Hybrid modelling and simulation of pipeless batch plants

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Abstract

In a pipeless batch plant, mobile reactors are transported between process stations. Typical process steps performed at these stations are filling, measuring, feeding and cooling/heating. In this paper, three hybrid models of a pipeless batch plant for the production of copolymers have been developed. The dynamics of the chemical reactions are modelled in detail by means of mass balances. The time points at which the process steps are applied to the reactor contents are determined by the state of the reaction. The simulation results can be used to determine the quality of the produced products, the throughput and lead time of the plant, and the degree of occupation of the process stations and reactors.

1. Introduction

In the fine chemicals industry as well as in the speciality polymer production, a trend appears towards high quality products in small production volumes. The future of the production of speciality chemicals, coatings and other performance products asks for flexibility of production in multi-purpose plants. For a chemical production environment, this flexibility in production can be achieved using the pipeless batch plant concept. In a pipeless batch plant, small reactors are transported between several process stations. The process stations perform the required process steps on the reactor contents. Typical examples of process steps are filling, measuring, feeding, cooling and heating. As a result of small reactor volumes, the reactions are well controllable, scaling-up is not an issue, and there is improved safety as compared to large scale batch reactors.

Pantelides et al. (1995) discuss a model for short-term scheduling of pipeless plants. The process times and transportation times are deterministic, and the time representations are discrete-time. Thus, the time horizon of interest is divided into *n* intervals of equal length, with all system events such as:

- start and end of processing a batch at a station,
- start and end of moving a vessel form one station to another,
- changes in vessel, station or utility availability, coinciding with interval boundaries.

The translation of this model into a discrete-event simulation model (Gonzalez and Realff, 1998a, 1998b), resulted in a more detailed model for the routing of the reactors between the process stations, and the process steps were made dependent on the starting and finishing of events rather than being forced to a rigid grid. The robustness of the schedules was determined using stochastic variations on processing and transportation times.

For reasons discussed in Section 2, a combined discrete-event/continuous time (hybrid) model of a pipeless plant may be desirable. In this paper, three hybrid modelling architectures of a pipeless batch plant for the production of copolymers are developed. First, the choice for hybrid simulation models for pipeless batch plants is motivated and the χ specification language is briefly described. Next, three different hybrid model architectures for a pipeless plant for the production of copolymers with a small intermolecular chemical composition distribution, i.e. homogeneous copolymers are developed using the χ language. Finally, simulation results are discussed.

2. Hybrid modelling of a pipeless batch plant

2.1 General

As stated in the introduction, for scheduling pipeless batch plants, processing times are usually assumed to be fixed. The obtained schedules are predictive, based on assumptions about plant operations (e.g. fixed processing and transportation times). However, due to unexpected events or stochastic variations on processing and transportation times, these predictive schedules may become infeasible.

Instead of a predictive schedule, the operation of the pipeless plant can be scheduled dynamically: During operation of the plant, the time schedule for process steps, such as filling, measuring, feeding and cooling/heating, is governed by the state of the reaction. The state of the reaction depends on factors such as the feeding amounts that can vary due to accuracy of the equipment, the time points of process steps that can vary due to traffic stagnations or occupied stations, and the temperature trajectory during the reaction. Therefore, the state of the reactor is not always predictable, and needs to be determined by means of analysis of a sample, that is taken from the reactor contents. The results of the analysis provide the required feed-back information on the state of the reaction.

In order to model a pipeless plant with feed-back information on the state of the reactions, the reactions need to be described in detail, using a set of differential algebraic equations (DAEs) derived from mass and heat balances. Depending on the modelling objective, the process steps performed at the process stations, and the routing of the reactor between the process stations can be modelled using continuous-time, discrete-event, or hybrid model specifications. In the developed models, the process steps performed at the process stations occur on a small time scale compared with the time scale of the reactions. Using time-scale abstraction (Mosterman, 1997), these process steps can be described by a discontinuous change at a point in time. The routing of the reactors between the process stations is modelled using discrete-event specifications.

