4.3 Dynamic Real-Time Optimization

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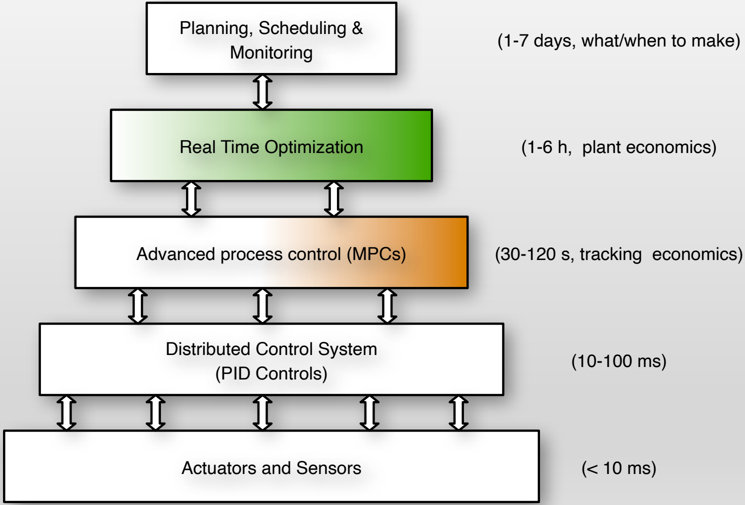
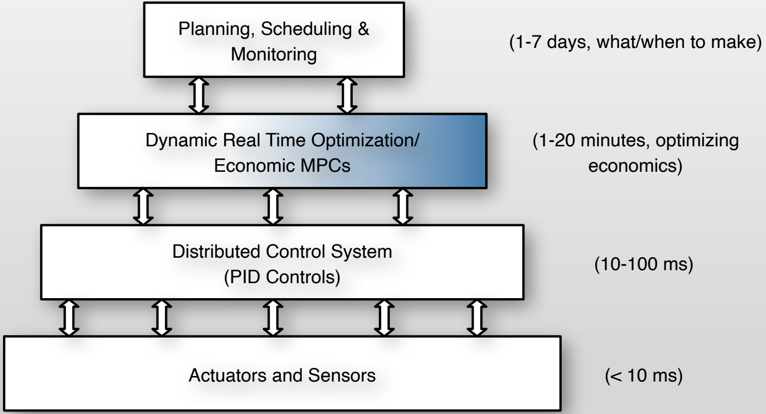
Outline

Hierarchical scheme of optimization, monitoring and control



Revised hierarchical architecture



Dynamic real-time optimization

Motivations and goals

Motivations

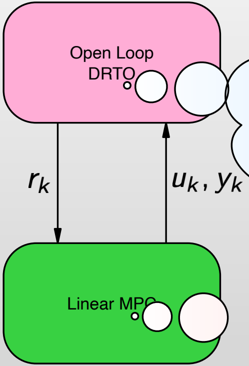
- Process plants are operating in an increasingly global and dynamic environment
- Account for transient behavior in the determination of economically optimal operating policies
- Inconsistency between the RTO and control layers (offset-free strategies needed)

Goals

- Optimize plant economics dynamically, taking into account changes in plant parameters (e.g. raw materials, energy price, throughput, etc.)
- Meet operating constraints

Two-layer approaches

Open-loop DRTO / MPC



Moving Horizon Open-Loop Dynamic Optimization

$$\min_{\mathbf{x},\mathbf{u},\mathbf{r}} \sum_{i=0}^{N-1} \ell(r_i, u_i)$$

subject to:

$$\begin{aligned} x_0 &= x(k) \\ x_{i+1} &= f(x_i, u_i), && i = 0, \dots, N-1 \\ r_i &= h(x_i, u_i), && i = 0, \dots, N-1 \\ r_i &\in \mathbb{Y}, \quad u_i \in \mathbb{U}, && i = 0, \dots, N-1 \end{aligned}$$

Tracking Linear MPC

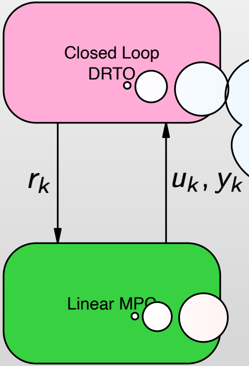
$$\min_{\mathbf{x},\mathbf{u}} \sum_{i=0}^{N-1} \|y_i - r_i\|_Q^2 + \|\Delta u_i\|_R^2$$

subject to:

$$\begin{aligned} x_0 &= x(k) \\ x_{i+1} &= Ax_i + Bu_i, && i = 0, \dots, N-1 \\ y_i &= Cx_i, && i = 0, \dots, N-1 \\ y_i &\in \mathbb{Y}, \quad u_i \in \mathbb{U}, && i = 0, \dots, N-1 \end{aligned}$$

Two-layer approaches

Closed-loop DRTO / MPC



Moving Horizon Closed-Loop Dynamic Optimization

$$\min_{\mathbf{x},\mathbf{r}} \sum_{i=0}^{N-1} \ell(r_i, u_i^{MPC})$$

subject to:

$$x_0 = x(k)$$
$$x_{i+1} = f(x_i, u_i^{MPC}), \quad i = 0, \ldots, N-1$$
$$y_i = h(x_i), \quad i = 0, \ldots, N-1$$
$$r_i \in \mathbb{Y}, \quad u_i^{MPC} \in \mathbb{U}, \quad i = 0, \ldots, N-1$$

