Problems of the equipment choice for existing multiproduct chemical plants

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Abstract. The problem of using the existing equipment to make a new product in a given volume by the due date is formulated as a two-level hierarchy of tasks. The upper level is the problem of finding product's batch size and scheduling parameters of the plant; the lower level is the problems of selecting the equipment units for the implementation of the batch processing stages. Example of solving the problem of making a new product in a given volume by the deadline for real multiproduct batch plant.

1. Introduction

The choice of equipment, which involves selecting the types and the number of equipment units for chemical process systems (CPS), their geometric dimensions and operation mode parameters, is a main challenge of designing a new chemical plant and updating the existing one, especially when it is necessary to change the range and volumes of products. The greatest difficulties arise in solving this problem for multiproduct batch chemical plants (MBCP), e.g., production of chemical dyes and intermediate products, additives for polymeric materials, pharmaceuticals, chemicals. The distinctive features of production systems of this type are an extensive range of products, a low-volume production character of its individual brands (up to 1000 tons per year), frequent changes in the product range and volumes.

The main structural unit of MBCP is a chemical process system, which is a combination of equipment units and technologies used for the manufacture of multiple brands of one kind. In batch processes, products are manufactured in batches, which pass all processing stages in a sequence. Standard equipment is used for the implementation of the processing stages to meet the requirements of the product specifications. In some stages (mainly, filtration and drying) units working in a continuous or semi-continuous mode are used.

The choice of equipment is one of the stages of process design when developing new equipment or re-designing the existing equipment for new product manufacturing. The main problem here is the choice of geometric dimensions (working volumes, working surfaces) and the number of equipment units used in any one processing stage for each CPS, operation mode parameters and equipment units for each stage to ensure the required productivity for each of the products of the specified range [1-5].

The problem of redesigning the existing equipment to meet new production targets is more popular, than the problem of designing a new MBCP. The equipment on the existing CPS can be used for manufacturing new products and/or improving productivity of the existing systems to meet the changing market requirements with minimum changes in the choice of equipment [6-8]. In this study,
we investigate the methodology of solving a typical problems of manufacturing a new product in a specified volume by the due date, which are often found in contemporary practice of design and engineering departments of operating MBCP.

2. The specifics of CPS for MCBP and methodology of choosing the equipment

Most of the approaches to the formulation and solution of the problems of choosing the equipment for MBCPs, which have been proposed in scientific literature, consider only some of the features of the equipment. The long-term experience (since 1975) of cooperative work with experts in MBCP design and operation, participation in designing and redesigning of dozens of real production systems have allowed us to formulate a set of features and characteristics that are crucial for the choice of equipment.

Material flows of the system can have a branch structure (it means that some processing stages can be implemented in parallel), which is often not identical for different products. For the mathematical representation of batch processing routes of each product \(i\), it is necessary to model a set of system stages for the equipment units and create a matrix \(\mathbf{M}_i\) of batch processing routes. The value of any element of matrix \(\mu_{iy}^e = j\) (the ordinal number of the stage) if the equipment units of stage \(j\) perform stage \#e of batch processing route \(y\) \((y = 1, \ldots, Y_i, e = 1, \ldots, E_{iy}, \text{where } Y_i \text{ is the number of batch processing routes of product } i, E_{iy} \text{ is the number of stages of route } y)\).

The batch processing time for the main equipment units, which working continuously, cannot be determined in advance; it depends on a batch size and dimensions of equipment units.

Filling / emptying operations of the main equipment units in some stages of the CPS can be combined with physical and chemical transformations (feeding slurry in a filter press, collecting filtrate, etc.).

In some stages of the system, batch sizes are subject to change: a batch can be divided into several equal portions to be processed sequentially or synchronously, or several batches can be combined and processed together. Such situations are typical of the CPS used in MBCPs; this can be explained by the desire of manufacturers to minimize the number of stages, use similar stages and the same equipment for different products even if the products differ in batch sizes and their material indices. We propose to describe a batch processing method for product \(i\) in the main equipment units in stage \(j\) of the system, using:

- mode indicator \(p^i_j\) for processing batches of products with parallel units (if \(p^i_j = 0\), a batch is processed at once, in sequence; if \(p^i_j = 1\) – in equal portions, synchronously)
- indicator \(r^i_j\) for resizing product batches in a stage (if \(r^i_j = 1\), no changes are made; if \(r^i_j > 1\), a batch is divided by \(r^i_j\) equal portions for step-by-step processing; if \(r^i_j < 1\), batches \(1/r^i_j\) are combined for co-processing).

