VERTICAL INTEGRATION OF PRODUCTION SCHEDULING AND PROCESS CONTROL

Progress, opportunities and challenges

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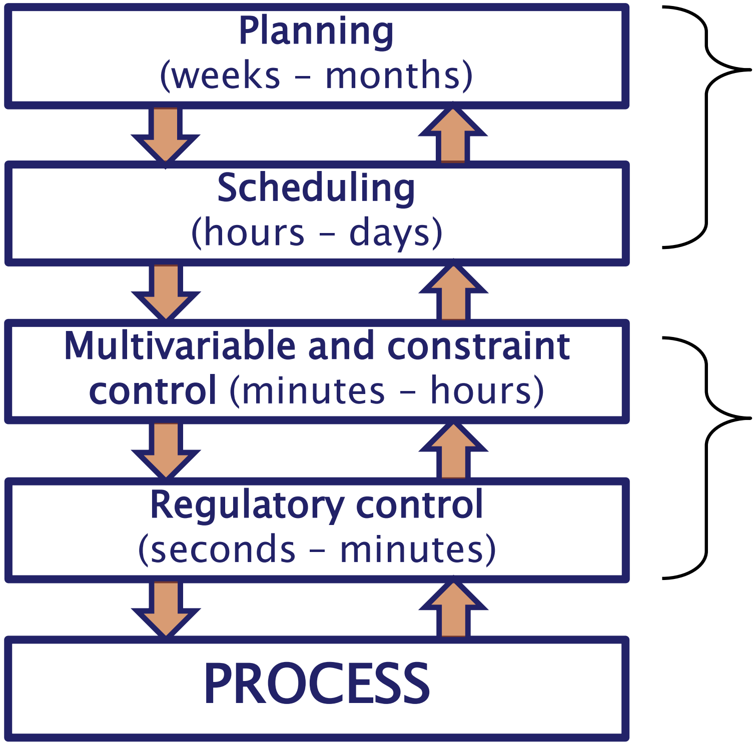
CPC/FOCAPO, Tucson, AZ, January 2017

Hierarchy of Process Operational Decisions



Planning (weeks – months)

Scheduling (hours – days)

Multivariable and constraint control (minutes – hours)

Regulatory control (seconds – minutes)

PROCESS

Production management

- Assume steady-state operation
- Typically carried out off-line
- **Business** function

Control

- Account for dynamics
- Online, in real-time
- **Operational** function

Historically: different time scales afforded separation

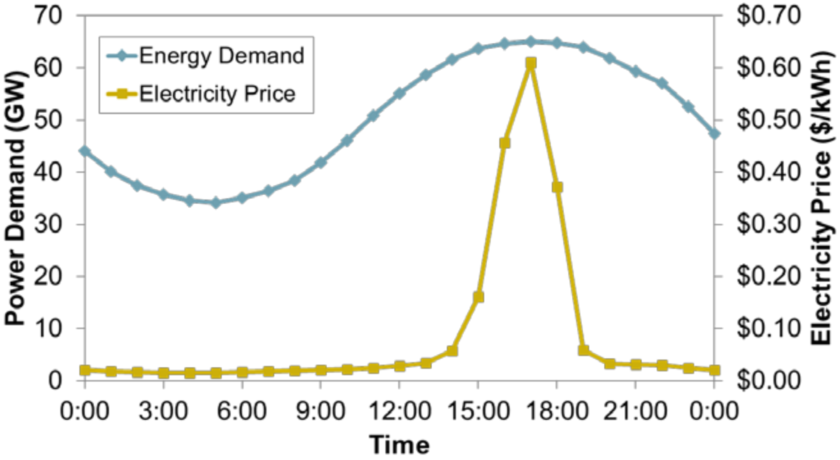
Production management and control carried out independently: different objectives, personnel

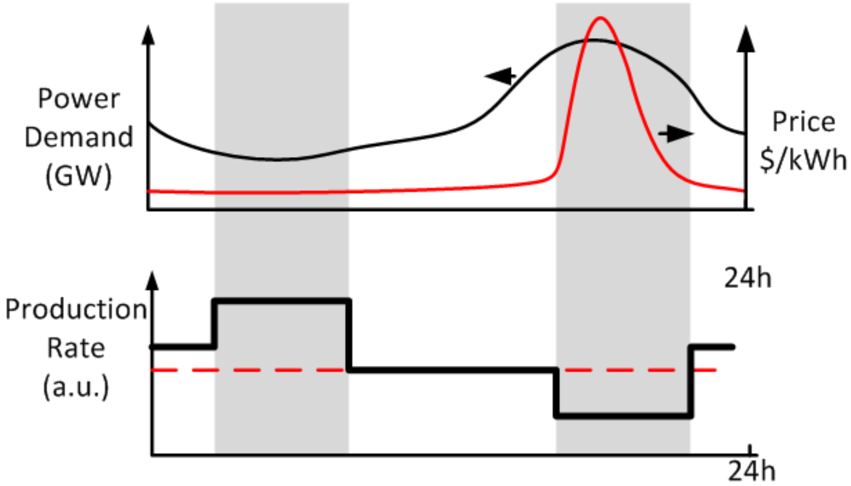
Seborg et al., Wiley, 2010, Baldea and Harjunkoski, Comput. Chem. Eng., 71, 377-390, 2014, Shobrys and White, Comput. Chem. Eng, 26, 149—160, 2002. Zhuge and Ierapetritou, AIChE J. 3304-3319, 2015.

Current Context: Fast-Changing Markets

Examples:

- Power prices can fluctuate considerably during the day
- Refinery can acquire crude from multiple shale wells



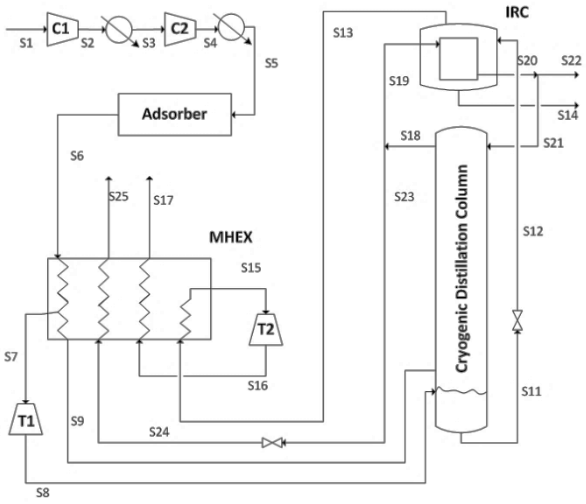


Exploiting these conditions:

- Production schedule features frequent changes in the production rate, product grade
- Use product and/or energy storage

ERCOT demand and day ahead settlement point prices for June 25, 2012 from www.ercot.com

