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Benchmark for Hierarchical Plantwide Control of Hybrid Chemical Processes: Control of Coupled Batch and Continuous Reactors

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Abstract

Chemical processes often exhibit a heterogeneous character and often have a highly complex behavior. In this work, a benchmark problem for hierarchical hybrid plantwide control is presented. The considered chemical process consists of coupled batch and continuous reactors. For this process, a hierarchical solution will be motivated. In order to compensate most disturbances, time-variant parameters, changes of the set point, and changes of the operating points, a control structure for each plant component is proposed. The benchmark high-level problem is to coordinate these component's control systems in a safe and optimal plantwide way.

Keywords: Hybrid Process, Plantwide Control, Hybrid Control, Hierarchical Control

1. Introduction

Industrial chemical processes are often operated in a number of plant components, which are connected by material or energy flows. Although most fundamental phenomena in chemical processes are continuous, chemical processes often feature a number of discrete event mechanisms which results in a hybrid control problem. In this contribution, we present a benchmark chemical process which consists of interacting continuous sub-processes and sub-processes performed in batch mode which imposes process discontinuities regarding the coordination of the entire chemical plant. The plant is controlled by both discrete and continuous control inputs. Moreover, some sensor information is available in form of discrete event signals only. The benchmark control problem is to design a plantwide optimal and safe control system which is robust to disturbances.

In hybrid control problems, which involve a large number of variables and highly nonlinear continuous dynamics, structured abstraction based approaches in combination with hierarchical methods seem a tractable way to overcome complexity, e.g. Raisch and Moor (2005); Skogestad (2004). In chemical industry, controllers for sub-processes often already exist. To increase productivity and safety, however, more effort in the control of the interaction of connected plant components is needed while "simplicity" should be retained. In Skogestad (2004), the advantages of a hierarchical structuring for plantwide control systems are described. A hierarchical approach can reduce control system complexity and, thus, the required effort in modeling and design. To follow this approach, we propose a low-level control system for the considered benchmark process.

The low level control system consists of controllers designed independently for each plant component. These controllers compensate the impact of most disturbances, time-variant parameters, changes of the set point and changes of the operating points. The high-level supervisory problem is to design a production rate controller for the entire plant, where the high-level controller changes the set points of the low-level control systems. This should guarantee acceptable performance, product quality and safety requirements. The major challenge in this high-level control problem is that some disturbances have a drastic impact on the plantwide dynamic behavior.

