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BATCH ANALYSIS

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Batch analysis is one of steps in the design and implementation of batch process plants – an S88 based – analysis of batch processes from the control point of view. It is between the conceptual design of the batch process (PFD or P&I) and the start of the design of the control system (design of instrumentation, control hardware and software). Its objective is to fill the gap almost always found between the formulation of requirements and the specification of the actual implementation by transforming user requirements into “process-based” detailed functional requirements. It has several advantages when these problems are handled, not by software engineers, rather by batch control analysts who are closer to the plant and has deeper knowledge of the process. In former batch systems this problem was solved instinctively by the engineers developing control software based on their earlier experience. Systematic design, however, allows finding an optimal or close to optimal solution in an easier and more manageable way. The method described in the paper is a new approach in batch engineering practice. Its exact formulation was made possible by the introduction of the S88. 01 standard. The application of the proposed approach can bring several benefits, like optimal control structure, well-structured and shorter software code, reduced debugging needs, simplified design and implementation as well as increased system reliability.

Keywords: batch control, systematic approach, S88. 01 models

Introduction

Majority of pharmaceutical and fine chemical processes are accomplished in batch or fed-batch operations. Batch processing involving the execution of several separate processing operations on a given amount of materials (batch) in a given order provides a great adaptability for rapidly changing market demands. While the control of batch processes carries much more difficulties than continuous processes do, present computer-based control systems and solutions allows efficient and flexible command of the batch production processes. At the same time, the design of batch control systems represents a rather complex problem for the process and control engineers [1-5].

Batch analysis is the phase in the design of a batch process control installation that covers the analysis of the control problem, the structuring of the process and equipment, the distribution of tasks between control levels (basic control, procedural control, coordination control) and the design of the recipe operation library including the control of abnormal situations (exception handling) in order to achieve optimal control [6, 7].

In the plant construction process, batch analysis is between definition of the user requirements and the design of instrumentation, hardware, and software. It is aimed at filling the gap found between the definition of requirements and the actual implementation in almost every project. For example the user may define only the following: crystallization must be executed automatically. To implement this into the control software, the programmer has to decide whether unit approach or equipment module approach should be used to solve the problem. It is better if these questions are answered, not by software engineers, rather by batch control analysts who are closer to the plant and know the process better.

Batch analysis is system independent, which means, that recommendations are defined without any limitations of the actual system. In the following steps such a control system must be chosen that allows implementation of the control strategies elaborated during the batch control analysis.

The original name of the method was batch analysis. Since nowadays this term is used for the evaluation of executed batches, we introduced an extended name “batch control analysis” in order to emphasize the difference. We feel this name even more clearly reflects the content, i. e. the analysis of the process and production system for developing an optimal control strategy and control system. In the followings both batch analysis and batch control analysis is used in the same sense.

Design and implementation of batch processes

The main steps of the construction of a batch processing system and their relations are represented in a simplified form on *Fig. 1* [8]. One of the important steps of this construction procedure is the batch analysis. The approach has been known in engineering practice for several years, however in spite of its significance it is less widely applied. The main objective of the approach is to provide a clear pathway between the user requirements and the actual implementation. Requirements defined by the user in the process descriptions do not contain the details necessary for configuring the DCS. It is desirable that this missing information be provided by a process expert – the batch analyst – who knows the process much deeper and better then the configuration expert who is more related to the informatics and control aspects. It is even better if the solution can be given in general form that is valid for other equipment as well, i. e. in form of strategies and basic principles, which could provide guidance for the instrumentation engineer as well as the hardware and software designer in other projects as well.

