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РАСЧЕТ СОСТАВОВ ПРОДУКТОВЫХ ПОТОКОВ СЛОЖНЫХ РЕКТИФИКАЦИОННЫХ СИСТЕМ НА ОСНОВЕ РАСШИРЕННОЙ ВЕРСИИ ПРИНЦИПА МАКСИМАЛЬНОЙ ЭНТРОПИИ

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Предложен метод расчета наиболее вероятных составов продуктов разделения атермальных смесей в сложных ректификационных системах, к которым относятся системы простых колонн с рециклами и без них, сложные колонны с боковыми отборами, системы со связанными тепловыми потоками и другие. В основе метода лежит расширенная версия принципа максимальной энтропии. В качестве критерия правдоподобия используется информационная энтропия сложного опыта с привлечением условной энтропии и условных вероятностей. Принятая аксиоматика позволяет получить наиболее вероятные распределения компонентов в продуктовых потоках системы, которое отвечает максимуму энтропии сложного опыта при соблюдении балансовых ограничений. Показано, что учет атермальных свойств смеси приводит к зависимостям, в которые входят энтропийные коэффициенты активности, связанные с условной энтропией, в характерной для термодинамики форме. Зависимости для идеальных смесей оказываются частным случаем полученных соотношений. Дан способ расчета энтропийных коэффициентов активности как функций относительных объемов молекул компонентов и мольного состава смеси. Предложенный метод ориентирован на проектный вариант расчета ректификационной системы. Он позволяет при заданных ограничениях на качество продуктов определить параметры, характеризующие протяженность процесса (число теоретических ступеней разделения в безотборном режиме), и составы продуктовых потоков. Учет атермальности смеси приводит к увеличению протяженности процесса и не оказывает существенного влияния на составы продуктов. Дано сопоставление результатов расчета составов продуктовых потоков типовой газофракционирующей установки с учетом и без учета атермальных свойств разделяемой смеси с данными промышленного эксперимента.

Ключевые слова: ректификация, атермальная смесь, сложная система, распределение компонентов, принцип максимальной энтропии, энтропия сложного опыта

COMPOSITIONS CALCULATION OF COMPLEX DISTILLATION SYSTEM PRODUCT FLOWS BASED ON THE EXTENDED VERSION OF THE MAXIMUM ENTROPY PRINCIPLE

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A method for calculating the most likely product compositions of athermal mixture separation in complex distillation systems, including systems of simple recycling and non-recycling columns, complex columns with side sampling, systems with joint heat flows, and others. The method is based on an extended version of the maximum entropy principle. The informational entropy of complex experiment involving conditional entropy and conditional probabilities is used as the like-

lihood criterion. The adopted axiomatic allows one to obtain the most probable component distributions in the product flows of the system, which corresponds to the complex experience maximum entropy in accordance with the balance restrictions. It has been demonstrated that athermal properties accounting of the mixture create dependencies that include entropic activity coefficients associated with the conditional entropy in a typical thermodynamics form. Dependencies are a special case of the correlations obtained for ideal mixtures. The method for calculating the entropy activity coefficients as functions of the components molecule relative volumes and the mixture molar composition has been provided. This method is focused on the design version of the distillation system calculation. It allows to determine the parameters characterizing the process length (the number of theoretical separation steps in the non-selective mode) and the product flow composition products under the product quality restrictions. The accounting of mixture athermal nature leads to an increased duration of the process and has a slight impact on the product compositions. A comparison is given of the results of the calculation of the composition of the product flows of a typical gas fractionating unit with and without taking into account the athermal properties of the mixture to be separated with the data of an industrial experiment.

