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AN INDUSTRIAL APPROACH FOR EFFICIENT MODELING AND ADVANCED CONTROL OF CHEMICAL BATCH PROCESSES

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Abstract: Chemical batch processes offer an attractive way of producing a variety of specialty products in a highly flexible manner. However, such processes are hard to control due to the absence of the notion of a steady state operation – necessitating the use of nonlinear models– and the fact that product qualities are only measured at the end of each batch. This paper proposes a new industrial modeling and control strategy that allows significant batch time reductions to be obtained, taking physical, safety and quality constraints into account. Application to an industrial reactor shows significant improvements over classical control strategies.

Keywords: Batch Processes, Modeling, Model based Predictive Control

1. INTRODUCTION

In recent years batch processes have regained popularity due to the possibility they offer to industry to produce relatively small quantities of a variety of products with a large added value (Bonvin (1998)). Examples of such products are fine chemicals, pharmaceutical products and certain classes of polymers.

In many situations up to 100 or more different products are produced in a single reactor. With no need to guarantee product type continuity between subsequent batch runs, these reactors offer larger production flexibility compared to continuous processes. This added flexibility represents the main advantage of batch processes and forms a significant competitive advantage in quickly fluctuating markets.

However, this flexibility directly translates into a higher level of complexity for the modeling and control of such processes. First of all, the transient behavior of batch processes necessitates the use of non-linear model based control methods in order to achieve optimal performance. Secondly, because of the wide variety of different products produced on a single reactor, the modeling effort is significantly larger compared to modeling continuous processes, since every product can result in different process dynamics. Finally, because product quality measurements are typically limited to lab analysis of batch-end product qualities, these measurements are not available for closing the control loop during individual batch runs. As a result tight control of pre-optimized temperature profiles (batch processes) and conservative feeding regimes (fed-batch processes) are typically used in order to obtain acceptable batch end-quality.

Academic research has put a lot of effort in the area of batch reactor modeling and control in recent years. For control purposes mostly the route of detailed mechanistic modeling is chosen in order to fully capture process nonlinearities over a wide operating range. These models are then typically used to compute optimal temperature and/or feeding profiles (e.g., Van Overschee and Van Brempt (2000)) after which tracking control

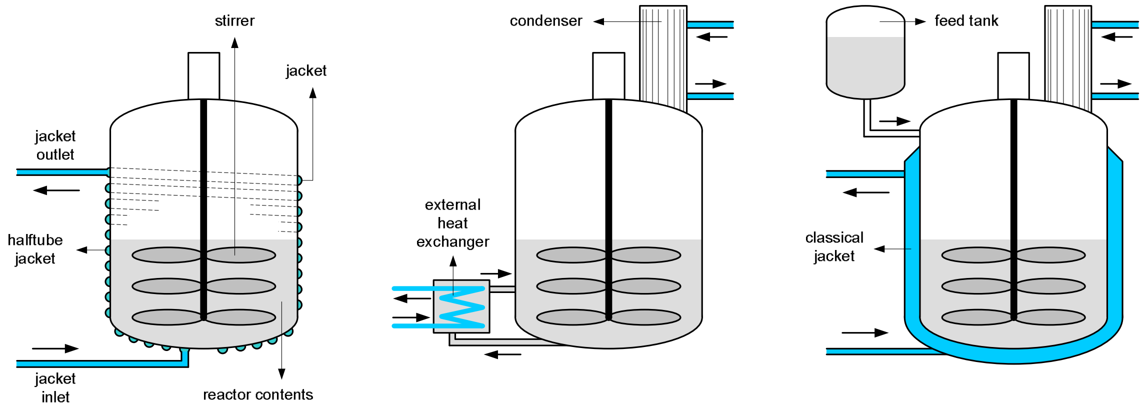

Fig. 1. Different types of batch reactors. **Left:** batch reactor with halftube jacket. **Middle:** Batch reactor with external heat exchanger and condenser. **Right:** Fed-batch reactor with condenser and classical jacket.

algorithms are used (e.g., Diehl et al. (2002)) to track the computed profiles despite disturbances and modeling errors. A good overview of the topic can be found in Bonvin (1998), Nagy and Braatz (2003), Smets et al. (2004) and references therein.

Industrially, very few solutions exist for modeling and control of (fed-)batch processes and none offer efficient modeling techniques for multi-product scenarios. This paper presents a unified industrial modeling and control framework, specifically designed for multi-product (fed-)batch reactors. The framework results in significant batch time reductions and improved quality control, as proven on a real-life industrial process.

