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Technical Equipment Configuration and Functioning Mode Optimizing for Chemical-engineering Systems of Multi-product Plants

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Abstract: The article is devoted to the method of technical equipment configuration and functioning mode for chemical-engineering systems of the designed multi-product chemical plant. The method is based on the representation of this problem (MINLP) as a task hierarchy: a task of system functioning mode selection (NLP) and tasks of technical equipment configuration for system stages (IP). The indispensable conditions for the task solvability and iteration algorithm for task concurrent solution are described. The task features in a case of functioning mode parameters and technical equipment configurations updating for the chemical-engineering system of the operating plant under the variation of its productivity scheme are considered: equipment of any stage may comprise parallel main apparatuses with different pursuits and basic dimensions; main apparatuses of any stage may successively process several synthesis steps of some product. A practical example of the offered method application is given.

Key words: Multi-product plants · Adjustment of functioning mode and technical equipment configuration

INTRODUCTION

Multi-product chemical plants (MCP), for example plants, which produce synthetic dyes and intermediates, pharmaceutical, chemical agents, are characterized by broad product*s* assortment and 4small yield (less than 1000 ton/year). Rather short turnout periods for the majority of the products and frequent changes in the volume of output are typical for the production of these plants.

The basic unit of MCP is a chemical-engineering system (CES) – it is a hardware-processing complex, oriented to the yield of several products, identical in the manner of production. The majority of CES MCP is intended for the sequential output of the products of fixed assortment and operates in a periodic mode, though can also use continuously working technical equipment.

The definition of the technical equipment configuration (TEC) for CES of the designed MCP corresponds to the selection of basic geometric dimensions (working volume or/and surface), the number of main apparatuses for system stages and characteristics of the system functioning mode, which ensure the specified assortment I and required yield of the products Q_i, $i = 1,...,I$ over the period Tp. This problem considered in many scientific publications, for example [1, 3-6].

We have suggested a mathematical model of multi-product CES functioning for the designed plant [7], which takes into account the following features of TEC and functioning of real plants:

- The concerned CES produces a single product at any point of time.
- The structure of CES material flows can ramify, i.e. the equipment of certain instrument stages can process batches of raw materials and intermediates at the same time.
- CES stages can be equipped with the following main apparatuses: vertical reservoirs with mixers (reactors and tanks for the implementation of such processes as solution, homogenization, slurring) andbatch or continuously working filters and dryers.

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- The processing cycle of the main apparatuses at any CES stage includes the following operations: charging, physicochemical conversions, discharging, cleaning.
- Charging and discharging operations of the main apparatuses of CES stages can be either separated in time with physicochemical conversions (for example, charging of a batch of raw materials and discharging of a batch of intermediates from the reactor) or can be combined with it (for example, slurry feeding into a flash dryer or discharging of filtrate from a pressure filter at the treatment filtration).
- The duration of any processing cycle operation at any CES stage is either a constant or known function of the processing volume.
- The difference between the duration of the same operations at the processing of different product batches and implementation of various processing cycles of each main apparatus is no significant.
- At certain CES stages it is possible to divide batches of raw materials and intermediates into equal portions for the sequential or synchronous processing.
- At certain CES stages several batches of raw materials and intermediates can be combined for co-processing.

MATERIALS AND METHODS

The methodology of TEC optimizing for CES MCP, which we have worked out, allows to represent that problem as a double-level hierarchy of tasks: on the top level the task of parameter optimizing of a system functioning mode is solved (task *PF*), on the bottom level we select the basic geometric dimensions and number of the main apparatuses for each system stage (tasks AS_j, $j = 1,\ldots,J$, where J – number of stages), see Fig. 1.

This decomposition of the general task allows to avoid difficulties, noted in scientific articles over the pending problem [1, 3-6, 8, 9], – and shows the necessity of the MINLP solution, which doesn't have a common strategy. Unlike considered earlier decomposition strategies [2, 8] *PF* is formulated as NLP andAS_j – as IP.

As an optimality criterion for *PF* solution we offer the cost of primary forms of energy (electricity, heat, cold), during the planning period of CES functioning andof AS_j, $j = 1,\ldots, J$ – depreciation charges from the cost of CES technical equipment at the same period.

