Methodology for the development of computer-aided design of technological equipment for chemical plants

V G Mokrozub*, S V Karpushkin and E N Malygin

Department of Computer-Integrated Systems in Engineering, Tambov State Technical University, 106, Sovetskaya St., Tambov, 392000, Russia

* mokr@mail.gaps.tstu.ru

Abstract. Design of multi-assortment chemical production (MCP) is a difficult task, the solution of which is carried out using the decomposition of the initial problem into a number of interrelated local subtasks that form a tree of tasks. The task tree defines the structure of the object-oriented component of the computer-aided design (CAD) system. The proposed methodology for developing CAD software is based on MCP procedural design model, information models that describe the structure of information necessary to solve local subtasks, information support for storing and processing information models.

1. Introduction

Multiple chemical production (MCP) is the production of semi-products, lacquers, paints, chemical reagents, drugs, additives to polymeric materials, etc. Their feature is the production of several technology-like products on one chemical-technological system (CTS), including main and auxiliary apparatus, pipelines and pipe fittings.

Designing is the most crucial stage of MCP life cycle, the results of which largely determine the efficiency of the operational phase. The initial data for the design are presented in the technical specification tz, the result of the design is the technical project tp, which is a documented set of MCP xtp characteristics (construction and performance characteristics of each element of the technological scheme, apparatus design and piping layout, equipment schedules and repairs).

X is set of all possible construction and performance characteristics of MCP, X1 is set of permissible values of these characteristics, TZ – set of possible technical tasks, V is a set of estimates ordered by the relation U ⊂ V × V. We introduce the efficiency function of allowable design solutions $FDP: TZ \times X \rightarrow V$ and function $EF: TZ \rightarrow V$.

The task of designing MCP can be represented as the task of choosing such an element $XTP \in X1 \subset X$, where

$$FDP(XTP,tz) \ U \ EF(tz) \ \forall tz \in TZ$$ (1)

In other words, $XTP$ is a solution to the design problem, if with any $tz \in TZ$ the estimation function $FDP(XTP,tz)$ is in relation $U$ to the limit value $EF(tz)$ for this $tz$.

In individual case $U$ represents a relation $\leq$, and $EF(tz)$ is the maximum allowable value of the estimation of the effectiveness of the design solution, for example, the cost of the project. In practice, one solution $xtp^* \in XTP$ is chosen from a set $XTP$. This solution is executed in the form of technical
documentation (technical project), \(tp\). If \(xtp^*\) is chosen in such a way that \(FDP(xtp^*,tz) = extr(EF(tz))\), then it considers the optimization problem.

The formulation and solution of individual design problems of MCP are considered in many scientific publications. Thus, in [1], a solution was proposed for the identification of the optimal determining sizes of CTS apparatus, in [2] the problem of locating of equipment in a production room was considered, work [3] was devoted to individual stages design, including water treatment, and in [4], scheduling of CTS work was considered at the design stage. In [5,6] and many other publications, the issues of designing devices of various types were considered, and in [7] methods of developing virtual simulators, including those for training CTS operators, were presented. In this case, the authors focus on the formulation and solution of problems of the form (1) and practically do not touch upon the development of a computer-aided design (CAD) methodology.

The purpose of the work is to present the methodology for the development of CAD software. In this case, the methodology is understood as the study of the organization of activities [8].

2. Structure of methodology for developing CAD MCP

We define the general design problem of MCP as \(z_0\). This problem is very complex and cannot be solved directly through formula (1). It is decomposed into a series of subtasks \(z_1, z_2, \ldots, z_k\), where \(k\) is the number of subtasks of the first level. Each task \(z_i, i = 1, k\) can, in turn, be decomposed into a number of second-level subtasks, etc. Thus, a task tree is constructed, the generalized structure of which is presented in figure 1.

![Generalized task tree structure](image)

Figure 1. Generalized task tree structure

The task tree presented in figure 1 is the basis for development of the structure of computer-aided design (CAD) system of MCP. In most cases, each subtask is a specific module (subsystem) of CAD. Coordinating and feedback links are set between the modules (figure 2). Coordinating communication is an information flow transmitted from an upstream module to a subordinate, feedback is an information flow transmitted from downstream modules to a higher one.

We define \(DZ = (Z, SZ)\) as task tree (goals) of MCP design, \(Z = \{z_i\}, i = 1, k\) – tasks, \(SZ = \{sz_{km}\}, k \in 1, I, m \in 1, I, k \neq m\) – subordination of tasks (edges). CAD is designed to solve problems \(Z\).

We define CAD as \(SYS\), which implements the task tree \(DZ\). Formation methodology of \(SYS\) is defined as \(Metsys: DZ \rightarrow SYS\). In turn, \(SYS\) represents a set of subsystems \(SYS = \{sys_r\}, r = 1, R\), \(sys_r\) – element of \(SYS\) system, \(R\) – number of subsystems.

