Innovative: International Multi-disciplinary Journal of Applied Technology
(ISSN 2995-486X) VOLUME 03 ISSUE 3, 2025

MATHEMATICAL MODELS OF THE RECTIFICATION COLUMN PROCESS IN THE OIL PROCESSING INDUSTRY.

Yakubov M.S.[1], Uzakov B.M.[2]

[1] Doctor of technical sciences, prof. Tashkent university of information technologies named after Muhammad al-Khorazmi

[2] Doctoral student of the Tashkent University of Information Technologies named after Muhammad al-Khwarizmi

Abstract:

The article developed a mathematical model of a closed flow in a rotating pipe, which allows determining the distribution of axial and azimuthal velocities. Also, a mathematical model of the diffusion and rectification processes in the temperature field of the rectification column of a mini-oil refining unit has been developed, which allows determining the effective rectification regime. In addition, a model of diffusion and rectification processes, competing in oil separation, has been created, which allows predicting the volume shares of light fractions of petroleum products.

Keywords: diffusion and rectification process, azimuthal velocity, fraction of petroleum products, rectification columns, vapor-liquid flows, heat generator, centrifugal field, kinetic energies.

1. Introduction

Modeling and optimization of oil refining processes are the main tasks of the effective and successful development of the fuel and energy complex. Research shows that fundamental theoretical and experimental issues in this area are being successfully resolved. Their application in the development, design and creation of an industrial model of the device allows to increase the efficiency of the work being carried out today and the technical characteristics of the devices. Two fundamental approaches are distinguished in the construction of mathematical models of technological processes: Theoretical and Formal-static. The theoretical approach is based on the use of mathematical descriptions of the physical and chemical processes occurring in the modeled technological device. [1]

2. Materials and Methods

We analyzed the rotational motion of a mixture of oil and gas condensate and presented a mathematical modeling of a stable axisymmetric flow with twisting in a rotating pipe. A mathematical model of the process occurring in a nozzle rectification column was developed on the example of a mini-oil refinery. A necessary condition for the operation of a rotating pipe is the presence of a rotating flow in it. The rotation of the flow inside a smooth-walled pipe is ensured by introducing gas (liquid) through a nozzle located tangentially to its inner surface. At the exit from the nozzle, a flow is formed and enters the rotating pipe with a high velocity. Having bypassed the inner surface of the pipe, the flow acquires a rotational motion characterized by tangential velocity. The greatest tangential velocities occur in the nozzle section of the pipe (in the cross section of the pipe passing through the nozzle center). Tangential velocities vary along the pipe radius and decrease towards the center. The twisting of the flow in a circle forces part of the heat, which is part of the internal energy of the system, to be converted into kinetic energy of the forward motion along the axis of rotation of the flow. The resulting forward velocity vector is perpendicular to the instantaneous tangential velocity vector of the circular motion of the particles in the flow and does not change the magnitude of the flow. We have analyzed the conversion of the kinetic energy of rotation into thermal energy.

The mathematical modeling of a steady-state axisymmetric flow rotating in a vortex tube or in the inlet of a stub distillation column is studied [1,2]. The general vector equation for the motion of a fluid with velocity and turbulence is as follows:

$$\overline{u} \times \overline{\omega} - \frac{\partial \overline{u}}{\partial t} = \nabla \overline{B} \qquad (1)$$

Let us consider an axisymmetric flow in cylindrical coordinates with $(\omega_r, \omega_h, \omega_\varphi)$ the corresponding velocity (u, v, ω) components and given turbulence components :

$$(r,h,\varphi)\ \omega_r = \frac{1}{h}\frac{\partial (h\omega)}{\partial h}, \omega_h = -\frac{\partial \omega}{\partial r}, \omega = \frac{\partial v}{\partial r} - \frac{\partial u}{\partial h}. \qquad (2)$$

If the velocity u and v components $\psi(r,\varphi)$ are expressed by the stream function as follows, the mass conservation equation holds: $u = \frac{1}{h}\frac{\partial \psi}{\partial h}, v = -\frac{1}{h}\frac{\partial \psi}{\partial r}.$ (3)

From this, the azimuthal component of the rotation is equal to:

$$\omega_\varphi = -\frac{1}{h}\left(\frac{\partial^2 \psi}{\partial r^2} + \frac{\partial^2 \psi}{\partial h^2} - \frac{1}{h}\frac{\partial \psi}{\partial h}\right). \qquad (4)$$

Here we get three scalar equations.