Some certain results of the solution of AS_j, $j = 1,\ldots,J$ are necessary for the solution of *PF*, see Fig. 1:

- The number of the main apparatuses for all of stages, necessary for the processing of each product's batches n_{ij}, $i = 1,\ldots,I$, $j \in J_i$, where J_i is a set of numbers of CES stages, which apparatuses processing batches of product i;
- The indicators of the processing manner for product batches at CES stages p_{ij}, $i = 1,\ldots,I$, $j \in J_i$ ($p_{ij} = 0$, if the main apparatuses of the stage j completely process batches of i-th product, loading them in turns; $p_{ij} = 1$, if all apparatuses synchronously process equal parts of batches);
- The factors of product batch size variations at CES stages r_{ij}, $i = 1,\ldots,I$, $j \in J_i$ ($r_{ij} = 1$, if at the stage j the batch size of product i does not change, $r_{ij} = \gamma$, $\gamma > 1$,

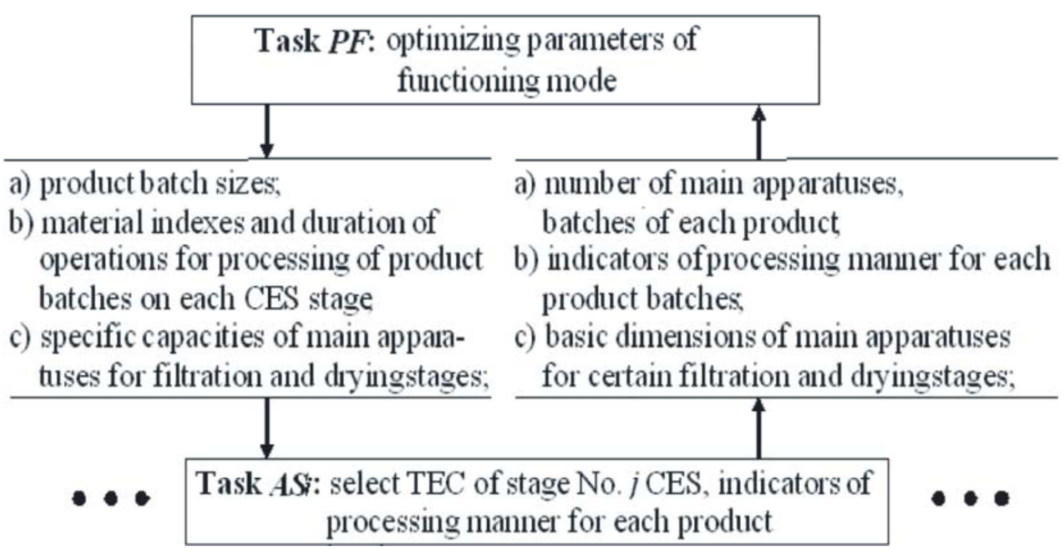

Fig 1: Tasks of TEC optimizing for CES MCP.

if the batch is divided into γ equal parts, processed in turns, $r_{ij} = 1/\gamma$, $\gamma > 1$, if γ complete batches are combined for co-processing);

- The basic dimensions of the main apparatuses for the stages $j \in Js_i/Jf_i$, where Js_i (subset of J_i) is a set of stage numbers, when the main apparatuses are filters or dryers; Jf_i (subset of Js_i) is a set of stage numbers, when the main apparatuses are pressure filters, intended for the selection of solid phase of slurry (the dimensions of apparatuses at the stages $j \in Js_i/Jf_i$ depend on the duration of products batches processing).

Therefore the method of coordinated solution of *PF* and AS_j, $j = 1,\ldots,J$ is provided for the prediction and iterative adjustment of values of the above-mentioned parameters.

Conditions for Tasks Solvability: We have formulated necessary conditions for *PF* and AS_j, $j = 1,\ldots,J$ solvability, which allow to detect in advance necessity and to define the directions of variations the quantity of parameters n_{ij}, p_{ij}, r_{ij}, $i \in (1,\ldots,I)$, $j \in (1,\ldots,J_i)$, using only given data, which can lead to the tasks feasible solutions:

The condition of "compatibility" of the selected assortment of products, i.e. the possibility of the implementation of all stages of all product synthesis in the main apparatuses, which are previously selected for the equipping of CES stages:

$$w_i^{\min} = w_i^{\max},\ i = 1,\ldots,I, \tag{1}$$

where $w_i^{\min}$, $w_i^{\max}$ – minimal and maximal allowed values for a batch size of product i (mass of the batch, passed through all processing stages), which are determined by the calculations of lower and upper bounds for basic dimensions of the CES stages' main apparatuses, upper bounds for the duration of product batch processing at the stages $j \in Js_i/Jf_i$ and lower bounds for the cycle periods of product processing (T_{ci*}).