The basis of \(SYS\) system's implementation of \(DZ\) task tree is the procedural model \(FZ\) [9], which determines the procedure for obtaining a technical project \(pr\) from the initial data of the technical task \(tz\). It uses knowledge of the subject area, which must be formalized for implementation in CAD. We denote the formalized knowledge as an information model of the subject area \(IM\), and then the procedural model \(FZ\) will be written as follows

\[FZ : tz \xrightarrow{IM} pr\]
We define the task of constructing a procedural model on the task tree as $MetFZ$, i.e.

$$MetFZ : DZ \rightarrow FZ.$$  

$IM$ information model is formed as a result of formalization of knowledge of the subject area of $Dom$. We define the task of creating an information model from the knowledge of $MetIM$ subject area, i.e.

$$MetIM : Dom \rightarrow IM.$$  

The information model is stored, maintained up to date and processed in the information storage, for example, in a relational database. Information support is developed for these purposes. We define the task of creating information support for CAD MCP, as $MetOI$, i.e.

$$MetOI : IM \rightarrow OI,$$

where $OI$ – information support for CAD,

$IM$ – information model of subject area.

Based on the above, the methodology for creation of CAD systems to fulfill the task tree $Metsys: DZ \rightarrow SYS$, can be written as a tuple

$$Metsys = < MetEZ, MetIM, MetIO >.$$  

3. Task of building a procedural model of MCP design

Building a MCP procedural design model is based on the methodology IDEF0At. The procedural model $FM$ is a set-theoretic representation of IDEF0 functional diagram.
As an example, we consider one of the main stages of the design of MCP - technological design. Figure 3 presents the task tree for technological design, in which two main tasks are highlighted: apparatus design and equipment layout.

The functional diagram of the upper level of technological design of MCP is presented in figure 4.

**Figure 4. Functional diagram of technological design**

Figure 5 shows the functional apparatus diagram of CTS. The procedural model $FZ$ is built on the basis of the functional diagrams presented in figures 4, 5. It is designed to convert the information flow defined by the technical task $tz$ into the information flow of the technological project $pr$.

In this case, the information model is used as a formal presentation of information (concepts, facts and rules) of the designed $IM$ object. We write the procedural model in the form:

\[
FZ : tz \xrightarrow{IM} pr, \quad pr = I_1 \cup I_2, \\
FZ = \langle FZ_1, FZ_2 \rangle, \\
FZ_1 : tz \cup I_2^1 \xrightarrow{IM_1} I_1, FZ_2 : tz \cup I_1 \xrightarrow{IM_2} I_2 \cup I_2^1, \\
FZ_1 = \langle FZ_{11}, FZ_{12}, FZ_{13} \rangle, \\
IM = IM_1 \cup IM_2, \quad IM_1 = IM_{11} \cup IM_{12} \cup IM_{13}, \\
FZ_{11} : tz \cup I_{12} \cup I_{13} \xrightarrow{IM_{11}} I_{11}, \\
FZ_{12} : tz \cup I_{11} \cup I_{13} \xrightarrow{IM_{12}} I_{12} \cup I_{12}^1, \\
FZ_{13} : tz \cup I_{11} \cup I_{12} \xrightarrow{IM_{13}} I_{13} \cup I_{13}^1.
\]
Calculation of number and sizes of apparatus at each stage

Optimization of constructive and operating characteristics of apparatus

Development of engineering and technological documentation of individual units of equipment

Typical equipment sizes

Mathematical models of processes, occurring in apparatus

Figure 5. Functional diagram of apparatus design of CTS

where $I_1$, $I_2$ – results (information flows) of solving the problem of apparatus design of CTS and equipment layout;

$FZ_1$, $FZ_2$ – procedural models of apparatus design MCP and equipment layout;

$IM_1$, $IM_2$ – information models of apparatus design and equipment layout;

$I_1$ – difficulties of problem solving for equipment placement and pipelines tracing (determination of the coordinates of apparatus and sections of pipelines) that require a re-solving of the problem of apparatus design $z_1$;

$FZ_{11}$, $FZ_{12}$, $FZ_{13}$ – procedural models for determining the number and size of devices at each stage of each CTS production, optimizing the design and performance characteristics of individual apparatus, development of design and technological documentation for individual units of equipment;

$IM_{11}$, $IM_{12}$, $IM_{13}$ – relevant information models;

$I_{12}$, $I_{13}$ – difficulties of problems solving of $z_{12}$ (conflicting requirements for the parameters of structures and mode of operation of individual apparatus) and $z_{13}$ (lack of reference information).

4. Task of building of information model MetIM

Each procedural model has a set of input data $X \in XV$ and a set of solution results $Y \subseteq YV$, where $XV$ and $YV$ are sets of acceptable values of $X$ and $Y$. In turn, $XV \subseteq DX$ and $YV \subseteq DY$, where $DX$ and $DY$ are sets (domains) of possible values of $X$ and $Y$. For example, an indication of the manufacturing material of the apparatus is part of the original data (technical task) during its design. The set $XV$ is a list of steel types that meet the requirements of the technical task, and $DY$ is the set of all steel types used in the development.