$$u\omega_z - u\omega_\varphi - \frac{\partial v}{\partial t} = \frac{\partial B}{\partial h}; \qquad (5)$$

$$u\omega_h - u\omega_z - \frac{\partial \omega}{\partial t} = 0; \qquad (6)$$

$$u\omega_\varphi - \omega_h - \frac{\partial \omega}{\partial t} = \frac{\partial B}{\partial r}. \qquad (7)$$

Here the equation can be rewritten as follows:

$$\frac{d(h\omega)}{dt} = 0. \qquad (8)$$

In this form, (8) expresses the continuity of circulation along a circular fluid contour with its center on the axis of symmetry and a plane normal to it.[2] For a steady flow, each fluid particle moves along a streamline along the surface formed by the rotation of a curve lying in the plane of the axis of symmetry of the flow. Then, from (8) and Bernoulli's theorem, we have:

$$\frac{1}{2}(u^2 + v^2 + \omega^2) + \frac{P}{\rho} = B(\psi); \qquad (9)$$

$$h\omega = A(\psi).$$

Here we obtain the equation for the current function from (4):

$$\frac{\partial^2\psi}{\partial r^2} + \frac{\partial^2\psi}{\partial h^2} - \frac{1}{h}\frac{\partial\psi}{\partial h} = h^2\frac{dB}{d\psi} - A\frac{dA}{d\psi}. \qquad (10)$$

Equation (10), which is applied to the entire flow field, is reduced to the Bessel equation through uncomplicated substitutions in the cylindrical domain.

$$\frac{d^2\Phi}{dh^2} + \frac{1}{h}\frac{d\Phi}{dh} + (K^2 - \frac{1}{h^2})\Phi = 0, \qquad (11)$$

having a general solution

$$\Phi = cJ_1(kh) + \text{Д}Y_1(kh), \qquad (12)$$

Here J_1 and Y_1 are Bessel functions of the 1st and 2nd kind; Φ is defined from the expression $\psi(z,h) = \frac{1}{2}uh^2 + h\Phi(r,h), k = 2\frac{\omega_1}{u_1}$

Finally, for the bullet velocity in a cylindrical sphere, we have:

$$\bar{u} = u_1 + \frac{1}{h}\frac{d}{dh}[chJ_1(kh) + \text{Д}hY_1(kh)]; \qquad (13)$$

for azimuthal velocity

$$\bar{\omega} = \omega_1 h + kcJ_1(kh) + kBY_1(kh), \qquad (14)$$

Here u_1 and ω_1 is the constant axial velocity of the fluid and the angular velocity of rotation as a whole.[3] Thus, as a result of the conducted studies, we obtain an expression for the distribution of axial and azimuthal velocities, thereby opening up the possibility of technological control of the process by converting part of the kinetic energy of the rotational motion into thermal energy.

In the modern petrochemical industry, the processes of separating mixtures and obtaining individual substances of varying purity occupy a leading place. At the same time, the tendency to obtain increasingly pure substances is clearly manifested. Among the separation processes, rectification occupies a leading place, and its quantitative share is about 90%. [1,2]. Rectification is based on the possibility of separating substances by converting them from liquid to vapor (evaporation) and vice versa (condensation).[4] Figure 1 shows the original scheme of a mini-oil refinery with a nozzle rectification column.

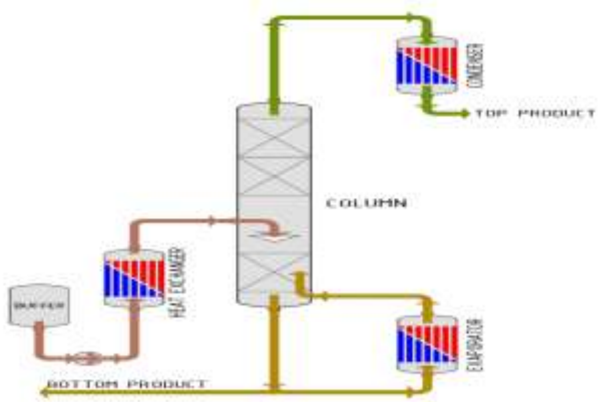

Figure 1. Schematic diagram of the main rectification column.