Example: DR Operation of Air Separation Unit

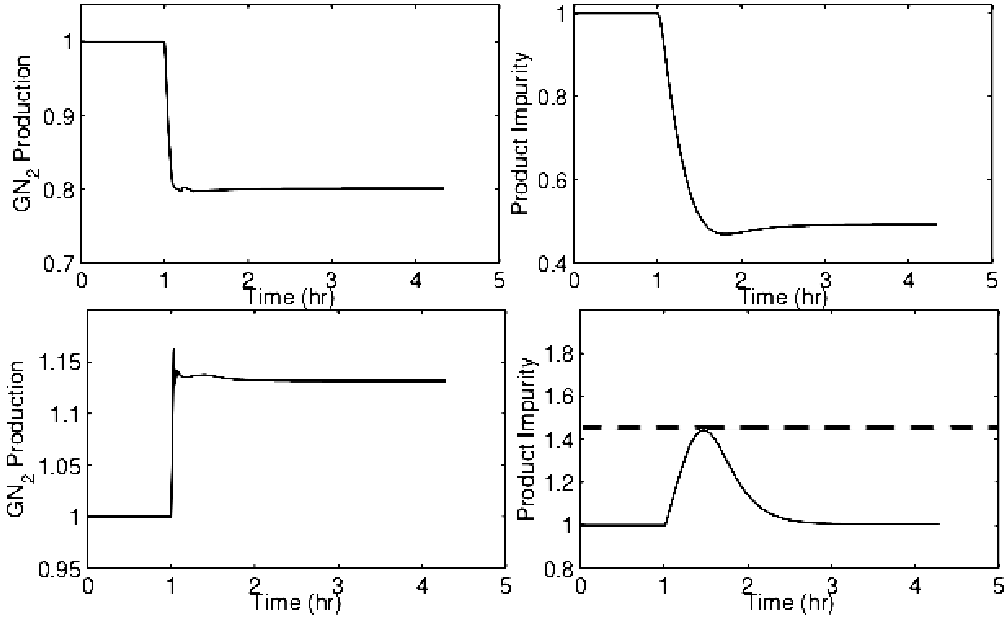


Demand response: production scheduled on an **<u>hourly basis</u>** to account for real-time energy pricing

- Production levels
- Liquid vs. gas products

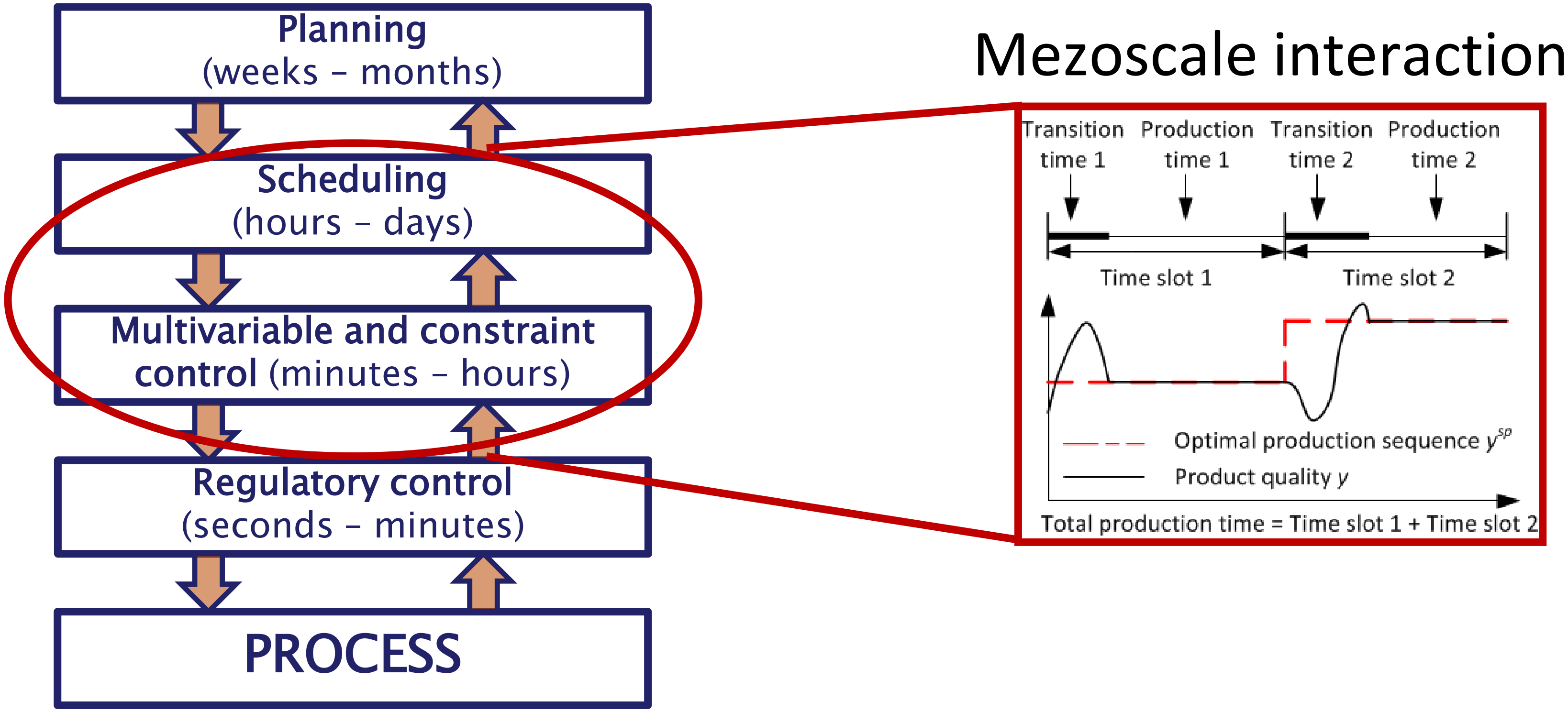
Process dynamics evolve in a comparable time scale

(**<u>time constant ~40 min</u>**)



Ierapetritou et al., Ind. Eng. Chem. Res., 41, 5262-5277, 2002; Miller et al., Ind. Eng. Chem. Res., 47, 1132-1139, 2008; Cao, Swartz, Baldea, Blouin, J. Proc. Contr., 54 (24), 6355–6361, 2015

Vertical Integration of Operation Decisions



Planning
(weeks – months)

Scheduling
(hours – days)

Multivariable and constraint control (minutes – hours)

Regulatory control
(seconds – minutes)

PROCESS

Mezoscale interactions

- Overlap in the time scales of production management and process control motivates considering the integrated problem

Goal: Mechanisms for synchronizing production scheduling with the control system, accounting for dynamics

Slot-Based Scheduling: Conventional

demand

price

static scheduling

sequence $z_{i,s}$

production time t^p_s

Mixed integer program

$$J_{scheduling} = \frac{1}{T_m}\left[\sum_{i=1}^{N_p}\pi_i\omega_i - \sum_{i=1}^{N_p}\sum_{s=1}^{N_s} z_{i,s}c_{storage,i}\left(T_m - t_s^f\right)\omega_i\right]$$

$$t_s^f = t_s^s + \sum_{i=1}^{N_p}\sum_{i'=1}^{N_p} z_{i',s-1}z_{i,s}\boxed{\tau_{i',i}} + t_{i,s}^p \quad t_{i,s}^p \le z_{i,s}T_{\max}^p \quad \forall i,s$$

$$\omega_i = \sum_{s=1}^{N_s} q_s t_{i,s}^p,\ \omega_i > \delta_i \mathrm{T}_m \quad \forall i \quad t_s^s = t_{s-1}^f \quad \forall s \ne 1$$

$$\sum_{s=1}^{N_s} z_{i,s} = 1, \quad \forall i \qquad \sum_{i=1}^{N_p} z_{i,s} = 1, \quad \forall s$$

MIP

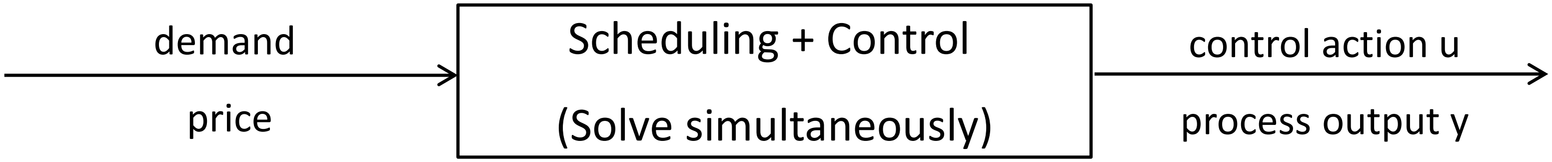
- Sequence $z_{i,s} \in \{0,1\}$
- Production time $\in$ R+

Static:

- Transition time is a pre-determined constant;
- Agnostic to process dynamics.