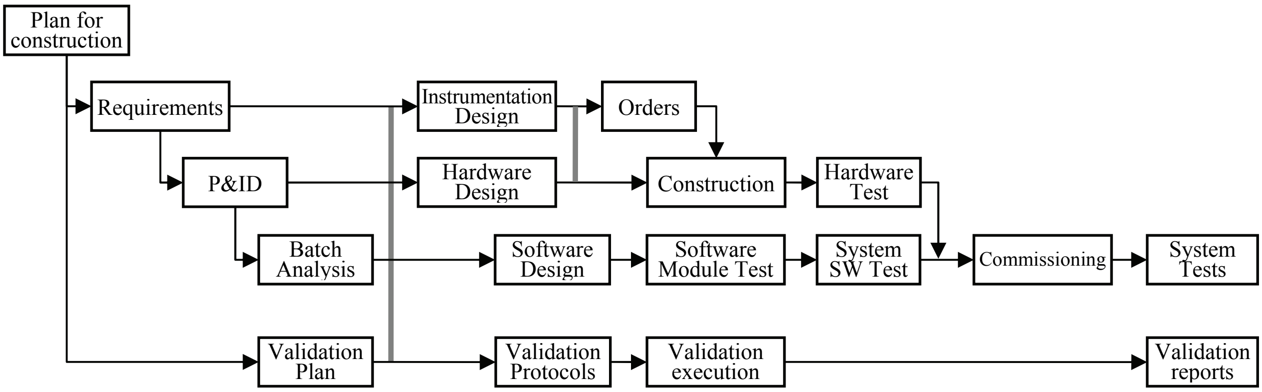

Figure 1: Construction of a batch plant

The batch analysis

Batch control analysis is one of steps in the design of plants executing batch process - an S88-based analysis of batch process from the control point of view in order to reach an optimal control structure, decompose the process and equipment, divide the control functions between control levels (basic control, procedural control, coordination control), design the operation library and the operations themselves including the exception handling. It is between the conceptual design of the batch process (PFD or P&I) and the start of the design of the control system (design of instrumentation, control hardware and software). Its objective is to fill the gap almost always found between the formulation of requirements and the specification of the actual implementation. It transforms user requirements into "process-based" detailed functional requirements. It has several advantages if these problems are handled, not by software engineers, rather by batch control analysts who are closer to the plant and know the process better.

In former batch systems this problem was solved instinctively by the engineers developing control software based on their earlier experience. Systematic design, however, allows finding an optimal or close to optimal solution in an easier and manageable way. The method described in the paper is a new approach in batch engineering practice. Its exact formulation was made possible by the introduction of the S88. 01 standard [9-11].

A very important feature of batch control analysis is system-independence. It means that the results of batch control analysis are independent of the actual control system. A good control system will not restrict the implementation of the results. Batch analysis must be launched in an early phase of construction process by deciding the control strategy to be applied (total automation, automated islands, etc.). In industrial practice, the tasks are allocated to the control experts only after the deciding fundamental process and machinery problems i. e. after fixing the concepts and topology of the plant. Naturally, at this phase the benefits of batch analysis are limited.

Steps of batch analysis

The batch control analysis consists of the following steps (see *Fig. 2*):

- Analysis of the process – a simplified description of the process for control purposes.
- Decomposition of equipment – Definition of hierarchy levels to be followed in the system (process and physical models).
- Decomposition of tasks:
  - Design of elements of procedural control (procedural control model, library of phases and operations).
  - Choice of control structure at the basic level.
- List of instrumentation.
- Specification of operator requirements.