Between several operations of loading or unloading portions of batches or whole batches (when they are combined) the equipment units can be partly filled; this condition is described in [9] as “waiting time”.

The main problem of choosing the equipment for MCBPs is typically formulated as the problem of mixed integer nonlinear programming (MINLP). The main problem to be solved here is to determine the CPS operation mode parameters, changing continuously with the discrete characteristics of the equipment units throughout the processing stages.

The proposed method of solving the problem of equipment choice for MCBP described in [8,10] involves splitting the general problem into the problem \(R\) of finding batch size values \((w_i, i = 1, \ldots, I)\) and scheduling parameters of the CPS, and the problem of choosing the equipment units for the implementation of the processing stages \(A_j, j = 1, \ldots, J\) i.e. a two-level hierarchy of tasks, see figure 1.

Here, \(I\) is the number of products manufactured by the system and \(J\) is the number of stages.

In contrast to previously considered strategies of splitting the general problem of choosing the equipment for MCPB [11,12], the proposed approach is based on the principle of distribution of the problem parameters by the nature of changes, i.e., distinguishing the system operation mode parameters changing continuously from discrete characteristics of the equipment. In other words, the
problem $R$ is formulated as a problem of nonlinear programming, and the problem $A_j$ is formulated as a problem of discrete optimization.

![Diagram](image)

**Figure 1.** Hierarchy of problems of the Equipment Choice for Multiproduct Chemical Batch Plants

We propose to use a lower bound estimate of the cost of all kinds of energy expended in batch processing operations for a specified product range in the planned volumes as a criterion for the optimal solution of the problem $R$, and the amount of depreciation of the equipment units in stage $j$ for the same period as a criterion for the optimal solution of the problem $A_j$ [13].

3. Formulation of the problems of choosing the equipment for the existing MCBP and algorithms for their solution

When solving the problem of manufacturing a new product in a given volume by due date, i.e., over a specified period of time $T_o$, the problems $R$ and $A_j, j = 1,...,J$ are solved only for this particular product. Even if several similar products are supposed to be placed on the same CPS, these problems are usually solved separately for each product, since the processes in this case have no influence on each other.

The first step to do is to determine the processing stages, select the equipment units which are suitable for the implementation of the task, create the structure of material flows, matrix $M$ and set $X_j, j = 1,...,J$ of the equipment units dimensions for the processing stages, including the newly introduced ones. It should be noted that the number of equipment units used in stage $j$ is usually limited to one or two units. Consequently, sets $X_j$ have one or two geometric dimensions.

Changes in the formulation of the problem $R$ are related to the design of new production are related to producing a single product is being considered. It is necessary to find a batch size ($w$) and determine the starting time ($t_{Bjkl}$) and completion time ($t_{Fjkl}$) for each operation ($l$) of each cycle ($k$) for the equipment units in each stage ($j$) to satisfy the criterion

$$ZR(w) = w \min_{j=1}^J \{r_j\} \sum_{j=1}^J \frac{\pi_j}{r_j} \sum_{k=1}^L \sum_{l=1}^\Psi \omega_{jkl} G_{jkl} (t_{Bjkl} - t_{Fjkl})$$ (1)

minimum when the constraints on the mathematical model of choosing the CPS operation mode parameters. In the formula (1): $\pi_l$ is a minimum integer greater than $x$; $Q$ is product volume, tons; $\pi_j = \begin{cases} 1, & \text{if } p_j = 0 \\ 1.05n_j, & \text{if } p_j = 1 \end{cases}$ is coefficient of energy consumption increase in stage $j$ during the synchronous batch processing of equal portions in several parallel equipment units (due to the increase in losses); $K_j = \frac{r_j}{\min_{j=1}^J \{r_j\}}$ is the number of cycles of the main equipment units in stage $j$ in one
operating cycle of the system; $\Omega^\psi$ is the cost per unit (1 J.) of energy resource type $\psi$ (electricity, heat, cold), rubles; $\Omega^\psi_{jkl}, j = 1, \ldots, J, k = 1, \ldots, K_j, l = 1, \ldots, L_jk$ are specific consumption rates of energy expended in the processing stages when implementing batch processing operations, W / kg; they can be calculated using the data on product specifications [13]; $L_{jk}$ is the number of batch processing operations during cycle $k$ in the main equipment units in stage $j$;