Pinto and Grossmann, Comput. Chem. Eng. 18 (9), 797-816, 1994

Scheduling and Control: Full Dynamic Approach



demand

price

Scheduling + Control

(Solve simultaneously)

control action u

process output y

Embed dynamic process model in scheduling calculation

$$J_{scheduling} = \frac{1}{T_m}\left[\sum_{i=1}^{N_p} \pi_i \omega_i - \sum_{i=1}^{N_p}\sum_{s=1}^{N_s} z_{i,s} c_{storage,i}\left(T_m - t_s^f\right)\omega_i\right]$$

$$t_s^f = t_s^s + \tau_s + \sum_{i=1}^{N_p} t_{i,s}^p \quad \forall s \qquad t_{i,s}^p \le z_{i,s} T_{\max}^p \quad \forall i, s$$

$$\omega_i = \sum_{s=1}^{N_s} q_s t_{i,s}^p, \; \omega_i > \delta_i \mathrm{T}_m \quad \forall i \qquad t_s^s = t_{s-1}^f \quad \forall s \ne 1$$

$$\sum_{s=1}^{N_s} z_{i,s} = 1, \quad \forall i \qquad \sum_{i=1}^{N_p} z_{i,s} = 1, \quad \forall s$$

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}) + \boldsymbol{G}(\boldsymbol{x})\boldsymbol{u}$$

$$\boldsymbol{y} = \boldsymbol{h}(\boldsymbol{x}) \qquad \boldsymbol{y}(\tau_s) = \sum_i z_{i,s} \boldsymbol{y}_i^{ss}$$

MIDO:

- Sequence $z_{i,s} \in \{0,1\}$
- Production time $\in$ R+
- u $\in$ U $\subset$ R+

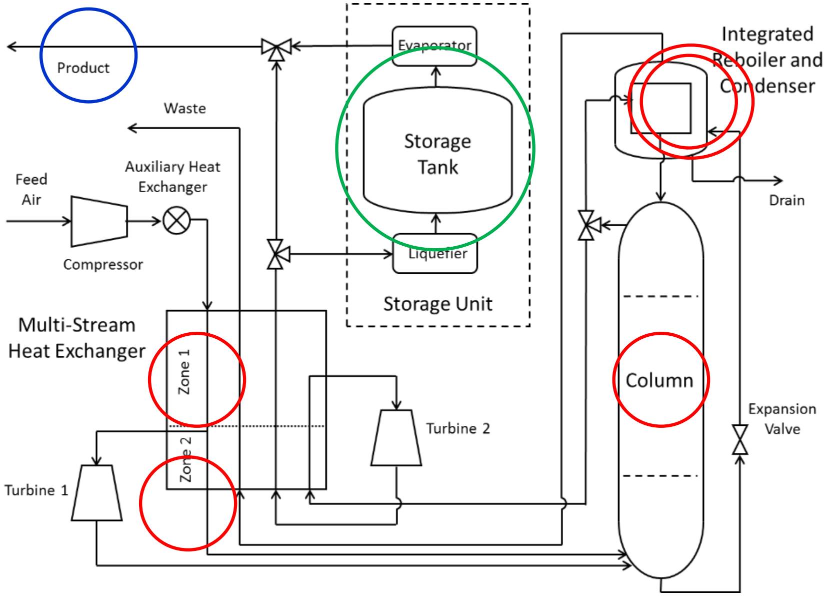
Disadvantages:

- Detailed dynamics: large-scale, computational difficulties
- Open-loop (optimal) control

Air Separation Example (cont'd)

Product Quality Constraints (QCs):

- Product purity (99.8%)
- Production flowrate (20 mol/s)



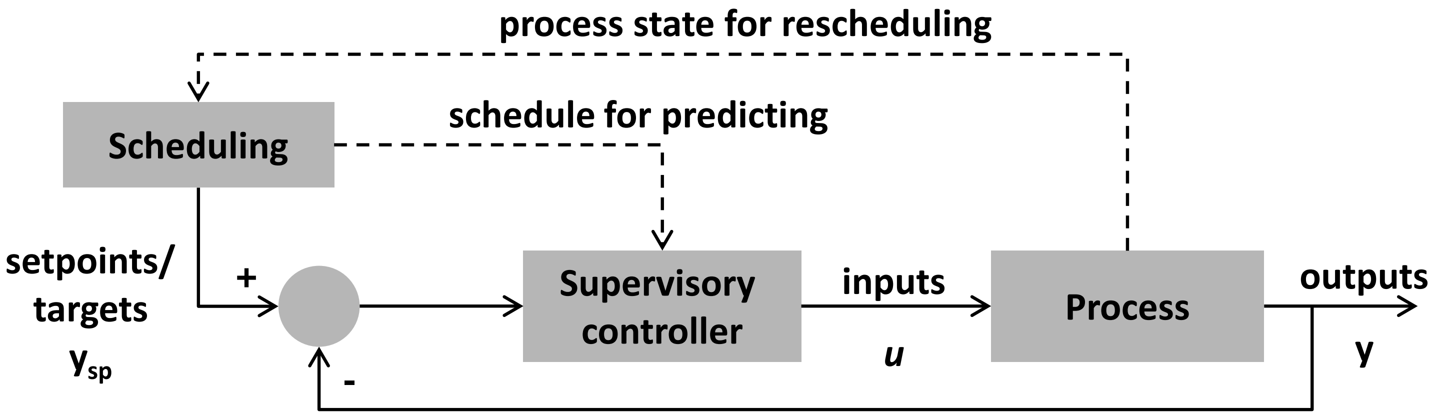
Process Constraints (PCs):

- Prevent tray flooding in the column
- Liquid level in the reboiler does not deplete
- All streams in the first zone of the PHX are in the gas phase
- All streams exiting the second zone of the PHX are in the liquid phase
- The temperature driving force in the reboiler/condenser is above the lower limit

Model: DAE System, 6094 eqns, 430 states, **97 h to solve for 72 h horizon**

Johansson, MSc Thesis, KTH/UT Austin, 2015, Pattison et al., Ind. Eng. Chem. Res., 55, 4562-4584, 2016

Main Challenge



Identify **computationally tractable, scheduling-relevant** representations of the process dynamics:

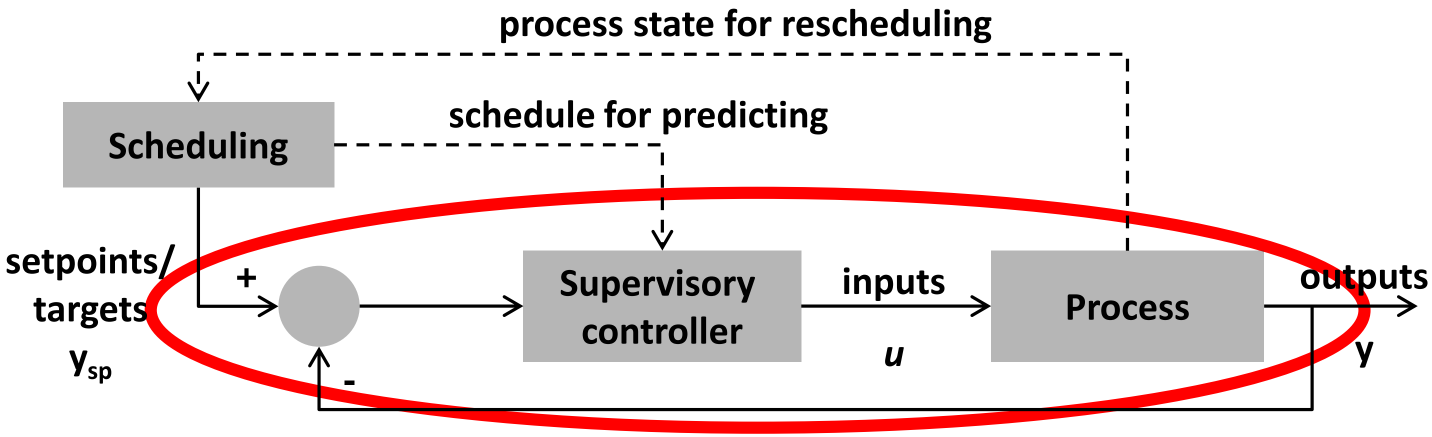
\- Capture **closed-loop** behavior and the presence of a controller

BENEFITS

- Scheduling: become aware of process state/dynamics
- Supervisory Control: become aware of future changes in production; improved response
- Rescheduling

Zhuge and Ierapetritou, Ind. Eng. Chem. Res. 51, 8550−8565, 2012. Baldea and Harjunkoski, Comput. Chem. Eng., 71, 377-390, 2014

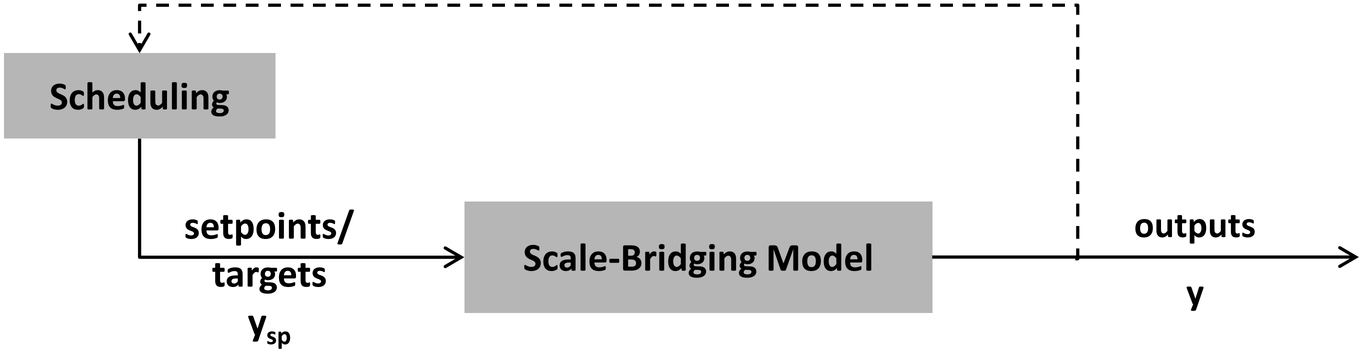
Concept 1: Scale-Bridging Model



Baldea and Harjunkoski, Comput. Chem. Eng., 71, 377-390, 2014

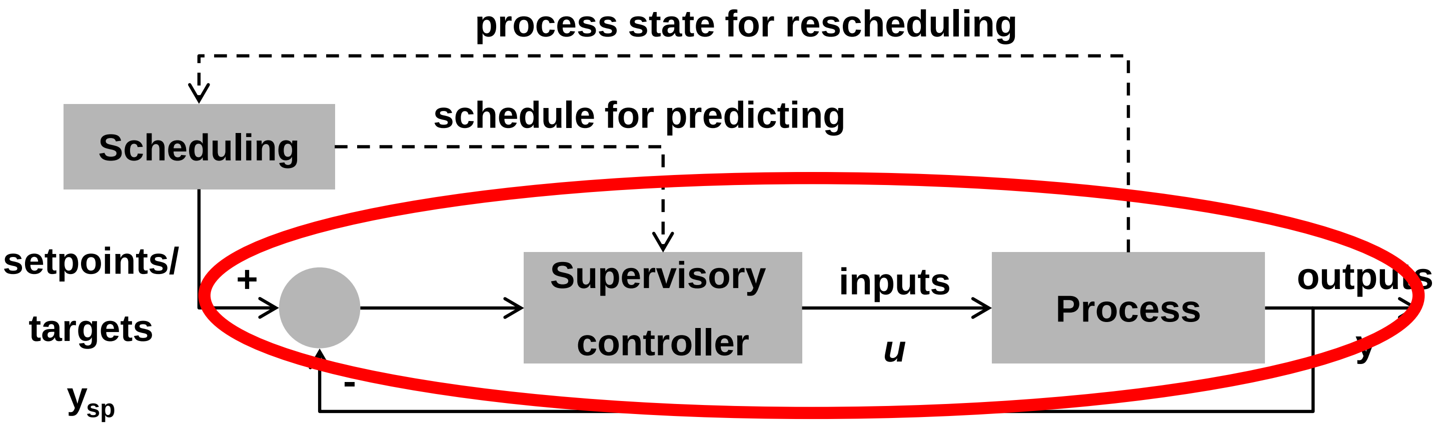
Scale-Bridging Model:

- Capture closed-loop input-output dynamics
- Embed in scheduling calculation



Baldea, Harjunkoski, Park, Du., AIChE J., 2015; Du, Park, Harjunkoski, Baldea. Comput. Chem. Eng., 79, 59-69, 2015

Scale Bridging Models: Challenges



process state for rescheduling

Scheduling

schedule for predicting

setpoints/ targets y_{sp}

+

-

Supervisory controller

inputs u

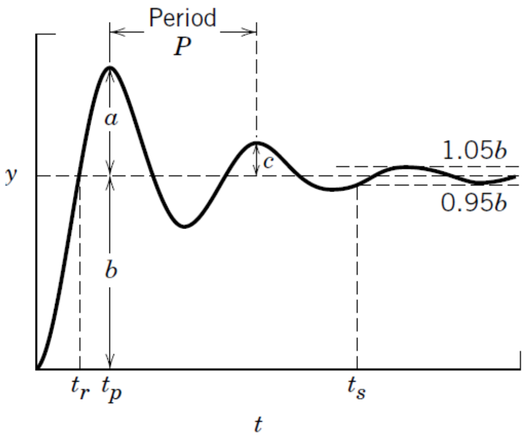
Process

outputs y

Baldea and Harjunkoski, Comput. Chem. Eng., 71, 377-390, 2014

Capture closed-loop input-output dynamics

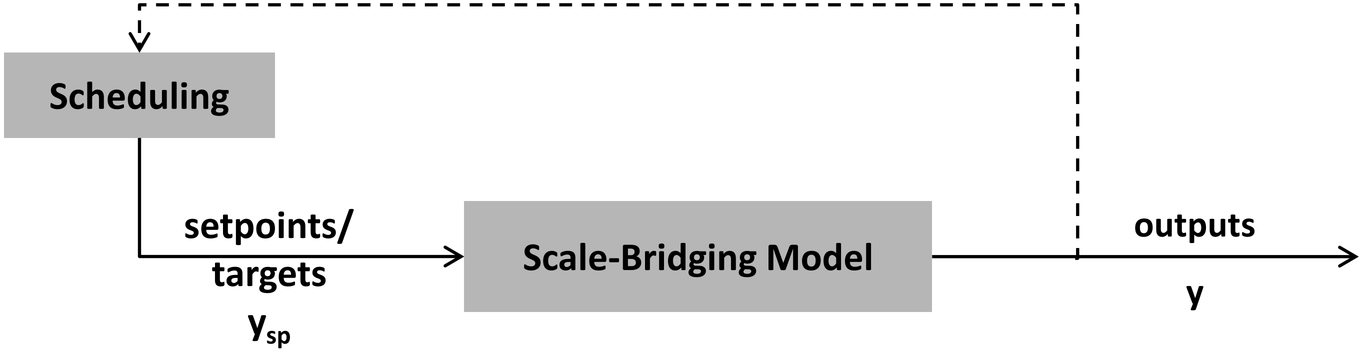
- Not a trivial task for a general nonlinear system
- Historically, research has focused on stability and speed of response, rather than the trajectory itself