Tracking Linear MPC

$$\min_{\mathbf{x},\mathbf{u}} \sum_{i=0}^{N-1} \|y_i - r_i\|_Q^2 + \|\Delta u_i\|_R^2$$

subject to:

$$x_0 = x(k)$$
$$x_{i+1} = Ax_i + Bu_i, \quad i = 0, \ldots, N-1$$
$$y_i = Cx_i, \quad i = 0, \ldots, N-1$$
$$y_i \in \mathbb{Y}, \quad u_i \in \mathbb{U}, \quad i = 0, \ldots, N-1$$

Single-layer approaches

Economic MPC

$$\min_{\mathbf{x},\mathbf{y}} \sum_{i=0}^{N-1} \ell(y_i, u_i)$$

subject to:

Economic NonLinear MPC

$$x_0 = x(k)$$

$$x_{i+1} = f(x_i, u_i), \qquad i = 0, \ldots, N-1$$

$$y_i = h(x_i), \qquad i = 0, \ldots, N-1$$

$$y_i \in \mathbb{Y}, \qquad u_i \in \mathbb{U}, \qquad i = 0, \ldots, N-1$$

NMPC formulation for reference tracking

Nominal formulation

Finite-horizon optimal control problem

$$\min_{\mathbf{x},\mathbf{u}} \|x_N - x_s\|_P^2 + \sum_{i=0}^{N-1} \|y_i - x_s\|_Q^2 + \|u_i - u_s\|_R^2 \qquad \text{subject to:}$$

$$x_0 = x(k)$$

$$x_{i+1} = f(x_i, u_i), \qquad y_i = h(x_i) \qquad i = 0, \ldots, N-1$$

$$y_i \in \mathbb{Y}, \qquad u_i \in \mathbb{U}, \qquad i = 0, \ldots, N-1$$

Equilibrium target

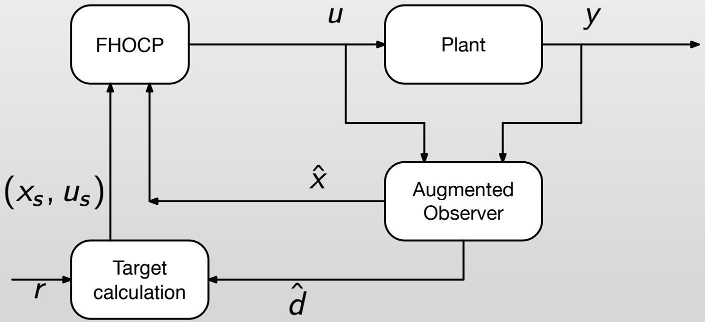
$$\min_{x_s, u_s, y_s} \|y_s - r\|_T^2 \qquad \text{subject to:}$$

$$x_s = f(x_s, u_s), \qquad y_s = h(x_s)$$

$$y_s \in \mathbb{Y}, \qquad u_s \in \mathbb{U}$$

NMPC formulation for reference tracking

Offset-free formulation: block diagram



NMPC formulation for reference tracking

Offset-free formulation: augmented model

Nominal and augmented model

- **Nominal** model:

$$x^+ = f(x, u)$$
$$y = h(x)$$

- **Augmented** model:

$$x^+ = F(x, d, u)$$
$$d^+ = d$$
$$y = H(x, d)$$

with **consistent dynamics**: $F(x, 0, u) = f(x, u)$ and $H(x, 0) = h(x)$

NMPC formulation for reference tracking

Offset-free formulation: target calculation

Equilibrium target

$$\min_{x_s, u_s, y_s} \|y_s - r\|_T^2 \qquad \text{subject to:}$$

$$x_s = F(x_s, \hat{d}_{k|k}, u_s), \quad y_s = H(x_s, \hat{d}_{k|k})$$

$$y_s \in \mathbb{Y}, \qquad u_s \in \mathbb{U}$$

NMPC formulation for reference tracking

Offset-free formulation: FHOCP

Finite-horizon optimal control problem

$$\min_{\mathbf{x},\mathbf{u}} \|x_N - x_s\|_P^2 + \sum_{i=0}^{N-1} \|H(x_i, \hat{d}_{k|k}) - y_s\|_Q^2 + \|u_i - u_s\|_R^2 \qquad \text{subject to:}$$

$$x_0 = \hat{x}_{k|k}$$

$$x_{i+1} = F(x_i, \hat{d}_{k|k}, u_i), \qquad i = 0, \dots, N-1$$

$$H(x_i, \hat{d}_{k|k}) \in \mathbb{Y}, \qquad u_i \in \mathbb{U}, \qquad i = 0, \dots, N-1$$

Economic MPC

Standard formulation

FHOCP where $\ell(\cdot)$ is **economic cost function**

$$\min_{\mathbf{x},\mathbf{u}} \sum_{i=0}^{N-1} \ell(H(x_i), u_i) \qquad \text{subject to:}$$

$$x_0 = x(k)$$

$$x_{i+1} = f(x_i, u_i), \qquad i = 0, \ldots, N-1$$

$$H(x_i) \in \mathbb{Y}, \qquad u_i \in \mathbb{U}, \qquad i = 0, \ldots, N-1$$

About the cost function

- $\ell(\cdot)$ measures the process economics during transient, not deviation from setpoints, which don't exist