The condition of the presence in sets XS_j, $j = 1,\ldots,J$ (basic dimensions of the standard main apparatuses, which are previously selected for the equipping of each CES stages), at least the dimension which is suitable for the processing of all product batches:

$$[X_j^L, X_j^U] \text{n} XS_j \neq \text{Ø},\ j = 1,\ldots,J, \tag{2}$$

where X_j^L, X_j^U are minimal and maximal allowed values for the basic dimension of main apparatuses for CES stage j, calculated by $w_i^{\min}$, $w_i^{\max}$, $i = 1,\ldots,I$.

The condition of the assurance of CES required capacity.

$$\sum_{i=1}^{I} Q_i \cdot T_{ci*} \big/ w_i^{\max} \leq Tp, \tag{3}$$

i.e. the capability of all product output in the sizes of Q_i, $i = 1,\ldots,I$ over the period Tp.

Note, that the fulfillment of the conditions (1)-(3) does not ensure the achievement of the task feasible solutions, but permits to discard at once an explicitly intolerable combination of values n_{ij}, p_{ij}, r_{ij}, $i = 1,\ldots,I$, $j \in J_i$.

For all situations, which result in no fulfillment of any conditions (1)-(3), we have worked out the guidelines on the variation of fixed values n_{ij}, p_{ij}, r_{ij}, $i \in (1,\ldots,I)$, $j \in J_i$, which could provide the fulfillment of relevant conditions. The expert opinion should be taken into consideration at the implementation of those guidelines: an expert estimates the acceptance of any guideline in terms of the implementation technology for the respective stages of products batches processing.

Algorithm for Combined Solution of Tasks: The iteration algorithm for the solution of the task *PF* and tasks AS_j, $j = 1,\ldots,J$ includes:

- The preliminary prediction values of the parameters n_{ij}, p_{ij}, r_{ij}, $i = 1,\ldots,I$, $j \in J_i$.
- The verification of the conditions (1)-(3) fulfillment and, in case of no fulfillment any of them, use guidelines on the variation of values n_{ij}, p_{ij}, r_{ij}, $i \in (1,\ldots,I)$, $j \in J_i$, which could provide the fulfillment of relevant conditions.
- The prediction of the main apparatuses basic dimensions X_j for the stage $j \in Js_i/Jf_i$. The solution of the task *PF*, i.e. the evaluation of product batch sizes w_i, $i = 1,\ldots,I$, which ensures the ordered yield of products Q_i, $i = 1,\ldots,I$ over the period Tp, subjected to the minimal cost of energy resources, which are consumed for the stages of product batch processing. This NLP can be solved by any method of constrained optimization.
- The solution of the tasks AS_j, $j = 1,\ldots,J$, i.e. the selection of the basic dimensions X_j, numbers N_j of the main apparatuses for each CES stage and values n_{ij}, p_{ij}, r_{ij}, $i = 1,\ldots,I$, $j \in J_i$, which ensures the possibility of each product batch processing in the main apparatuses of all stages $j \in J_i$ andminimal cost of technical equipment. The algorithm for the solution of these IP's provides the selection of the minimal basic dimension from the sets XS_j, $j = 1,\ldots,J$, which is

sufficient for relevant constrains andvariation values of the parameters n_{ij}, p_{ij}, r_{ij}, $i \in (1,...,I)$, $j \in J_i$ for the assurance of faulted constrains.

- The return to pt.3 occurs if the values n_{ij}, p_{ij}, r_{ij}, $i = 1,...,I$, $j \in J_i$, obtained in the course of the solution of tasks AS_j, $j = 1,...,J$, mismatch with their preliminary prediction.

To estimate the efficiency of the offered method for TEC definition of the designed MCP CES we have used the information about the main equipment and functioning mode of operating plants, producing synthetic dyes (above 20 CESs). As a result of the iterative algorithm application for all CES we have managed to optimize the TEC stages and system functioning mode: the cost of the main equipment decreases an average in 15%, the cost of the primary forms of energy – in 10%.

Retrofit Design of Operational Plant: The operational MCP productivity scheme (assortment, capacities or/and periods of product outlet) is often modified in connection with the change of market conditions.