Seborg, Edgar, Mellichamp, Doyle, Process Dynamics and Control (3rd Ed.), Wiley, 2011

Scale-Bridging Models: Derivation

- SBM is the **explicit form** of the closed-loop dynamics of process with its supervisory controller



Scheduling

setpoints/ targets y_{sp}

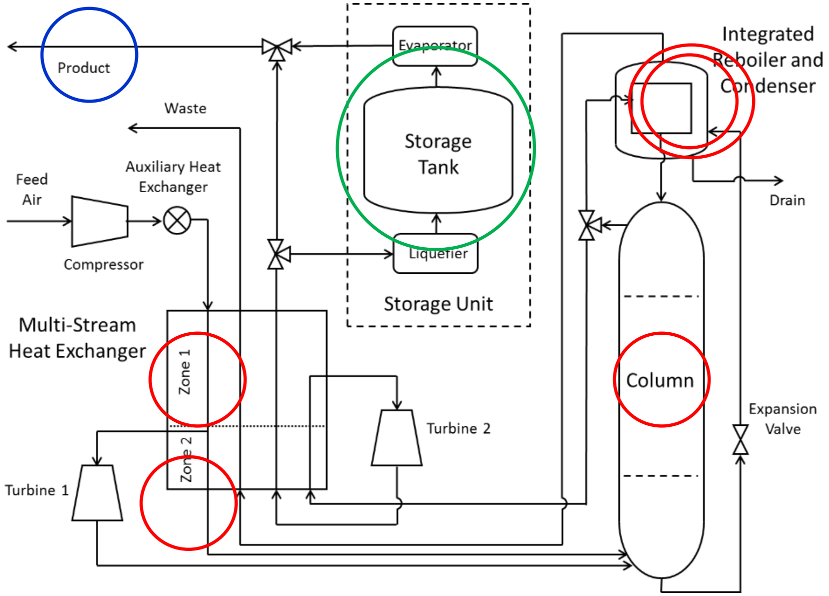
Scale-Bridging Model

outputs

y

- Low dimensional: $n_y \ll n_x$
- Process operates in closed-loop: stability guarantees
- Derivation of SBM:
  - input-output linearization (Du et al., CCEng 2015) **Later in this talk**
  - via model predictive control (Baldea et al., AIChE J, 2015)
  - empirical, using routine operating data **Poster F93 tonight**

Air Separation Example (cont'd)



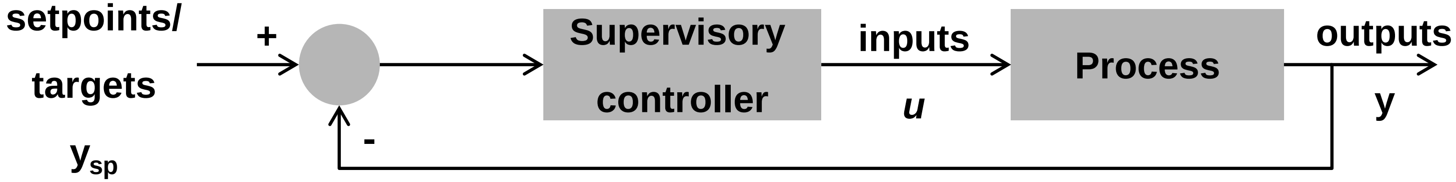
Poster F93 tonight

Problem	Variables	Operating cost ($)	CPU time (h)
Constant production rate	-	22,187	-
Full-order model	430 differential 5,764 algebraic	21,520 (-3.0%)	97*
Data-driven SBM	51 differential	21,584 (-2.7%)	1.2*

*gPROMS ProcessBuilder 1.0, Intel Core i7 @3.40GHz, 16GB RAM, Windows 7 x64

Scale-Bridging via Input-Output Linearization

- SBM is the **explicit form** of the closed-loop dynamics of process with its supervisory controller



setpoints/

targets

$\mathbf{y_{sp}}$

+

-

Supervisory controller

inputs

$\boldsymbol{u}$

Process

outputs

y

- Use feedback linearization to design a control law that imposes a closed-loop behavior of the type:

$$\sum_{i=0}^{r}\tau_i \frac{d^i y_j}{dt^i} = y_j^{sp}$$

(this is the SBM)

- Input u calculated from inverse of process model (Hirschorn, 1979)

$$\dot{x} = f(x) + g(x)u$$
$$y = h(x)$$

$$u = \frac{y_{sp} - y - \sum_{i=1}^{r}\tau_i L_f^r h(x)}{\tau_r L_g L_f^{r-1} h(x)}$$

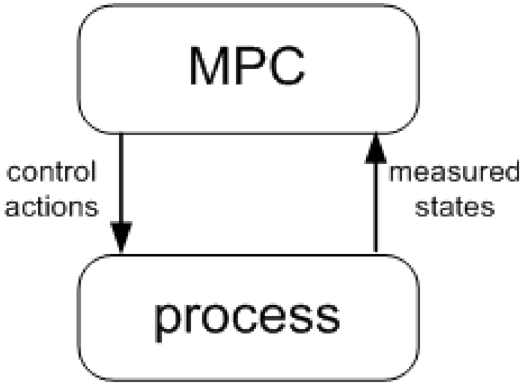
Kravaris and Kantor, IECR, 29, 2295-2310, 1990; Daoutidis and Kravaris, Chem. Eng. Sci., 49, 433—447, 1994