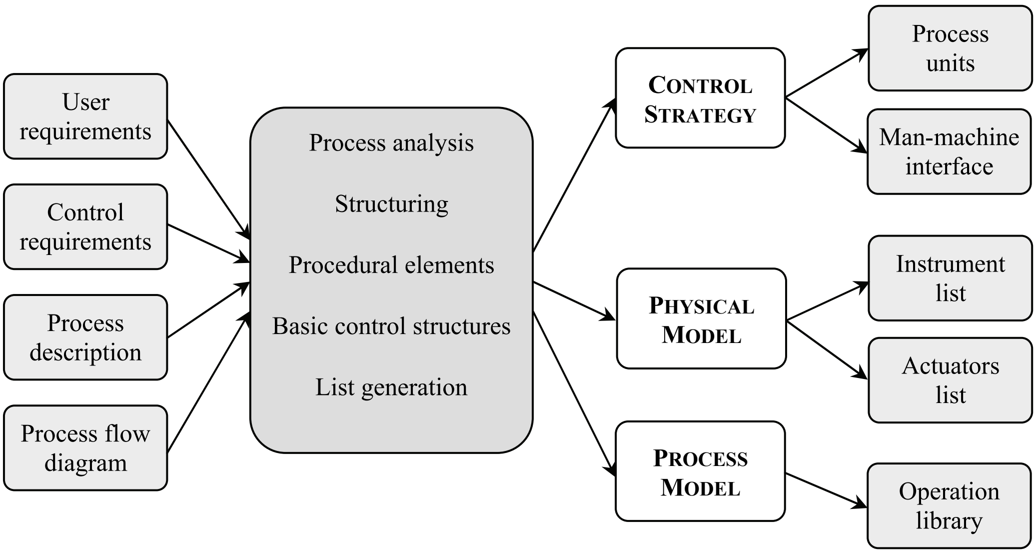

Figure 2: Steps of the batch control analysis

Process analysis

The work is started from a general, brief process description. This document should include the followings:

- short description of the technological process,
- description of the most important operations,
- description of the main process units,
- description of the process chemistry,
- summary of the most important requirements for the process (e. g.: the necessity of high-accuracy temperature control),
- safety, health and environmental protection considerations.

The role of process safety risk analysis must be emphasized here. It is definitely to be included in this step since it provides information significantly influencing the further design process.

It is decisive in this phase that a simplified process diagram has to be available. It should show all the equipment essential from process control point of view (reactors, dryers, tank park, utilities, shared-use equipment). To avoid misunderstanding, a common terminology has to be agreed. Nowadays the usage of the S88. 01 standard is a general requirement.

Structuring

Well-considered, well-done structuring makes further work significantly easier. Bad compromises accepted during structuring will hit back. It is only a question of time and in some phase of the following work the poorly selected hierarchy will become unusable. It is not worthwhile to give up a decomposition justified by system engineering for illusory, short-range advantages. If structuring is too difficult to do or involves lots of compromises, it suggests that there are shortcomings in the previous design phase (e. g.: in the process or equipment concepts).

The first step of structuring is the definition of the process model (see *Fig. 3*). The process model as defined by ISA S88 is a four-level hierarchical model composed of process/ process stages/ process operations/ process actions. The complete production process is first divided into process stages, then into process operations. This later one is not equivalent to a recipe operation. The only requirement is that process operations must allow describing the complete process. The process model will serve later as a basis for determining the necessary recipe operations.

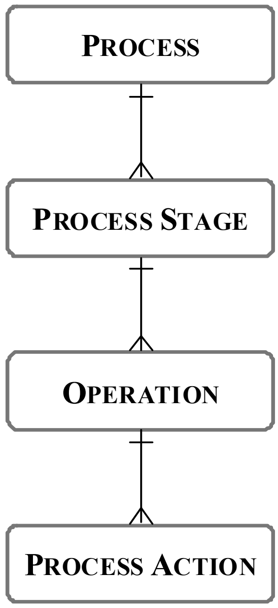

Figure 3: The process model

The practical use of the process model is very obvious. For illustration, *Fig. 4* depicts the representation and the use of the operations in the process model.

Code	Process operation	Parameters	Process measurement				Process mode	Required manipulating element	Comments
			Critical	Important	Informative	Safety			
P1_1	Acetone charging	111 l acetone		$FIQS_{aceton}$			Auto		
P1_2	Water charging	222 l DEMIwater		FIQ_{water}			Auto		
P1_3	Temperature setting	20 – 25 °C		$TITCA_{react}$ $NTC_{reactor}$	$TTC_{jack-in}$ $TT_{jack-out}$	PTS_{jack}	Auto		