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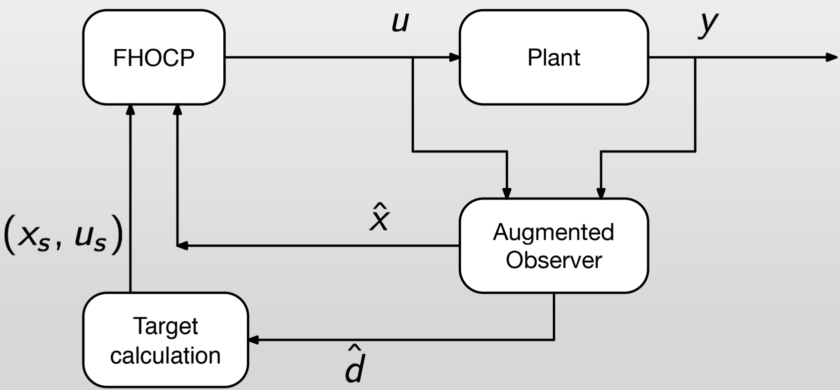
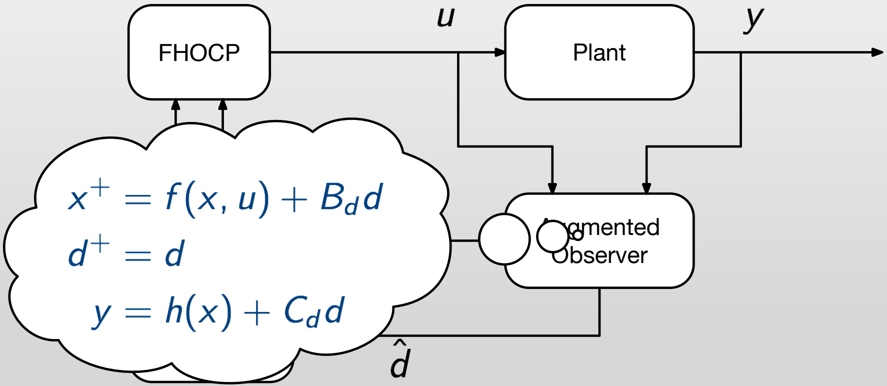
Economic MPC

Offset-free formulation



Economic MPC

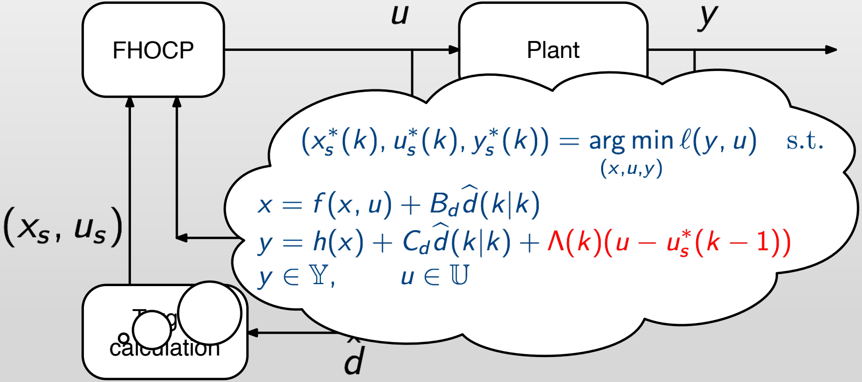
Offset-free formulation



$$x^{+} = f(x,u) + B_d d$$
$$d^{+} = d$$
$$y = h(x) + C_d d$$

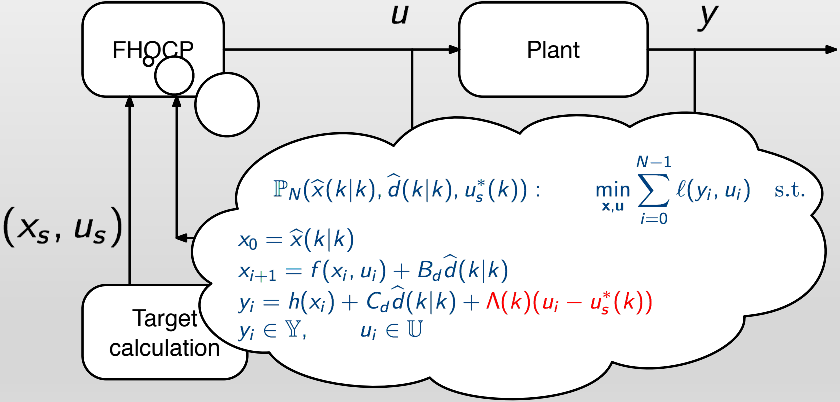
Economic MPC

Offset-free formulation



Economic MPC

Offset-free formulation



Open-source software tool for NMPC

Presentation

https://github.com/CPCLAB-UNIPI/MPC-code

Welcome to the MPC-code!

We present a multipurpose, easy-to-use code for Model Predictive Control (MPC) design, analysis and simulation. The major goal of this code is to provide the user with a general, versatile MPC framework that can be adapted to problems in different areas...