Key words: distillation, athermal mixture, complex system, component distribution, maximum entropy principle, entropy of complex experience

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ENTROPIC ACTIVITY COEFFICIENT

As it has been mentioned before, the maximum likelihood criterion, along with Shannon's entropy, also includes conditional entropy and conditional probabilities while accounting the athermal mixture properties. By conditional probability should be meant the probability of randomly detected particle of one type in an athermal mixture, provided that, in the case of an ideal mixture, a particle of another type will be detected in its place. In the reference [16] we can see the relationship between conditional probabilities and relative micro-particle sizes; and the continuity of relation of conditional probability to the component mole fraction a in a binary mixture has been established:

$$p_{12} = qx_2,\ p_{21} = qx_1. \quad (1)$$

Here p_{12} is the conditional probability that particle 2 will be detected in the sequence of particles randomly extracted from the athermal mixture in place of particle 1 in the case of an ideal mixture; p_{21} is the same for second type of particle; x_1, x_2 are the mole fractions of components 1 and 2 in the mixture; q is the athermal coefficient of a binary mixture, which characterizes the degree of athermality of the mixture and does not depend on the composition just the same like the δ relative particle size.

For an ideal binary mixture $\delta = 1$, $q = 0$ are used. For another extreme case, when the particles differ in size by an arbitrarily large value $\delta = 0$, $q = 1$ are used.

Since the relation between the conditional probability and the athermal coefficient is very simple (1), it is more convenient to use athermal coefficients, rather than relative particle sizes in practical calculations. To go from δ to q, we have compiled a table of athermal coefficients and proposed a transition to multicomponent mixtures [16]. In the latter case, a matrix of athermal coefficients is compiled according to the table q_{ik} $(i,k=\overline{1,m})$ based on the analysis of the relative particle size values of each pair of multicomponent mixture components δ_{ik} $(i,k=\overline{1,m})$. The volume of the largest particle is always considered as a unit.

With the athermal coefficients and the multicomponent mixture composition, it is possible to calculate the conditional probabilities

$$p_{ik} = \frac{q_{ik}x_k}{x_i + x_k(1-q_{ik})} \Bigg/ \sum_{k=1}^{m} \frac{q_{ik}x_k}{x_i + x_k(1-q_{ik})},\quad i,k=\overline{1,m}, \quad (2)$$

where $q_{ii} = 1$.

The formula (2) shows that values p_{ik} depend on the concentrations. However, when it is about solving the problem of the component distribution in the product flows system, conditional probabilities will be assumed to be fixed at each step of the iterative calculation procedure.

By knowing the conditional probabilities, one can calculate the conditional entropies related to each component

$$H_i = -\sum_{k=1}^{m} p_{ik} \ln p_{ik}\ , \ i = \overline{1,m}\,, \tag{3}$$

and the component entropic activity coefficients [17]

$$\gamma_i = \exp(-H_i)\ , \ i = \overline{1,m}\,. \tag{4}$$

To calculate the entropic activity coefficients, according to (2)–(4), it is necessary to have a matrix of athermal coefficients and composition of the mixture.

MOST PROBABLE COMPONENT DISTRIBUTION

Let's consider a distillation system designed to separate the original m-component athermal mixture into p products (flows). Let's define the consumption of the j product, reduced to one mole of the source mixture (relative molar selection of the product), – ε_j ($j = \overline{1,p}$); molar concentration of the i component in the source mixture – z_i ($i = \overline{1,m}$); the molar concentration of the i component in the j product – x_{ij} ($i = \overline{1,m}$, $j = \overline{1,p}$).

Let's formulate the problem of the most probable distribution of components between the product flows of a complex distillation system. Following Jaynes's model, and taking into account the peculiarities of the similar problem formulation in distillation ideal mixtures [14], we will present the source information in the following form: the molar concentration of the i component in the j product

$$\sum_{j=1}^{p} \varepsilon_j x_{ij} = z_i\ , \ i = \overline{1,m}\,, \tag{5}$$

$$\sum_{i=1}^{m} x_{ij} = 1\,, \quad j = \overline{1,p-1}\,, \tag{6}$$

$$\varepsilon_j \sum_{i=1}^{m} a_{ij} x_{ij} = \langle a_j \rangle\,, \quad j = \overline{1,p-1}\,, \tag{7}$$

where $a_{ij} = a_{ij}^0 - a_{ip}^0$; a_{ij}^0 is a phenomenological coefficient that evaluates the problem's characteristic property of the i component under the conditions (temperature and pressure) of the j product; $\langle a_j \rangle$ is an average value (mathematical expectation) of coefficients a_{ij}^0 for the j product.