Using a hybrid model, hazardous operating conditions can be detected early, by means of simulation. Also, the validity of the simulation results of the plant can be higher than that of a discrete-event model. Furthermore, it is possible to calculate the quality of the product (i.e. the intermolecular chemical composition distribution (CCD)) during simulation. In case that, in reality, due to unexpected events, a copolymer doesn't meet its required specification, its production may be terminated immediately. Then, production resources are not unnecessarily occupied for the production of a useless product and production losses can be decreased. In the models, the quality of the product can be calculated during simulation, and so it is possible to terminate the production of this regarding copolymer and to correspond with the reality. The simulation results can be used to calculate the degree of occupation of the process stations and reactors, the throughput and the lead time of the entire plant. This information is required at the design stage of a pipeless plant in order to determine the number of process stations and the number of reactors. Scheduling algorithms can be developed and tested in order to optimise the efficiency of the pipeless plant. These scheduling algorithms can be implemented directly in the developed χ models (e.g. see Fey, 2000).

2.2 The χ specification language

The χ language is developed by the Systems Engineering Group at the Eindhoven University of Technology. It has been designed from the start as a hybrid language that can be used for specification, verification (Bos and Kleijn, 2002), simulation (Van de Mortel-Fronczak, 1995) and real-time control of discrete-event systems (Hofkamp, 2001), continuous-time systems and combined discrete-event/continuous-time systems. The language is based on mathematical concepts with well defined semantics (Bos and Kleijn, 2002). The discrete-event part of χ is based on Communicating Sequential Processes (Hoare, 1978), the continuous-time part on differential algebraic equations (DAEs). Processes are parameterised and can be grouped into systems; discrete and continuous channels are used for inter-process communication and synchronization. High level data types are available such as arrays, lists and sets along with many associated operators. The χ simulator is described by (Van Beek, 2000). It has been successfully applied to a large number of industrial cases, such as an integrated circuit manufacturing plant (Van Campen, 2001), a brewery, and a fruit juice blending and packaging plant (Fey, 2000). With χ,

it is possible to specify a simulation model of a pipeless plant elegantly. The real-time software implementation can be specified in χ, re-using the software of the simulation model.

3. A pipeless plant for copolymer production

This section describes the modelling and simulation of a pipeless batch plant for the production of copolymers. First, the chemical copolymerisation process is discussed. The plant layout and the functionality of the process stations is described. Then, three different architectures for a pipeless plant for copolymer production are developed using the hybrid χ language.

3.1 Copolymerisation Process

In the developed pipeless plant, copolymers of styrene (S) and methyl acrylate (MA) are produced. These copolymers are obtained by a free-radical solution polymerisation in toluene. For initiation of the reaction, 4,4'-azo-bis-4-cyanopentanoicacid is used. The copolymerisation reactions are described by means of a set of differential and algebraic equations derived from mass balances.

For a given pair *A* and *B* of co-monomers, the value of F_A (instantaneous mole fraction of monomer *A* in the formed copolymer) for the copolymer formed early in the reaction is determined as a function of the initial value of f_A (mole fraction free monomer *A*) via the Mayo-Lewis equation (Mayo, 1944) which defines F_A as function of polymerisation rate, rate constants and fraction of free monomer. Figure 1 shows the Mayo-Lewis plot for the monomer pair styrene – methyl acrylate.

For most copolymerisations, $F_A \neq f_A$, so that one monomer is consumed preferentially, causing f_A to change as the overall monomer conversion increases. This leads to composition drift. For the monomer pair styrene – methyl acrylate, styrene is preferentially build into the copolymer. In a batch process, styrene is consumed faster than methyl acrylate. Homogeneous copolymers of styrene and MA can be produced by feeding styrene to the reaction mixture, so that the molar ratio of styrene and MA at the locus of polymerisation is kept constant. Adjusting the molar ratio of styrene and MA in a (semi-) batch process asks for a model based on mass balances for styrene and methyl acrylate.

3.2 Plant Layout

Figure 2 shows a schematic overview of the pipeless batch plant for copolymer production. The process stations and reactors are depicted by different images. The arrows represent the routing of the mobile reactors between the process stations. Buffer 1 stores the reactors that are ready to be used. At the filling station, the required initial amounts of monomer and initiator are added to the reactor. After the addition

