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RESEARCH ARTICLE

Algorithm and software for the optimal technological design of a system of simple distillation columns

Nadir N. Ziyatdinov@, Ilia I. Emelyanov, Alina A. Ryzhova, Petr S. Chernakov

Kazan National Research Technological University, Kazan, 420111 Russia
@Corresponding author, e-mail: nnziat@yandex.ru

Abstract

Objectives. *The formalized problem of the optimal design of distillation column systems belongs to the class of mixed integer nonlinear program problems. Discrete search variables are the number of trays in the rectifying and stripping sections of columns, whereas the continuous ones are the operating modes of columns. This study aimed to develop an algorithm and a software package for the optimal technological design of a system of simple distillation columns based on the criterion of total reduced capital and energy costs using rigorous mathematical distillation models.*

Methods. *The solution to this problem is based on the branch and bound method. A computer model of the distillation column system was developed in the environment of the Aspen Hysys software package. The Inside–Out module was used as the distillation model. The developed algorithm is implemented in the software environment of the Matlab mathematical package. To solve the conditional optimization problem, a sequential quadratic programming method-based model was used. The interaction between software add-ins in Matlab and Aspen Hysys is implemented using a Component Object Model interface.*

Results. *Approaches to obtain the lower and upper bounds of the optimality criterion and the branching method for the implementation of the branch and bound method have been developed. In addition, an algorithm for the optimal design of a distillation column of a given topology based on the branch and bound method has been developed. Furthermore, using Matlab, a software package that implements the developed algorithm and is integrated with the universal modeling software AspenHysys has been created.*

Conclusions. *An algorithm and a software package have been developed and implemented that allows automating the design process of distillation column systems and integration with advanced mathematical programming packages, respectively. The performance of the algorithm and software package has been evaluated using the optimal design of the debutanization column as an example.*

Keywords: *distillation, branch and bound method, optimization, design, Matlab, AspenHysys*

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НАУЧНАЯ СТАТЬЯ

Алгоритм и программный комплекс оптимального технологического проектирования простых ректификационных колонн

Н.Н. Зиятдинов[@], И.И. Емельянов, А.А. Рыжова, П.С. Чернаков

Казанский национальный исследовательский технологический университет, Казань, 420111 Россия
[@]Автор для переписки, e-mail: nnziat@yandex.ru

Аннотация

Цели. *Формализованная задача оптимального проектирования систем ректификационных колонн относится к классу задач дискретно-непрерывного нелинейного программирования. Дискретными поисковыми переменными являются число тарелок в укрепляющей и исчерпывающей частях колонн, а непрерывными – режимы работы колонн. Цель работы – разработать алгоритм и программный комплекс оптимального технологического проектирования системы простых тарельчатых ректификационных колонн по критерию суммарных приведенных капитальных и энергетических затрат на основе строгих математических моделей ректификации.*
Методы. *Решение поставленной задачи базируется на методе ветвей и границ. Компьютерная модель системы ректификационных колонн построена в среде программного комплекса Aspen Hysys. В качестве модели ректификации использован модуль Inside-Out. Разработанный алгоритм реализован в программной среде математического пакета Matlab. Для решения задачи условной оптимизации использован модуль, основанный на методе последовательного квадратичного программирования. Взаимодействие программной надстройки, построенной в Matlab, с Aspen Hysys реализовано с помощью COM-интерфейса.*
Результаты. *Разработаны подходы к получению нижних и верхних границ критерия оптимальности и способ ветвления при реализации метода ветвей и границ. Разработан алгоритм оптимального проектирования ректификационной колонны заданной топологии на основе метода ветвей и границ. В математическом пакете Matlab создан программный комплекс, реализующий предложенный алгоритм и интегрированный с универсальной моделирующей программной AspenHysys.*
Выводы. *Разработан алгоритм и реализован программный комплекс, позволяющий автоматизировать процесс проектирования систем ректификационных колонн и интеграцию с передовыми пакетами математического программирования. Работоспособность алгоритма и программного комплекса апробирована на примере оптимального проектирования колонны дебутанизации.*

Ключевые слова: *ректификация, метод ветвей и границ, оптимизация, проектирование, Matlab, AspenHysys*