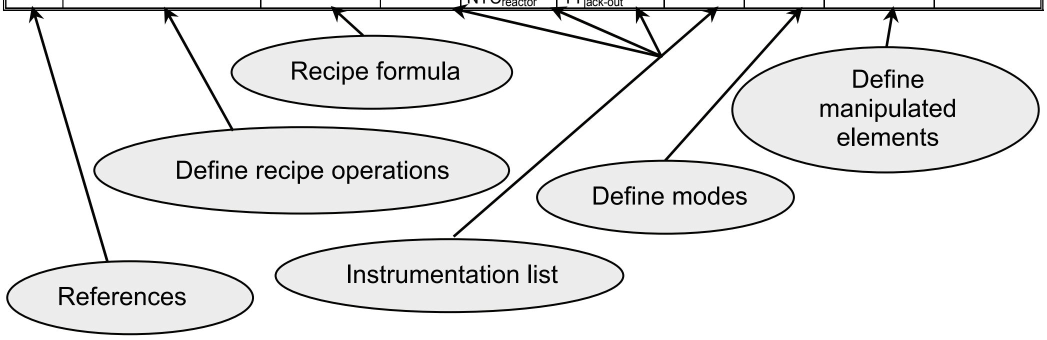

Figure 4: The application of the process model

The purpose of the application of each previous column is easily conceivable:

- *Code* - for reference (coordination links),
- *Process operation* - these operations will serve later as the basis for recipe operations,
- *Process measurement* - the following groupings: critical (influencing the quality), important for the process, informative and safety provides the requirements for the designer of the instrumentation. Considerable cost reduction can be achieved by choosing suitable types of instruments.
- *Required manipulated element* - operations under automatic control require automatic manipulated elements.
- *Other* - special requirements, coordination requirements, etc.

The second step is the definition of the physical model (*Fig. 5*). The main function of the physical model is to define the relations of the process equipment unambiguously. The prerequisite for assuring transparency and order is that each element belongs to one and only one higher-level element. Later on, the hierarchy of the control system will follow this model. Every control module will be responsible for handling its own physical elements, therefore it must know which elements of the physical model are allowed to be manipulated directly and which are not.

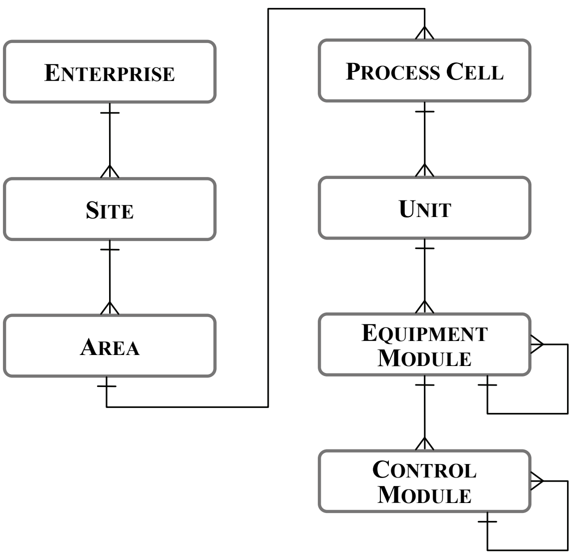

Figure 5: The physical model

While the decomposition an intuitive procedure, several general rules can be applied.

It must be assured in the structuring of the process system, that:

- functions must be clear and separable,
- they do not be tied to one product,
- it is practical that subordinate elements can accomplish their task independently in an asynchronous way in order to allow precise control for the higher level,
- the connections to other elements are minimized,
- its borders are clearly defined,
- in case of units a corresponding recipe should exist [12].

Structuring an equipment group requires the basic knowledge of the supplementary operations. Several control modules together can build an equipment module or another control module.

The physical model has an important role in maintaining a clear naming and tagging convention, as well. The notation: process cell/ unit/ equipment module/ control module identifies any element of a system precisely.

During the whole course of the construction of the process system all of the structuring and grouping steps should follow some of these models. For example, the process graphics can be organized according to the process model. The support system for maintenance tasks should follow the physical model, etc.

Design of procedural elements

Procedural control is the most characteristic level of batch process control. It involves the execution of equipment-specific operations in a predetermined order to achieve the production objectives of the process. The procedural control applies the elements of the hierarchical procedural control model to accomplish the required control of the batch process. The procedural control model is shown in *Fig. 6*.