$$
g_{jkl}^O = \left\{ g_{jkl} \left( \Lambda^D_j \right)^{-1}, j = 1, \ldots, J, k = 1, \ldots, K_j, l \in \Lambda_jk \cup B_{jk} \right\},
$$

material indexes of operations implemented in processing stages: the volume $v_{jkl}$, m$^3$/t, or (and) mass $m_{jkl}$, kg/t of materials to be processed to produce 1 ton of a product; $A_{jk}, B_{jk}, \Gamma_{jk}, \Delta_{jk}, I_{jk}$ are sets of numbers of processing operations of cycle $k$ for the equipment units in stage $j$ (operations of filling, “waiting time during filling”, physical and chemical transformations, emptying, “waiting time during emptying”, respectively); $\Lambda^D_j = \max \left\{ 1, r_j \right\}$, $\Lambda^U_j = \max \left\{ 1, r_j \right\}$ is the number of filling and emptying operations of equipment units in stage $j$ during one cycle of main units operation; $j', j''$ are numbers of the system stages before $j$ and after it.

The mathematical model for the choice of the system operation mode parameters and equipment for its stages satisfies the following conditions.

Constraints on changing the values $w$:

$$0 < w \leq Q. \quad \text{(2)}$$

The condition of product manufacturing in the given volume by the indicated date

$$T_c + \left[ Q \left( \min \left\{ r_j \right\} w \right)^{-1} - 1 \right] T_p \leq T_0, \quad \text{(3)}$$

where $T_c = \max_{j=1,J} \left\{ \sum_{e=1}^{E_j} \theta_{e,w} \right\}$ is duration of the manufacturing cycle (time interval from the start of the first operation of the first stage until the last operation of the last stage of batch processing $\left( \min_{j=1,J} \left\{ r_j \right\} \right)^{-1}$, hrs; $T_p = \max_{j=1,J} \theta_j$ is inter-cycle period of the system, i.e., the minimum possible time interval between the start (completion) of manufacturing cycles implemented sequentially, hrs;

$$\theta_j = \begin{cases} K_j \left( t_{jlkj}^F - t_{jlkj}^B \right) \left( n_j \right)^{-1}, & \text{if } n_j > 1, p_j = 0 \\ t_{jlkj}^F - t_{jlkj}^B, & \text{otherwise} \end{cases}$$

is duration of operation cycle of equipment units in stage $j$ (the minimum possible interval between the start of the first operation of the first cycle and the completion of the last operation of the last cycle for the equipment units used in the stage), hrs; $n_j$ is the number of equipment units in stage $j$.

Formula for determining the values $t_{jkl}^B$ and $t_{jkl}^F$

$$t_{jkl}^B = t_{jkl}^F - \tau_{jkl}, \quad j = 1, J, \quad k = 1, K_j, \quad l = 1, L_{jk}, \quad \text{(4)}$$

where $\tau_{jkl}$ is the duration of operation $l$ of processing cycle $k$ in stage $j$, hrs, see more in [9].

Synchronization conditions of operation cycles of equipment units in system stages
Conditions (5), (6) are designed to test the correctness of values \( r_j \), \( j = 1,J \), i.e. the possibility of practical realization of the proposed changes in the batch size during their processing in the CPS stages. It is obvious that the number of operation cycles of the main equipment units in any stage of the system, the number of filling and emptying operations in a single cycle in any stage of the system can only be an integer.

\[
t_{jk}^B = t_{j',k',j'}^B, \quad t_{jk}^F = t_{j',k',j'}^F, \quad j = \mu_{ye}, j' = \mu_{ye}, y = 1,|Y|, e = 2,|E_y|, k = 1,|K_j|, l \in A_{jk} \cup I_{jk},
\]

where \( k' \) is the number of the operation cycle in stage \( j' \), during which the equipment unit is emptied, which corresponds to the filling operation \( l \) during the operation cycle \( k \) of equipment units in stage \( j \); \( l' \) is the number of emptying operations during cycle \( k' \) of equipment units in stage \( j' \), which corresponds to a filling operation \( l \) during operation cycle \( k \) of equipment units in stage \( j \).

