Rudnev N., Abyzgildin A.

Ufa State Petroleum Technological University

SOFTWARE FOR COMPUTING AND OPTIMIZING PETROCHEMICAL PROCESSES BASED ON GRAPHIC MODELS AND OBJECT ORIENTED ANALYSIS

(optimization, petrochemical, chemical, mathematics models, object -oriented, graphic model)

INTRODUCTION

It is necessary to mark, that the complexity of software permanently grows, that is called not only tendency to create the universal program on all probable inquiries of the chemical-engineers, but also more and more increasing complexity of chemical-processes. Therefore it is necessary to give more attention to analysis of composite chemical processes when we are designing programs.

The system for development mathematical models of chemical processes should use the new information technologies and to have ability to rebuilt quickly, to develop without extra costs and being adapted to needs of the engineers and designers of chemical processes.

Recently designed method of the analysis of petrochemistry composite systems with usage of method of graphic models allows essentially to simplify the representation of chemical flow diagrams without a loss of information.[1] Besides, the given method is convenient for usage on a computer.

Calculation, simulation and optimization of petrochemical processes programs are of great importance for the chemical engineers. The designing of the universal programs of chemical process simulation with usage of a method of graphic models is of great interest.

The effective overlapping of graphic models of chemical processes with mathematical models in one program with application of the modern concepts of programming can help to build the computational programs having a simple user interface and broad functional capabilities for calculation and simulation. The pilot project of such program and some results of usage of this program are described below.

BASIC

There are some manufacturers of software for calculation, optimization, analysis and synthesis of petrochemical processes: AspenTech [2], SimSci Corp. [3], HyproTech [4]) produce a large set of software products, attempting to envelop all areas of application of computer facilities in an petroleum refining and petrochemical industry.

From the programs of simulation, optimizations of processes and apparatus in the chemical technology take the beginning programs of synthesis**.** The development of the programs of synthesis and expert systems is connected that the large experimental material and libraries of different algorithms is accumulated, and the programs of synthesis XTC should have the large database and algorithms, as it is marked Kafarov V.V. Association data with algorithms allow to proceed to a new level of designing of processes.

In the literature there are publications on a problem of synthesis of manufacturing processes, but in the present moment in commercial usage there are only programs of synthesis of systems of heat exchangers and rectification.

Recently designed method of the analysis of composite systems in USPTU by a method of graphic models allows essentially to simplify the representation of flow diagrams without a loss of information. Besides, the given method is convenient for usage on a computer systems.

The effective overlapping of graphic model of chemical processes with mathematical in one program with application of the modern concepts of programming can help to build the computational programs that have a simple, well understandable user interface and broad functional capabilities for calculation and simulation.

In those programs, in which we use image of petrochemical flow diagrams and apparatus (simulation programs, control etc.) there is a composite graphic interface. Three approaches are usually applied to a scheming in such programs:

- user makes flow diagram independently, using a set of primitives (for the map of apparatus, pipe lines, reinforcement etc.) that are storing in the program;
- user receives ready chemical flow diagram of concrete process and can not independently make changes in scheme;
- the program synthesizes flow diagram by principals and algorithms.

The first approach is more convenient for users and is more universal, but only large companies can develop the programs, using a set of primitives, because the set of objects is very large, for example, for the program DESIGN II, the set of primitives reaches 60 units.

The analysis of flow diagrams of chemical processes with usage of graphic models allows representing the scheme of any complexity, using a minimum set of graphic primitives. Figure 1 presents the graphic model of hydrocleaning process which enters a structure of the industrial complex of catalytic reforming - L-35-11/1000 (NOVOIL).

According to a new way of the map the flow diagram of any complexity represents a tree - graph with apparatus, placed on branches. Any composite flow diagram can be figured by a small amount of graphic primitives, and in a computer storage it is necessary to create object model of such scheme. [5]

Usage of graphic models is more preferential to mining the interface of the programs as contrasted to by existing methods, as it saves time and allows to simplify the program without loss of information saturation.

Now the most widespread and powerful method of engineering and analysis of software are the object-oriented approach.