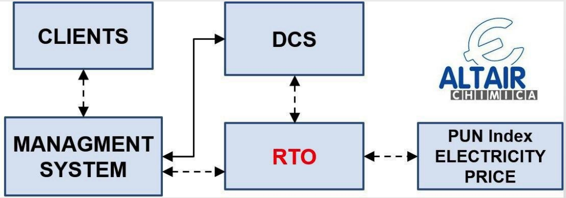
- **Python** Amply validated, fast, easy-to-use, open-source, customization.
- **CasADi** Open-source symbolic calculation through algorithmic differentiation, numeric optimization oriented.
- **IPOPT** Standard in the class of open-source nonlinear programming (NLP) solvers.

Industrial case study

Problem definition: project scheme

Enhancing the factory management of **Altair Chimica SPA** with:

automation, digitalization, machine learning and *process computerization*



Project major components

- **Management System**: handle the orders from clients and make the sale plan by hand
- Distributed Control System (**DCS**)

Goals

Develop a **RTO system** to model and **optimally schedule** the production plan

- exchange input and output data with the DCS at fixed times
- hierarchically superior to controllers: works as a **fully automatic operator**

Industrial case study

Problem definition: Nomenclature

n_p products. Each j-th has

- Production rate: $x_j = [x_j^0, \dots, x_j^i, \dots, x_j^{n_h-1}]$
- Sales plan: $S_j = [S_j^0, \dots, S_j^i, \dots, S_j^{n_h-1}]$

n_h are the hours in the **optimization horizon**, i.e. $n_h = 24 \times 7 = 168$ h in a week.

Sales plan features

- From the selling department and used within the problem as **input parameters**
- Defining $t_{s,d}$, with $d = 1, \dots, 7$ as the selling time of each day
  - the only non-zero components of S_j are the ones for $i = t_{s,d}$
  - sale is satisfied iff the stock of product j contains enough material at time $t_{s,d}$

Batch vs Continuous products

- $n_b < n_p$ products are produced with batch reactors
- The corresponding x_j is zero throughout most of the horizon

Industrial case study

Problem definition: Nomenclature

Storable vs Non-Storable products

Storable

- Stock of product j is **function of x_j and S_j**
- Stock is **bounded by physical constraints**
- **Mass balance** from the initial stock σ_j^0:

$$\sigma_j^{i+1} = \sigma_j^i + x_j^i - S_j^i - a_j(x)^i \quad \forall\, i = 0, \dots, n_h$$

Non-Storable

- Some products cannot be stocked due to specific **safety or logistic reasons**
- **Cannot be stocked or sold** $\rightarrow$ must be consumed within the facility
- **Mass balance** collapse to:

$$0 = x_j^i - a_j(x)^i \quad \forall\, i = 0, \dots, n_h$$

Self-consumption $a_j(x)$

Some of the products are **consumed** within the industrial site **to obtain other chemicals**

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Industrial case study

Batch Scheduling: the methodology through an example

The sales plan

	$t_{s,1}$	$t_{s,2}$	$t_{s,3}$	$t_{s,4}$	$t_{s,5}$	$t_{s,6}$	$t_{s,7}$
P_1	0	$S_{P_1}^{t_{s,2}}$	0	$S_{P_1}^{t_{s,4}}$	0	0	0
P_2	0	0	0	$S_{P_2}^{t_{s,4}}$	0	0	0
P_3	0	0	0	0	$S_{P_3}^{t_{s,5}}$	0	0

Example

- 7-day plan
- 3 batch products and 3 reactors
- All initial stocks empty

$t_{s,2}$

	Day 1	Day 2	Day 3	Day 4	Day 5	Day 6	Day 7
R_1							
R_2							
R_3							

Industrial case study

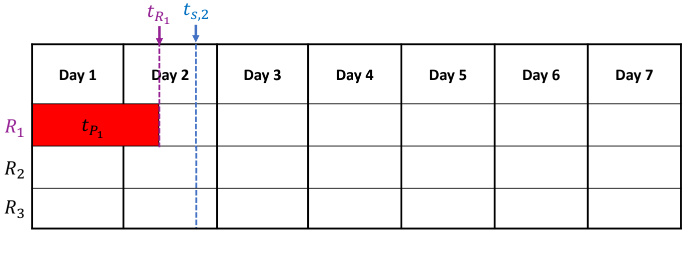
Batch Scheduling: the methodology through an example

The sales plan

	$t_{s,1}$	$t_{s,2}$	$t_{s,3}$	$t_{s,4}$	$t_{s,5}$	$t_{s,6}$	$t_{s,7}$
P_1	0	$S_{P_1}^{t_{s,2}}$	0	$S_{P_1}^{t_{s,4}}$	0	0	0
P_2	0	0	0	$S_{P_2}^{t_{s,4}}$	0	0	0
P_3	0	0	0	0	$S_{P_3}^{t_{s,5}}$	0	0

Comments

- Consider $S_{P_1}^{t_{s,2}} > W_P$
- 1 batch reaction for P_1 in R_1
- Reactor time $t_{R_1} < t_{s,2} \rightarrow$ ✓



Industrial case study

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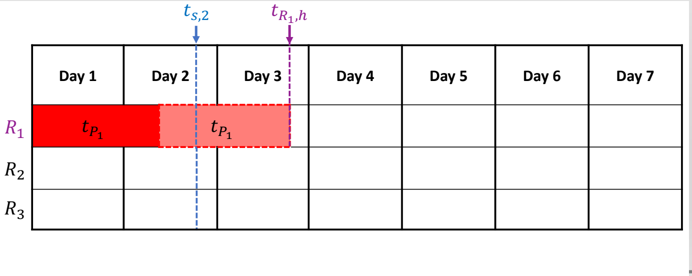
The sales plan

