SIMULATION MODEL OF A POLYMERIZATION PLANT

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ABSTRACT

The control systems in production plants are structured hierarchically into several layers, each operating on a different time scale: business-management, production and process level. In this article simulation model of the polymerization plant was presented to help developing a production control. The model was designed in Matlab, Simulink and Stateflow simulation environment. With the model it is possible to simulate the execution of scheduled jobs in production and to investigate and verify the plant wide control algorithms. In the model the process of retrieving the production Performance Indicators (pPI) is included, which are used to obtain information about current status of the production process. These indicators are also used to control the production process. Hierarchical closed-loop control scheme was proposed. Some preliminary results demonstrate the usefulness of the proposed methodology.

Keywords: production model, production control, performance indicators.

1. INTRODUCTION

The modern business environment demands an instant response to customers’ needs, a short product lifecycle, minimal inventories, short lead times, the concurrent processing of different products and short delivery times, as well as compliance with different regulations, environmental constraints, safe and reliable production measures, energy and material criteria, social pressures, changes in the workforce, etc. Advanced manufacturing requires quick and accurate decisions and actions at all management levels in a factory, and a high degree of decision-making autonomy within particular business and production processes in a factory. The demand for high cost-effectiveness has turned modern industry away from the planned production concept to an order-driven one. This has entailed a new concept of management based on an online estimation of the current situation together with efficient decision-making and execution. Great importance has been placed on the interaction and coordination of all the business and production activities in a company. These demands have established the importance of a production control system, used to perform at least two essential production-management activities: the transformation of a company’s objectives into results (products) and the optimization of production.

Production is a complex process, consisting of several interconnected operations restricted by various constraints. To be able to control the production process a lot of information has to be handled. The control systems in production plants are structured hierarchically into several layers, each operating on a different time scale (business-management level, production-management level and process level control) (Anthony 1965).

In general, an appropriate model of a production process is needed in order to cope with its behavior and to build a control system. However, this behavior is often extremely complex. When the behavior is described by a mathematical model, formal methods can be used, which usually improve the understanding of systems, allow their analysis and help in implementation. Within the changing production environment the effectiveness of production modeling is, therefore, a prerequisite for the effective design and operation of manufacturing systems.

It this paper the model of the polymer-emulsion batch-production process is presented. The polymerization process consists of three main stages: preparation of raw materials, the reaction process and the product analysis. Batches are produced successively using variety of equipment. The main purpose of designing the production-process model is the capability of simulating the execution of scheduled jobs in production and of investigating and verifying the plant-wide control algorithms. The demands on the procedural model of the case-study production process have many specifics that are not easy to implement in commercially available modeling and simulation tools. To avoid this trap, Matlab, Simulink and Stateflow simulation environment were used.

A number of information-technology products have been developed to collect and process a vast amount of production data. However, the production-management-level functions are covered only partially. The problems regarding a production manager’s decision-making process that still remain are: how to extract the relevant information from a vast amount of disposable production data in order to make the correct decision; and how to design a plant-wide production-control system that is capable of maintaining near-optimal production and eliminating a production manager's/operator's subjective assessments.

Usually the most important production objectives (such as profitability, production efficiency, plant productivity, and product quality) cannot be directly measured from current production data. For this reason their translation into a set of output production-process variables, i.e., *production-performance indicators – pPI*, should be provided (Folan and Brown 2005).

Plantwide control deals with the structural decisions of the control systems, including what to control and how to pair the variables to form the control loops (Stephanopoulos and Ng 2000). Decomposition of the problem is the underlying principle, leading to the classification of the control objectives (regulation, optimization) and the partitioning of the process for the practical implementation of the control structures. Hierarchical feedback implementation of a control is used here, where *optimization layer* computes set-points for the controlled variables and *control layer* implements this in practice, with the aim of achieving that (Larsson and Skogestad 2000).

In the next section production process and its model are described. In section 3 the development of control system is described. This building and testing of control is done on a model. Finally, some conclusions are given in section 4.

2. PRODUCTION PROCESS MODEL

2.1. Emulsion polymerization production process

The polymer-emulsion batch-production process is a typical representative of process-oriented production. The production effectiveness, to a large extent, relies on the quality of the production-control system. The production layout consists of several reactors, dosing vessels, storage tanks and equalizers, which are used for the production of different products.