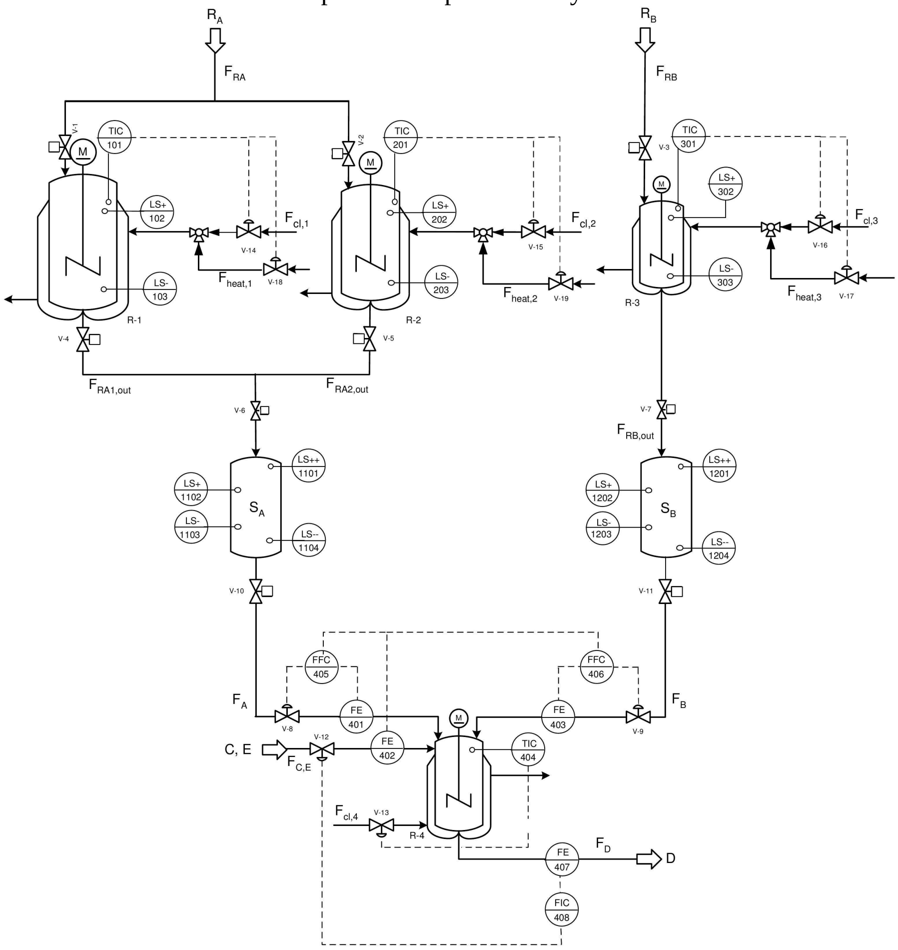

Fig. 1. Flowsheet of the coupled reactors

2. Problem Statement

Discontinuously operated plants are widely used in chemical process industries for the production of fine, or specialty chemicals. The reactors discharge their final product into buffer tanks used to transfer it continuously to the subsequent plant devices. For those units, it is highly desirable to have optimal control and operation schedules (Barton et al. (2000, 2006)). These schedules determine the stand-by times between the batch reactor phases, as well as the flow rates between the different devices in order to maximize the average plant productivity and to have an un-interrupted production without incidents.

The proposed benchmark process consists of a continuous reactor and several batch reactor units which are influenced by continuous and discrete event control inputs. Fig. 1 depicts the flowsheet of the process. Although the model process is less complex than many real world processes it exhibits most of the problems encountered in coupled batch and continuous reactors. The overall process can be divided into two major coupled production steps. In the first step, intermediate products are produced in batch reactors. When the batch has finished and a required purity of the intermediate products is achieved, the reactors are discharged into storage tanks. The intermediate products are then fed into a continuously stirred reactor where they react with another reactant.
The core of the plant is a set of 3 parallel batch reactors (denoted by R-1 to R-3 in Fig. 1). In the first process step, the intermediate product *A* in reactors R-1 and R-2 and the intermediate product B in the reactor R-3 are manufactured. The component A possesses a lower molecular mass than B, and thus, the combined volume of reactors R-1 and R-2 is larger than the volume of reactor R-3. Furthermore, in order to compensate for a larger demand of A during the startup as well as for disturbances, reactors R-1 and R-2 may be used simultaneously. To compensate larger demands of A quickly, reactor R-2 features a smaller volume and consequently a smaller cycle time than reactor R-1.
In the batch reactors R-1 to R-3, two parallel exothermic reactions take place correspondingly. The corresponding reactions are: $R_A \xrightarrow{k_A} A$ and $R_B \xrightarrow{k_B} B$ with the first reaction being faster than the second one. They both are accompanied by the parallel reactions: $R_A \xrightarrow{k_{W_A}} W_A$ and $R_B \xrightarrow{k_{W_B}} W_B$ which produce the waste product W_A and W_B, respectively. If the final concentrations of A and B are lower than $c_{A,min}$ and $c_{B,min}$ at the end of the corresponding batches, the batches are spoilt. When the reactions for the production of A and B are completed under the compliance of the purity requirements, the product of each reactor is discharged and stored in two parallel buffering tanks S_A and S_B. Each tank features a maximal volume, which may not be exceeded. The aim of the buffer tanks is to ensure an un-interrupted supply of the educts to the continuous section of the plant, which, in this case, consists of a continuous reactor R-4. In this reactor, the final product D is produced via the exothermic reaction: $A + B + C \xrightarrow{k_1} D$, also an undesired parallel reaction takes place: $4A + E \xrightarrow{k_2} C$, where the component E represents a contamination of the feed stream of *C* into the continuous reactor. Thus, a contamination with E leads to an increased need of the intermediate product A.