For the analysis of the dedicated area and construction of object-oriented model of chemical process flow diagram and design the program was applied the CASE package - Rational-Rose (the object-oriented analysis, designing and programming). [6]

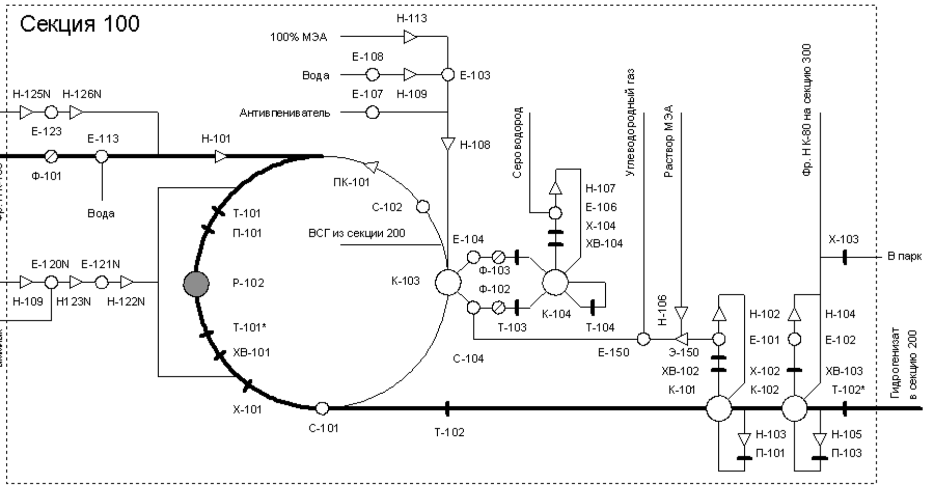


Figure 1 Graphic Model of Hydroclearning Process

As a notation - Unified Modeling Language (UML) or Booch Notation were be used. [5]

At programming the object-oriented approach was applied twice:

- at first, for the analysis of dedicated area;
- at second, for construction of structure of the program and allocation of the main classes and modules.

From the point of view of the object-oriented technology the analysis of chemical processes flow diagrams with the help of graphic models gives:

- hierarchic structure of petrochemical production;
- a set of abstraction permitting to the expert to operate with a large array of information;
- complex representation about petrochemical plant or large industry unit;
- decomposition technique for the given dedicated area.

The overlapping of the object-oriented technology and method of graphic models allows to construct information structure for storage of any information about petrochemical processes. For building in program were selected only schemes of the combined industrial units (3-4 processes) or schemes of one process. Algorithm of building of flow diagram by a method of graphic models following:

- definition of the main flows;
- arrangement apparatus on the main flows;
- building peripheral flows;
- arrangement of apparatus on peripheral flows.

Any composite flow diagram can be figured by a small amount of graphic primitives, and in a computer storage it is necessary to create object model of such scheme.

The graphic model of flow diagram is submitted in a computer memory by objects of the TApparat class and descendants, TSchem and descendants and objects of the TProduct class, figure 2.

According to the diagram on figure 3 all information about an apparatus is contained in object (1) of class TApparat, the same object contains a list of all (3) entering and leaving it products (2) and data about the place on the scheme. Product line (5) contains a list of all (4) apparatus, through which he passes. The general flow diagram is represented by a list (6) of product lines with the apparatus, arranged on them.

During developing a graphic interface the initial concepts and structure were not changed, and only have acquired set of details. It has allowed to save a significant amount of time. The designed graphic interface allows building graphic models of any chemical and petrochemical processes.

Figure 2
Hierarchy of the main classes of apparatus and denotation them on flow diagram