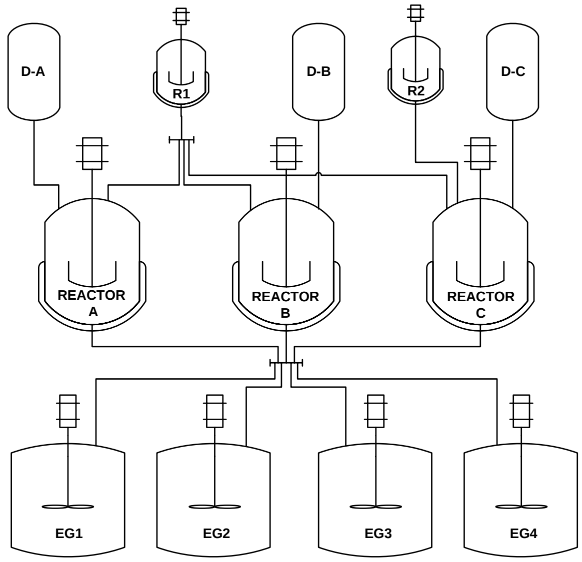


Figure 1: Simplified technological scheme of the polymerization plant

Simplified technological scheme of the polymerization plant is presented in the Figure 1. The technological process is defined with a recipe, i.e., the sequence of operations that have to be performed for the production of a particular product. Various recipes performed simultaneously can share some common resources. The polymerization process for the production of one batch of emulsion can be represented by the state-transition diagram that is depicted in Figure 2 and consists of three main stages: (i) the preparation of raw materials, (ii) the reaction process and (iii) the product analysis and reactor discharge. The optional stage of the product equalization takes place in the equalizator.

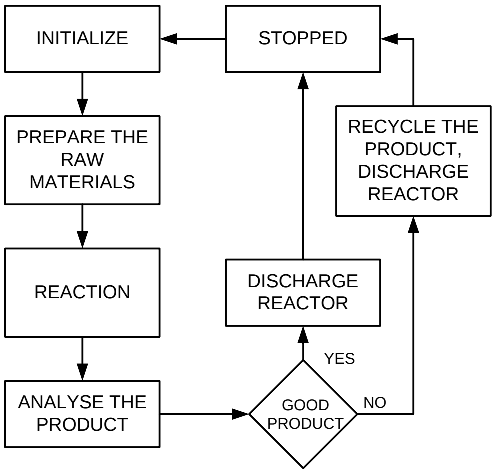


Figure 2: State-transition diagram of the polymerization process

The polymerization plant produces three groups of products (*H*, *KM* and *PA*). There are four different types of products in a product group *H* (*Homopolymers*). They follow the same process but have some differences in proportions of the raw materials and are produced in reactors A, B or C.

First input material is prepared in dosing tanks (D-A, D-B or D-C) and in reactor R1 or R2. Then the initiation starts. The reactions take place in the reactors A, B or C. After the reaction is finished more batches are mixed together in equalizer in order to equalize their properties and to obtain similar quality of a final product.

Raw materials for the second group of products (*Copolymer KM*) are prepared in dosing tank D-B and reactors R1 and R2. In this case the reaction can be performed only in reactor B.

At the end again equalization of more batches is done. Product *PA* (*Polyacrylate*) is produced in reactor E, but since this part of the process is independent of other one, it is not included in the production process model. Before the successive batch can be produced reactors have to be cleaned.

The main characteristic of this batch-production process is the production of successive batches using a variety of equipment in which intermediate products appear during each batch stage and must be used in successive stages as soon as possible. In each step certain physical actions (heating, blending) and chemical reactions are involved. The utilization of the whole production process depends on the execution of a list of production jobs.

There are many variables that are controlled during the polymerization process at the lowest (process) level of control: temperature of the reaction, reflux temperature, flow rate of monomers, pressure in the reactor, etc. Our point of interest is the control at the production level, where scheduling, plant-wide optimization etc. are performed. The variables to control here can be the quality of products, productivity, production costs…

2.2. Production process model of a polymerization plant

The demands on the model for the case-study production process have many specifics that are not easy to implement in commercially available modeling and simulation tools. To avoid this trap, the model was designed in an academically well-established Matlab, Simulink and Stateflow simulation environment.

The developed production process model of the polymerization plant represents the production process and its attributes (utilization of resources, production gain, product quality, production costs, etc) in the form needed for production management. This means that we have modeled physical realities of the process as well as production costs and quality aspects of the process. The model is structured in six logical units that are interconnected as depicted in Figure 3.