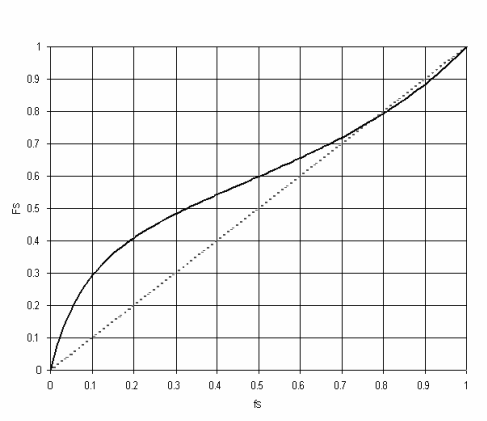

Figure 1: Mayo-Lewis plot for styrene and methyl acrylate

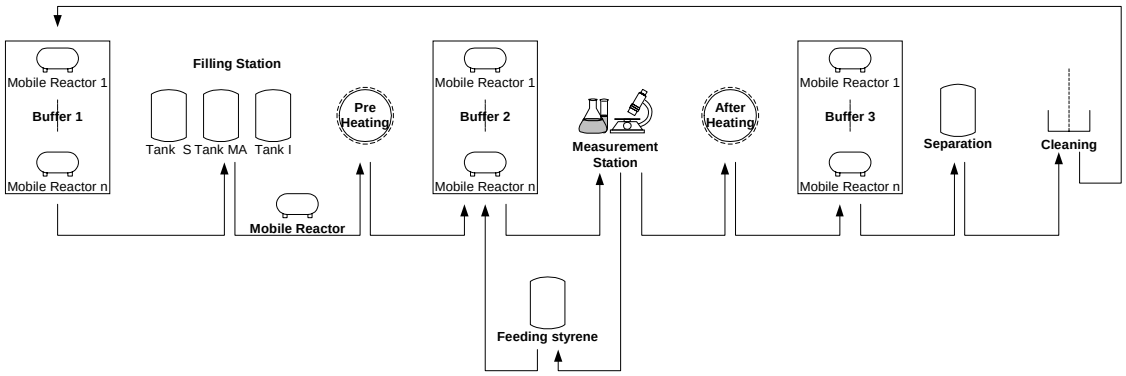

Figure 2: Layout of the pipeless batch plant

of the initiator, the reaction starts. The pre-heating station heats the reactor contents up to a level of 80 ºC. Buffer 2 stores the reactors that are waiting for sampling. At the measurement station, a sample is taken from the reactor contents. If after analysis of the sample it turns out that the reaction is completed for less than 95%, an additional feeding of styrene is required in order to keep the fraction styrene in the copolymer (F_S) in the small desired range. Analysis takes approximately 4 minutes. Therefore, the data of the sample analysis is the data that was valid 4 minutes before. Using a forecast of the measured quantities, the feeding amount can be calculated. At the feeding station, the calculated feeding amount of styrene is added to the reactor contents. After feeding, a predictive model is used to calculate the next measurement time point and the reactor is transported to Buffer 2 again.

If after analysis of the sample taken at the measurement station, it turns out that more than 95% of the reaction is completed, the reactor is transported to the after heating station, where the reactor contents is heated to a level of 80 ºC again in order to speed up the last stage of the copolymerisation. Then, the reactor is stored for 1 hour in Buffer 3 for after-reaction. After that, the reactor contents is removed from the reactor at the separation station. Finally, the reactor is cleaned in the cleaning station. From the cleaning station, the reactor is transported to Buffer 1.

3.3 Three architectures of the plant

Figures 3, 4, and 5 show three different architectures of the pipeless batch plant. The circles represent processes, which describe the functionality of the process stations. The arrows represent synchronous communication channels, interconnecting the various processes. The reactions are modelled in reactor processes. The reactors are transported from one station process to another station process.

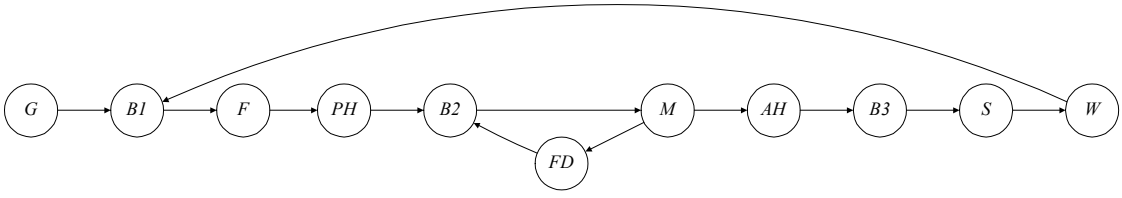

Figure 3: Flow-line with two back-tracking loops

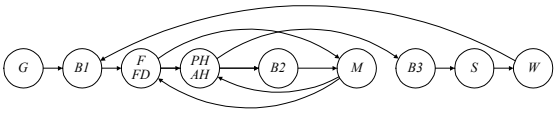

Figure 4: Flow-line with back-tracking and by-passing loops

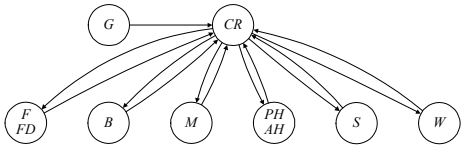

Figure 5: A job-shop architecture of the pipeless batch plant

The transportation time between the stations is taken into account as follows: when a reactor is sent from one station process to another, the reactor is put in a list. After the transportation time between these two stations has expired, the reactor is sent from the list to the intended station process. The lists are modelled in transport processes. For reasons of clarity, the transport processes and the reactor processes are omitted in the figures.