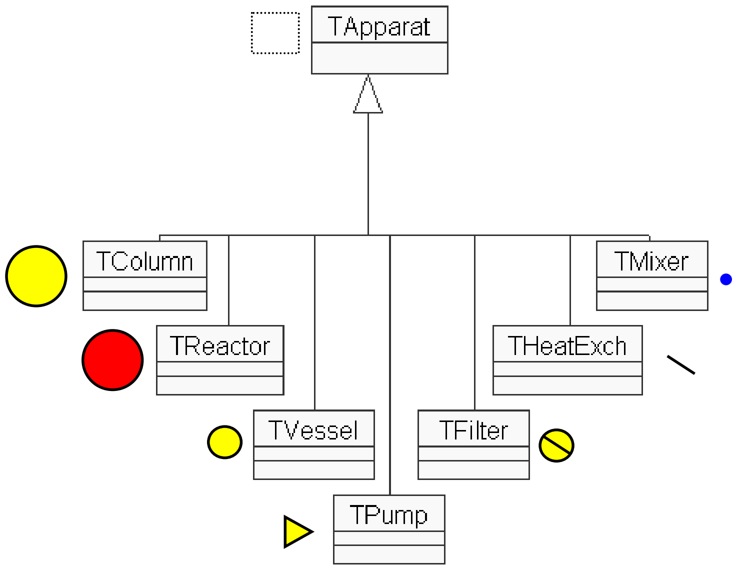
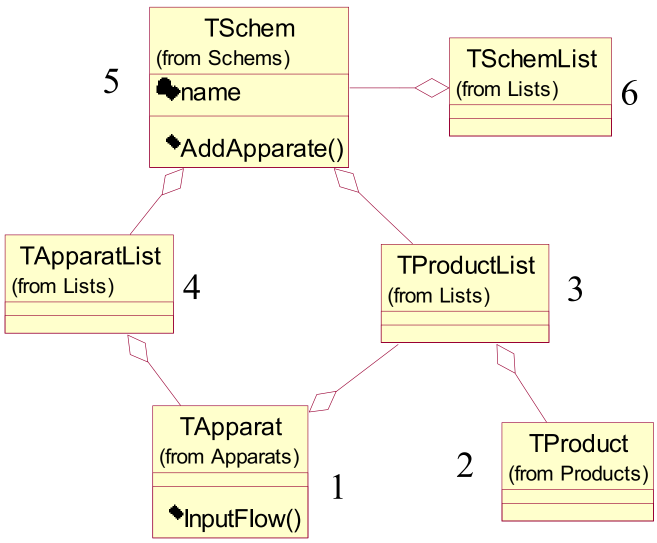


Figure 3
General structure for data storage of flow diagram in the program



There were constructed graphic model and object-oriented model of catalytic reforming which enter a structure of the industrial complex of Catalytic reforming - L-35-11/1000 (NOVOIL). In figures 4 and 5 the graphic models of sections 100 and 200, build in program are presented.