Equations (5) follow from the material balance of the system, and (6) – conditions for the normalization of concentrations. The equation (6), recorded for the flow p, was not included in the operand because it is not independent.

Equations (7) are typical of the entropic modeling method [13, 14]. They introduce the component properties and fix the separation degree in the system when setting the task. The number of equations (7) corresponds to the number of restrictions that should be imposed on the system (apart from material balances and specified product selections) so that the task acquire physical significance. It is assumed that the coefficients a_{ij}^0 in equations (7) depend on the type of molecules and external parameters (temperature and pressure) at the product sampling points. The problems with phase transformations of ideal mixtures can be expressed through phase equilibrium constants and the relative volatility component coefficients:

$$a_{ij} - a_{nj} = \left(a_{ij}^o - a_{ip}^o\right) - \left(a_{nj}^o - a_{np}^o\right) =$$
$$= \ln\sqrt{K_{ij}^o K_{ip}^o} - \ln\sqrt{K_{nj}^o K_{np}^o} = \ln \alpha_{ij}\ \ i = \overline{1,m}\,, \ \ j = \overline{1,p-1}\,, \tag{8}$$

where K_{ij}^0 is a phase equilibrium constant of the i component for the conditions of the j product; K_{nj}^0 is the same for the reference component n with the arbitrary choice; α_{ij} is an effective coefficient of relative volatility of the i component for the j product.

The expression (8) is also true for athermal mixtures, if the phase equilibrium constant is taken not the ratio of equilibrium concentrations, but the ratio of product concentrations to entropic activity coefficients [17, 18].

Therefore, the solution of this problem lies in the determination of the product flow compositions x_{ij} given ε_j, z_i, a_{ij}, $\langle a_j \rangle$. Since generally the number of dimensionalities is greater than the number of equations (5)–(7), it is possible to find only the most probable (likely) component distribution law. To evaluate the uncertainty of the determinates we will use an extended version of the maximum entropy principle, in which the likelihood criterion is the complex experience entropy

$$H = -\sum_{j=1}^{p}\left[\varepsilon_j\left(\sum_{i=1}^{m} x_{ij}\ln x_{ij} + \sum_{i=1}^{m} x_{ij} H_{ij}\right)\right]. \tag{9}$$

Here H_{ij} is a conditional entropy related to the i component in the j flow.

Formally, the problem is as follows: when the values are known z_i ($i = \overline{1,m}$) and ε_j ($j = \overline{1,p}$), as well as given values a_{ij} ($i = \overline{1,m}$, $j = \overline{1,p}$), $\langle a_j \rangle$ ($j = \overline{1,p-1}$), p_{ik}^j ($i,k = \overline{1,m}$, $j = \overline{1,p}$), the task is to find such values x_{ij} ($i = \overline{1,m}$, $j = \overline{1,p}$), which would afford the maximum entropy (9) subject to restrictions (5)–(7).

We use the Lagrange multiplier method to solve the problem. Introducing undetermined multipliers σ_i ($i = \overline{1,m}$), $\mu_j\varepsilon_j$, λ_j ($j = \overline{1,p}$) for restrictions (5)–(7), you can come up with the following solution:

$$-\varepsilon_j(1 + \ln x_{ij}) + \varepsilon_j H_{ij} + \sigma_i \varepsilon_j + \mu_j \varepsilon_j + \lambda_j \varepsilon_j a_{ij} = 0\,,$$
$$i = \overline{1,m}\,, \ \ j = \overline{1,p}\,. \tag{10}$$

In the used notation $\lambda_p = \mu_p\varepsilon_p = 0$. After that, we have a closed system of equations (5)–(7) and (10) to determine the unknown concentrations and Lagrange multipliers.