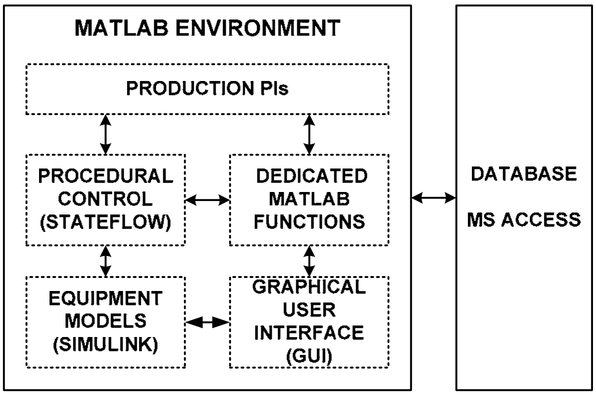


Figure 3: The structure of the production process model

2.3. Equipment models

The *equipment models* are created with simple Simulink models that incorporate I/O control signals. The models of the chemical reactors do not include the exact mathematical formulation of the chemical reactions involved in the polymerization process (as at this level of interest are not necessary), but they do include the equations of temperature, mass flow and level dynamics. The model of reactor R-A is demonstrated in Figure 4. On the upper part of the picture there is an integrator which describes mass flow and the lower part represents the model of a temperature.

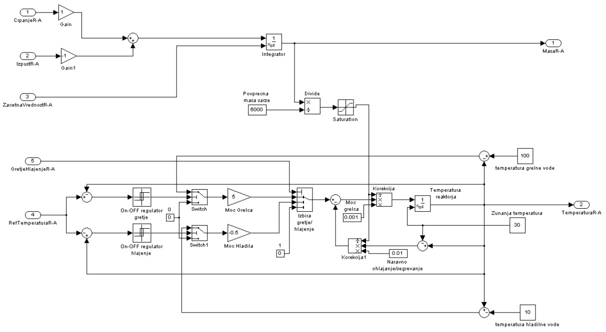


Figure 4: Simulink model of reactor R-A

2.4. Procedural control

Procedural control of the equipment was implemented using Stateflow charts. It supervises the execution of tasks and calculation of indicators about the production process status. The scheme of procedural control is depicted in Figure 5. The production jobs are scheduled according to the demands from the business management level (due times, desired product cost and quality, etc) and other production constraints (production rate, availability of resources, etc).

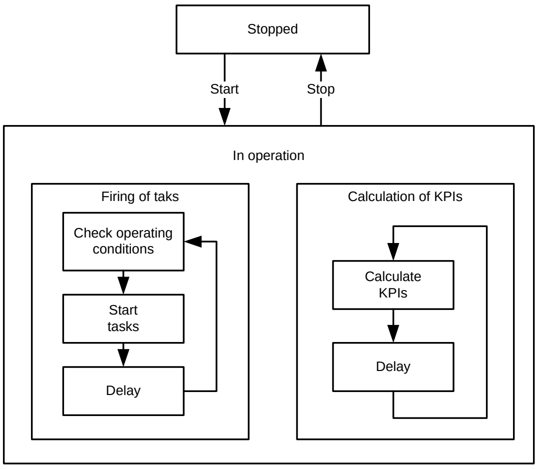


Figure 5: Procedural model scheme

2.5. Dedicated Matlab functions

Dedicated Matlab functions are used to evaluate other properties (e.g., the product quality) of the chemical reactions. These functions were designed and calibrated on the basis of statistical analyses of the production data and on knowledge about the production process obtained by interviewing production operators and technologists.

2.6. Production Performance Indicators

There are number of measured signals that can be used to get an insight into the process system state. The main problem is how to extract the relevant information from a vast amount of disposable production data in order to be used for making correct decisions in production control. The problem lies in the fact that the most important global production objectives such as profitability production efficiency, plant productivity and product quality usually cannot be directly estimated from current production data. For this reason their translation into set of output production-process variables should be provided. Production Performance Indicators (pPIs) are introduced to overcome this problem. In our case three pPIs were selected: *Productivity - P*, *Product quality - Q_P* and *Production costs - PC*. None of these pPIs is directly measurable, but an estimation of their current values can be made using the combination of the measurable output production-process variables. The procedure for the pPIs calculation has two characteristic parameters:

- calculation frequency f_{PI} which defines the time frames in which the pPIs are evaluated and
- calculation window T_{PI} that defines which production history data are used for the evaluation of the pPIs.