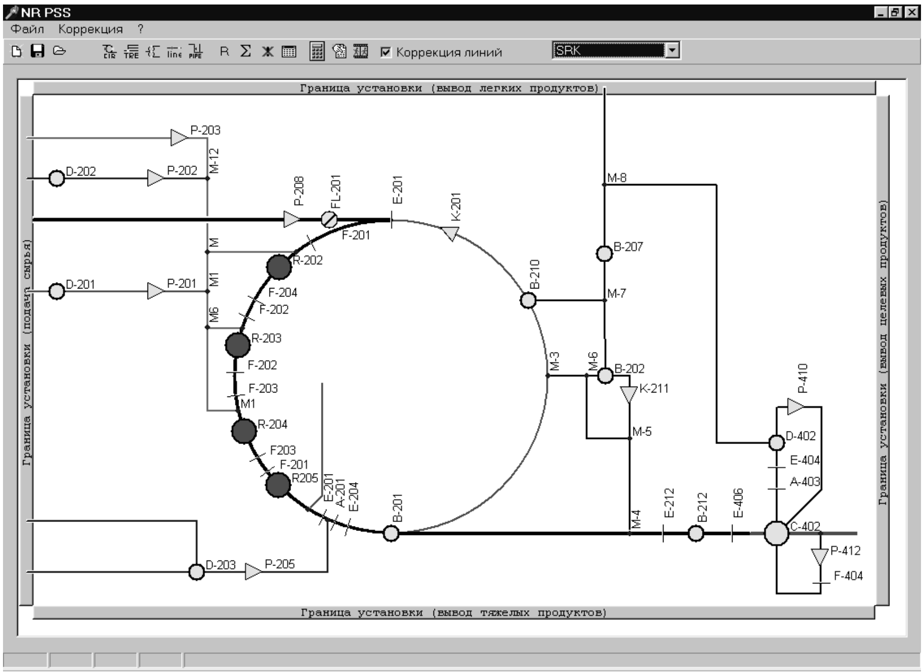


Figure 4 Graphic Model of Catalytic Reforming Process

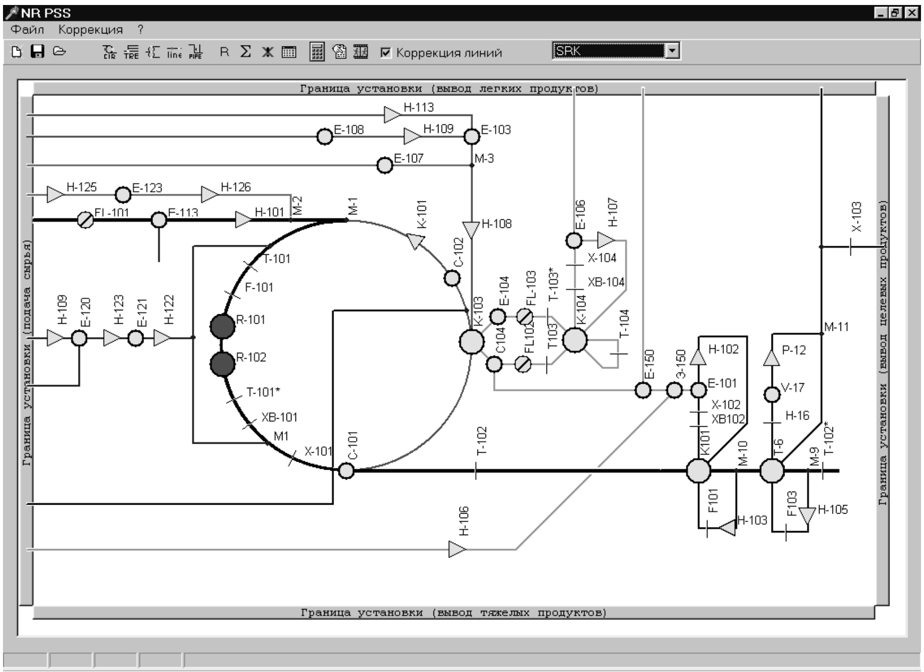


Figure 5 Graphic Model of Hydroclearning Process

While developing GUI the capability was stipulated to supplement a set of graphic primitives for the map of apparatus, pipe lines, reinforcement. The small modification of GUI and extension of a set of graphic primitives will allow to plot flow diagrams from any grain size and different problems (automation, pipeline systems etc.).

When we design mathematical models in programs [2, 3, 4] the following units can be used: the library of thermodynamic methods, library of models of apparatus, library of components and different algorithms of calculation and optimization. The quality, and consequently price of such program, as a rule, is determined by quantity of libraries and methods accessible to the user.

In the given activity an attempt of entering all accessible methods, algorithms and data into the computer wasn't undertaken**.** The problem was put as follows: to create such structure of the program, that makes it possible to expand the library of mathematical methods and algorithms.

For maintenance a full access to mathematical methods in the program properties were used methods immanent to the object-oriented. All techniques of calculation, algorithms, mathematical models of separate apparatus can be removed or placed at the program separately. Also, in the program the chemical components database is accessible.

For conversion of parameters of flows (entered the user or for application in some mathematical models) to "standard" there is a separate module, as the standard the C system is selected. For the program the following dimensions (table 1) are adopted, for example.

To calculate any unit for flow diagram, for example, apparatus, it is necessary to know all input and output flows.

If there are recycles on flow diagrams, the problem to calculate the apparatus with recycle flow become more complicated, the calculation of flow diagram becomes iterative. At composite flow diagram quantity of iterations can increase on some orders, and the calculating time can exceed reasonable value, despite of power of a computer. The structure analysis of flow diagrams was applied to reduce dimension of problems, which is based on graph theory and algorithms from graph theory [7]. The purpose of structure analysis is the finding a gaps of cycles, including an optimum gap of cycles. The different algorithms for a computer are applied for this purpose. The new algorithm of finding gaps of flows on schemes for compilation the sequence of calculation of apparatus and units is offered. This algorithm is done on the basis of graphic models. In the designed program named - "GMTP" the technique of building flow diagrams on several stages is realized. While building a graphic model, the person himself determines contours and subsystems on flow diagram. The given activity for the user is not difficult and does not require knowledge of graph theory or mathematical methods realized in the program - the expert outgoes only from the technological bases of a petrochemical process. The direction of stream on the scheme is not underlined, but the user while building a graphic model, determines a streamline. The apparatus that placed on flows automatically arranged. Figure 6 is present the simplified graphic model of hydroclearning process which enters in a structure of the industrial complex of catalytic reforming - L-35-11/1000 (NOVOIL).