	$t_{s,1}$	$t_{s,2}$	$t_{s,3}$	$t_{s,4}$	$t_{s,5}$	$t_{s,6}$	$t_{s,7}$
P_1	0	$S_{P_1}^{t_{s,2}}$	0	$S_{P_1}^{t_{s,4}}$	0	0	0
P_2	0	0	0	$S_{P_2}^{t_{s,4}}$	0	0	0
P_3	0	0	0	0	$S_{P_3}^{t_{s,5}}$	0	0

Comments

- $S_{P_1}^{t_{s,2}} > W_P \rightarrow 2^\circ$ batch of P_1 has to be scheduled
- 2° batch reaction for P_1 in R_1
- Tentative reactor time $t_{R_1,h} > t_{s,2} \rightarrow$ ✗



Industrial case study

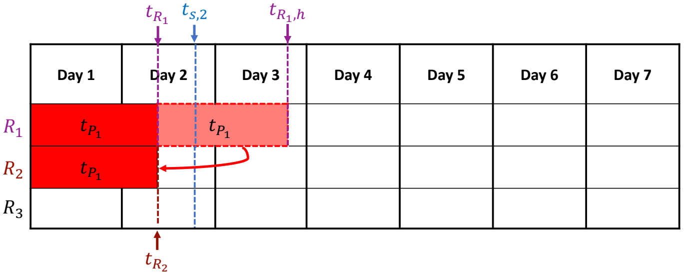
Batch Scheduling: the methodology through an example

The sales plan

	$t_{s,1}$	$t_{s,2}$	$t_{s,3}$	$t_{s,4}$	$t_{s,5}$	$t_{s,6}$	$t_{s,7}$
P_1	0	$S_{P_1}^{t_{s,2}}$	0	$S_{P_1}^{t_{s,4}}$	0	0	0
P_2	0	0	0	$S_{P_2}^{t_{s,4}}$	0	0	0
P_3	0	0	0	0	$S_{P_3}^{t_{s,5}}$	0	0

Comments

- R_2 is enrolled
- 1 batch reaction for P_1 in R_2
- Reactor time $t_{R_2} < t_{s,2} \rightarrow$ ✓



Industrial case study

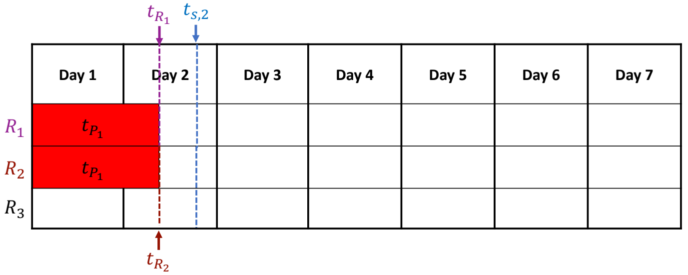
Batch Scheduling: the methodology through an example

The sales plan

	$t_{s,1}$	$t_{s,2}$	$t_{s,3}$	$t_{s,4}$	$t_{s,5}$	$t_{s,6}$	$t_{s,7}$
P_1	0	$S_{P_1}^{t_{s,2}}$	0	$S_{P_1}^{t_{s,4}}$	0	0	0
P_2	0	0	0	$S_{P_2}^{t_{s,4}}$	0	0	0
P_3	0	0	0	0	$S_{P_3}^{t_{s,5}}$	0	0

Comments

- The first sale is satisfied correctly
- $t_{R_1} = t_{P_1}$, $t_{R_2} = t_{P_1}$, $t_{R_3} = 0$



Industrial case study

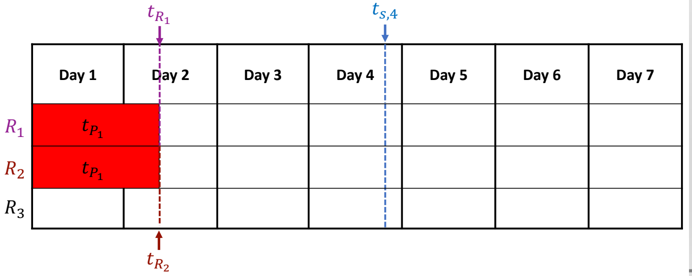
Batch Scheduling: the methodology through an example

The sales plan

	$t_{s,1}$	$t_{s,2}$	$t_{s,3}$	$t_{s,4}$	$t_{s,5}$	$t_{s,6}$	$t_{s,7}$
P_1	0	$S_{P_1}^{t_{s,2}}$	0	$S_{P_1}^{t_{s,4}}$	0	0	0
P_2	0	0	0	$S_{P_2}^{t_{s,4}}$	0	0	0
P_3	0	0	0	0	$S_{P_3}^{t_{s,5}}$	0	0

Comments

- $S_{P_2}^{t_{s,4}} > W_P$ and $S_{P_1}^{t_{s,4}} \leq W_P$
- 2 batch for P_2 and 1 batch for P_1 required
- P_2 has the priority



Industrial case study

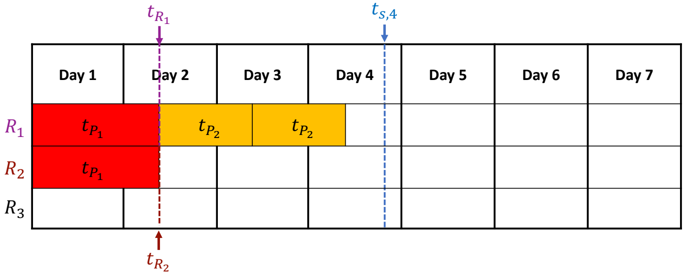
Batch Scheduling: the methodology through an example