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INTRODUCTION

One of the main processes in the chemical, petrochemical, and oil and gas processing industry is distillation. This process is characterized by high energy and metal consumption [1–5]. Therefore, at the design stage of distillation columns and systems, it is necessary to make decisions aimed at minimizing these costs while meeting design requirements [6–12]. Currently, simplified methods [1, 5], thermodynamic methods [4, 13], and methods based on rigorous mathematical models [9, 10, 14–16] are used to solve such design problems. The essence of a simplified approach, as implemented in the methods of Fenske–Underwood–Gilliland and Lvov is to determine the minimum reflux number by which the optimal number of column and food trays is calculated to yield a given quality of output product. Simplified methods have low accuracy. Thermodynamic methods focus on minimizing energy costs and do not fully take into account capital costs. As a result, the task of developing effective methods for designing distillation column systems (DCS) that are optimal according to technical and economic criteria is important. The latter, in turn, requires the use of rigorous mathematical models and optimization methods. In this case, given the quality of products obtained, the optimal design task is to find a compromise between capital and operating costs, a sum that determines the optimality criterion [16]. An effective tool for computer modeling and optimization in chemical technology is the use of chemical process simulator (CPS) built on strict mathematical models of distillation processes, which are based on the laws of conservation of energy, mass, and momentum, the so-called mass, equilibrium, summation, and heat (MESH) models. These models are contained in the libraries of all leading CPS, such as Aspen Plus [17], AspenHysys [18], Unisim [19], and ChemCad [20, 21], allowing the investigation, design, and management of technological processes at all stages of their life cycle [22]. The CPS also contain effective nonlinear programming methods, including sequential quadratic programming and modified Lagrange function methods. However, these optimization methods can only solve problems of continuous nonlinear programming with discrete values of constructive and operational technological parameters. Because the problem of optimal DCS design is solved in the space of both continuous and discrete search variables, the development of DCS design methods remains relevant.

MATHEMATICAL SUBSTANTIATION OF THE PROBLEM OF OPTIMAL DESIGN OF DCS

The optimal design problem formulated above belongs to the class of mixed integer nonlinear program (MINLP) problems [6, 16], where the discrete search variables are the number of trays in the rectifying and stripping sections of the projected columns, whereas the continuous ones are the parameters that determine the operating modes of the columns. Let us present this problem in a formalized form:

$$f = \min_{x^j, u^j, m_s^j} \sum_{j=1}^{N} f^j\left(x^j, u^j, m_s^j\right), \tag{1}$$

$$\varphi_k^j(x^j, u^j, m_s^j) = 0,\ s = 1, 2,\ j = 1,\ldots,N,\ 1 \le m_s^j \le m_s^{j,\max},\quad k = 1,\ldots,\ m_s^{j,\max}, \tag{2}$$

$$\psi^j(x^j, u^j) \le 0,\ j = 1,\ldots,N, \tag{3}$$

$$F^{j_g} - D^g = 0,\ F^{r_g} - W^g = 0,\ j_g, r_g = 1,..,N, \tag{4}$$

$$\varphi_k^j(x^j, u^j, m_s^j) = \left\{ \begin{array}{l} \varphi_{s_0}^j(x^j, u_0^j), s = 1 \\ \varphi_{s_1}^j(x^j, F^j), s = 2 \\ \varphi_{s_k}^j(x^j), 1 \le k \le m_s^j \\ \varphi_{m_s^j+1}^j(x^j, u_{m_s^j+1}^j), s = 2 \end{array} \right\}, \tag{5}$$

where $f^j(x^j, u^j, m_s^j)$ in Equation (1) is a cost function that includes the total given capital and operating costs of the *j*th column; Equation (2) is a mathematical model of the *j*th column; x^j, u^j represent state and control variables of the *j*th distillation column; N represents the number of columns in the system; j represents the ordinal number of the distillation column; s represents the index of the column section (s = 1–rectifying section; s = 2–stripping section); m_s^j represents the number of trays in each section of the *j*th distillation column with values ranging from 1 to $m_s^{j,\max}$; $m_s^{j,\max}$ –the maximum number of trays; in Equation (5), $\varphi_{1_0}^j(x^j, u_0^j)$, $\varphi_{s_k}^j(x^j)$, $\varphi_{2_1}^j(x^j, F^j)$ and $\varphi_{m_2^j+1}^j(x^j, u_{m_2^j+1}^j)$ are mathematical models of the dephlegmator, *k*th trays, food trays, and boiler of the *j*th column, respectively; the inequalities in Equation (3) are design constraints; Equation (4) is a ratio describing the DCS structure, which means that when $F^{j_g} - D^g = 0$ the feed flow of the j_gth column is the distillate of the *g*th column; when $F^{r_g} - W^g = 0$, the feed flow of the r_gth column is the bottom product of the *g*th column; j_g, r_g = 1,..., N, j, g = 1,..., N –the numbers of the columns. Furthermore, for the simplicity of the algorithm under consideration, Equations (4) and (5) will be omitted.