This type of mass transfer technique allows to realize the hydrodynamic principle of gas-liquid interaction in inclined grids and to increase the time of passage of the vapor-liquid flow through the stable temperature zone. The rapid development of numerical methods and their application in various fields of science has led to mathematical modeling and computational experiments on modern computer systems. Since the oil in the rectification column is separated into components along the height of the column (i.e., only vertically), this problem can be considered one-dimensional (Fig. 1). In this case, the diffusion process can be described by t a function $u(x,t),$ representing the combination at a time instant x. According to the Nernst law, $(t,t+\Delta t),$ the mass of gas flowing through the cross section during a time interval is equal to x

$$dQ = -Д\frac{\partial u}{\partial x}(x,t)Sdt = WSdt, \qquad (15)$$

$$W = -Д\frac{\partial u}{\partial x}$$

Here $Д$ is the diffusion coefficient, S is the cross-sectional area of the tube, $W(x,t)$ is the diffusion flux density, which is equal to the mass of gas flowing through a unit area per unit time. According to the definition of concentration, the amount of gas in a volume V is equal to .[5] From this, we obtain that the change in the mass of gas in the tube section when $Q = u\cdot V;$ the concentration Δu changes (x_1, x_2) is equal to . $\Delta Q = \int_{x_1}^{x_2} C(x)\Delta u\cdot Sdx,$ Here $C(x)$ is the porosity coefficient.[6,7] We formulate the $(t_1,t_2):$ equilibrium equation for the gas mass in the area over time (x_1,x_2).

$$S\int_{t_1}^{t_2}[D(x_2)\frac{\partial u}{\partial x}(x_2,\tau) - D(x_1)\frac{\partial u}{\partial x}(x_1,\tau)]d\tau = S\int_{x_1}^{x_2} C(\xi)[u(\xi,t_2) - u(\xi,t_1)]d\xi.$$

From this we form an equation.

$$\frac{\partial}{\partial x}(D\frac{\partial u}{\partial x}) = C\frac{\partial u}{\partial t} \qquad (16)$$

Diffusion equation. If the diffusion coefficient is constant, the diffusion equation takes the following form. $u_t = a^2 u_{xx},$ Here $a^2 = \frac{D}{C}.$ If the porosity coefficient and $C = 1,$ diffusion coefficient are constant, the diffusion equation takes the following form: $u_t = Du_{xx}.$ We find the solution of equation (16) the domain $t > 0$ with T initial condition $u(x,y,z,o) = \varphi(x,y,z)$ and boundary condition $u_t = a^2\Delta u$ where $u\big|_{\Sigma}$, Σ is the boundary of the domain. Let us consider an auxiliary problem: find a nontrivial solution of the equation T. $u_t = a^2\Delta u = 0$ Next to T $t > 0$

(17)

By separating the variables in the usual way, $v(M)$ satisfying the homogeneous boundary condition $u\big|\sum = 0$ and presented in the form of a product , we arrive at the following conditions that define the functions $u(M,t) = v(M)T(t) \neq 0.$ and $T(t)$.

$$\left.\begin{array}{l}\Delta v+\lambda v=0T, v(M)\neq 0\\ v=0 на \sum\end{array}\right\} \quad (18)$$

$$T'+a^2\lambda T=0 \quad (19)$$

We take the problem of determining the eigenvalues for the function V. Let $\lambda_1,\lambda_2,......,\lambda_n,...$ the eigenvalues of problem (18) $v_1,v_2,......,v_n,...$ be its eigenfunctions. The functions $\{v_n\}$ form an orthogonal system.[8,9] The corresponding functions $T_n(t)$ have the form $T_n(t)=C_n e^{-a2\lambda_n t}$, and the auxiliary problem has a non-trivial solution.

$$u_n(M,t)=C_n v_n(M)e^{-a2\lambda_n t}, \quad (20)$$

The general solution to the initial problem can be expressed as follows:

$$u_n(M,t)=\sum_{n=1}^{\infty}C_n e^{-a2\lambda_n t}v_n(M), \quad (21)$$

Satisfying the initial condition

$$u_n(M,O)=\varphi(M)=\sum_{n=1}^{\infty}C_n v_n(M), \quad (22)$$

we find the coefficients

$C_n=\frac{\int_T \varphi(M)v_n(M)d\tau_M}{\|v_n\|^2}$ Here $\|v_n\|=[\int_T v_n^2(M)d\tau_M]^{\frac{1}{2}}$ is the norm of the function Vп . Thus, expression (21) represents the solution to the problem.[10, 11] The rectification process is based on the separation of substances by converting them from liquid to vapor (evaporation) and vice versa (condensation). This occurs because each substance has its own saturated vapor pressure.[12] According to the model considered above, the mass of gas flowing through the cross section $(t,t+\Delta t)$, X during a time interval is equal to:

$$dQ=R\frac{\partial u}{\partial x}(x,t)Std=PStd; \quad (23)$$

$$M=R\frac{\partial u}{\partial x},$$

Here R is the rectification coefficient , S is the cross-sectional area of the tube, P(x, t) is the rectification flux density, which is equal to the mass of gas passing through a unit area per unit time.[13] According to the definition of concentration, the amount of gas in a volume V is equal to:

$$Q=u\cdot V.$$

It follows that when the concentration Δu changes , (x_1,x_2) the change in the mass of the gas in the pipe section is equal to: $\Delta Q = \int_{x_1}^{x_2} C(x)\Delta u \cdot Sdx,$, Here $C(x)$ - porosity coefficient. for the gas mass in the area (x_1, x_2) over time (t_1, t_2) is as follows.[14]

$$S\int_{t_1}^{t_2}[R(x_2)\frac{\partial u}{\partial x}(x_2,\tau) - R(x_1)\frac{\partial u}{\partial x}(x_1,\tau)]d\tau =$$

$$= S\int_{\tau}^{x_2} C(\psi)[u(\psi,t_2) - u(\psi,t_1)]d\psi,$$

From this we obtain the equation

$$-\frac{\partial}{\partial x}(R\frac{\partial u}{\partial x}) = C\frac{\partial u}{\partial t}, \qquad (24)$$

it describes the rectification process. The solution to equation (24) is similar to the solution to equation (16):

$$u(M,t) = -\sum_{n=1}^{\infty} C_n e^{-a2\lambda_n t} v_n(M), \qquad (25)$$

As a result of the developed program and its numerical implementation using the "MathCAD" program, we obtain graphs of two diffusion and rectification processes in oil cracking. [15]

3. Results

A mathematical model of the flow of a mixture of oil and gas condensate twisted in a rotating pipe was developed, which made it possible to determine the distribution of axial and azimuthal velocities of the flow in a rotary rectification column. On its basis, control parameters were determined that characterize the energy efficiency of the rectification column in automatic mode. A mathematical model of the diffusion and rectification processes in the temperature field of the rectification column of a mini-oil refinery was developed. Based on this model, an effective rectification mode was determined. Mathematical modeling of the process in the rectification column of a mini-oil refinery allows for effective control of the process of separating oil into specific fractions in the temperature field.

4. Discussion

The study presents a comprehensive mathematical approach to modeling the rectification (distillation) column process, which is crucial in the separation of binary mixtures, such as ethanol and water. The use of both differential and algebraic equations to represent mass and energy balances across the stages of the column provides a solid foundation for simulation and optimization. Notably, the incorporation of the Antoine equation and Raoult's Law enables a more accurate representation of vapor-liquid equilibrium, which is central to the rectification process.

An important aspect of the model lies in its flexibility to simulate both equilibrium and non-equilibrium stages, offering insight into the practical design and control of industrial distillation columns. The paper's use of numerical methods, particularly for solving ordinary differential equations and implementing finite-difference schemes, highlights how computational tools are vital in predicting system behavior where analytical solutions may not be feasible.

Furthermore, the paper demonstrates the significance of model validation through experimental data comparison. Although the results show good alignment between simulated and empirical values, it is important to recognize the sensitivity of the model to various assumptions, such as ideal mixing and constant molar overflow. Deviations from these assumptions in real-world settings could potentially lead to inaccuracies, emphasizing the need for model adjustments or hybrid approaches combining empirical and theoretical models.

The results also open avenues for further research, especially in enhancing the model to handle multi-component mixtures, incorporating dynamic changes in operation (such as feed composition variation), and implementing control strategies based on real-time optimization. As environmental and energy-efficiency concerns become increasingly relevant, optimizing the rectification process using such mathematical models is not only beneficial for productivity but also for sustainable chemical processing.

5. Conclusion.

In conclusion, the mathematical modeling of rectification columns presented in this study provides a foundational framework for understanding and optimizing separation processes in chemical engineering. By utilizing systems of ordinary and partial differential equations, along with algebraic relationships, the models effectively describe both the steady-state and dynamic behaviors of the column. These models not only enhance our theoretical understanding but also facilitate practical improvements in design and operation through simulation and control. Ultimately, such mathematical representations serve as essential tools for improving process efficiency and product quality in industrial rectification applications.