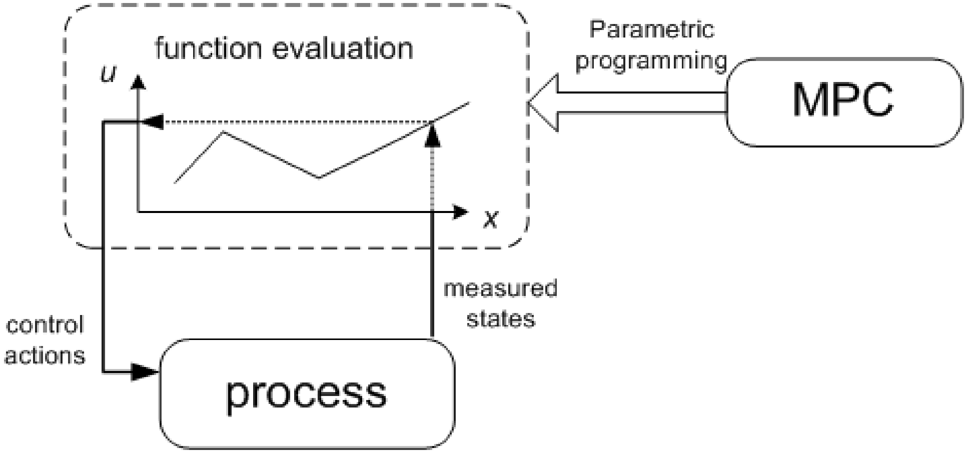
Concept 2: Explicit MPC

On-line Optimization via off-line Parametric Optimization

Conventional MPC

- Expensive online computation





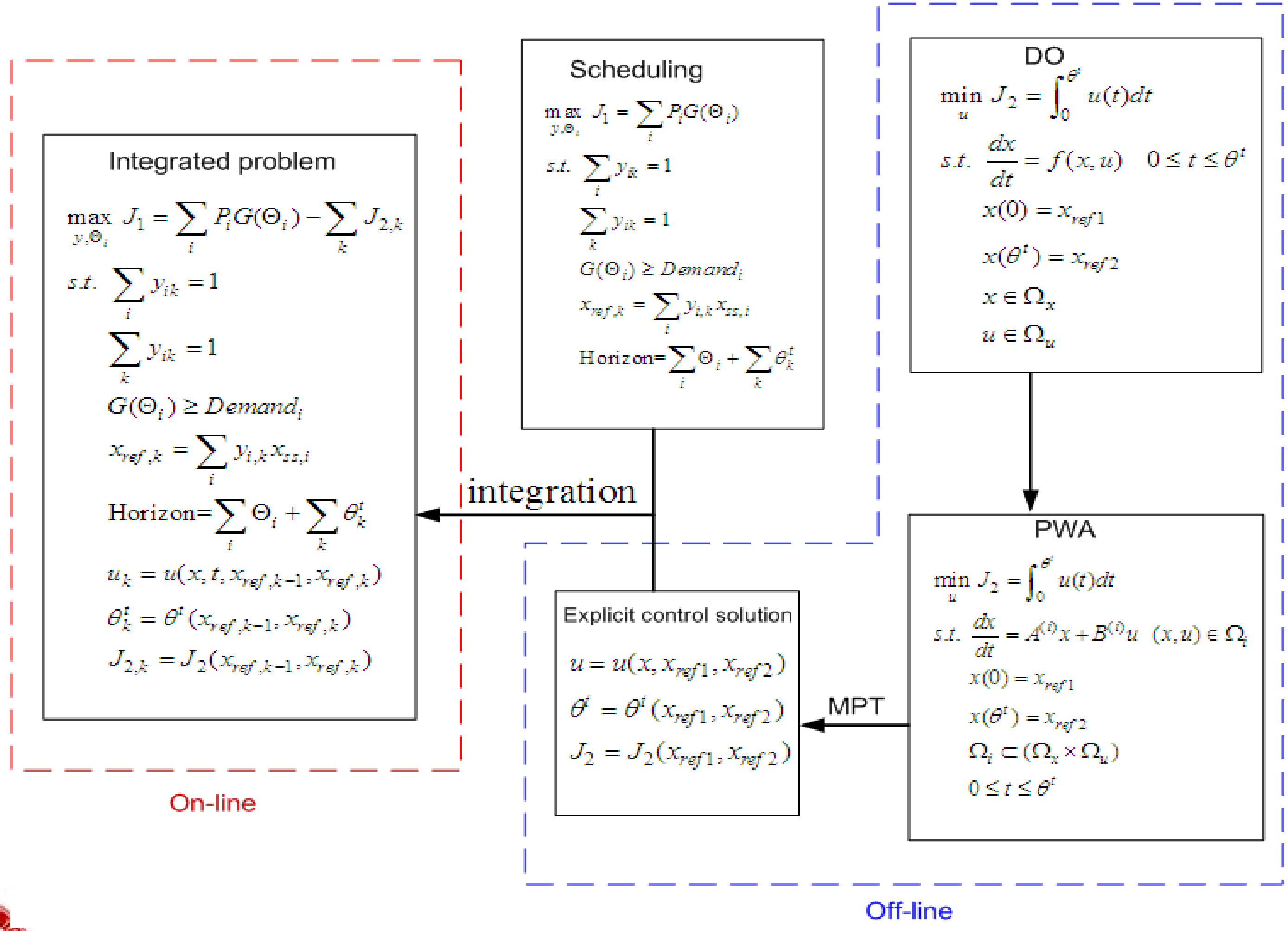
Advantages of mp-MPC

- Online optimization for fast dynamic
- Reduce the computational complexity when integrated with scheduling level

Bemporad, A.; Bozinis, N. A.; Dua, V.; Morari, M.; Pistikopoulos, E. N. *Comput. Chem Eng. 8, 301-306, 2000.*

Concept 2: Explicit MPC

- Transforms the MINLP of the original integrated problem into a MILP
- Applies to both continuous and batch processes