Productivity is defined as the amount of all products that were produced in a certain production period, and this amount is defined with:

$$P = \frac{\sum_{i=1}^{n} k_i \cdot M_i}{T} \tag{1}$$

where k_i represents the correction factor, M_i is the batch quantity, T is the observed time window and n is the number of observed batches. We take into consideration all the batches that were completely or partly produced in the defined production period and calculate the average amount of products that were produced in an hour. The correction factor defines the percentage of the production time of each batch that fits into the observed production period.

Another important indicator of production efficiency is the *mean product quality*, Q_P, which is calculated as the mean value of the quality factors of the batches that were completed in the observed production period. It is calculated with:

$$Q_P = \frac{\sum_{i=1}^{n} Q_i}{n} \tag{2}$$

where Q_i is the quality of a single batch and n is the number of observed batches.

The production costs indicator consists of *variable costs* such as raw-materials, energy, and other operating costs and *fixed costs*. The *mean production costs* (per kilogram of final product), *PC*, are calculated as the sum of all the costs related to production in the observed production period divided by the total number of products produced in that production period:

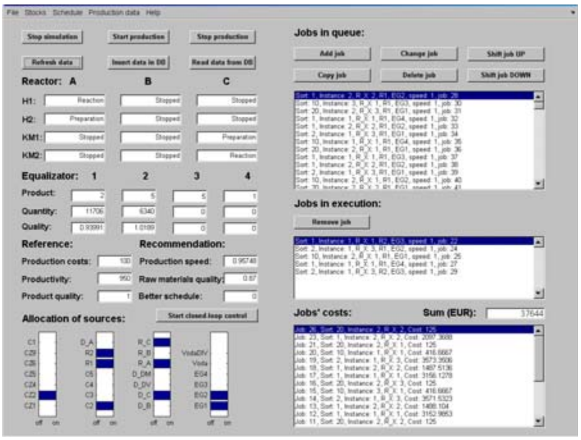
$$PC = \frac{\sum_{i=1}^{n} k_i \cdot C_i + T \cdot C_f}{\sum_{j=1}^{m} k_j \cdot M_j} \tag{3}$$

Here k_i is the correction factor for the job costs, C_i the job cost, T the production period, C_f the fixed costs, n the number of observed jobs, M_j the batch quantity, k_j a correction factor for the batch quantity and m the number of observed batches.

Those pKPIs represents the outputs of our production model. On the other hand there are more manipulated variables, i.e., physical degrees of freedom, which represent the inputs into the model. Selection of these variables is usually not much of an issue, since these variables usually follow as a direct consequence of the design of the process itself. Production jobs are scheduled according to the demands from the business management level and *Job schedule – BS* can be considered as one input variable into the production-process model. There are two other input variables that define the production process which are the *Production speed - S*, which defines the production rate, and the *Raw materials' quality - Q_{RM}*.

2.7. Graphical User Interface

The GUI (Figure 6) enables the user to simulate the production process; the user can manipulate online the *Job schedule*, the *Production speed* and the *Raw materials' quality*. On the other hand, the GUI presents the current state of the equipment (reactors, equalizator, etc.) and enables statistical analyses and a visual representation of the historical production data.



Reactor:	A	B	C
H1:	Reaction	Stopped	Stopped
H2:	Preparation	Stopped	Stopped
KM1:	Stopped	Stopped	Preparation
KM2:	Stopped	Stopped	Reaction

Equalizator:	1	2	3	4
Product:	2	5	5	1
Quantity:	11706	6340	0	0
Quality:	0.93991	1.0189	0	0

Reference:		Recommendation:	
Production costs:	100	Production speed:	0.95748
Productivity:	950	Raw materials quality:	0.87
Product quality:	1	Better schedule:	0

Jobs' costs: Sum (EUR): 37644

Figure 6: GUI of the simulation model

2.8. Database

The simulated data are stored in an MS Access Database and are available for online and offline processing.

3. USE OF PRODUCTION PROCESS MODEL

The model was validated by the production manager and it reflexes the actual situation in the production process. Later model was used to design and to test the production control system.

The control is being performed on different levels of decisions. The idea of hierarchical control levels is related to the so-called self-optimizing control that was presented by Skogestad (2000, 2004). Generally speaking, for every system we have available degrees of freedom (decisions), u, that we want to use in order to optimize the system operation. With the proper selection of the controlled variables, c, and the set-points, c_s, for these variables it is possible to operate in a near-optimal regime just by preserving these variables at defined set-points. With this approach the complex optimization problem can be translated to a simpler control problem.