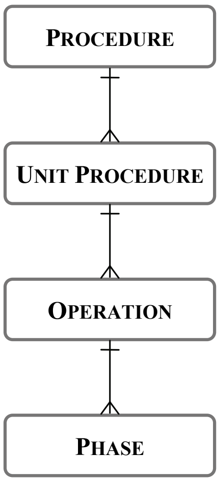

Figure 6: Procedural control model

The procedure itself defines the strategy of the main process action. The strategy of final processing e. g. can be – solution, crystallization, centrifuging, drying.

The unit procedure is an ordered sequence of the operations belonging to the unit. In case of a centrifuge procedure these are the filling, spinning, washing, spinning, and removal operations.

The operation is the sequence of the main processing phases. The execution of an operation results in significant chemical or physical changes of the processed material leading to the required production objectives. The phases of the crystallization e. g. – filling, heat up, cooling and removal.

The phase is the lowest level of procedural control (according to IEC 488 it can be further divided into steps and transitions). The phase executes the process actions by commanding the operation of basic control level or other phases. The data collection is also accomplished during the phase execution. The phase execution provides commands for the control loops, moves the system to new state according to the state-transition diagram, changes the parameters, etc.

The recipe operation is an element of ISA S88 recipe model (recipe procedure/ unit-procedure/ operation/ phase). The recipe operation is a more generalized form of process operation, which can be used for a number of different processes. The relationship between process and recipe operations is illustrated in *Table 1.*

The library of recipe operations and recipe phases has to be developed during the batch control analysis. At this time required recipe procedural elements have to be generated from the elements of the process model in such a way that the procedural elements must be generic allowing the accomplishment of more process elements and thus allowing that the production task be defined by compiling a recipe from these elements. A few points of view for the development a recipe operation are the following:

- Any process operation (phase) can be generated by assembling one or more recipe operations (phases) serially or parallel.
- Functions used more than once have to be identified. The fewer and the simpler recipe operations required to cover the problem, the better the implementation will be. A simple method for reducing the number of operation is shown in *Fig. 7* and *8*.
- The simpler available recipe operations are the more difficult is to build a recipe; however, the system will be more flexible. An optimum has to be found to reach the necessary flexibility with the most complex operations.
- The tool for fitting recipe operations to the actual process application is the use of recipe parameters. The more the available parameters there are, the more flexible the system will be, however at the same time, the more difficult it is to build a recipe and understand and explain an operation and its parameters.

The recipe operation library is a collection of recipe operations from which the process engineer can build the master recipe. Its content is expanding continuously. As new processing tasks emerge the library selection grows. The library contains also the operation descriptions which are used for developing the operations by the control and software engineers as well as when building a recipe by the process engineer.

Typical problems in the operation development are the following:

- Very few and complex operations result in a less flexible system.
- Operation parameters are used to solve discrete control functions of the basic control. The operation parameters should belong to the process engineer, not to the system integrator.

Table 1: Relationship of process and recipe operations

Process operation	Recipe operation	RO No
Quick heat up	Thermal operations	01
Quick cool down		
Linear heat up		
Linear cool down		
Temperature hold		
Refluxing	Reflux	09
Solvent removal	Atmospheric distillation	04
Evaporation		
Solvent removal in vacuum	Vacuum distillation	05
Evaporation in vacuum		
Solvent charging	Liquid charging	16
Water charging		
Solid charging	Solid charging	17
Inertization	Inertization	10
Filling from drum	Filling	12
Discharging into drum	Discharging	13
Discharging to incinerator		
Discharging by pump		
Circulation		
Transfer into other unit	Transfer	18