This paper is organized as follows. Section 2 proposes the new modeling framework for multi-product batch reactors that lies at the basis of the new framework. Section 3 then describes the control strategy that is used for obtaining batch time reductions and quality control after which the implementation within the existing INCA® (IPCOS Novel Control Architecture) framework and industrial validation is discussed in Section 4. Section 5 concludes the paper.

2. BATCH REACTOR MODELING

2.1 Disadvantages of existing methods

In chemical engineering, control-oriented modeling problems are typically tackled either in a black-box or empirical way or by means of rigorous modeling.

Black-box techniques are often the method of choice for continuous processes, since they avoid the large cost of constructing fully-rigorous dynamic process models. However, for batch processes, traditional linear black-box techniques require reformulation of the control algorithm, but most significantly, require extensive on-site testing to produce the necessary models. Batch processes go through a trajectory of set-points and are therefore always in transient behavior. This wide range of operating conditions necessitates the use of nonlinear models. This prohibits the use of linear black-box techniques to be used from a cost perspective and for technical reasons, since these require the process to stay around a steady state. When applicable however, black-box techniques offer a way to obtain dynamical models in relatively small amounts of time and with relatively little process knowledge.

Rigorous models, on the other hand, include a very detailed description of the process and can involve hundreds of state variables and kinetic parameters. Due to the complexity, rigorous modeling is very expensive in terms of human effort and expertise. The modeling costs are often prohibitively high for a model-based control project. However, such models most often have a wider validity range than black-box models, enabling the design of more reliable and flexible model-based controllers.

In this section a new modeling methodology is introduced, called *hybrid batch modeling*, which aims to combine the advantages of both approaches. *Hybrid batch modeling* allows reliable dynamical batch models with good extrapolation properties to be obtained in a fast way. In this new approach the part of the complex mechanistic model that can be constructed with little effort is kept or mapped in a new set of simplified first-principles equations, whereas the reaction kinetics, which are harder to model rigorously, are condensed in an empirical nonlinear function, resulting in an observable low-order model that can be used for control purposes.

It should be noted that the *hybrid batch modeling* approach considered in this paper is not to be confused with the more classical meaning of hybrid modeling, which involves discrete-valued states (e.g., Potočnik et al. (2004)).

symb.	meaning	unit
A_c	condenser area	m^2
A_j	internal reactor contact area	m^2
C_{pf}	specific heat of feed	kcal kg^{-1} K^{-1}
C_{pr}	specific heat of react. content	kcal kg^{-1} K^{-1}
F_f	feed flow rate	kg s^{-1}
m_r	mass of reactor content	kg
Q_c	condenser duty	kcal s^{-1}
Q_f	feed flow heat content	kcal s^{-1}
Q_j	jacket cooling/heating duty	kcal s^{-1}
Q_r	chemical reaction heat	kcal s^{-1}
T_c	condenser wall temperature	°C
T_f	feed flow temperature	°C
T_j	cooling jacket temperature	°C
T_r	reactor content temperature	°C
U_c	condenser heat transfer coeff.	kcal m^{-2} s^{-1} K^{-1}
U_j	jacket heat transfer coeff.	kcal m^{-2} s^{-1} K^{-1}
n_m	conversion	mole/mole

Table 1. Explanation of the symbols used in Section 2.2.

2.2 Hybrid Batch Modeling

Since most batches are operated mainly based on temperature measurements, while product properties (concentrations, quality parameters) are most often not measured during the batch, the main aim of the new hybrid batch modeling strategy is to accurately model reactor temperatures based on energy balances.

This energy balance is constituted of several components. In most cases, the reactor is jacketed and a thermal fluid is used to control the temperature inside the reactor. In some cases the reactor is equipped with a condenser, which often can absorb more heat than the jacket, but which cannot be used for heating. On the other hand, the reaction energy of the process and the energy content of the feed flow (in fed-batch reactors) are other important components in the overall energy balance. The overall temperature model can hence be written as follows:

$$m_r C_{pr} \frac{dT_r}{dt} = Q_j + Q_c + Q_f + \ldots + Q_r. \qquad (1)$$

By including or excluding certain components at the right hand-side of the equation a wide variety of batch processes (see Fig. 1) can be captured with this model structure. Other contributions might enter the equation depending on the reactor environment, the batch recipe, . . . For the sake of brevity, we refer to Table 1 for the meaning of the different symbols used in this section.