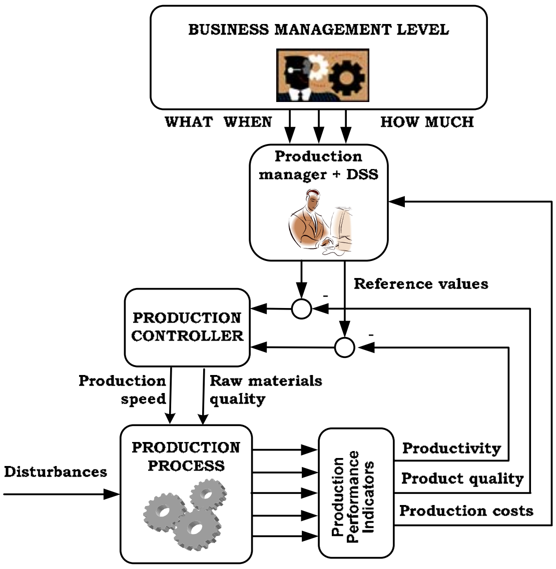


Figure 7: Hierarchical closed-loop control scheme for the polymerization process plant

Figure 7 presents the generalized, hierarchical control-loop scheme for our production process based on the self-optimizing control approach and pPIs. On the optimization level, represented by the upper control loop, the production manager optimizes the production process by selecting appropriate reference values for the pPIs in the control loop on the lower production-control level. The production manager's choice of proper pPIs set-point values depends on her/his experiences and skills, the demands from a higher business-management level and on the current state of the production process. The process of defining the set points can be improved by using the production DSS, where an estimation of the current production costs can be made using a cost model and the online production data. Once the reference values for the pPIs are defined, they are maintained by the production controller. To define appropriate controller usually also a model is needed. The described control structure reduces the complexity of the control problem; while at the upper control loop production manager with a help of a cost model make decisions about the set-point values for the chosen pPIs (e.g., on a daily basis), the lower control loop is managed automatically by the production controller more frequently (e.g., on a hourly basis).

3.1. Control of the polymerization plant

While controlling the plant, the minimization of production costs is the highest priority, and the majority of control actions are made to fulfill this demand.

On the process-optimization level the cost optimization is performed by the production manager, who is making a decisions based on the current value of the *Production costs*, the *Job schedule*, with a help of a production cost model, to define the optimal set points for the *Product quality* and *Productivity* indicators. The production costs' model acts as a kind of decision support system (DSS) for the definition of references for the pPIs.

Sensitivity analysis of the pPIs was done in order to get the production costs' model. The pPIs were evaluated at 20 working points and connected together by extrapolation. Figure 8 shows the relation between *Production costs*, *Product quality* and *Productivity* pPIs, i.e. the dependence of the *Production costs* regarding *Productivity* and *Product quality*. These are dependencies for the case for unified production, i.e., a production where a series of batches of the same or similar final products are performed on each reactor. Another cost model would be achieved for different production.

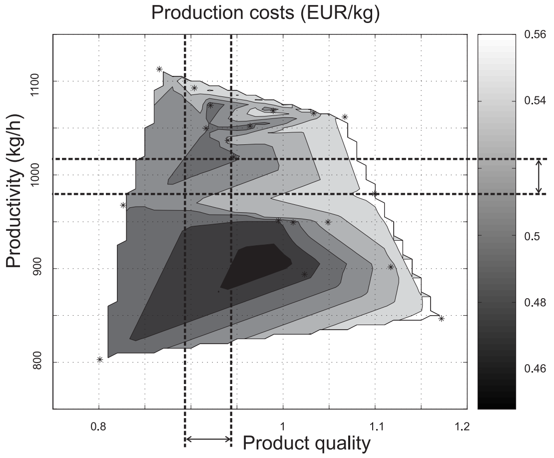


Figure 8: Cost model – *Production costs* in relation to *Productivity* and *Product quality* for unified production

Once the pPIs' reference values are defined (e.g., from the area defined with dashed lines) they are maintained by the production controller, which controls the execution of the production jobs' schedule by adjusting the available degrees of freedom for the chosen production processes, which are *Production speed* and *Raw materials' quality*.