The offered formulation of the task *PF*, in case of the correction of functioning mode parameters for CES of operational MCP andof the tasks AS_j, $j = 1,...,J$ – correction of TEC for CES stages in connection with a changing system productivity scheme, is provided for the following directions of TEC modification:

- The replacement of existing main apparatuses at certain CES stages or introduction of new main apparatuses in TEC stages (for the fulfillment of conditions (1)-(3));
- The introduction of new instrument stages for the implementation of synthesis steps of new products and the selection of the main apparatuses for their equipping (among reserve or reacquired apparatuses).

In addition, the analysis of practical work of Russian MCP RD departments, in terms of the retrofit design of operational CES with changing of its productivity scheme, brings us to the necessity of taking into account the following possibilities of changes in TEC system stages, which are not considered in the scientific publications:

- TEC of any CES stage can include parallel main apparatuses with different pursuits and different basic dimensions; moreover each of them can be exploited for the processing of batches of some particular products and not be used for the processing of the rest;
- The main apparatuses of some CES instrument stages can successively process several synthesis steps of some products, for example dissolving of raw materials, chemical change and product selection.

Note, that the decision on the successive processing of several synthesis steps of some products with the main apparatuses of some CES instrument stages regards the stages $j \in Jb_i$, $i \in (1,...,I)$, which are implemented in vertical reservoirs with mixers, because the main apparatuses of other stages (filters, dyers) are one-purposed and cannot be used for other processes.

A mathematical model of the CES TEC functioning for operational MCP, when its productivity scheme is modified, includes the following correctives in contrast with [7]:

- As a result of the possibility (i), it is provided the formation for each CES stage j the sets F_{ij}, $i = 1,...,I$ of numbers of the main apparatuses, which operate at the processing of each product batches, as well as the dependence of any parameters of the apparatuses on their pursuits (specific capacities of filter or dyer, frame or cell depth of pressure filters, maximal filling degree of periodic dyer volume);
- We take into account that the number of the stage j main apparatuses, under their turnaround numbering, corresponds to the maximal component of sets F_{ij}, $i = 1,...,I$, i.e.

$$N_j = \max_{i=\overline{1,I}} \{f \mid f \in F_{ij}\},\ j = 1,...,J\ ;$$

- As a result of the possibility 2), it is provided the formation of the sets v_{ij^c}, $i \in (1,...,I)$, $j \in Jb_i$, $c = 1,...,C_{ij}$, which contained the values of material indexes for the stages of the same product synthesis, implemented in the main apparatuses of the instrument stage j (C_{ij} –number of those stages) andcorresponding changes in the constraints over the main apparatuses basic dimensions for those stages.

The goal of the *PF* task solution in that case also corresponds to the minimal cost of energy, used for product batch processing during the period *Tp*, but the goal of the AS_j task solution changes: it is necessary to process every product batches over the minimal cost of the additional main apparatuses at *j* stage of CES. The possibility of extrication of the main apparatuses is not considered, because they usually remain in TEC of CES and can be used over the next changing of their productivity scheme.

Note, that the possibility of divide/joint product batches at the same CES stages is especially important for the solution of the tasks AS_j, j = 1,...,J under the conditions of the limitation base of equipment of operational MCP. For example, in situation

$$\max_{f\in F_{ij}} \{X_{jf} \mid X_{jf} \in XS_j\} < u_{ij} \cdot \frac{v_{ij^c} \cdot w_i}{\varphi^*_{ij^c}},$$
$$i \in (1,...,I), j \in Jb_i, c \in (1,...,C_{ij})$$

(dimension X_{jf} of the maximal main apparatus, suitable for the equipment at stage j of CES is too small for the processing of batches of product i) it is possible to reduce the coefficient of the product batch size

$$u_{ij} = \frac{p_{ij} + (1-p_{ij}) \cdot n_{ij}}{n_{ij}} \cdot \frac{1}{r_{ij}} \qquad (4)$$

(to divide the product batch into equal portions for consecutive processing), if an expert (technologist) will consider this operation possible. Here w_i is a batch size of product i, $\varphi^*_{ij^c}$ is a limit level of filling for the main apparatuses of the instrument stage j under the implementation stage c of the synthesis of product i.

The change of the productivity scheme of operational CES often associates with the contract performance to yield a particular new product in the fixed quantity by the specified date, i.e. for the fixed duration of this product yield. Tasks PF and AS_j, j = 1,...,J in that situation are solved only for a particular single product.