Flow-line with backtracking: Figure 3 shows the flow-line with backtracking architecture. The order-generator, process G, represents the consumer market by generating orders. An order consists of an order-number, the production recipe and the time at which the order enters the system. The recipe consists of the initial amount of the monomers (which specifies the composition of the produced copolymer), the reaction parameters, e.g. initiation, propagation and termination rate constants. Processes F, PH, M, FD, AH, S, and W represent the stations for filling, pre-heating, measuring, feeding, after heating, separation and washing respectively. Processes B1, B2, and B3 represent the Buffers 1, 2, and 3.

From a flow-line to a job-shop architecture: From the simulation results of the flow-line, it becomes clear that the flow-line architecture is not very efficient. Most of the process stations are only used during small periods of time. Some stations perform more or less the same production steps on the reactor. For example the filling and feeding stations both add a certain amount of monomer to the reactor. Performing these production steps at the same process station, results in a model that is more flexible with respect to the routing, and which requires less process stations. Figure 4 shows a flow-line with combined stations for filling and feeding, and pre-heating and after-heating.

In case of different production recipes, new process stations, and more flexibility of the routing between the process stations may be necessary. In that case, a job-shop architecture of the plant, as shown in Figure 5 may be more suitable. In this architecture, an additional controller (CR), which controls the routing of the reactors between the process stations, is required.

3.4 Simulation results

Figure 6 shows the results of a simulation with 2 reactors. In these reactors, two copolymers with different compositions of styrene and methyl acrylate are produced. For the first produced copolymer in reactor R1 and the second produced copolymer in reactor R2, the fraction styrene in the copolymer (F_S) is kept between 0.55 and 0.6. For the first produced copolymer in R2 and the second produced copolymer in R1, F_S is kept between 0.4 and 0.45. Note that the simulation results are independent of the architecture of the model.

Figure 7 shows a copolymer composition deviation of the produced copolymer within the desired range of $0.55 \leq F_S \leq 0.6$. Note that the width of the range is a parameter of the recipe. Almost 97% of the produced copolymer falls in the desired range. More homogeneous copolymers can be obtained by feeding more frequently. However, when the frequency of feeding becomes too high, the analysis time or the transportation times between the measurement and feeding station and the buffer can be larger than the allowed time between two feedings.

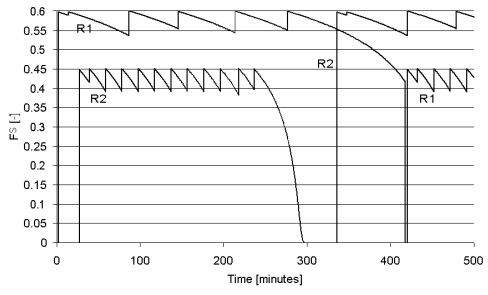

Figure 6: Results of a simulation with 2 reactors

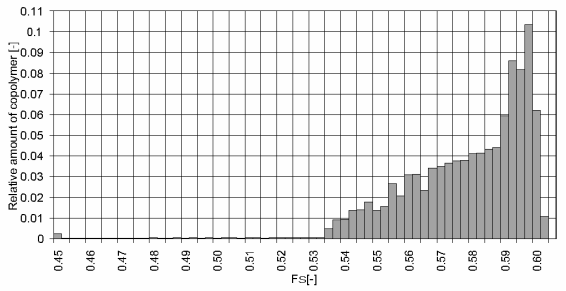

Figure 7: CCD of a produced copolymer

4. Conclusions

In the developed hybrid models of a pipeless batch plant for the production of copolymers, the dynamics of the chemical reactions have been described in detail. The required process steps and the accompanying time points are determined by the state of the reaction. The control algorithm specified in the model uses only the results of the analysis of the sample taken in the measurement station, to calculate the required feeding amount, and the time point of the next measurement. Therefore, the model is quite realistic. The developed models are the basis for further development of optimised dynamic schedulers.

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