Various methods exist for solving MINLP problems, among which one of the most effective is the method of branches and boundaries [16]. However, this method is not fully formalized because its application to a specific problem necessitates the development of a branching procedure on a tree graph, as well as the formalization of tasks of finding the upper and lower estimates of the optimality criterion. This fully applies to the design problem under consideration, where the main difficulty lies in developing an approach to calculate the lower estimate of the optimality criterion. To do this, it is necessary that all search variables, including the number of trays, can take continuous values. Then, the problem of finding the lower estimate of the criterion will be reduced to a nonlinear programming problem. Solving the minimization problem with continuous search variables will give a better solution than with discrete variables, i.e., a lower bound. The latter is infeasible since the discrete search variable in the number of plates in columns cannot be fractional. In [16], we proposed a technique that allows us to switch from discrete to continuous variables based on the problem under consideration.

To obtain a lower estimate for each column plate, we proposed introducing an additional fictitious structural parameter into the equation of the relationship between the equilibrium and working concentrations of the *i*th component of the *k*th tray α_{sk}^j:

$$y_{is}^{jk} = y_{is}^{j,k+1} + \alpha_{sk}^j E_{is}^j (y_{is}^{*jk} - y_{is}^{j,k+1}). \tag{6}$$

This parameter accepts a value of 0 or 1. If $\alpha_{sk}^j = 0$, the tray is missing; otherwise, if $\alpha_{sk}^j = 1$, the tray is present.

Taking into account the introduced modification, Equations (1)–(3) will take the form of Equations (7)–(9):

$$f = \min_{x^j, u^j, \alpha_s^j} \sum_{j=1}^{N} f^j(x^j, u^j, \alpha_s^j), \tag{7}$$

$$\varphi^j(x^j, u^j, \alpha_s^j) = 0, \tag{8}$$

$$\psi^j(x^j, u^j) \le 0, \; j = 1, \ldots, N, \tag{9}$$

$$\alpha_s^j = [0,\ 1],$$

where α_s^j represents a vector whose components are α_{sk}^j, $k = 1, \ldots, m_s^{j,\max}$.

Thus, the task of the optimal design of DCS is reduced to determining the optimal values of structural parameters and control variables. The continuity of the values of structural parameters α_{sk}^j allows us to calculate the lower estimates of the optimality criterion.

To solve the problem Equation (7) by the method of branches and boundaries, sets of M_s^{jl} plates are introduced in the rectifying and stripping sections of the *j*th column (s = 1, 2), where the structural parameter α_{sk}^j accepts a value of 0 or 1. The number of plates is determined in the previous steps of the branch and boundary method. Let us consider the formulation of the problem at the *l*th step:

$$f^l = \min_{x^j, u^j, \alpha_{sk}^j} \sum_{j=1}^{N} f^j(x^j, u^j, \alpha_s^j), \quad k \notin M_s^{jl}, \tag{10}$$

$$\varphi^j(x^j, u^j, \alpha_s^j) = 0,$$

$$\psi^j(x^j, u^j) \le 0, \; j = 1, \ldots, N, \; s = 1,\ 2,$$

where the set α_{sk}^{j} = [0, 1] at $k \in M_s^{jl}$, found in the previous iterations, is constant; at the same time, α_{sk}^{j} at $k \notin M_s^{jl}$ are binary search variables.