Previously selected instrumental CES stages, which main apparatuses are suitable for the implementation of the stages of new product synthesis, determine the structure of material links between them and their supposed TEC, including newly introduced stages in CES (sets XS_j, j = 1,...,J). Note, that in this case the amount of the main apparatuses, suitable for the equipment of CES stages, is not large (two-three apparatuses, usually – one), therefore the verification of the conditions (1)-(3) and their fulfillment often result in the obtaining of feasible solutions of the tasks PF and AS_j, j = 1,...,J. For example, for the tasks to yield intermediate 1,3 phenilendiamin with using of the equipment of one of the operational MCP in Tambov region (Russia), the variations of the values n_j, p_j, r_j, $j \in (1,\ldots,J)$, are necessary for the fulfillment of the conditions (1)-(3), ensured the possibility of the yield of the intermediate in the ordered quantity of 170 ton for the period of 2640 hours, without implementation of the additional main apparatuses.

The tasks AS_j in the situation of a new single product processing with using of the operational CES equipment, are solved under the fixed size of the product batch w, which is found as a result of PF task solution: it is necessary to find out whether it is possible to process the batches of such a size with the use of the main apparatuses of the particular CES stage j, considering the possibilities of variations of the value u_j, see (4), and/or using additional apparatuses.

For the answer to that question it is necessary to check the constraints to the dimensions of the main apparatuses, for example, to the main apparatuses of the stages $j \in Jb_i$ – constraints

$$w \cdot u_j \geq \max_{c=\overline{1,C_j};f=\overline{1,N_j}} \left\{ \frac{\varphi_{j^c*} \cdot X_{jf}}{v_{j^c}} \right\},$$
$$w \cdot u_j \leq \min_{c=\overline{1,C_j};f=\overline{1,N_j}} \left\{ \frac{\varphi^*_{j^c} \cdot X_{jf}}{v_{j^c}} \right\} \qquad (5)$$

and for the stages $j \in Jf_i$, equipped with pressure filters for the selection of the solid phase of slurry, – constraints ar

$$w \cdot u_j \leq \min_{c=\overline{1,C_j};f=\overline{1,N_j}} \left\{ \frac{\delta_{j^c f} \cdot X_{jf}}{v_{j^c}} \right\}, \qquad (6)$$

where $\delta_{j^c f}$ – thickness of settling (half of the height for a filter frame or chamber).

Practical Example: The offered method for the retrofit design of operational MCP CES, when its productivity scheme is modified, is tested by the examples of the changing of real operational CES productivity. With its application we solve the tasks of retrofit design, necessary for the processing of direct dyes fixed assortment to the plant, designed for the processing of dispersed dyes, as well as the tasks of the processing organization for any dyes and intermediates with the use of the main apparatuses of the same plant. As an example, let us consider CES, formed from the reserve equipment of the same plant for yielding of the following products over the period of Tp = 2520 hours:

- Direct yellow dye SV 2KM – Q_1 = 25 ton;
- Direct blue dye SV 2KM – Q_2 = 20 ton;
- Direct black dye M – Q_3 = 200 ton.

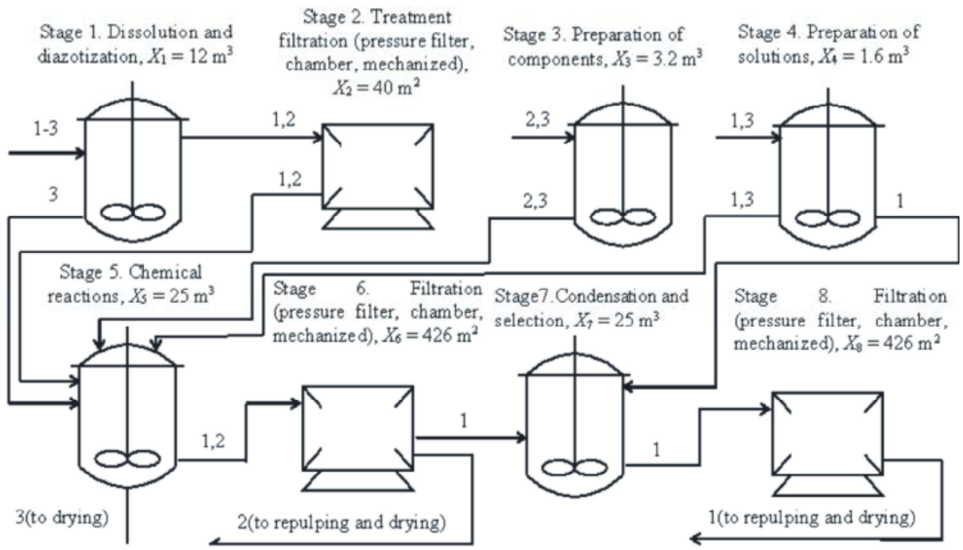

Fig 2: Structure of material flows, names of stages, types and basic dimensions of main apparatuses to CES for processing direct dyes.