References

[1]. Redkozubov S.A. Vartanov K.S. Mathematical modeling of the process in the rectification column //Estestvennye i teknicheskie nauki. -2007. - #5. - S. 242-247.

[2]. Oil and gas enterprises innovative development " foreign countries experience Lecture thesis // " Enterprises strategic planning and development " Sixth All-Russia Symposium , April 12-13 , 2005. Section 3 " Russia and foreign in enterprises strategic planning experience " M:01. 05 .

[3]. Vu Trieu Minh, Ahmad-Majdi Abdul-Rani. Modeling and Control of Distillation Column in a Petroleum Process // Mathematical Problems in Engineering, 2009(5). DOI:10.1155/2009/404702.

[4]. Sheikus, A. Distillation process optimization using continuous mobile control actions by redistributing the feed flow // Advanced Information Systems, (2019). 3(3). –PP.30–36. https://doi.org/10.20998/2522-9052.2019.3.04.

[5]. Ramezani Mohammad Hossein, Sadati Nasser. Hierarchical optimal control of a binary distillation column // Optimal Control Applications and Methods, 2019. 40(1) –PP.172-185. https://doi.org/10.1002/oca.2473.

[6]. Krämer Korbinian. Optimization-based Synthesis of Hybrid Separation Processes Fortschr. Dissertation. -Ber. VDI Reihe 3 Nr. 934. Düsseldorf: VDI Verlag, 2012. -245p.

[7]. Jiang Zheyu. Multicomponent Distillation - Mathematical Modeling, Global Optimization, and Process Intensification. - Purdue University Graduate School, 2019. Thesis (Dissertation Doctor of Philosophy). https://doi.org/10.25394/PGS.7543439.v1 .

[8]. Uzakov B.M, Xoshimov B.M, O‘zbekiston neft-gaz tomonidan ishlab chiqarishni moliyalashtirish boy‘icha xorijni o‘rganish. //Muhammad al-Xorazmiy nomidagi TATU Farg’ona filiali “Al-Farg‘oniy avlodlari” elektron ilmiy jurnali ISSN 2181-4252 Tom: 1 | O’g’il: 1 |10-19 betlar| 2024 yil.

[9]. Uzokov B.M. Adaptation of operational management models of technological processes based on technical and economic indicators.// Electronic scientific journal "Descendants of Al-Fargani" of the Fergana branch of TATU named after Muhammad al-Khwarizmi ISSN 2181 - 4252 Volume: 1 | Issue: 2 | 2023.

[10]. Yakubov M.S, Uzakov B.M., Modeling of processes of oil refining under operational

management on indicators of quality of products. // "Descendants of Al-Farghani" electronic scientific journal of Fergana branch of TATU named after Muhammad al-Khorazmi. ISSN 2181 -4252 Vol: 1 |Iss: 1 | 2023 year.

[11]. M.S. Yakubov, B.M. Uzokov Modeling of oil refining processes under operational management based on product quality indicators. // Scientific-technical journal (STJ FerPI, FarPI ITZh, NTZh FerPI, 2023, Vol.27, special issue No.2).

[12]. Uzakov B.M. Activity of oil refining enterprises improvement of management system // European Journal of Economics, Finance and Business Development ISSN (E): 2938-3633 Volume 2, Issue 5, May - 2024

[13]. M.S. Yakubov, B.M. Uzokov Modeling of oil refining processes under operational management based on product quality indicators // Scientific-technical journal (STJ FerPI, FarPI ITZh, NTZh FerPI, 2023, Vol.27.special issue No.2) (40-46 betlar)

[14]. Uzakov B.M. Neft maxsulotlarini ekstraksiyalash jarayonini modellashtirish va boshqarish usullarini tahlili.// “Texnika va raqamli texnologiyalarni amaliyotda qo‘llanilishi va ularning innovatsion yechimlari” xalqaro ilmiy-texnik konferensiya materiallari. Farg‘ona 4-5- may 2023 yil. (459-462 betlar)

[15]. Yakubov M.S, Uzakov B.M., Xoshimov B.M, Farg‘ona neftni qayta ishlash zavodi uchun avtomatlashtirilgan tizimini matematik modeli va algoritmlash jadvalini rejalashtirish vazifalari// Muhammad al-Xorazmiy nomidagi TATU Farg‘ona filiali “Al-Farg‘oniy avlodlari” elektron ilmiy jurnali ISSN 2181-4252 Tom: 1 | Son: 2 | 2024-yil