The basic dimensions of parameters in the program

Table 1. /

Title of parameter	Allowed for input by user	Internal standard in the program
Temperature	^{o}C, K	K
Pressure	Pa, MPa, KPa, kg/cm^2	Pa
Consumption	kg/hr, m^3/hr, k-mole/hr	k-mole/hr
Composition	% mass, % vol	% mass, % vol
Volume	l, m^3	m^3

The following algorithm of a gap of flows is offered:

1. Each apparatus has even 1 entering and 1 leaving flow, we will call them conditionally "main" for the apparatus, they have an index accordingly, 0 and 1. The flows in the apparatus are realized as objects, which have the link to the apparatus, place on input and output flows. The apparatus can have some extra entering or leaving flows, their indexes in the apparatus will be - 3, 4, 5, 6... For example (see figure 6), the separator C-

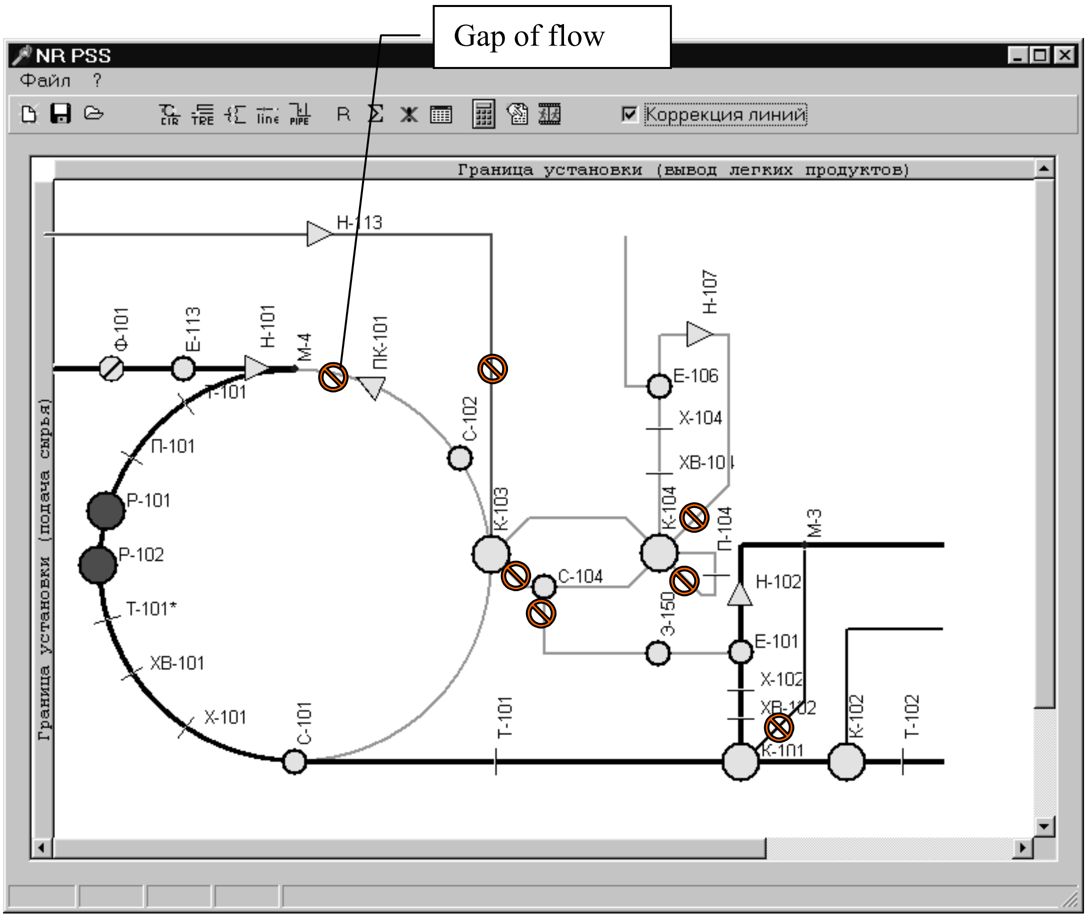


Figure 6 Simplified Graphic Model of Hydroclearning process with gaps of flows

101 has the main flow from a refrigerator X-101, main leaving flow in the heat exchanger T-101 and extra flow routed to the column K-103.