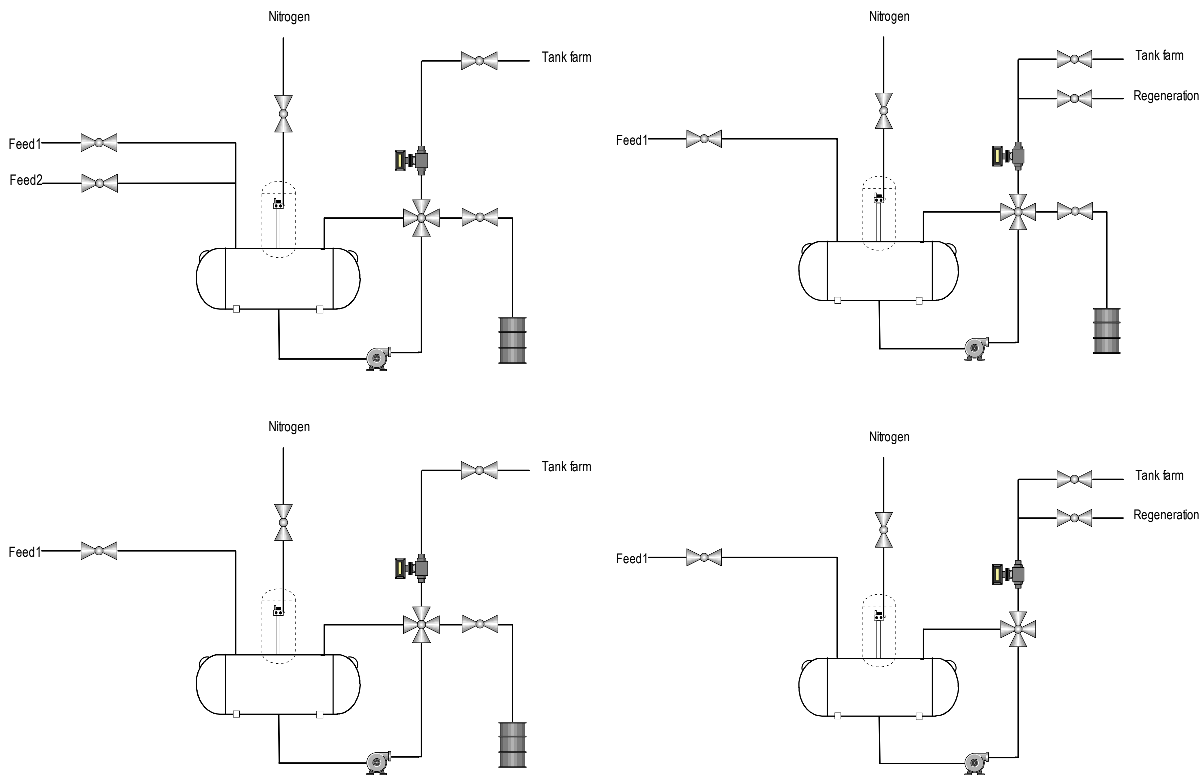

Figure 7: Tank constructions (they are not identical)

Fig. 7. shows four different tank constructions. None of them is the same. However the similarity of them is striking. Instead of developing the individual operations (filling, discharging, homogenization, inertization, etc.) for the four different tank arrangements, one single virtual tank is formed as a superstructure of the four vessels (Fig. 8). In the next step one set of operations is developed and the deviations are handled in the software.

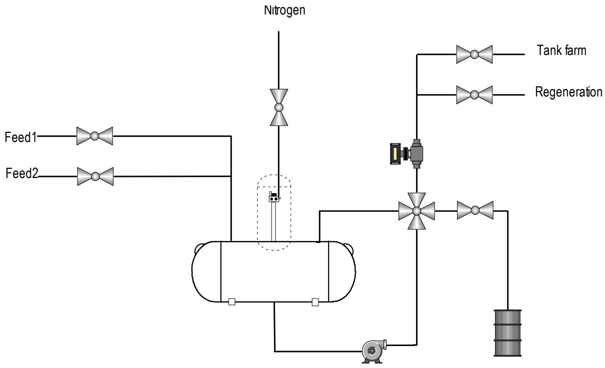

Figure 8: Virtual tank

Design of the basic control structures

The necessary basic control elements are implicitly defined in the procedural control (valve operations, motor operations, etc.). A well-tried practical approach for solving similar problems is developing typical (standard) solutions, then testing them and finally applying them repeatedly.