To obtain the lower estimate Equation (10), we solve the following problem:

$$\mu^l = \min_{x^j, u^j, \alpha_{sk}^j} \sum_{j=1}^{N} f^j\left(x^j, u^j, \alpha_s^j\right),\ k \notin M_s^{jl}\ , \tag{11}$$

$$\varphi^j(x^j, u^j, \alpha_{sk}^j) = 0\ ,\ j = 1,\ldots,N\ ,$$

$$\psi^j(x^j, u^j) \le 0\ ,\ j = 1,\ldots,N\ ,$$

$$0 \le \alpha_{sk}^j \le 1,\ \text{for all}\ k \notin M_s^{jl}\ .$$

The value of the upper estimate of the optimality criterion is determined by the values of parameters α_{sk}^{*j} obtained from the solution of the problem in Equation (11) at the value $\bar{\alpha}_{sk}^{j}$ obtained in the previous iterations. To do this, we solve Equation (12) under the conditions that, for $k = 1,\ldots p_s^j$, $\bar{\alpha}_{sk}^j = 1$, where $p_s^j = \left[\sum_{k \notin M_s^{jl}} \alpha_{sk}^{*j}\right] + \sum_{k \in M_s^{jl}} \bar{\alpha}_{sk}^j$ is the set of the nearest integer sum of the structural parameters, and for the remaining k $\bar{\alpha}_{sk}^j = 0$, the following problem is solved:

$$\eta^l = \min_{x^j, u^j} \sum_{j=1}^{N} f^j(x^j, u^j, \bar{\alpha}_{sk}^j)\ , \tag{12}$$

$$\varphi^j(x^j, u^j, \bar{\alpha}_{sk}^j) = 0\ ,\ j = 1,\ldots,N\ ,\ k = 1,\ldots,m_s^{j,\max}\ ,$$

$$\psi^j(x^j, u^j) \le 0\ ,\ \ j = 1,\ldots,N\ .$$

The branching rule is as follows. The number of trays of each section (*s* = 1, 2) of each column (*j* = 1,…,*N*) is divided into two subsets. In the first subset, parameters for α_{sk}^j for which *k* lies in the interval ($\left[\frac{m_s^{jl}}{2}\right]+1,\ m_s^{jl}$) vary, and the parameters for α_{sk}^j for which *k* belongs to the interval (1, $\left[\frac{m_s^{jl}}{2}\right]$) are equal to 1, where m_s^{jl} represents the number of trays for which $k \notin M_s^{jl}$. In the second subset, the values of parameters α_{sk}^j for which *k* lies in the interval (1, $\left[\frac{m_s^{jl}}{2}\right]$) vary, and α_{sk}^j is 0 for those for which *k* varies in the interval ($\left[\frac{m_s^{jl}}{2}\right]$ +1, m_s^{jl}).

At each iteration, the two problem Equations (11) and (12) are solved to determine the lower and upper estimates of the optimality criterion. The obtained values of the objective function are compared. If, in the *l*th step, the difference between the upper and lower estimates is less than the specified accuracy ε, the solution found is considered optimal. Otherwise, for further branching, the vertex with the lowest lower score is selected from all hanging vertices.

Aspen Hysys was chosen to solve the problem of the optimal design of DCS with a given topology, as it can be integrated with advanced mathematical programming packages and can model complex petrochemical processes, including DCSs; it contains libraries of many rigorous models of technological equipment with advanced calculation algorithms and a built-in optimization module; and it has a friendly interface that provides a simple and concise representation of a technological scheme. However, because of the software closeness of the optimization module and a limited set of tuning parameters of optimization methods in the Aspen Hysys, it cannot create a program of the proposed algorithm.

SOFTWARE PACKAGE AND ALGORITHM FOR DESIGNING OPTIMAL DCS

To automate the process of designing an optimal system of distillation columns, the software implementation of the algorithm is performed in the Matlab mathematical package. It has a built-in programming language, advanced optimization methods, and is a convenient and relatively simple package for managing the calculation process in the Aspen Hysys. It also enables the development of an interface linking these software tools using Component Object Model/ActiveX technology. In the Aspen Hysys environment, a preliminary assembly of the projected DCS is performed, and its calculation is based on the values of search variables generated in the algorithm implemented in Matlab.

Figure 1 shows the structure of the developed software package for designing an optimal system of distillation columns.

We describe an expanded algorithm for implementing the developed software package.