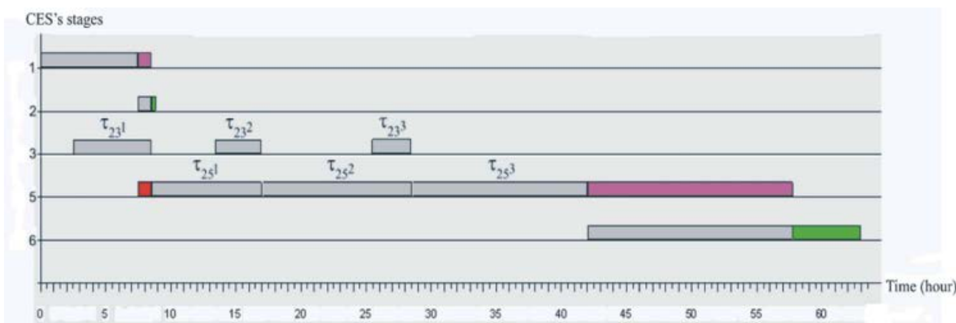

Fig 3: Diagram of CES working cycle, processing product 2.

Fig. 2 shows the structure of the CES material flows at the processing of products, names of instrumental stages, types and basic dimensions of the main apparatuses. All of CES stages are equipped with a single main apparatus.

In the apparatuses of stages 3, 4, 5 and 7, at the processing of products 1) and 2), more than one stage of their synthesis is implemented. When processing product 1), in the apparatus of stage 4 primarily prepare copper-ammoniac complex for the reaction of three azotizing at stage 5 and then – the solution of glucose for dye selection at stage 7. In the apparatus of stage 5 the following reactions are implemented successively: diazotization of DNS-acid, azocoupling and three azotizing. In the apparatus of stage 7 the following stages are implemented successively: solution of three azotize product paste, condensation and dye selection. When processing product 2), in the apparatus of stage 3 the following stages are implemented successively: solution of R-salt (for the first azocoupling), solution of I-acid (for the second azocoupling) and preparation of metalized agent (for metallization and dye selection). In the apparatus of stage 5 three aforesaid chemical reactions are implemented successively.

In the course of the control over the fulfillment of the conditions (1)-(3) we have detected the necessity for the preparation of sodium acetate solution in the apparatus of stage 3 at once for two batches of the third product (r_{33} = 1/2). The results of *PF* task solution are presented in Table 1.

Fig. 3 presents the diagram of one working cycle of those CES main apparatuses at the processing of product 2), received in the course of *PF* task solution.

As_j, j = 1,...,8 task solutions in that case lead to the verification of the fulfillment of conditions (5), (6) under the fixed batch sizes of products and basic dimensions of the main apparatuses on CES stages.

Table 1: Parameters of functioning mode to CES for processing direct dyes.

No. product	Batch size, ton	Intercycle period, hour	Cycle of CES working, hour	Number of batches, output at cycle	Duration of processing, hour
1	1.006	51.2	117	1	1338.7
2	1.299	50.28	63.03	1	867.5
3	4.25	10.4	15.4	2	249.7

RESULTS AND DISCUSSION

One of the main scientific results, discussed in this article, is to present the problems of TEC for MCP CES as a hierarchy of tasks, at the top level that determines the optimum settings for the operation mode of CES, on the ground - TEC for stages of systems. This avoids the problem formulation in the form of MINLP, conventional methods of effective solutions which has not yet been proposed.

An iterative algorithm for joint solving tasks upper and lower levels of the hierarchy, providing for the use of the necessary conditions for the solvability of tasks. The application of these conditions can significantly reduce the amount of computation required.

In addition, it should be noted correction mathematical model of the designed CES functioning for retrofit design of operational plants. As a result of this correction first considered the possibility of incorporating the CES stage parallel main apparatus, having unequal performance and basic geometrical dimensions, as well as the consistent implementation in the same set of several synthetic steps of the same product.

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