Integrated problem

$$\max_{y,\Theta_i} J_1 = \sum_i P_i G(\Theta_i) - \sum_k J_{2,k}$$

$$s.t.\ \sum_i y_{ik} = 1$$

$$\sum_k y_{ik} = 1$$

$$G(\Theta_i) \geq Demand_i$$

$$x_{ref,k} = \sum_i y_{i,k} x_{ss,i}$$

$$\text{Horizon} = \sum_i \Theta_i + \sum_k \theta_k^t$$

$$u_k = u(x, t, x_{ref,k-1}, x_{ref,k})$$

$$\theta_k^t = \theta^t (x_{ref,k-1}, x_{ref,k})$$

$$J_{2,k} = J_2(x_{ref,k-1}, x_{ref,k})$$

integration

Scheduling

$$\max_{y,\Theta_i} J_1 = \sum_i P_i G(\Theta_i)$$

$$s.t.\ \sum_i y_{ik} = 1$$

$$\sum_k y_{ik} = 1$$

$$G(\Theta_i) \geq Demand_i$$

$$x_{ref,k} = \sum_i y_{i,k} x_{ss,i}$$

$$\text{Horizon} = \sum_i \Theta_i + \sum_k \theta_k^t$$

DO

$$\min_u J_2 = \int_0^{\theta^t} u(t)dt$$

$$s.t.\ \frac{dx}{dt} = f(x,u) \quad 0 \leq t \leq \theta^t$$

$$x(0) = x_{ref1}$$

$$x(\theta^t) = x_{ref2}$$

$$x \in \Omega_x$$

$$u \in \Omega_u$$

PWA

$$\min_u J_2 = \int_0^{\theta^t} u(t)dt$$

$$s.t.\ \frac{dx}{dt} = A^{(i)}x + B^{(i)}u \quad (x,u) \in \Omega_i$$

$$x(0) = x_{ref1}$$

$$x(\theta^t) = x_{ref2}$$

$$\Omega_i \subset (\Omega_x \times \Omega_u)$$

$$0 \leq t \leq \theta^t$$

MPT

Explicit control solution

$$u = u(x, x_{ref1}, x_{ref2})$$

$$\theta^t = \theta^t (x_{ref1}, x_{ref2})$$

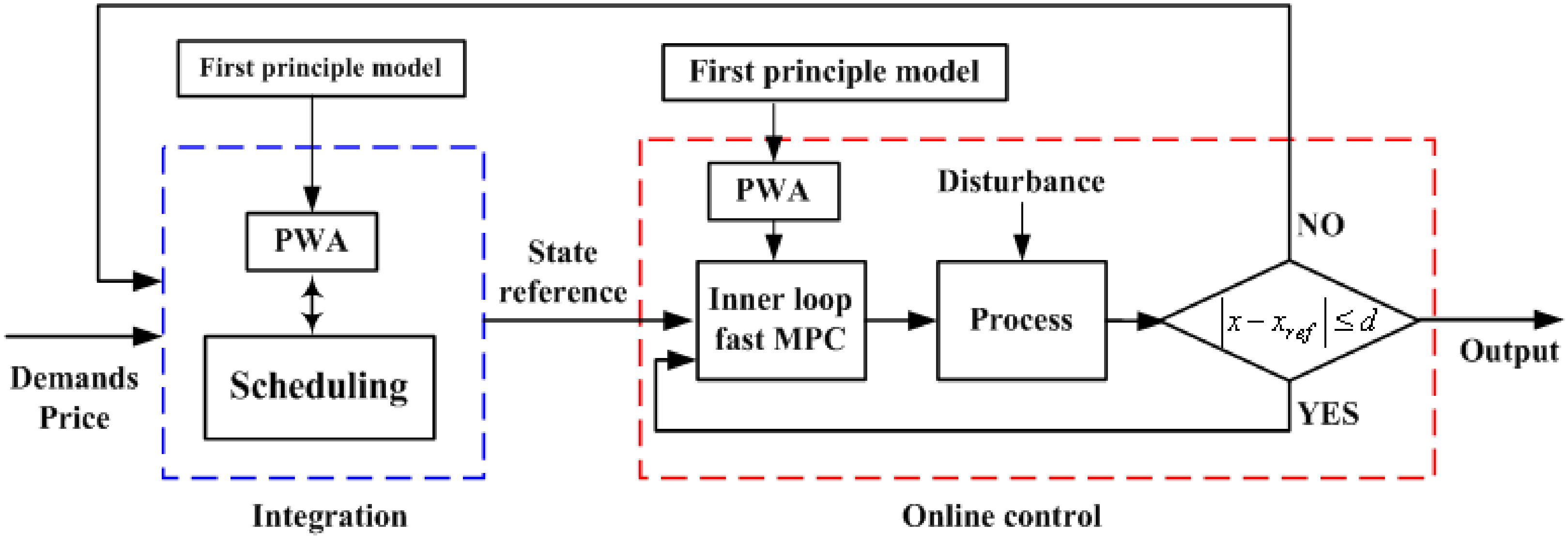
$$J_2 = J_2(x_{ref1}, x_{ref2})$$

On-line

Off-line

Zhuge, J., Ierapetritou, M. *Aiche Journal. 60(9), 3169-3183, 2014.*

Concept 3: Fast MPC



Integration of scheduling and fast MPC

- PWA approximations of nonlinear dynamic, simplify control computation
- Integrated problem incorporating PWA system
- Inner and outer loops for the integration of scheduling and control.

Zhuge, J., Ierapetritou, M. *Aiche Journal. 61(10), 3304-3319, 2015.*
Dias, L. S., Zhuge, J., Ierapetritou, M. Aiche Journal. 62(10), 3822-3823, 2016

Fast MPC - Algorithm

Step 1: Transfer nonlinear dynamic into PWA using optimization methods

$$LTI^{(i)}: x(k+1) = A_i x(k) + B_i u(k) + C_i$$

$$\text{if } x(k) \in \Omega_i = \{x : V_i x \le W_i\}$$

$$\text{where } \bigcup_i \Omega_i = \Omega_x \text{ and } \Omega_{i_1} \cap \Omega_{i_2} = \varnothing \text{ if } i_1 \neq i_2$$

Step 2: Set initial states and initial manipulated variables (x^0,u^0)

Step 3: Locate corresponding PWA for current states.

$$\text{if } x \in \Omega_i = \{x : V_i x \le W_i\},\ i \in S_i = \{1, 2, \ldots N_i\},$$

$$\text{then select } LTI^{(i)} : \bigcup_i \Omega_i = \Omega_x \text{ and } \Omega_{i_1} \cap \Omega_{i_2} = \varnothing \text{ if } i_1 \neq i_2$$

Step 4: Solve MPC problem

$$\min_{x_k, u_k} \sum_{k=1}^{N-1} \left(x_k^T Q x_k + u_k^T R u_k \right) + x_N^T P x_N$$

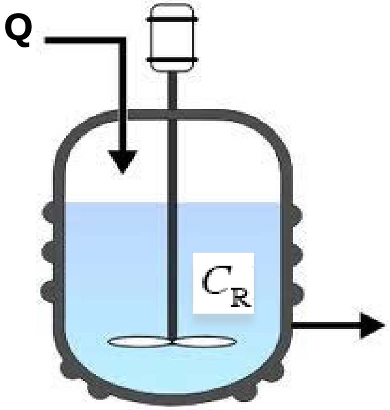
$$s.t. \begin{cases} x_1 = x^0 \\ x_{k+1} = A_i x_k + B_i u_k + C_i, \text{ if } (x_k, u_k) \in \Omega_i,\ k = 1, \ldots, N-1 \\ x_{\min} \le x_k \le x_{\max}, \quad k = 1, \ldots, N \\ u_{\min} \le u_k \le u_{\max}, \quad k = 1, \ldots, N \end{cases}$$

Step 5: k=k+1, go to step 3

Zhuge, J., Ierapetritou, M. *Aiche Journal. 61(10), 3304-3319, 2015.*
Dias, L. S., Zhuge, J., Ierapetritou, M. Aiche Journal. 62(10), 3822-3823, 2016

Case study: cyclic production SISO CSTR

- **Reaction** $3R \xrightarrow{k} P, -\mathscr{R}_{\mathrm{R}} = kC_{\mathrm{R}}^{3}$
- **Dynamic model** $\frac{\mathrm{d}C_{\mathrm{R}}}{\mathrm{d}t} = \frac{Q}{V}(C_{\mathrm{o}} - C_{\mathrm{R}}) + \mathscr{R}_{\mathrm{R}}$
- **Control input u:** feed flow Q
- **State variable x:** concentration of R



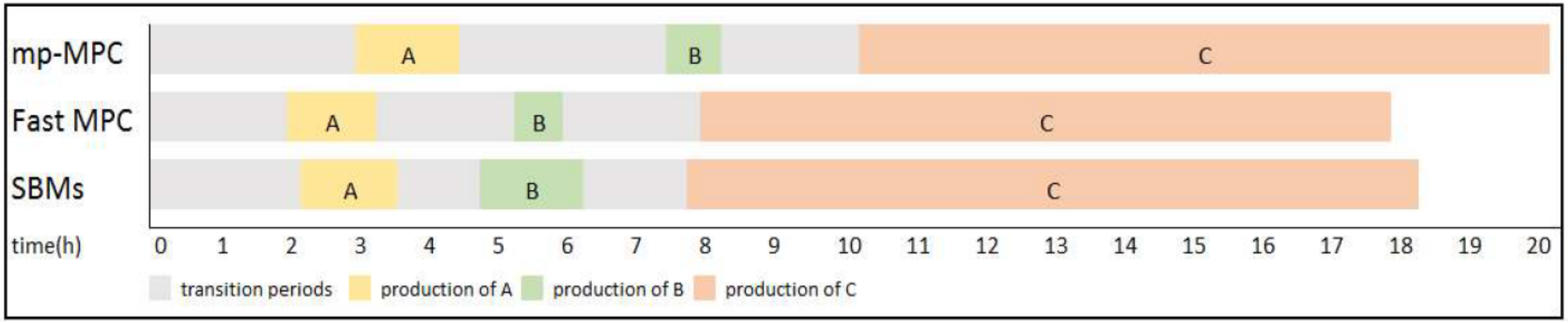
- **Three products** with steady state information and market information