The solution of the obtained system of algebraic equations is similar to [14]. Using (5), from the expressions (10) it is possible to exclude the multipliers σ_i

$$x_{ij} = z_i \exp(\mu_j + \lambda_j a_{ij} + H_{ij}) \Big/ \sum_{j=1}^{p} \varepsilon_j \exp(\mu_j + \lambda_j a_{ij} + H_{ij}),$$

$$i = \overline{1,m}, \; j = \overline{1,p}. \tag{11}$$

In order to determine multipliers $\mu_j\varepsilon_j$ we could use equations (6) or (7), however, we will go the other way. In the practice of calculations, it can happen there are no values $\langle a_j \rangle$ given that limit the degree of separation according to the original formulation of the problem, but the concentration of individual components in the system product flows. Therefore, instead of p-1 equations (7), we introduce p-1 equations (11), recorded for given concentrations x_{kl}. These new restrictions can be brought to a linear equation system for $\exp(\mu_j)$

$$\sum_{j}^{p-1} \varepsilon_j C_{fj} \exp(\lambda_j a_{mj}) \exp(\mu_j) = -\varepsilon_p C_{fp} \exp(\lambda_p a_{mp}) \exp(\mu_p),$$

$$f = \overline{1, p-1}, \tag{12}$$

where f is the ordinal number of a given concentration for each flow;

$$C_{fj} = \begin{cases} \exp\left[\lambda_j (a_{kj} - a_{mj}) + H_{kj}\right], & \text{if } j \neq l, \\ \left(1 - \dfrac{z_k}{x_{kl}\varepsilon_l}\right) \exp\left[\lambda_l (a_{kl} - a_{ml}) + H_{kl}\right], & \text{if } j = l. \end{cases}$$

When solving system of linear equations (12), we find

$$\exp(\mu_j) = \frac{\varepsilon_p}{\varepsilon_j} \exp(\lambda_p a_{mp} - \lambda_j a_{mj}) \exp(\mu_j) \frac{D_j}{D_p},$$

where $D_p = \det\left\| C_{fj} \right\|$; $D_j = -\sum_{f=1}^{p-1} A_{fj} C_{fp}$; $f = \overline{1, p-1}$; A_{fj} – algebraic matrix complement with elements C_{fj} in the determinant D_p.

Substituting the value $\exp(\mu_j)$ into the equation (11), taking into accounting (4) and (8), we get the final solution:

$$x_{ij} = z_i \alpha_{ij}^{\lambda_j} \gamma_{ij} D_j \Big/ \varepsilon_j \sum_{j=1}^{p} \alpha_{ij}^{\lambda_j} \gamma_{ij} D_j, \quad i = \overline{1,m}, \; j = \overline{1,p}, \tag{13}$$

where

$$C_{fj} = \begin{cases} \alpha_{kj}^{\lambda_j} \gamma_{kj}, & \text{if } j \neq l, \\ \left(1 - \dfrac{z_k}{x_{kl}\varepsilon_l}\right) \alpha_{kl}^{\lambda_l} \gamma_{kl}, & \text{if } j = l. \end{cases}$$

For $p = 2$, we have formulas to calculate the compositions of the athermal mixture product separation in a simple (two-product) column.

The distribution (13) corresponds to the linerithmic relation

$$\lambda_j = \ln\left(\frac{x_{ji}\gamma_{ji}}{x_{pi}\gamma_{pi}} \cdot \frac{x_{pk}\gamma_{pk}}{x_{jk}\gamma_{jk}} \right) \Big/ \ln \frac{\alpha_{ji}}{\alpha_{jk}}, \quad i,k = \overline{1,m}, \quad i \neq k,$$

$$j = \overline{1, p-1},$$

which is a generalization of the known in the distillation theory of the Fenske-Underwood equation. The latter is obtained as a special case for ideal mixtures with $\gamma_{ji} = 1$ ($i = \overline{1,m}$, $j = \overline{1,p}$). Therefore, the Lagrange multipliers λ_j have the physical significance of the minimum number of theoretical contact stages necessary to separate the source mixture into products from j to p from the point of view of the equilibrium distillation theory.