Thus, the information model ($IM$) can be represented as a tuple:

$IM = <X,Y,DX,DY,IZ>$,

where $X$ – list of initial data necessary for the implementation of the procedural model;

$Y$ – list of results of its implementation;
DX – domain of possible values of initial data (information) required to perform the procedural model;
DY – domain of possible values of the results of procedural model;
IZ – additional information that is required during the implementation of the procedural model.

We note that X and Y are not initial data, but only a list of source data (structure). Information is entered into X and Y in the process of executing a specific procedural model. DX, DY, IZ sets, unlike X and Y, contain both the structure and the information itself, which is entered before procedural models, or rather, can be entered and refined continuously (information support process).

5. Task of information supply MetOI creation
In modern CAD systems, the functioning and integration of individual subsystems into a single system is carried out through a single information support (space) according to the scheme presented in figure 6.

![Figure 6. Scheme CAD MCP subsystem interaction](image)

As specified above, the structure of information necessary for solving design problems of an MCP is determined by the information model. The list of initial data needed to perform the procedural model X, and the list of results of the procedural model Y must correspond to each project, while the domain of possible values of the initial data DX, the domain of possible values of results of the procedural model DY and additional information IZ, required in the process of performing the procedural model, does not depend on the implemented project.

Currently, one of the promising areas of development of CAD is the use of artificial intelligence methods [10, 11], allowing us to accumulate and maintain knowledge of the subject area.

It follows from the above that the information support of CAD MCP should ensure the storage and processing of the following information:
- MCP projects (calculation results, text and graphic documents);
- subject area data (reference books of equipment, individual elements of equipment, materials and their properties, etc.);
- knowledge of the subject area.

6. Conclusions
MCP design is a complex task that is solved by decomposing the initial (global) task into a series of interconnected local subtasks that form a task tree. The task tree defines the structure of the object-oriented component of MCP CAD. The main elements of the proposed methodology for the development of MCP CAD systems are:
- procedural design model of MCP. The procedural model is built on the basis of the task tree and IDEF0 functional diagram.
- information models for solving local subtasks. These models include the initial data, the results of problem solution, the domains of the initial data and results, additional information;
- information support intended for storing and processing information models in the selected information storage. The stored information is classified into: MCP projects, data of subject area, subject area knowledge.
Acknowledgments
This work was financially supported by Ministry of Science and Higher Education of the Russian Federation within the basic part (project 8.7082.2017/8.9).

References

[1] Malygin E N, Karpushkin S V and Borisenko A B 2005 A mathematical model of the functioning of multiproduct chemical engineering systems *Theor. Found. Chem. Eng.* **39** 429

[2] Egorov S Ya and Sharonin K A 2017 Automated decision making in the problem solving of objects layout for chemical and refining industries using expert software systems *Chem. Petr. Eng.* **53** 396

[3] Nemtinov V A, Nemtinova Yu V and Salushcheva A V 2011 Automated synthesis of water treatment stages in systems of circulating water supply at industrial enterprises *Theor. Found. Chem. Eng.* **45** 667

[4] Egorov A F, Belkov V P, Savitskaya T V and Comissarov Yu A 2004 Odnovremennyy sintez i sostavleniye raspisaniya vypuska produktov mnogoassortimentnykh khimicheskikh proizvodstv [Simultaneous synthesis and scheduling of production of multi-range chemical plants] *Izv. VUZov: Khimiya i khimicheskaya tekhnomologiya* [Izv. Universities: Chemistry and Chem. Techn.] **47** 93

[5] Dvoretskii D S, Dvoretskii S I, Polyakov B B and Ostrovskii G M 2012 A new approach to the optimal design of industrial chemical-engineering apparatuses *Theor. Found. Chem. Eng.* **46** 437

[6] Mokrozub V G, Manuilov K D, Gorshkov V V and Gorshkova T S 2016 Structure of information model of steel tanks *Chem. Petr. Eng.* **52** 613

[7] Dedov D L, Krasnyanskiy M N, Obukhov A D and Arkhipov A E 2017 Design and development of adaptive simulators using 3d modeling *Int. J. Appl. Eng. Res.* **12** 10415

[8] Novikov A M and Novikov D A 2007 *Metodologiya* [Methodology] (Moscow: SINTEG)

[9] Mokrozub V G, Nemtinov V A and Mokrozub A V 2017 Procedural Model for Designing Multiproduct Chemical *Chem. Petr. Eng.* **53** 326

[10] Mokrozub V G and Nemtinov V A 2015 An approach to smart information support of decision-making in the design of chemical equipment *Chem. Petr. Eng.* **51** 487

[11] Ostroukh A V, Krasnyanskiy M N, Obukhov A D, Karpov S V and Dedov D L 2015 Development of automated information systems for monitoring of intellectual activity results *Pros. Int. Multidisc. Sci. GeoConf.: Surveying Geology and Mining Ecology Management* **1** 101