The sales plan

	$t_{s,1}$	$t_{s,2}$	$t_{s,3}$	$t_{s,4}$	$t_{s,5}$	$t_{s,6}$	$t_{s,7}$
P_1	0	$S_{P_1}^{t_{s,2}}$	0	$S_{P_1}^{t_{s,4}}$	0	0	0
P_2	0	0	0	$S_{P_2}^{t_{s,4}}$	0	0	0
P_3	0	0	0	0	$S_{P_3}^{t_{s,5}}$	0	0

Comments

- 2 batch reaction for P_2 in R_1
- Reactor time $t_{R_1} + 2 * t_{P_2} < t_{s,4} \rightarrow$ ✓



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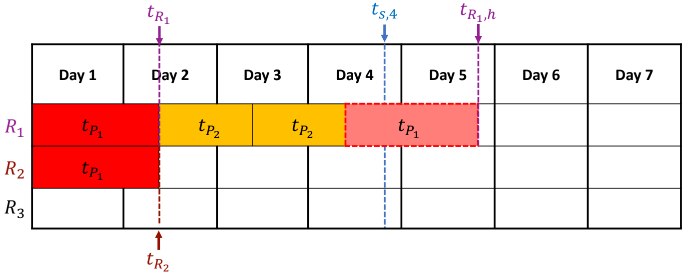
Batch Scheduling: the methodology through an example

The sales plan

	$t_{s,1}$	$t_{s,2}$	$t_{s,3}$	$t_{s,4}$	$t_{s,5}$	$t_{s,6}$	$t_{s,7}$
P_1	0	$S_{P_1}^{t_{s,2}}$	0	$S_{P_1}^{t_{s,4}}$	0	0	0
P_2	0	0	0	$S_{P_2}^{t_{s,4}}$	0	0	0
P_3	0	0	0	0	$S_{P_3}^{t_{s,5}}$	0	0

Comments

- 1 batch reaction for P_1 in R_1
- Tentative reactor time $t_{R_1,h} > t_{s,4} \rightarrow$ ✗



Industrial case study

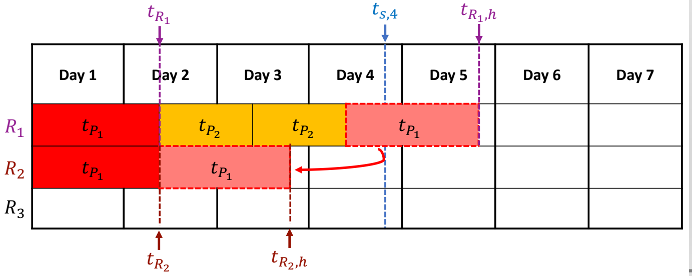
Batch Scheduling: the methodology through an example

The sales plan

	$t_{s,1}$	$t_{s,2}$	$t_{s,3}$	$t_{s,4}$	$t_{s,5}$	$t_{s,6}$	$t_{s,7}$
P_1	0	$S_{P_1}^{t_{s,2}}$	0	$S_{P_1}^{t_{s,4}}$	0	0	0
P_2	0	0	0	$S_{P_2}^{t_{s,4}}$	0	0	0
P_3	0	0	0	0	$S_{P_3}^{t_{s,5}}$	0	0

Comments

- 1 batch reaction for P_1 in R_1
- Tentative reactor time $t_{R_1,h} > t_{s,4} \rightarrow$ ✗
- R_2 is enrolled
- Tentative reactor time $t_{R_2,h} < t_{s,4} \rightarrow$ ✓



Industrial case study

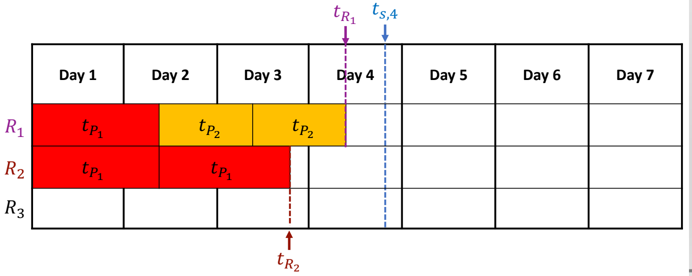
Batch Scheduling: the methodology through an example

The sales plan

	$t_{s,1}$	$t_{s,2}$	$t_{s,3}$	$t_{s,4}$	$t_{s,5}$	$t_{s,6}$	$t_{s,7}$
P_1	0	$S_{P_1}^{t_{s,2}}$	0	$S_{P_1}^{t_{s,4}}$	0	0	0
P_2	0	0	0	$S_{P_2}^{t_{s,4}}$	0	0	0
P_3	0	0	0	0	$S_{P_3}^{t_{s,5}}$	0	0

Comments

- The second sale is satisfied correctly
- $t_{R_1} = t_{P_1} + 2 * t_{P_2}$, $t_{R_2} = 2 * t_{P_1}$, $t_{R_3} = 0$