An important phase of the design process is the design of interlocks. These will assure the a basic level of process safety to prevent accident triggered by the errors of the higher level, more complex and therefore less reliable software elements. These interlocks provide the safety functions at lowest level, close to the process equipment. They also support the safe operation in manual-mode in case of operator interventions.

The batch operation requires the understanding and implementation of procedural interlocks which operate only in the active state of the corresponding procedural elements.

List of instruments and manipulated elements

After defining the operations and the basic control requirements for the instrumentation (i. e. what kind of measurements and manipulating elements are necessary from process point of view) and their importance with respect to the process (critical, important, informative, safety, etc.), each instrument can be defined. Therefore the necessary elements of the loops can be designed and selected optimally considering functionality and cost aspects.

Definition of operator requirements

At this phase, based on the ratio of automatic and manual modes (given in the Mode column of the process model definition), the operator requirements and the corresponding human-machine interface for the field and control-room operations can be designed. The more manual activities are involved the more complex field HMI is required. It must be decided here that how many operators will operate the plant, how many operator stations will be necessary, what is the function of each station (which consol is allocated for each particular process system), who is responsible for a given section of the system.

The structure of displays, i. e. the system of operator displays as well as the tree-diagram for the display transitions must be designed. To provide a unified display system, standards are to be developed for colour coding, equipment symbols (equipment library) and for the general layout of the displays (template).

The operator messages must be prioritized. They can be:

- Alarm messages – standard functions are usually available,
- Warnings – a typical warning e. g. is a message of exceeding the planned operation time,
- Call for acknowledgement – e. g. for continuing a recipe.

SUMMARY

Engineering approaches similar to that of batch control analysis were necessary in the past as well, of course. Engineers developing the control system did this work instinctively based on their earlier experience. Systematic design – based on the batch control analysis – however, makes the engineering design simpler, more effective and more straightforward to achieve an optimal or close to optimal solution. According to our experience, in many cases the control software of systematically structured systems is shorter by 50 % than that of instinctively structured solutions. The method reduces not only programming efforts but also the number of software errors by the same ratio, and it results in a system which is simpler to start-up and is more reliable with a much lower number of abnormal occurrences coming from software.

It is also not negligible that batch control analysis provides control and process engineers with much deeper knowledge of the process. That has an advantageous effect throughout the design and implementation of the new batch processes.

REFERENCES

1. DIXON-DECLEVE S.: World Refining, *2001*, 12(9), 8
2. FISHER G. T.: Batch Control Systems: Design, Application and Implementation, ISA, North Carolina, *1990*
3. LIPTAK B. (Ed.): Instrument Engineer's Handbook, Process Control Volume, Chilton Book Company, *1995*
4. RAVEMARK D. E. , RIPPIN D. W. T.: Optimal design of multi-product batch plant, Comp. Chem. Eng. , *1998*, 22, 177-183
5. REAKLAITIS G. V.: Overview of scheduling and planning of batch process operations, Proc. NATO-ASI on Batch Processing Systems engineering, *1992*

6. THOMAS G. F.: Batch Control System: Design, Application, and Implementation, ISA, *1990*
7. MOLNAR F., CHOVAN T.: Integration of package units, WBF European Conference, Brussels, *2000*
8. MOLNAR F, CHOVAN T., NAGY T.: Batch Control Analysis, WBF European Conference, Mechelen, *2002*
9. MOLNAR F.: BATCH ANALYSIS (in Hungarian), Magyar Elektronika, *1999*, 06, 18-12
10. ISA-S88. 01-1995 Batch Control. Part 1: Models and Terminology, Internal Society for Measurement and Control, *1995*
11. BRANDL D.: S88. 01 - The Standard for Flexible Manufacturing and Batch Control, White paper, Sequencia Corporation
12. VERWATER-LUKSZO Z.: A practical approach to recipe improvement and optimization in the batch processing industry, Computers in Industry, *1998*, 36, 279-300
13. PARSALL J., LAMB L.: Applying S88 – Batch Control from a User's Perspective, ISA, *2000*