2. The calculation of apparatus under the scheme is conducted sequentially, pursuant to a direction of product lines under the statement of item 1. The calculation starts with boundary of the unit, from the main product line. For example (see figure 6), first is calculated the filter Ф-101, then vessel E-113 etc.

3. The algorithm of detour of apparatus is realized as recursions with several limitations.

3.1. If in the apparatus two leaving flows main and extra, the next apparatus for calculation will be on the main flow, the calculation of the apparatus on an extra flow implements later. For example (see figure 6), after calculation of the separator C-101 the apparatus T-101, K-101, K-103, T-102 are calculated, and only then pass to recycle to a column K-103, then the apparatus C-102, ПК-101 are calculated.

3.2. If the apparatus has two entering flows and while calculating we meet an apparatus through an extra flow, in this point the solution will stop and will be a flow gap at calculation of flow diagram. For example (see figure 6), after calculation of the compressor ПК-101, it would be necessary to calculate a unit of mixture of raw material and hydrogen gas - M-4, but as the calculation of this apparatus was already made, we only reassign parameters of an extra flow to the M-4 and the solution in this point stopped. Pursuant to item 2 we come back to calculation of other apparatus on product line from the K-103 to the K-104.

3.3. Criterion of breaking will be quantity of calculations of the apparatus on the scheme. When all apparatus on the scheme will be calculated n times, we can once again calculate the scheme, or, if the accuracy of the reached solution satisfies us, we stop the calculations.

Having algorithm of a structure analysis it is possible to calculate the scheme in static conditions or with constant parameters.

The problem of optimization of petrochemical process to find a minimum of a function [7]:

$$F(f_1, f_2, f_3 \dots f_n) \rightarrow min \qquad (1)$$

If there is limitations such as equalities

$$\varphi_i(f_1, f_2, f_3 \dots f_n) = 0 \qquad (2)$$
$$i=1, \quad ,m \quad m<n$$

And such as inequalities

$$\psi_i(f_1, f_2, f_3 \dots f_n) = 0 \qquad (3)$$
$$i=1, \dots ,p$$

where, f_i - varied parameters of the scheme.

As varied parameters can be selected: the technological mode conditions, parameters of raw and auxiliary flows of the scheme, parameters of apparatus.

The different mathematical methods are applied for solving optimization problem. One of the most simple methods of minimization of a function is the method of scanning. The largest lack of this method is the plenty of iterations to find an extreme point. To advantages of a method it is possible to attribute that if the behavior of a function on an interesting segment is not known and there can be some minimum or maximum points, the given method allows finding all these points.

At the solution optimization problem it is not always possible to forecast behavior of a function, so application of the given method is justified. The selection variable for optimization implements by user. With the help of object model of flow diagram it is possible easily to realize direct access to fields of the object data (apparatus, flow) that in turn allows the user to change during optimization any variables on scheme.

Among available models and algorithms of calculations in the given program were realized the computational methods of thermodynamic properties of gases: ideal, Lee-Kesler, Redlih-Kvong, Soave-Redlih-Kvong.

CONCLUSION

With usage of a structure analysis it is possible to calculate hydraulic resistance of flow diagram. Individual mathematical models of several apparatus were also constructed.

In practice all methods, described in the article, were realized in the program under a title "GMTP" (graphic models of technological processes). The program is the 32-bit application and operates under Windows 98/NT. The program is registered in the Russian patent agency under № 990857.

REFERENCES

[1] Abyzgildin A.U., Abyzgildin U.M., Hafizov A.R. "About the description of technological inheriting by the way of graphs" VINITI Journal 31.10.94. - № 4264-B94.

[2] www.aspentech.com

[3] www.simsci.com

[4] www.hyprotech.com

[5] Grady Booch "Object-oriented Analysis and Design with Applications. Second Edition" Addison-Wesley Longman, Inc., 1994.

[6] www.rational.com

[7] Ostrovski G.M., Volin U.M. Simulation of composite cmemical systems M.:, "Chemistry", 1975. - 312.

[9] № 990857 ROSPATENT.