Since the final calculated dependencies contain only the difference of phenomenological coefficients a_{ij}^0, their point of reference does not affect the structure of the final formulas, but leads only to a new reference system of Lagrange multipliers introduced for restrictions (7). This work provides the reference coefficients a_{ij}^0 with their values sampled at temperature and pressure of p flow. It is convenient to use such a reference system when the concentrations of target components in flows are set from 1 to p-1. If under the statement of the problem the component concentration in one of the intermediate product flows of the system is not fixed, then the point of reference of the coefficients a_{ij}^0 would be more convenient to transfer to the temperature and pressure of this flow [14].

ALGORITHM AND CALCULATION SAMPLE

The dependencies (13) are focused on the design version of the complex system calculation. Together with (6) they allow us to determine the conditional depth of system elements (sections of complex column) λ_j and distribution of components in product flows x_{ij} at known parameter values z_i, ε_j, α_{ij}, q_{ik} ($i,k = \overline{1,m}$, $j = \overline{1,p}$), as well as predetermined concentrations of target components x_{kl} in p-1 separation products. The coefficients of the component relative volatility at the beginning of the calculation are taken for the temperature of the output flowed at the approximate estimation. Having determined the composition of the output flows, these temperatures are elaborated and, if necessary, recalculated.

Since the entropic activity coefficients in expressions (13) depend on the product flow compositions, which are yet to be determined, the calculation algorithm becomes iterative:

1) originally, all activity coefficients are taken equal to one, i.e. the mixture is considered ideal;

2) parameter values are found λ_j as a result of solving the system of equations (6) and (13);

3) the composition of product flows is calculated according to the formulas (13);

4) the activity coefficient values are specified by formulas (2)–(4), using the compositions calculated in the previous step;

5) the calculation is repeated, starting from point 2, until there is a coincidence of the compositions obtained in two successive iterations with a preset accuracy.

Below you can find a comparison of the calculation results of the product flow composition of an ordinary gas fractioning unit (complex system) according to the offered model (6), (13) with the data of an industrial experiment. The installation consists of three distillation columns and divides the initial hydrocarbon mixture into four products: j = 1 – propane fraction (ε_1 = 0.279, T_1 = 325 K, P_1 = 1.67 MPa), 2 – isobutane fraction (ε_2 = 0.113, T_2 = 327 K, P_2 = 0.80 MPa), 3 – butane fraction (ε_3 = 0.225, T_3 = 344 K, P_3 = 8.3 MPa) and 4 – pentane fraction (ε_4 = 0.383, T_4 = 387 K, P_4 = 0.65 MPa). The source mixture composition, the experimental compositions of the separation products, as well as other primary source data are given in table. 1. The volumes of the component molecules needed to calculate the relative particle size δ_i are determined by the method of molecular models [20].

Table 1

Initial and experimental data

Таблица 1. **Исходные и экспериментальные данные**

i	Component	δ_i	α_{i1}	α_{i1}	α_{i1}	z_i	x_{i1}	x_{i2}	x_{i3}	x_{i4}
1	CH_4	0.201	288.4	280.9	227.3	0.0101	0.0362	-	-	-
2	C_2H_4	0.414	66.7	65.4	56.0	0.0094	0.0337	-	-	-
3	C_3H_6	0.560	21.1	20.8	18.6	0.2656	0.8710	0.1999	0.0000	0.0000
4	и-C_4H_{10}	0.770	9.2	9.1	8.3	0.1117	0.0409	0.7999	0.0327	0.0067
5	н-C_4H_{10}	0.707	7.0	7.0	6.4	0.2272	0.0180	0.0002	0.9313	0.0329
6	и-C_5H_{12}	0.853	3.2	3.2	3.0	0.0947	0.0002	0.0000	0.0325	0.2280
7	н-C_5H_{12}	0.853	2.6	2.6	2.5	0.1169	-	-	0.0034	0.3032
8	C_6H_{14}	1.000	1.0	1.0	1.0	0.1644	-	-	0.0001	0.4292