The different subcomponents $Q_j, Q_c, \ldots$ are modeled separately, whereby an appropriate choice is made between rigorous and black-box modeling, based on the following criteria:

(1) minimization of number and intrusiveness of required reactor experiments,
(2) easy adaptation of existing models towards new products on the same reactor.

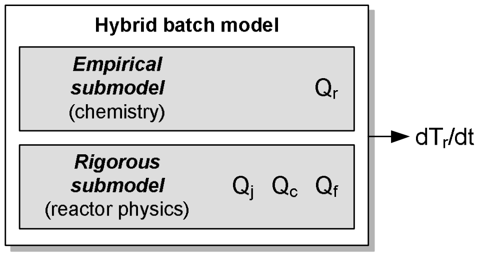

Fig. 2. Hybrid batch model structure.

Therefore the thermodynamics of the reactor, for which the physical relations are well known and understood, are modeled in a mechanistic way. This reduces the need for experiments and eliminates remodeling of these components for each new product. The chemical reactions taking place during the process, are mostly not well understood and the kinetics of it are unknown. This part of the process is therefore modeled empirically. Figure 2 gives a schematic depiction of the hybrid modeling approach.

In what follows, a brief overview of the different rigorous submodels is given:

- Q_j represents the heat exchanged through the jacket wall and is given by $U_j A_j (T_j - T_r)$. Depending on the jacket configuration, nonlinear dependencies on the cooling flow rate can also be incorporated.
- Q_c denotes the heat exchanged via the condenser and is given by the similar expression $U_c A_c (T_c - T_r)$.
- Q_f represents the energy contribution of the feed flow to the reactor and is given by $F_f C_{pf} (T_f - T_r)$.

These submodels can be constructed based on physical knowledge of the reactor, historical data and simple, non-intrusive reactor experiments and in general guarantee reliable extrapolation beyond the operating range within which calibration data is available.

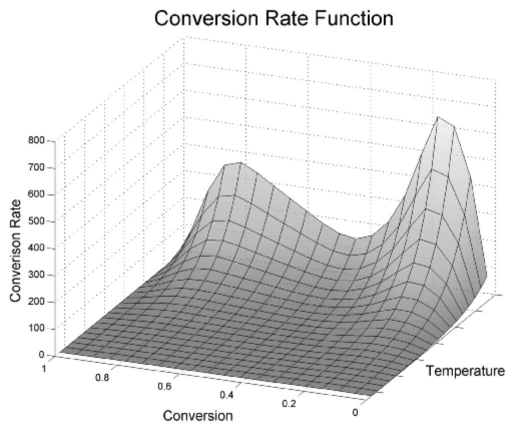

Fig. 3. Example of estimated function $f_Q(n_M, T_r)$.

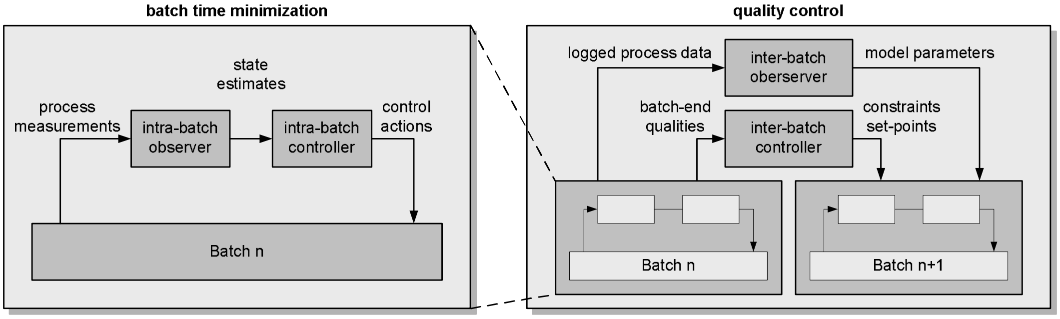

Fig. 4. Cooperation between inter- and intra-batch observers and controllers for batch time reduction and end-quality control.

As mentioned above and depicted in Figure 2, the reaction energy Q_{r} is modeled empirically. In most cases reaction kinetics strongly depend on temperature as dictated by Arrhenius' law. Also, depending on the specific reaction taking place, the reaction energy can be strongly dependent on the conversion (representative of the progression of the chemical reaction). Therefore the heat generation can be expressed as a function of the conversion and temperature:

$$Q_{\mathrm{r}} = f_{\mathrm{Q}}(n_{\mathrm{M}}, T_{\mathrm{r}}).$$

This function can be estimated based on readily available historical data of the batch process and limited additional experiments. The above relationship also allows easy estimation of the instantaneous reactant excess, which facilitates end-of-batch quality control, as will be clarified in the next section.