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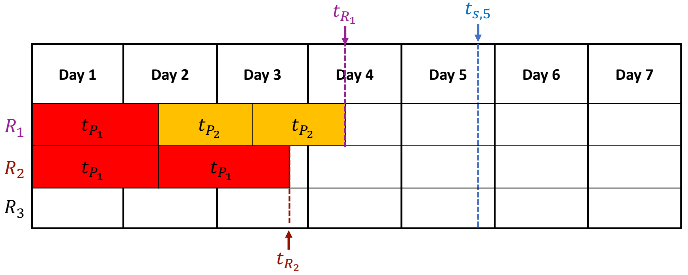
Batch Scheduling: the methodology through an example

The sales plan

	$t_{s,1}$	$t_{s,2}$	$t_{s,3}$	$t_{s,4}$	$t_{s,5}$	$t_{s,6}$	$t_{s,7}$
P_1	0	$S_{P_1}^{t_{s,2}}$	0	$S_{P_1}^{t_{s,4}}$	0	0	0
P_2	0	0	0	$S_{P_2}^{t_{s,4}}$	0	0	0
P_3	0	0	0	0	$S_{P_3}^{t_{s,5}}$	0	0

Comments

- $S_{P_3}^{t_{s,5}} < W_P$
- 1 batch for P_3 required



Industrial case study

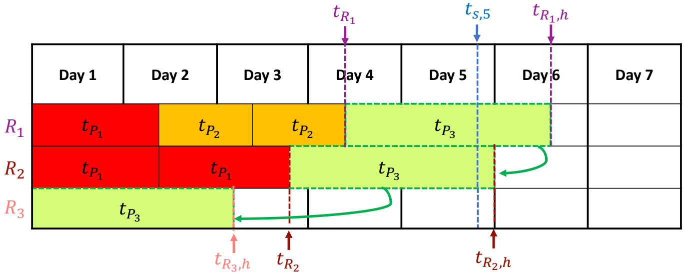
Batch Scheduling: the methodology through an example

The sales plan

	$t_{s,1}$	$t_{s,2}$	$t_{s,3}$	$t_{s,4}$	$t_{s,5}$	$t_{s,6}$	$t_{s,7}$
P_1	0	$S_{P_1}^{t_{s,2}}$	0	$S_{P_1}^{t_{s,4}}$	0	0	0
P_2	0	0	0	$S_{P_2}^{t_{s,4}}$	0	0	0
P_3	0	0	0	0	$S_{P_3}^{t_{s,5}}$	0	0

Comments

- $t_{R_1,h} > t_{s,5} \rightarrow$ ✗
- $t_{R_2,h} > t_{s,5} \rightarrow$ ✗
- R_3 is enrolled $\rightarrow t_{R_3,h} < t_{s,5} \rightarrow$ ✓



Industrial case study

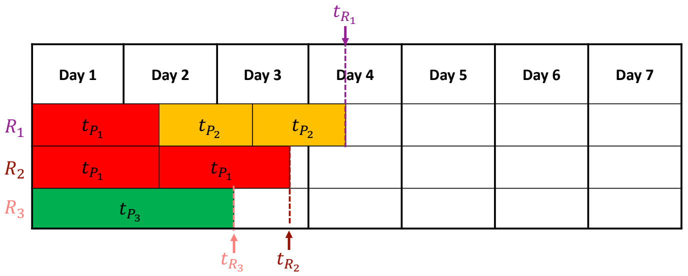
Batch Scheduling: the methodology through an example

The sales plan

	$t_{s,1}$	$t_{s,2}$	$t_{s,3}$	$t_{s,4}$	$t_{s,5}$	$t_{s,6}$	$t_{s,7}$
P_1	0	$S_{P_1}^{t_{s,2}}$	0	$S_{P_1}^{t_{s,4}}$	0	0	0
P_2	0	0	0	$S_{P_2}^{t_{s,4}}$	0	0	0
P_3	0	0	0	0	$S_{P_3}^{t_{s,5}}$	0	0

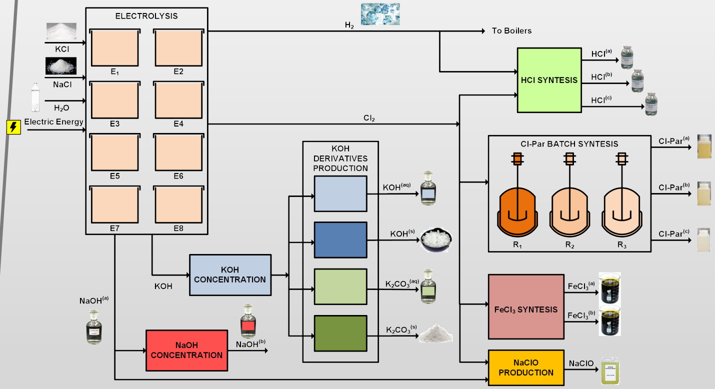
Comments

- All the sals are correctly satisfied
- $t_{R_1} = t_{P_1} + 2 * t_{P_2}$, $t_{R_2} = 2 * t_{P_1}$, $t_{R_3} = t_{P_3}$



Industrial case study

ALTAIR plant for chlorine derivatives



Details

16 products ($n_p = 16$)

- 12 continuous-time
- 1 non-storable and non salable (Cl_2)
- 3 batch ($n_b = 3$)

Optimization horizon

$n_h =$ **168 h**

Decision variables

$n_x = (n_p - n_b)n_h =$ **2184**

Constraints

- 12 on stocks
- 5 safety and others

total along n_h, > 3000

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Dynamic optimization problem details