Step 0. Inputting initial data: the initial number of trays and specifications that are used as search variables; boundaries of changes in the values of specifications and structural parameters of plates; initial approximations of

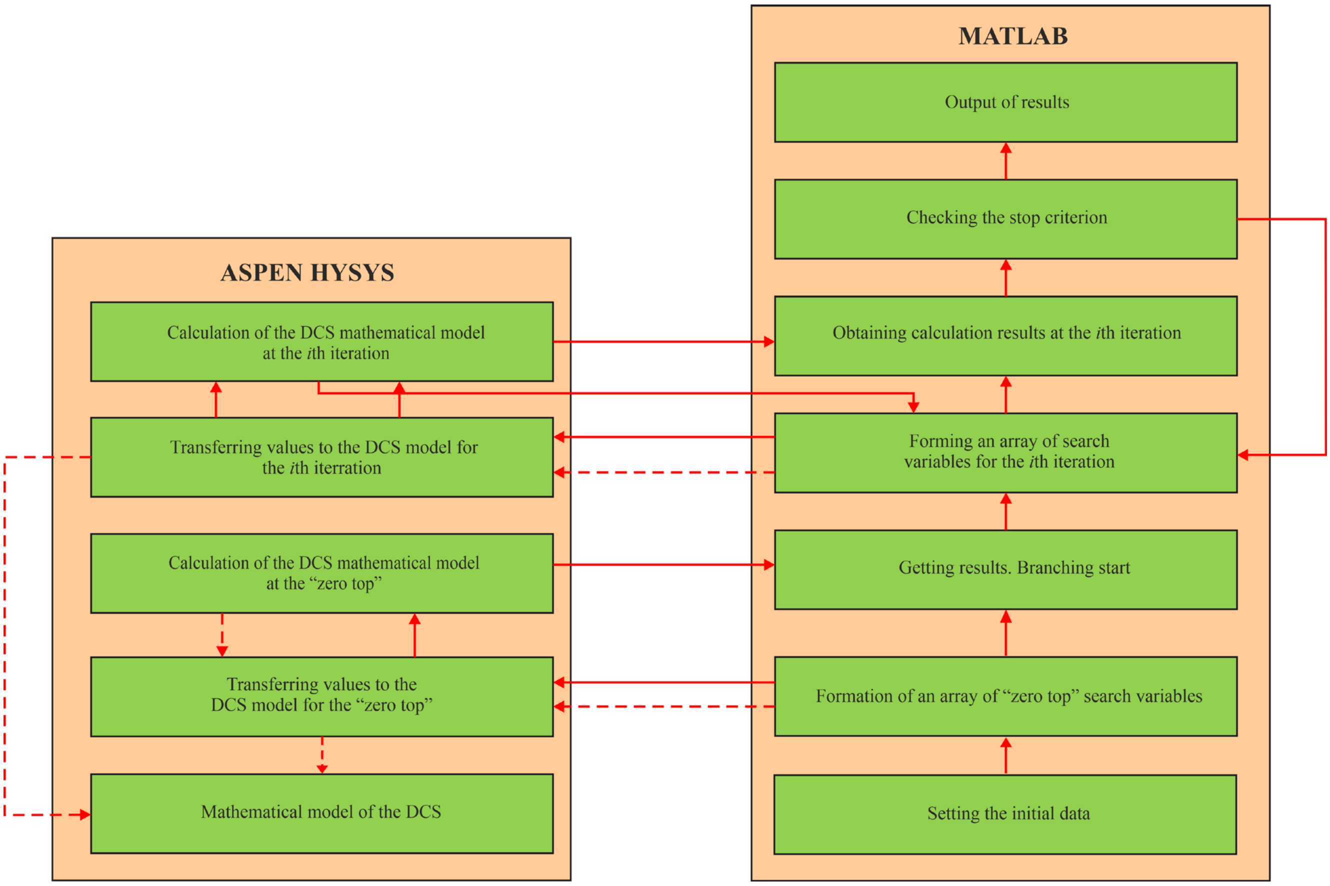

Fig. 1. The structure of the software package.

the values of specifications and structural parameters of trays; cost coefficients; the mathematical model's calculation accuracy of the distillation column and optimization method; refrigerant and steam temperatures.

Step 1. Formation of an array of search variables: the lower and upper estimates of the criterion at the zero vertex, obtained by solving Equations (11) and (12).

Step 2. Splitting of a promising vertex by choosing the smallest upper bound $\overline{\eta} = \min\{\overline{\eta}, \eta_l^d\}$, l = 1, 2, where d represents the iteration index, and l represents the index of the descendant of the vertex of the branch tree at the iteration d, by solving Equation (11) and (12).

Step 3. Exclusion of unpromising vertices $\mu_l^t > \overline{\eta}$, l = 1, 2, t = 1, d.

Step 4. Searching for a promising vertex $\{l^*, t^*\}$ among the remaining ones $\mu_{l*}^{t*} = \min_{\mu_l^t \in M} \mu_l^t$.