3. BATCH REACTOR CONTROL

This section describes how the *hybrid batch models* that are described in the previous section are used to develop an advanced model based batch control strategy. The benefits of advanced process control for batch processes consist of batch time reductions resulting in increased production capacity together with reduced process variability (i.e., better batch reproducibility) resulting in improved batch-end product quality.

Batch time reduction and reduced process variability are obtained by means of intra-batch control, while after each batch an inter-batch controller updates process operation parameters (set-points, constraints) in order to obtain optimal product qualities despite changing feed stocks and other disturbance factors. This approach is illustrated in Fig. 4.

First, we give a brief introduction to Model based Predictive Control (MPC, see e.g., Qin and Badgewell (2003)) .

3.1 Model based Predictive Control

Model based Predictive Control (MPC) is an optimization based control paradigm that computes an optimal sequence of future control actions at every sample instant, based on a dynamical plant model. Only the first control action of this computed sequence is applied to the process after which the optimization is repeated at the next sample instant. MPC has become the de facto industrial standard for Advanced Process Control (APC) in the last few decades (Qin and Badgewell (2003)) and has also attracted widespread attention from academia. In its most general form, MPC uses non-linear state space models:

$$x_{k+1} = f(x_k, u_k), \tag{2a}$$
$$y_k = g(x_k), \tag{2b}$$

where u_k, x_k, y_k respectively denote the control input, the state and output (measurement) vectors of the dynamical system. At every sample time k, based on a dynamical model of form (2), a MPC controller computes an optimal control sequence $u_k, \ldots, u_{k+N_c-1}$, by solving an optimization problem of the following form:

$$\min_{u_k,\ldots,u_{k+N_c-1}} \sum_{i=0}^{N_c-1} \|u_{k+i} - u_{k+i,\mathrm{ref}}\|_R^2$$
$$\sum_{i=1}^{N_p} \|y_{k+i} - y_{k+i,\mathrm{ref}}\|_Q^2, \tag{3a}$$

subject to

$$\underline{u}_{k+i} \leq u_{k+i} \leq \overline{u}_{k+i}, \quad i = 0, \ldots, N_c - 1, \tag{3b}$$
$$\underline{y}_{k+i} \leq y_{k+i} \leq \overline{y}_{k+i}, \quad i = 1, \ldots, N_p, \tag{3c}$$

with N_c and N_p respectively denoting the control and prediction horizon, $u_{k+i,\mathrm{ref}}, y_{k+i,\mathrm{ref}}$ denoting input and output reference signals and $\underline{u}_{k+i}, \overline{u}_{k+i}, \underline{y}_{k+i}, \overline{y}_{k+i}$ representing lower and upper bounds on inputs and outputs at time $k + i$. Relations between inputs and outputs within the optimization are given by model equations (2), leading to non-linear optimization.

Although the above formulation has become relatively standard in academia, industrial implementations most often still use impulse or step response models or linear state space models. Neural net based models have been implemented in recent years but these models still belong to

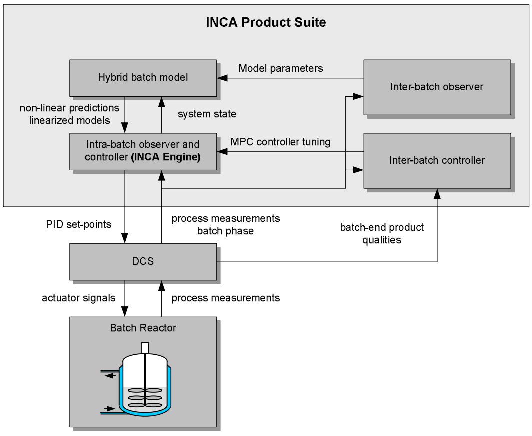

Fig. 5. Integration of the control framework within the INCA® Product Suite.

the black-box category. For batch control, where a wide range of operating conditions is typically encountered within a single batch run, the use of non-linear process models is required to obtain stable process operation when applying model-based control.