3. Plant under Low-level Control

The major challenge in the presented benchmark process is to coordinate the coupled plant components, whereas control concepts for the single plant components can be easily obtained. In fact, all proposed low-level control concepts are quite simple and widely used in chemical industries. Based on the single control components, we propose a hierarchical control structure which reduces the coordination control problem significantly in terms of complexity.

Batch Reactors

To produce one batch of the intermediate products in one of the batch reactors, a sequence of five production steps has to be performed: filling, heating, cooling while reaction takes place, cooling the reaction products at the end of reaction, and discharging. In the proposed control strategy, every production step can be controlled independently, i.e., at the end of each step an event is generated which enables the next production step. Filling, heating, the cooling process after the reaction has finished and

discharging are controlled by discrete valve positions, while cooling during the reaction can be controlled by continuous coolant inflows $F_{cl,i}$, i = 1; 2; 3 into the reactor shell.
The coolant inflow has been chosen such that the coolant consumption is minimized while temperature constraints and product quality requirements at the end of the reaction are satisfied. The optimization problem can be expressed in the following way:

$$\min_{F_{cl,i}} \int_0^{t_{f,i}} F_{cl,i}(t)dt \qquad (1)$$

$$T_{L,i} \leq T_{R-i} \leq T_{U,i};\ c_A(t_{f,i}) \geq c_{A,min},\ \text{for } i = 1,2;\ c_B(t_{f,3}) \geq c_{B,min},\ \text{for } i = 3.$$

This optimization problem has been solved iteratively in two optimization steps. First, the coolant consumption has been minimized for a given reaction duration $t_{f,i}$ such that the reactor temperature T_{R-i}, i = 1,2,3, remains between an upper and lower bound, $T_{L,i}$ and $T_{U,i}$ respectively, and the concentration of the intermediate product at the end of the reaction exceeds a minimal concentration $c_{A,min}$ and $c_{B,min}$ for reactors R-1, R 2 and R-3. Then, the reaction duration has been varied where for smaller $t_{f,i}$ the coolant consumption gets smaller. $t_{f,i}$ has been reduced iteratively until the minimal reaction time still meeting the safety and quality requirements has been reached.
The optimization problem for fixed $t_{f,i}$ has been solved by a NLP approach, where the control profiles has been parameterized by piecewise constant functions. The obtained profile for the coolant inflow $F_{cl,1}(t)$ of reactor R-1 is shown in Fig. 3. The resulting concentration profiles in reactor R-1 are depicted in Fig. 4. In this setting, the only relevant information for the high-level controller is the cycle time $t_{f,i}$ of each reactor.

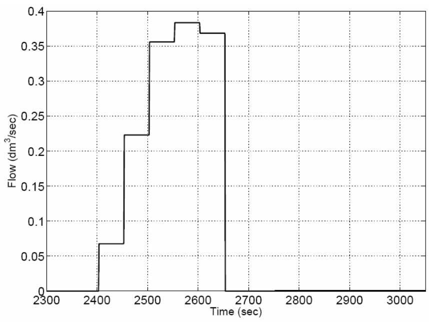

Fig. 3. Coolant flow $F_{cl,1}(t)$ during reaction to produce intermediate product *A* in Reactor R-1.

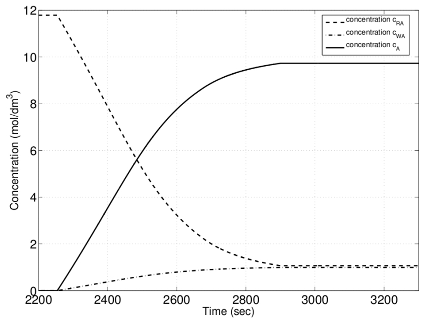

Fig. 4. Concentration profiles of reactant R_A, intermediate product A and waste product W_A in reactor R-1.