Table 2

The calculation results of a complex system

Таблица 2. **Результаты расчета сложной системы**

i	**Ideal mixture** λ_1 = 56.707; λ_2 = 51.185, λ_3 = 7.685				**Athermal mixture** λ_1 = 61.697; λ_2 = 54.764, λ_3 = 9.076			
	x_{i1}	x_{i2}	x_{i3}	x_{i4}	x_{i1}	x_{i2}	x_{i3}	x_{i4}
1	0.0362	0.0000	0.0000	0.0000	0.0362	0.0000	0.0000	0.0000
2	0.0337	0.0000	0.0000	0.0000	0.0337	0.0000	0.0000	0.0000
3	**0.8710**	0.1999	0.0000	0.0000	**0.8710**	0.1999	0.0000	0.0000
4	0.0397	**0.7999**	0.0420	0.0021	0.0418	**0.7999**	0.0403	0.0015
5	0.0193	0.0002	**0.9313**	0.0320	0.0172	0.0002	**0.9313**	0.0335
6	0.0001	0.0000	0.0203	0.2353	0.0000	0.0000	0.0225	0.2340
7	0.0000	0.0000	0.0064	0.3014	0.0000	0.0000	0.0059	0.3018
8	0.0000	0.0000	0.0000	0.4292	0.0000	0.0000	0.0000	0.4292

Table 2 shows the calculation results of this system including and excluding the accounting of separated mixture athermal properties. The effective coefficients of the component relative volatilities of the in both cases are assumed to be identical. The preset concentrations are specified in bold letters. The results analysis show that accounting of the mixture athermality leads, first of all, to increased values of the Lagrange multipliers. λ_j, characterizing duration of the process, and has no significant impact on the composition of the products. At the same time, the distributions calculated considering the athermal properties of the mixture and assuming that mixture is ideal are similar to the data of an industrial experiment.

CONCLUSION

The offered calculated composition of the athermal mixture separation products in complex distillation systems is quite similar to the thermodynamic method. The method is based on an extended version of the maximum entropy principle, with the introduction of complex experience information entropy as the likelihood criterion. The extended version allows to carry out the multicomponent distillation calculation of both ideal and non-ideal (athermal) mixtures on a uniform methodological basis.