Condition (7) stipulates the necessity of matching the duration of operations of receipt and transfer of materials from the previous stages.

The problem \( A_j \) for the case of new product manufacturing on the existing equipment is solved if the batch size \( w \) has a fixed value, which is found when solving the problem \( R \). It is necessary to find whether the equipment used at the stage \( j \) can be used for processing of the same size batches if the method of processing is changed (values \( n_j, r_j, p_j \)) and whether it is possible to use additional equipment units. The answer to this question requires verification of the constraints on relationship \( w/x_j \) values (\( x_j \) is the basic geometric dimension of the main equipment units in stages \( j \), m³, m²). For example, if stage using bulk capacity vessels with mixers as main equipment units

\[
\phi_j \left( v_j u_j \right)^{-1} \leq w(x_j)^{-1} \leq \phi_j^* \left( v_j^* u_j \right)^{-1}, \quad j \in \Sigma_b,
\]

where \( \phi_j, \phi_j^* \) are the minimum and maximum permissible degree of filling equipment units in stage \( j \) with the processed mass, \( u_j = \left[ p_j + (1 - p_j) n_j \right] \left( n_j r_j \right)^{-1} \) is the change factor of the batch size in stage \( j \); \( v_j = \min_{k=1,|K_j|,l=1,L_{jk}} \left\{ v_{jkl} \right\}, \quad v_j^* = \max_{k=1,|K_j|,l=1,L_{jk}} \left\{ v_{jkl} \right\} \).

Constraints for other stages (filtration, drying) see in [8].

In addition, changes in the values of variables \( n_j, x_j \) are limited by:

\[
x_j \in X_j,
\]

\[
n_j - \text{integer}.
\]

Parameters \( r_j \) and \( p_j \) can take the following values:

\[
p_j = \begin{cases} 0, & \text{if } n_j = 1 \\ 0 \text{ or } 1, & \text{if } n_j > 1 \end{cases}
\]

\[
r_j = \begin{cases} 1 - \text{batch size does not change} \\ \gamma, \gamma > 1, \text{integer} - \text{batch splitting into } \gamma \text{ chunks} \\ 1/\gamma, \gamma > 1, \text{integer} - \text{combining } \gamma \text{ chunks} \end{cases}
\]
It is desirable to manufacture a new product with minimum costs of the equipment, so we propose to use the following function as the optimality criterion for the solution of the problem $A_j$

$$Z_j^A = N\left(T_o\left(T_w\right)^{-1}\right)n_j\sigma(\kappa_j, x_j), \quad (13)$$

where $N$ is a standard rate of return for chemical equipment (0.15); $T_w$ is annual effective worktime fund of the system, $\sigma(\kappa_j, x_j)$ is dependence of equipment cost in stage $j$ on their type ($\kappa_j$) and size ($x_j$), see in [13].

The process of joint solution of the problems $R$ and $A_j$, $j = 1,...,J$ when making a new product on the existing equipment is reduced to the iterative procedure of clarification of the initially assumed values $n_j$, $r_j$, $p_j$, $j = 1,...,J$:

1) prediction of values $n_j$, $r_j$, $p_j$, $j = 1,...,J$ and $x_j \in \Sigma_k/\Sigma_f$ ($n_j = 1$, $r_j = 1$, $p_j = 0$, $j = 1,...,J$; $x_j = \max X_j$, $j \in \Sigma_k/\Sigma_f$);

2) solution of the problem $R$, i.e. finding the value of a batch size $w$ and values of the start and completion time of operation cycles $t_{\text{hl}}^k$, $t_{\text{kl}}^k$, $j = 1,...,J$, $k = 1,...,K$, $l = 1,...,L_{jk}$ of equipment units for each stage, satisfying the minimum of function (1) under constraints (2)–(7);

3) solution of the problems $A_j$ for each stage of the system, i.e. the choice of the number of units and their geometric dimensions ($x_j$, $n_j$, $j = 1,...,J$) in stages given the possibility of changing the values $n_j$, $r_j$, $p_j$, $j \in \{1,...,J\}$, providing minimum values of functions (13) under conditions (8)–(12);

4) return to 2), if the values of $n_j$, $r_j$, $p_j$, $j = 1,...,J$ and $x_j \in \Sigma_k/\Sigma_f$ obtained in 3) do not coincide with the predicted values.