Step 5. Checking the end of the solution. If the end condition is met,

$$\eta_{l*}^{t*} = \overline{\eta} \text{ and } \left|\mu_{l*}^{t*} - \eta_{l*}^{t*}\right| / \mu_{l^*}^{t^*} \le \varepsilon,$$

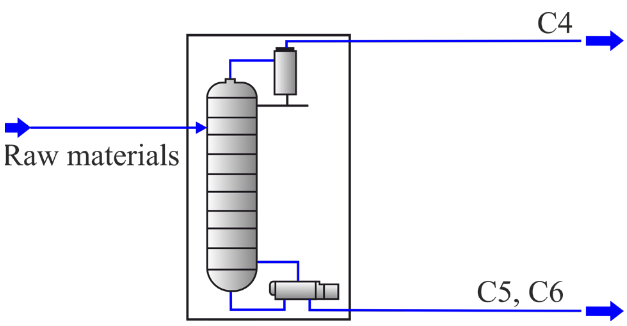

Fig. 2. Diagram of the debutanizing column.

where ε represents the accuracy of the solution, the completion of the algorithm, and the output of the results. Otherwise, go to step 2.

The effectiveness of the developed algorithm and software package was tested on the example of designing an optimal distillation column of debutanization (Fig. 2). To solve the problem in the Aspen Hysys environment, a MESH model of the distillation column was selected, including the Inside-Out method, which is an effective method in terms of time and accuracy of the obtained solution.

Problem statement: with the given parameters of the feedstock (Table 1), it is required to find such values of search variables (the number of plates in

Table 1. Raw material flow parameters

Parameter	Value
Pressure, bar	5
Temperature, °C	80
Mass flow, kg/h	10000
Mass fraction of *n*-butane	0.35
Mass fraction of *n*-pentane	0.30
Mass fraction of *n*-hexane	0.35

stripping and rectifying sections of the column, the value of the reflux ratio, and the temperature in the cube of the column) that the criterion given the total capital and operating costs has a minimal value and to restrict the quality of the partial products: the content of *n*-butane in the distillate is greater than 0.99 mass fraction but less than 0.01 in the cube of the column. The pressure at the top of the column was assumed to be equal to 4 bar, taking into account the possibility of condensation of the upper products by submerged water. The efficiency of the plates for the distillation column was assumed to be equal to 1, the initial approximation of the fictitious structural parameter is 0.7, the specified accuracy ε of the solution is equal to 0.05, and the initial approximation of the number of trays in the column is 30.

The progress of solving the problem is shown in Table 2 and Fig. 3. The optimum corresponds to the vertex 41. Tables 3 and 4 show the data of the material balance of the column and parameters and technical and economic indicators of the column, respectively.

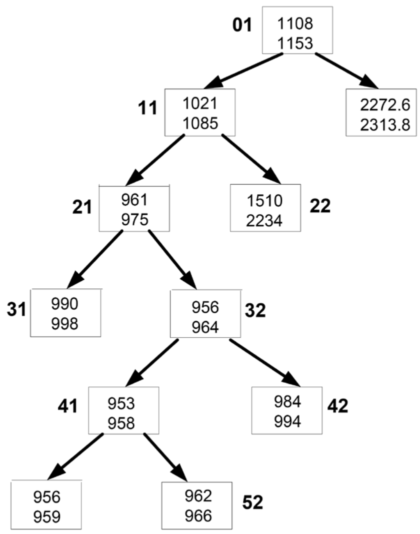

Fig. 3. Tree graph of the solution of the problem (at the vertices of the graph, the lower and upper estimates of the optimality criterion are given).

Table 2. Progress in solving the problem

Vertex No.	Lower estimate, c.u./h	Upper estimate					Accuracy
		Number of trays		Reflux ratio	Criterion c.u./h		
		Rectifying section	Stripping section				
01	1107.9	8	7	2.31	1153.3		0.039
11	1021.1	11	7	2.12	1085.0		0.054
12	2272.6	4	7	5.02	2313.7		0.017
21	960.9	10	10	1.81	974.7		0.014
22	1509.6	11	4	4.74	2233.8		0.320
31	990.3	12	10	1.82	997.7		0.007
32	956.0	9	11	1.83	963.6		0.0078
41	952.6	9	13	1.81	957.9		0.005
42	983.9	9	9	1.93	993.9		0.010
51	955.8	9	12	1.82	958.9		0.003
52	962.3	8	13	1.86	966.3		0.004