ЛИТЕРАТУРА

1. **Jaynes E.T.** Probability theory: The logic of science. Cambridge: Cambridge University Press. 2003. 727 p.
2. **Латыпов А.Ф.** Принцип максимума энтропии для стационарного течения газа в канале. *ПМТФ*. 2011. Т. 52. № 3. С. 68–73.
3. **Фрадков А.Л., Шалымов Д.С.** Законы эволюции нестационарных процессов, подчиня-ющихся принципу максимума энтропии. *Труды СПИИРАН*. 2014. Вып. 3(34). С. 14–32. DOI: 10.15622/sp.34.2.
4. **Maron A.I.** Assessment of service quality for complex technical devices based on the Jaynes' information principle. Business Informatics. 2016. N 4 (38). P. 47–51. DOI: 10.17323/1998-0663.2016.4.47.51.
5. **Presse S., Ghosh K., Lee J., Dill K.A.** Principles of maximum entropy and maximum caliber in statistical physics. *Rev. Mod. Phys.* 2013. V. 85. N 3. P. 1115–1241. DOI: 10.1103/RevModPhys.85.1115.
6. **Drory A.** Failure and Uses of Jaynes' Principle of Transformation Groups. *Found. Phys.* 2015. V. 45. N 4. P. 439–460. DOI: 10.1007/s10701-015-9876-7.
7. **Favretti M.** Remarks on the Maximum Entropy Principle with Application to the Maximum Entropy Theory of Ecology. *Entropy*. 2018. V. 20. N 1. P. 11. DOI: 10.3390/e20010011.
8. **Banavar J.R., Maritan A., Volkov I.** Applications of the principle of maximum entropy: from physics to ecology. *J. Phys.: Cond. Mat.* 2010. V. 22. N 6. DOI: 10.1088/0953-8984/22/6/063101.
9. **Harte J., Zillio T., Conlinsk E., Smith A.B.** Maximum entropy and the state-variable approach to macroecology. *Ecology*. 2008. V. 89. N 10. P. 2700–2711. DOI: 10.1890/07-1369.1.
10. **Phillips S.J., Anderson R P., Schapire R.E.** Maximum entropy modeling of species geographic distributions. *Ecolog. Model.* 2006. V. 190. N 3–4. P. 231–259. DOI: 10.1016/j.ecolmodel.2005.03.026.
11. **Bowler M.G.** Species abundance distributions, statistical mechanics and the priors of MaxEnt. *Theor. Popul. Biol.* 2014. V. 92. P. 69–77. DOI: 10.1016/j.tpb.2013.12.002.
12. **Harte J., Newman A.** Maximum information entropy: A foundation for ecological theory. *Trends Ecol. Evol.* 2014. V. 29 (7). P. 384–389. DOI: 10.1016/j.tree.2014.04.009.
13. **Балунов А.И., Майков В.П.** Энтропия и информация в теории ректификации. *Изв. вузов. Химия и хим. технология*. 2003. Т. 46. Вып. 9. С. 54–67.
14. **Балунов А.И., Майков В.П.** Расчет составов продуктовых потоков сложных ректифи-кационных систем на основе принципа максимальной энтропии. *Изв. вузов. Химия и хим. технология*. 2013. Т. 56. Вып. 9. С. 96–102.
15. **Балунов А.И., Майков В.П.** Оптимальный отбор продуктов в процессе ректификации. Энтропийно-информационный анализ. *Изв. вузов. Химия и хим. технология.* 2013. Т. 56. Вып. 4. С. 97–106.
16. **Майков В.П., Балунов А.И.** Условная энтропия в описании свойств атермальности. *Изв. вузов. Химия и хим. технология.* 2004. Т. 47. Вып. 8. С. 76–81.
17. **Балунов А.И., Майков В.П.** Расширенный принцип максимальной энтропии для опи-сания процесса фазовых превращений в атермальной системе. *Изв. вузов. Химия и хим. технология.* 2014. Т. 57. Вып. 12. С. 93–99.
18. **Балунов А.И., Майков В.П.** Описание процесса многокомпонентной ректификации на основе расширенного принципа максимальной энтропии. *Изв. МГТУ «МАМИ»*. 2014. Т. 3. № 4 (22). С. 31–44.
19. **Волков Д.Н., Вилков Г.Г.** Энтропийное моделирование сложных ректификационных колонн. *НТВ Поволжья*. 2013. № 5. С. 134–139.
20. **Гордон А., Форд Р.** Спутник химика. М.: Мир. 1976. С. 127.