3.1. Storage Tanks

The level of both storage tanks, h_{SA} and h_{SB} can be controlled by discrete inlet (V-6,V-7) and outlet valves (V-10, V-11). In the storage tanks, in addition to the upper and lower level thresholds ($h_{uu,j}$, $h_{ll,j}$, $j = S_A, S_B$) two intermediate measurement thresholds ($h_{u,j}$, $h_{l,j}$, $j = S_A, S_B$) are introduced (see Fig. 1). Based on this measurement, the task for the low-level controller is to prevent the storage tanks from over- and under filling $h_{ll,j} \leq h_{Sj} \leq h_{uu,j}$. A simple solution that prevents infinite fast switching is shown in Fig. 5. Closing the outlet valves V-10 and V-11 will cause an interruption of the supply for the subsequent reaction and is, therefore, not allowed. The underfilling of both storage tanks should be prevented by the high-level supervisor by manipulating the production rate of the entire plant. An example profile for the tank level in storage tank S_A is shown in Fig. 6.

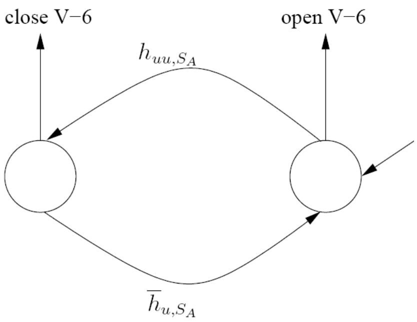

Fig. 5. *Automaton for switching valve V-6 to control filling of storage tank S_A.* The event $h_{uu,SA}$ is generated when the tank level in tank S_A has reached the upper threshold and event $h_{u,SA}$ is generated when the intermediate threshold $h_{u,SA}$ has been passed from above.

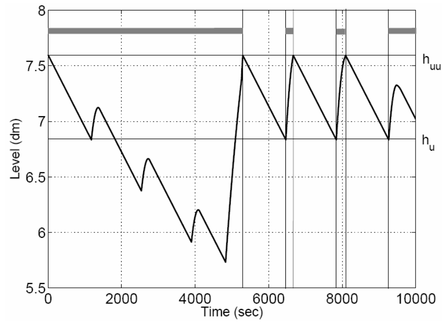

Fig. 6. *Tank level profile in storage tank S_A.* The storage tank is completely filled with *A* in the beginning. First, three batches produced in reactor R-2 are discharged into the storage tank three times in a row. Then, reactor R-1 is discharged. The cycle time of reactor R-1 is ca. three times larger than the cycle time of reactor R-1. Bars mark time intervals when valve V-6 is open.

3.2. Continuous Reactor

The control problem for the continuous reactor R-4 is to track the reference value for the outflow rate of the final product F_D and the temperature $T_{R\text{-}4}$. The reference values $F_{D,sp}$ and $T_{R\text{-}4,sp}$ are adjusted by the high-level controller to be designed. Control inputs are the inflow rate of the cooling liquid $F_{cl,4}$ into the reactor shell and the valve positions controlling the inflow rates of all reactants F_A, F_B and $F_{C,E}$. Measured variables are the outflow F_D and the temperature $T_{R\text{-}4}$ in the reactor. The concentration of reactant C in the inflow C,E which is impured with E can be measured with a small sampling rate. The proposed low-level control system for reactor R-4 consists of a temperature control system and an outflow control system and is shown in Fig. 7.