Table 3. Parameters of fed and obtained products

Raw materials flow parameters	Flow No.		
	Raw materials	C4	C5, C6
Pressure, bar	5	4	4.5
Temperature, °C	80	42.6	102
Mass flow rate, kg/h	10000	3444	6556
Composition	Mass fract.		
Butane	0.35	0.99	0.01
Pentane	0.30	0.01	0.45
Hexane	0.35	0	0.53

Table 4. Parameters and technical and economic indicators of the column

Indicators	Rectifying section	Stripping section
Number of trays in section	9	13
Reflux ratio	1.8	–
Cube temperature, °C	42.6	102
Section diameter, m	1.1	0.9
Section height, m	5.4	7.8
Interdisciplinary distance, m	0.6	0.6
Heat duty, kcal/h	−516280	658352
Capital costs, c.u./h	112.4	
Operating costs, c.u./h	845.6	
Optimality criterion, c.u./h	958	

CONCLUSIONS

An algorithm for the optimal design of a distillation column of a given topology, based on the method of branches and boundaries, is presented. A software package based on the Matlab mathematical programming package has also been implemented, which allows automating the design process and integration with Aspen Hysys. The effectiveness of the developed algorithm and software package was tested on the example of a distillation column of debutanization.

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Authors' contribution

N.N. Ziyatdinov – formulation of research goals and objectives, development of a method and algorithm, general management of the research process.

I.I. Emelyanov – development of a software package, experimental research, processing of the obtained experimental data.

A.A. Ryzhova – processing of the obtained experimental data, preparation of materials for publication.

P.S. Chernakov – preparation of materials for publication.

The authors declare no potential or actual conflicts of interest.

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About the authors:

Nadir N. Ziyatdinov, Dr. Sci. (Eng.), Professor, Head of the Department of Process System Engineering, Kazan National Research Technological University (68, Karl Marx ul., Kazan, 420015, Republic of Tatarstan, Russia). E-mail: nnziat@yandex.ru. https://orcid.org/0000-0002-2314-8935

Ilia I. Emelianov, Cand. Sci. (Eng.), Associate Professor, Department of Process System Engineering, Kazan National Research Technological University (68, Karl Marx ul., Kazan, 420015, Republic of Tatarstan, Russia). E-mail: ilyaemelyan@gmail.com. https://orcid.org/0000-0003-0257-0739

Alina A. Ryzhova, Postgraduate Student, Department of Process System Engineering, Kazan National Research Technological University (68, Karl Marx ul., Kazan, 420015, Republic of Tatarstan, Russia). E-mail: alinagainullina0@yandex.ru. https://orcid.org/0000-0001-5918-8296

Petr S. Chernakov, Student, Department of Process System Engineering, Kazan National Research Technological University (68, Karl Marx ul., Kazan, 420015, Republic of Tatarstan, Russia). E-mail: systech2@yandex.ru

Об авторах:

Зиятдинов Надир Низамович, д.т.н., профессор, зав. кафедрой системотехники, ФГБОУ ВО «Казанский национальный исследовательский технологический университет» (420015, Россия, Республика Татарстан, Казань, ул. К. Маркса, д. 68). E-mail: nnziat@yandex.ru. https://orcid.org/0000-0002-2314-8935

Емельянов Илья Игоревич, к.т.н., доцент, доцент кафедры системотехники, ФГБОУ ВО «Казанский национальный исследовательский технологический университет» (420015, Россия, Республика Татарстан, Казань, ул. К. Маркса, д. 68). E-mail: ilyaemelyan@gmail.com. https://orcid.org/0000-0003-0257-0739

Рыжова Алина Альбертовна, аспирант, кафедра системотехники, ФГБОУ ВО «Казанский национальный исследовательский технологический университет», (420015, Россия, Республика Татарстан, Казань, ул. К. Маркса, д. 68). E-mail: alinagainullina0@yandex.ru. https://orcid.org/0000-0001-5918-8296

Чернаков Петр Станиславович, студент, кафедра системотехники, ФГБОУ ВО «Казанский национальный исследовательский технологический университет» (420015, Россия, Республика Татарстан, Казань, ул. К. Маркса, д. 68). E-mail: systech2@yandex.ru

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