Soft and *Hard* constraints

- *Soft*:
  - **2 on HCl**: $HCl^{(b)}$ can be sold after dilution to cover sales for missing $HCl^{(a)}$, $HCl^{(c)}$ can be sold after dilution to cover sales for both $HCl^{(a)}$ and $HCl^{(b)}$
  - **1 on $FeCl_3$**: $FeCl_3^{(b)}$ can be sold directly as $FeCl_3^{(a)}$ with a little profit loss
- *Hard*: stock bounds, electrical bounds for production of $NaOH^{(a)}$ and KOH by electrolysis

Objective Function

$$f(x) = \sigma^{n_h}_{HCl^{(a)}} + \sigma^{n_h}_{HCl^{(b)}} + \sigma^{n_h}_{HCl^{(c)}}$$

Initial condition

- $f(x_0) = 18$ tons
- Two types of *hard* constraints are violated

Optimal solution

- $f(x_{opt}) = 39.1$ tons
- Two types of *soft* constraints are violated

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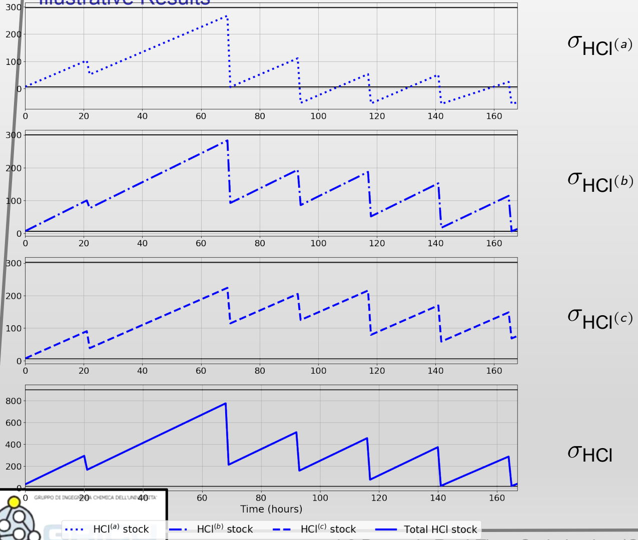
Illustrative Results



Stocks of $HCl^{(a)}$, $HCl^{(b)}$ and $HCl^{(c)}$

Main comments:

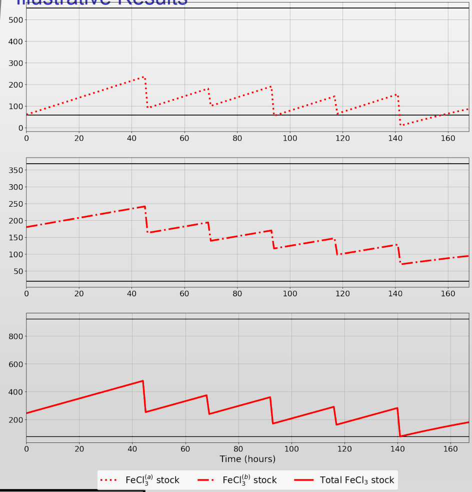
- **Stocks “zigzag” behavior** is given by the sales concentrated on $t_{s,d}$
- **Stock of $HCl^{(a)}$ is lower than the minimum bound** (*soft* constraint)

  ↓ ↓

  $HCl^{(b)}$ or $HCl^{(c)}$ have to be diluted and sold as $HCl^{(a)}$
- **Sum of stocks of the three HCl is ok** (*hard* constraint)

Industrial case study

Illustrative Results



$\sigma_{FeCl_3^{(a)}}$

$\sigma_{FeCl_3^{(b)}}$

σ_{FeCl_3}

Stocks of $FeCl_3^{(a)}$ and $FeCl_3^{(b)}$

Main comments:

- **Stocks "zigzag" behavior** is given by the sales concentrated on $t_{s,d}$
- **Stock of $FeCl_3^{(a)}$ is lower than the minimum bound** (*soft* constraint)

  ↓ ↓

  $FeCl_3^{(b)}$ has to be sold as $FeCl_3^{(a)}$ with a profit loss
- **Sum of stocks of the two $FeCl_3$ is ok** (*hard* constraint)

Industrial case study

Conclusions

- **DRTO algorithm** to best manage production rates based on the sales plan
- **Project** for an integrated digitalization of an industrial site according to **Industry 4.0 paradigms**
- Products continuous vs batch, storable to be sold vs consumed in real-time within the industrial site
- **Preliminary scheduling** procedure for batch productions to avoid MIP
- **A smooth implementation of a LP** to obtain always a numerically feasible solution. The scheduling procedure gives parameters used into the LP
- A post-analysis of the optimal solution gives a **feedback to the operator**
- A key instrument in a full computerization and digitalization project of the company

DRTO: Conclusions

- Direct optimizing control is a promising approach to optimization of dynamic economic performance of chemical processes
- Modeling is about making educated approximations to arrive at a model of acceptable complexity that is adequate for optimization in the presence of uncertainty
- Advances in large-scale nonlinear programming solvers and sensitivity lead to formulation of nonlinear model-based dynamic optimization that are feasibly executed within allowed time
- DRTO/EMPC scheme are likely to replace or at least complement the more conventional hiearchical RTO/LMPC architecture

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