3.2 Intra-Batch Control

At this control layer, a MPC controller based on the *hybrid batch model* is employed, called the *intra-batch controller*. Based on process measurements (temperatures, flows, ...) the *intra-batch observer* estimates the current state of the system, after which the *intra-batch controller* computes an optimal control action to be applied to the batch process. The cost function of the MPC optimization problem (3) is tuned such that the batch is operated as fast as possible (with the aim of obtaining batch-time reductions) within all constraints. In order to allow a computationally feasible on-line implementation, the optimization problem (3) is solved approximately in the following two-step procedure:

(1) a non-linear prediction is performed, using the full non-linear *hybrid batch model* and the optimal control sequence computed at the previous sample time,
(2) a dynamic optimization is performed using linear time-varying (LTV) dynamical models, based on linearizations of the *hybrid batch model*.

In this way the MPC optimization problem (3) is solved in an SQP fashion, making optimal use of the structure present in this dynamic optimization problem.

3.3 Inter-Batch Control

At the top control layer, an *inter-batch controller* is employed to guarantee optimal product qualities. These qualities are only known at the end of each batch run and can therefore not be used at the *intra-batch* control level. Therefore, after each batch run, the *inter-batch controller* updates the set-points or constraints of the MPC controller in order to stay within the imposed product specifications. For example, this can be done by updating the maximum temperature constraint, for processes where temperature-dependent reaction specificities (Berber (1995)) influence the production of undesired byproducts. In other cases a constraint can be imposed on the reagent excess, which is easily predicted based on the *hybrid batch model*, limiting the production of byproducts formed in second order reactions. Based on lab results obtained at the end of each batch, these constraints and set-points are updated to compensate the influence of unmeasured disturbances and influences such as catalyst activity, feed stock quality, reactor cleanliness, etc.

In parallel with the *inter-batch controller*, an *inter-batch observer* is used to update the model parameters based on process measurements of the previous batch run. In this way the model is kept up to date when reactor dynamics change due to fouling, wear, season-dependent cooling conditions, etc...

4. INDUSTRIAL IMPLEMENTATION AND VALIDATION

The control approach described in this paper was implemented at a production facility where an amine catalyst product is produced via a fed-batch reaction. The reactor configuration is similar to the batch reactor with halftube jacket shown in Fig. 1. The reaction utilizes a pre-fed reaction catalyst, multiple feed streams, and internal heat transfer coils. Since this is a production facility, it was critical that testing for model development be minimized, the controller work well when first implemented, and the controller seamlessly integrate into the existing control system architecture.

The framework described in this paper was implemented within the INCA® (IPCOS Novel Control Architecture) environment as depicted in Fig. 5. Process measurements and PID set-points are exchanged with the on-site DCS through an OPC connection. The different subcomponents of the framework are implemented in an extended version of the INCA® Suite that allows improved integration with the non-linear hybrid batch models.

The INCA® batch controller is seamlessly integrated in the batch sequencing system (also called the batch recipe manager by some vendors). When each batch is scheduled, the operator specifies if the batch will be controlled by the INCA controller and the controller reads the requisite batch parameters such as maximum temperature. The

Fig. 6. Qualitative view of the control behavior of the INCA® batch controller on the batch process at the Air Products and Chemicals Inc. plant. Cooling and quality constraints are depicted as dash-dotted lines.

INCA controller automatically assumes control of the batch when the batch reaches the correct phase. At the end of each batch run, the limiting impurity is measured and adjustments are made to the controlling constraint. Eventually, this functionality will be automated via the inter-batch observer. The plant LIMS system will automatically forward the batch-end quality measurements to the DCS and then into the INCA control suite. This functionality will permit the production rate to be maximized as the catalyst ages and the reactor fouls.

This implementation of the INCA® Batch Controller resulted in significant batch reaction time reductions and thus delivered substantial benefits for this product. Fig. 6 shows qualitative control behavior on this process. The intra-batch controller maximizes the feed flow while satisfying the imposed constraints; different constraints can be active at different points in time.

5. CONCLUSIONS

In this paper an industrial approach towards modeling and control of batch processes is presented. The framework is based on *hybrid batch models*, that consist of rigorous and empirical submodels, which are combined with non-linear MPC to obtain significant batch time reductions and improve process variability. Product qualities are controlled in an inter-batch fashion by updating constraints or set-points of the MPC control layer based on batch-end quality measurements. The new approach is integrated within the existing in-house developed INCA® software environment and allows seamless integration with the batch sequencing system and the LIMS system. This implementation has been validated on an industrial process, creating significant benefits for the customer.

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