Product	u [L/h]	x [mol/L]	Demand [kg/h]	Inventory cost [$/kg]	Product price [$/kg]
A	400	0.3032	20	1.8	130
B	1000	0.393	25	2	125
C	2500	0.5	10	1.7	120

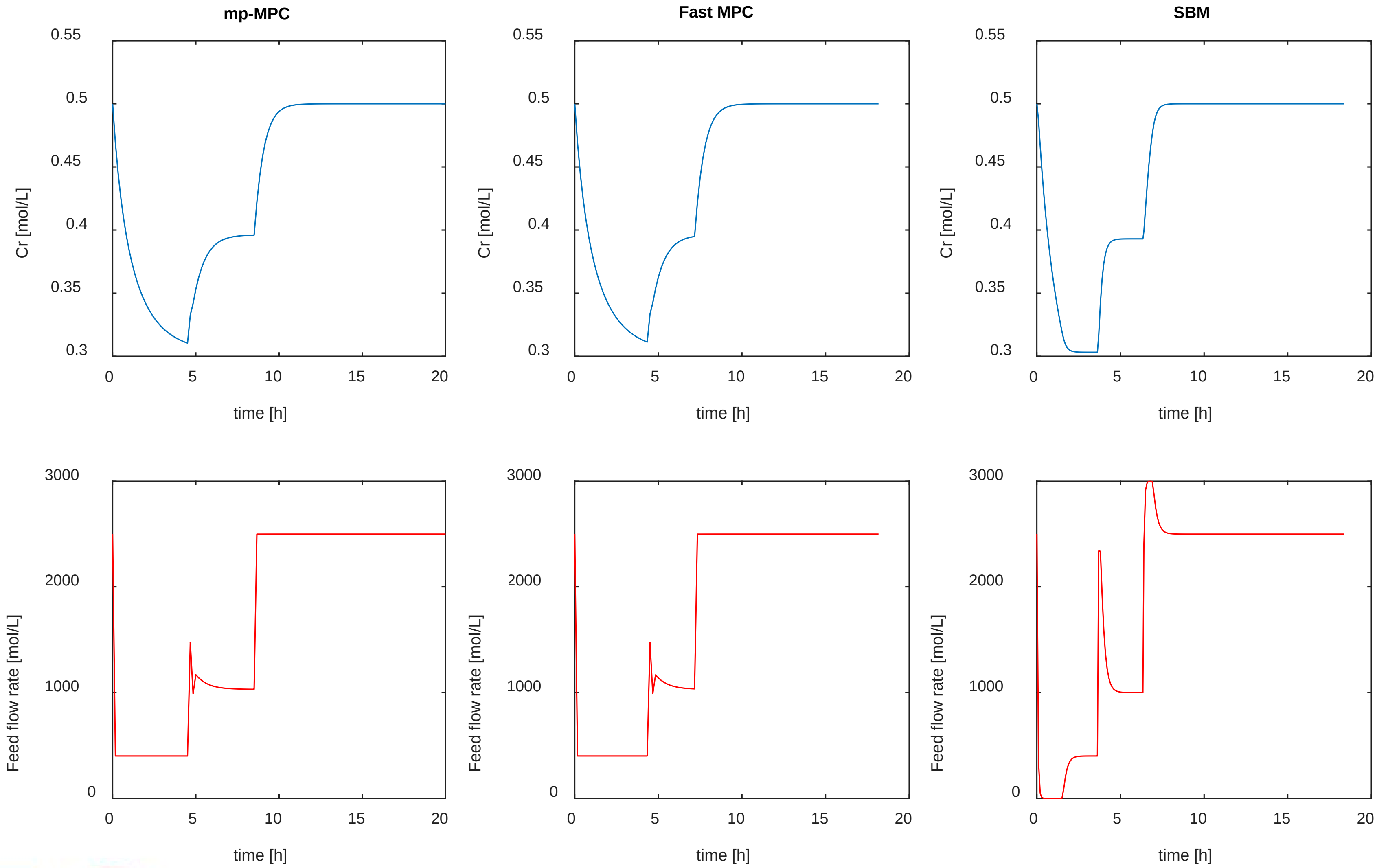
Flores-Tlacuahuac, A., Grossmann, I. Ind Eng Chem Res, 45, 15, 2006.

Case study: Results

	mp-MPC	**Fast MPC**	**SBM-based**
CPU Time (s)	83	1	5
Optimal sequence	A-B-C	A-B-C	A-B-C
Cycle time	20.29	18.04	18.37
Revenue ($)	79646.44	88886.62	94743.61
Raw material cost ($)	15547.48	16405.73	18772.19
Inventory cost ($)	6214.34	5468.120	8241.69
Profit ($)	57884.61	67012.77	67729.72



Case study: dynamic profiles



Case study: Results

- **mp-MPC:** higher computational time, lower profits
- **Fast MPC:** capable of handling large size control problems
- **SBM-based:** highest profit due to shorter transition times. Higher raw material costs due to more aggressive control action.

Conclusions and Discussion

- **Integrated scheduling and control**
  - Required when frequency of scheduling decisions overlaps with dynamic modes of the plant: fast changing markets
  - CONTROL DOES MATTER: execution of production schedules and economic performance is highly dependent of the choice of control system
  - Frameworks can be adapted to more complex problems involving batch and continuous process (ASU example earlier, Zhuge and Ierapetritou, 2014. Touretzky et al., 2016)

Quo Vadis, Integrated Scheduling and Control?

- **Practical applications:**
  - Chemical and petrochemical processes, electric grid, powerplants (Pistikopoulos et al.), other players (e.g., buildings) (Touretzky and Baldea, 2014, 2016, Risbeck et al., 2016…)
- **Applications**: broader perspective
  - Demand response: Interaction of industrial energy users with the grid: optimal plant operation from the <u>user</u> perspective ***<u>does not imply</u>*** optimal operation from the <u>grid</u> perspective (Baldea, Springer Verlag, 2017)

Perspective and challenges

- **First challenge:** Development of systematic and general approach for deriving <u>scheduling-relevant low order process models</u>
  - High fidelity representation of process dynamics are high-dimensional, stiff and potentially discontinuous (recall ASU)
  - High computational costs for performing the integrated scheduling/control calculations online

Perspective and challenges (cont'd)

- **Second challenge:** Closing the scheduling loop
  - Implementing **feedback** mechanisms that inform rescheduling decisions in the presence of process faults and disturbances
  - Consideration of stability and feasibility
  - Moving horizon implementation, defining rescheduling triggers, state space scheduling formulations

Touretzky et al., AIChE J., 2017, Subramanian, K. et al, Comput. Chem. Eng. 47, 97–110, 2012.

Perspective and challenges (cont'd)

- **Third challenge:** Considerations of uncertainties
  - Plant-model mismatch, changes in market demand and prices, changes in flows and composition, etc.
  - Addressing the uncertainty problem simultaneously in both scheduling and control levels
  - **Integration of scheduling and robust control:** on-going work

Poster F57 tonight

Perspective and challenges (cont'd)

- **Fourth, fifth…:** data integration, organizational silos within a company, closer relationships between industry and academia, defining meaningful
  "Tennessee Eastman"-like benchmark problems

More Developments (Posters Tonight)

APPLICATION: **Pattison and Baldea,** Closed-loop scheduling with process faults: framework and an air separation unit example *(Poster F93)*

THEORY: **Dias and Ierapetritou,** Integration of production scheduling and model predictive control under process uncertainties *(Poster F57)*

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- DOE: DE-EE0005763, DE-OE0000841
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MGI:

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