The problem $R$ in the formulation (1)-(7) is a one-dimensional optimization problem on the interval $w \in [0,Q]$. To solve this problem, we propose to use a step-by-step method [14] with an initial approximation $w = Q/T_o$, initial operating step 0.05 (50 kg), accuracy of determining the value of batch size 0.001 (1 kg) and the value of the exploratory step 0.0005 (0.5 kg).

The problem $A_j$ for a specific stage $j$ consists in checking whether constraints of the form (8) are fulfilled for the type $\kappa_j$ of the equipment units used in this stage under fixed values of their size and number. If the conditions are not fulfilled, it is necessary to select an option by changing the batch processing method (values $r_j$, $p_j$), integer $n_j$ and the equipment size $x_j$, providing the minimum value of function (13) under conditions (8)-(12).

4. Illustrative example

As an example of manufacturing a product in the given volume by due date we consider the problem of producing a brown anionic dye for leather in the volume $Q = 90$ tons over the operating time period $T_o = 2040$ hrs (85 days of twenty-four hour operation), using the equipment units of the CPS #1, #2, and #4 in the workshop #2 of Sivash AKZ on request of JSC “Ecochimproekt”, Tambov, Russia. Figure 2 shows the structure of material flows, processing stages, numbers, types and dimensions of equipment units. It should be noted that due to lack of small-size bulk capacity vessels with mixers, two stages of product synthesis (dissolution and diazotization) are implemented in sequence in equipment units in stages 1 and 3.

When solving problems $A_j$, it was found that working volumes and conditions of filling equipment units in stages 2, 4, 6 and 9 do not satisfy the constraints (8). To satisfy the constraints it was decided to combine two batches for joint processing in these stages ($r_2 = r_4 = r_6 = r_9 = 1/2$). Under the minimum number of equipment units in each stage ($n_j = 1$, $j = 1,10$) the minimum processing period, see (3), exceeded 3200 hours (134 days), and it was stage 8 (filtration) that limited the values of intercycle period. To solve this problem, given the availability of reserve equipment units, it was decided to perform synchronous processing of two batches in two parallel units in stages 7 and 8 ($n_7 = n_8 = 2$, $r_7 = r_8 = 1/2$, $p_7 = p_8 = 1$). Two identical filters were used in stage 8, and one additional unit # 1-31 with the working volume of 16 m$^3$ suitable for delivery of dye slurry into the filter press was used in
stage 7. The unit used in stage 10 was able to take the entire volume of the repulped concentrate (both batches), i.e. $r_{10} = 1/2$.

![Diagram of chemical process system](image)

**Figure 2.** The structure and main equipment characteristics for the stages of chemical process system, release brown anionic dye for leather

The results of solving the problem $R$ after correcting the values $n_j, r_j, p_j, j \in (1,...,10)$ were as follows: the batch size $w = 0.853$ tones; the number of batches manufactured for the operating cycle of the system $\left(\min\{r_j\}\right)^{-1} = 2$; the duration of the system cycle $T_c = 84.4$ hrs; the inter-cycle period $T_P = 36$ hrs; the production cycle $T_o = 1944.4$ hrs (81.02 days).

### 5. Conclusions

The proposed mathematical formulations and methods of solving problems of choosing the equipment for the existing MCBP ensure informed decision-making on manufacturing new products in specified amounts by the indicated deadline using the existing production equipment.

The solution of this problem enables to choose the main equipment units of the existing MCBP to implement all processing stages of a new product synthesis and determine scheduling parameters for all the equipment units. This will ensure the execution of the order on new product manufacturing with minimum utilities and depreciation costs.

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