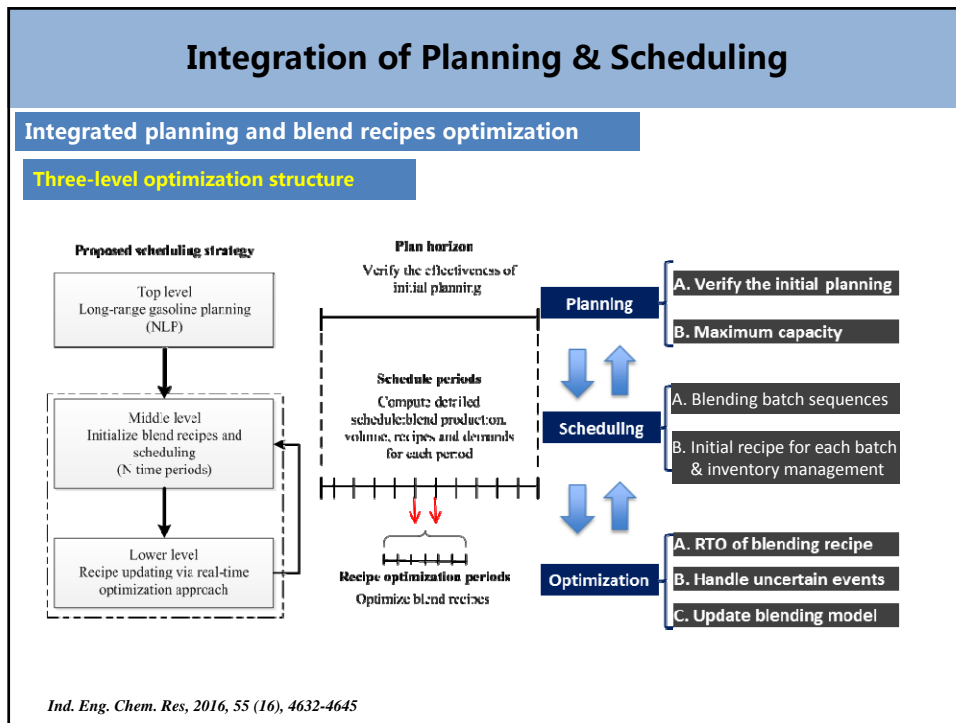
Locally weighted learning

Improved recursive strategy

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



Model	R ²	RMSEP	Mean-error	Max-error
PLS	0.8329	0.1925	0.1460	0.6888
PLS-Bias	0.7699	0.2259	0.1477	0.9638
LW-PLS	0.8431	0.1865	0.1451	0.7095
RPLS	0.8303	0.1940	0.1467	0.7010
RPLS-OD	0.8313	0.1934	0.1465	0.6988
ORL-PLS	0.8580	0.1774	0.1338	0.5933



Integration of Planning & Scheduling

Integrated planning and blend recipes optimization

The necessity for integration

Blend recipe calculated by scheduling level

Period	1	2	3	4	5	6	7
SZORBD	0.152	0.443	0.444	0.445	0.48	0.444	0.14
OCTMD	9.76E-04	0.364	0.184	0.349	0.375	0.139	0.694
REFOR	0.349	0.152	0.195	0.157	0.006	0.213	4.34E-04
NOARO	0.444	0.017	0.175	0.025	0.009	0.2	0.035
SZORBG	0.053	0.023	0.002	0.024	0.13	0.004	0.13

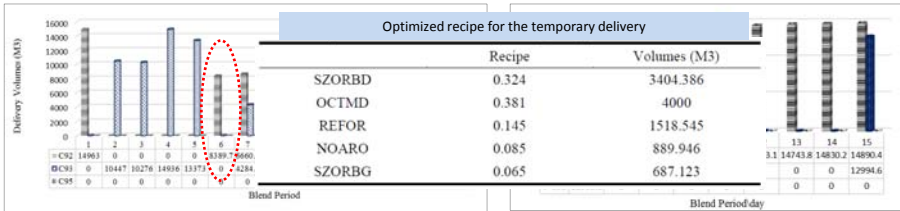
Period	8	9	10	11	12	13	14	15
SZORBD	0.444	0.441	0.444	0.223	0.444	0.403	0.44	0.44
OCTMD	0.152	0.363	0.049	0.606	0.147	0.459	0.175	0.173
REFOR	0.208	0.068	0.258	0.04	0.212	0.001	0.199	0.201
NOARO	0.192	0.004	0.248	0.001	0.195	0.008	0.183	0.184
SZORBG	0.003	0.123	0.002	0.13	0.002	0.128	0.003	0.003

blend recipes by Real-time optimization

1	2	3	4	5	6	7
SZORBD	0.449	0.446	0.45	0.448	0.45	0.449
OCTMD	0.276	0.275	0.277	0.276	0.277	0.358
REFOR	0.126	0.169	0.124	0.127	0.167	0.109
NOARO	0.108	0.068	0.108	0.108	0.065	0.017
SZORBG	0.041	0.041	0.041	0.041	0.041	0.1

8	9	10	11	12	13	14	15
SZORBD	0.443	0.456	0.448	0.401	0.45	0.449	0.448
OCTMD	0.289	0.301	0.276	0.378	0.277	0.276	0.276
REFOR	0.13	0.119	0.169	0.107	0.124	0.125	0.127
NOARO	0.038	0.024	0.065	0.015	0.108	0.108	0.107
SZORBG	0.099	0.1	0.041	0.099	0.041	0.041	0.041

Response to temporary delivery

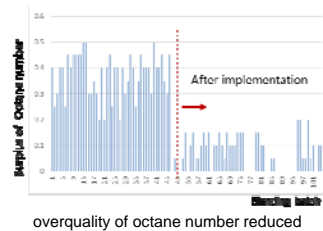


Integration of Planning & Scheduling

Integrated planning and blend recipes optimization

Implementation Results :

- Jinling Pec. (3.6Mt/a Gasoline product) in Nanjing City as validation
 - 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**.



Embedded AI



Embedded CI



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

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Thanks for your attention