REFERENCES

1. **Jaynes E.T.** Probability theory: The logic of science. Cambridge: Cambridge University Press. 2003. 727 p.
2. **Latypov A.F.** Entropy maximum principle for a steady gas flow in a channel. *JAMTP*. 2011. V. 52. N 3. P. 385–389 (in Russian).
3. **Fradkov A.L., Shalymov D.S.** Evolution laws for non-stationary processes that follow the MaxEnt principle. *SPIIRAS Proceedings*. 2014. N 3(34). P. 14–32 (in Russian). DOI: 10.15622/sp.34.2.
4. **Maron A.I.** Assessment of service quality for complex technical devices based on the Jaynes' information principle. Business Informatics. 2016. N 4 (38). P. 47–51. DOI: 10.17323/1998-0663.2016.4.47.51.
5. **Presse S., Ghosh K., Lee J., Dill K.A.** Principles of maximum entropy and maximum caliber in statistical physics. *Rev. Mod. Phys.* 2013. V. 85. N 3. P. 1115–1241. DOI: 10.1103/RevModPhys.85.1115.
6. **Drory A.** Failure and Uses of Jaynes' Principle of Transformation Groups. *Found. Phys.* 2015. V. 45. N 4. P. 439–460. DOI: 10.1007/s10701-015-9876-7.
7. **Favretti M.** Remarks on the Maximum Entropy Principle with Application to the Maximum Entropy Theory of Ecology. *Entropy*. 2018. V. 20. N 1. P. 11. DOI: 10.3390/e20010011.
8. **Banavar J.R., Maritan A., Volkov I.** Applications of the principle of maximum entropy: from physics to ecology. *J. Phys.: Cond. Mat.* 2010. V. 22. N 6. DOI: 10.1088/0953-8984/22/6/063101.
9. **Harte J., Zillio T., Conlinsk E., Smith A.B.** Maximum entropy and the state-variable approach to macroecology. *Ecology*. 2008. V. 89. N 10. P. 2700–2711. DOI: 10.1890/07-1369.1.
10. **Phillips S.J., Anderson R P., Schapire R.E.** Maximum entropy modeling of species geographic distributions. *Ecolog. Model.* 2006. V. 190. N 3–4. P. 231–259. DOI: 10.1016/j.ecolmodel.2005.03.026.
11. **Bowler M.G.** Species abundance distributions, statistical mechanics and the priors of MaxEnt. *Theor. Popul. Biol.* 2014. V. 92. P. 69–77. DOI: 10.1016/j.tpb.2013.12.002.
12. **Harte J., Newman A.** Maximum information entropy: A foundation for ecological theory. *Trends Ecol. Evol.* 2014. V. 29 (7). P. 384–389. DOI: 10.1016/j.tree.2014.04.009.
13. **Balunov A.I., Maikov V.P.** Entropy and information in theory rectification. *Izv. Vyssh. Uchebn. Zaved. Khim. Khim. Tekhnol.* 2003. V. 46. N 9. P. 54–67 (in Russian).
14. **Balunov A.I., Maikov V.P.** Calculation of distillation products composition for complex rectification systems based of maximum entropy principle. *Izv. Vyssh. Uchebn. Zaved. Khim. Khim. Tekhnol.* 2013. V. 56. N 9. P. 96–102 (in Russian).
15. **Balunov A.I., Maikov V.P.** Optimal sampling of products during rectification. Entropic and information analysis. *Izv. Vyssh. Uchebn. Zaved. Khim. Khim. Tekhnol.* 2013. V. 56. N 4. P. 97–106 (in Russian).
16. **Maikov V.P., Balunov A.I.** Conditional entropy in description of atermal properties. *Izv. Vyssh. Uchebn. Zaved. Khim. Khim. Tekhnol.* 2004. V. 47. V 8. P. 76–81 (in Russian).
17. **Balunov A.I., Maikov V.P.** Extended principle of maximal entropy for description of process of phase transformations in atermal system. *Izv. Vyssh. Uchebn. Zaved. Khim. Khim. Tekhnol.* 2014. V. 57. N 12. P. 93–99 (in Russian).
18. **Balunov A.I., Maikov V.P.** Description of multicomponent rectification based on extended principle of maximum entropy. *Izv. MGTU «MAMI».* 2014. V. 3. N 4 (22). P. 31–44
19. **Volkov D.N., Vilkov G.G.** Entropic modeling of complex distillation columns. *NTV Povolzh'ya*. 2013. N 5. P. 134–139 (in Russian).
20. **Gordon A.J., Ford R.A.** The chemist's companion: a handbook of practical data, techniques, and references. 1972. New York: Wiley. 537 p.

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