The production controller is placed in the lower hierarchical control loop in Figure 7. To design a controller a model of the production process is needed. The part that has to be controlled is a multivariable system that can be linearized for a commonly used working area. It has two input variables (*Production speed* and *Raw materials' quality*) and two output variables (*Productivity* and *Product quality*).

Model predictive control (MPC) is well suited to solving this constraint problem (Morari and Lee 1999, Qin and Badgwell 2003). First linear process model was obtained by using the identification process over the production-process model. In the identification process, input-output data that were obtained from several simulation runs were used. Here it is assumed that the process is linear. In such a situation an approach where one input is changing while another one is fixed can be used. In the first experiment the *Raw materials' quality* was fixed and the influence of *Production speed* on the outputs of the system (*Productivity* and *Product quality*) was studied. The same experiment was repeated, but in this case the *Production speed* was fixed and the influence of *Raw materials' quality* was studied. The model parameter estimation was made using the identification method in which the least-square criterion was minimized. The input-output dependencies are therefore given with first-order models, where the *sampling time* T_S was 5 hours:

$$G = \begin{bmatrix} \dfrac{31.84}{z-0.938} & \dfrac{-4.43}{z-0.834} \\ \dfrac{-0.04}{z-0.932} & \dfrac{0.052}{z-0.94} \end{bmatrix},\ T_S=5\ h \qquad (4)$$

This multivariable model *G* was used for the MPC controller design, where the MPC Toolbox from the Matlab environment (Bemporad *et al.* 2006) was used.

The main challenge was the tuning of MPC controller's cost function parameters. The MPC toolbox supports the prioritizations of the outputs. In this way, the controller can provide accurate set-point tracking for the most important output, sacrificing others when necessary, e.g., when it encounters constraints. In our case the controller has to consider the input and output constraints as defined with next equations:

$$\begin{matrix} 0.5 \le S \le 1.3 \\ 0.85 \le Q_{RM} \le 1.2 \end{matrix} \quad \text{and} \quad \begin{matrix} 700 \le P \le 1300 \\ 0.87 \le Q_P \le 1.3 \end{matrix} \qquad (5)$$

Different weights were used to prioritize the input and output variables. To solve the optimization problem, a prediction horizon of 100 hours and a control horizon of 40 hours were used.

Closed-loop control was tested in several simulation runs. Figure 9 presents the results of an experiment where the set-point for *Productivity* was changed two times and the set-point for *Product quality* was changed just once. In the experiment a normal batch schedule for the production of three products, each of them produced in one reactor, was used. MPC managed to achieve the prescribed set-points for the controlled pPIs (*Productivity* and *Product quality*). With the increasing set-point for the *Productivity* the *Production costs* indicator is also increasing, and with the decreasing set-point for the *Product quality* the *Production costs* decrease. The *Production costs* indicator is not as smooth as the other two pPIs, which reflects the influence of the stops in production on the production costs. With an increased time horizon for the pPI evaluation such leaps in the pPI values are reduced, but also the pPI's dynamic is reduced, and consequently the performance of the MPC controller is also reduced. From the pPI responses on changed set-points for *Product quality* and *Productivity* the time constant of such a pPI model can be estimated at around 50 hours.

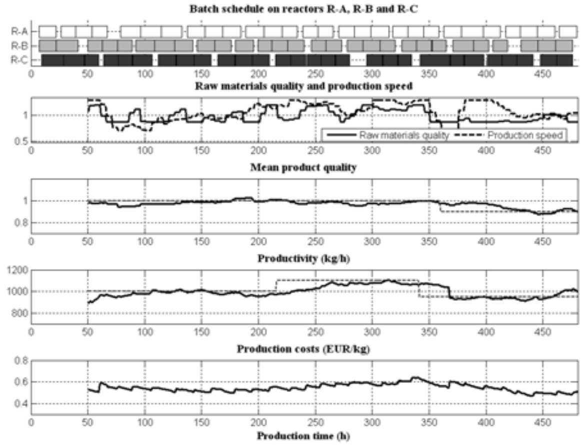


Figure 9: Batch schedule, input and output variables for one simulation run for normal production

4. CONCLUSIONS

Simulation model of a polymerization plant in the form needed for production control is presented. Production Performance Indicators are used to get an insight into the process system state. Hierarchical closed-loop control system was developed using this model and can be further implemented in the real industrial plant. The main challenge here would be the reorganization of an existing information system, in order to have available all needed variables.

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