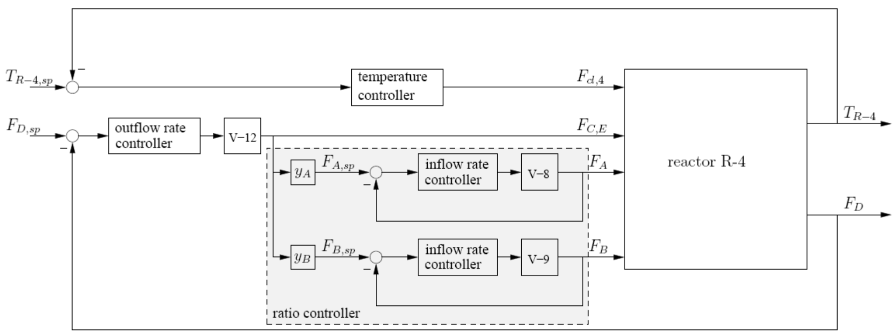

Fig. 7. Low-level control system for reactor R-4.

The control system for the outflow rate F_D consists of a PI controller manipulating the inflow rate $F_{C,E}$ and a ratio control system adjusting the inflow rates F_A and F_B depending on $F_{C,E}$ (see Fig. 8) in order to allow the equimolar reaction $\mathrm{A}+\mathrm{B}+\mathrm{C}\rightarrow\mathrm{D}$. The ratio controller is simply formed by two PI controllers for the inflow rates F_A and F_B. The set points for these controllers are calculated by the current inflow rate $F_{C,E}$ multiplied with factors y_A and y_B. The latter depend on the concentration of reactant C in the feed C,E. All PI controllers are enhanced by anti-reset windup structures. Note that the outflow-rate control system can only work properly if the supply of reactants *A* and B from the previous production steps is guaranteed. The second low-level control goal is to track the reference signal $T_{R\text{-}4,sp}$ for the temperature. The temperature controller is synthesized as a PI controller with anti-reset windup.

4. High-Level Problem Statement

On the basis of the low-level control layer, we can now formulate the benchmark plantwide control problem. A high contamination of the feed stream of C,E with E results in a high demand for A. If the production rate F_D were fixed, it could happen that the storage tank S_A runs empty in the case of an unexpected increase of the concentration of E in the feed. To prevent an interruption of the entire process, it is therefore necessary to adjust the reference value $F_{D,sp}$ for the production rate appropriately. Additionally, changes in the production rate also require an adjustment of the temperature reference value $T_{R\text{-}4,sp}$ in Reactor R-4 to ensure the specified product quality. This is necessary because the reaction rates k_1 and k_2 of the desired reaction $A + B + C \rightarrow D$ and the undesired reaction $4A + E \rightarrow C$ depend on temperature.

The high-level control inputs are the reference value for the production rate F_D and the temperature $T_{R\text{-}4}$ in reactor R-4. The information available for the high-level controller includes the cycle time of each batch reactor and, therefore, the time before the next batch is finished, discrete events issued from the threshold sensors in the storage tanks and the concentration of E in the feed C,E. The high-level control problem is to maximize the average production rate while preventing an interruption of the process, guaranteeing the required product purity and respecting all plant dynamics and constraints. This optimization problem can be formulated in the following way:

$$\max_{T_{R-4},F_{D,sp}} \quad \frac{1}{\tau}\int_0^{\tau} F_{D,sp}(t)dt$$
$$h_{ll,S_A} \leq h_{S_A} \leq h_{uu,S_A};\, h_{ll,S_B} \leq h_{S_B} \leq h_{uu,S_B};\, c_D \geq c_{D,\min};\, T_{R-4} \leq T_{R-4,\max}, \tag{2}$$

where τ is the overall operating time. The considered high-level problem is, of course, scalable to more complex problems, e.g. if the production costs for the batch reactors are included in the overall cost function.

5. Conclusions

We have presented a hybrid chemical production plant and suggested standard low-level control schemes, which are widely used in industries. The remaining high-level problem has been suggested as a realistic benchmark for hybrid control. A complete and detailed description of all model equations including all process and low-level controller parameters will be provided in a separate document available for download.

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