Technical Physics, 2026, Vol. 71, No. 1

03

Computer simulation of hydrocarbon liquid flow for the synthesis of petrochemical products

© S.V. Polyakov, T.A. Kudryashova, N.I. Tarasov

Keldysh Institute of Applied Mathematics, Russian Academy of Sciences,
125047 Moscow, Russia
e-mail: kudryashova@imamod.ru

Received April 29, 2025
Revised June 26, 2025
Accepted June 26, 2025

An important problem of oil refining related to the production of diesel fuels with specified properties is considered. The technology of production of hexadecane isomer in a laboratory setup is chosen as an example. A material based on aluminophosphate is used as a catalyst. An original complex three-dimensional mathematical model is proposed for this physico-chemical problem. The model includes a quasi-hydrodynamic system of equations for calculating the flow of a multicomponent two-phase medium and convection-diffusion-reaction equations for calculating the dynamics of concentrations of the feedstock and reaction products. The numerical implementation of the model uses methods of splitting into physical processes and finite volumes. To speed up the calculations, a parallelization procedure based on the domain decomposition technique is applied. Numerical experiments demonstrate the efficiency of the developed computing technology.

Keywords: oil refining, catalytic isomerization reactions, quasi-hydrodynamics, convection–diffusion, three-dimensional computer modeling.

DOI: 10.61011/TP.2026.01.62839.92-25

Introduction

Theoretical study of characteristics of liquid and gas streams in oil production systems started in the 1950s with a focus on applications to processes in vertical wells. At that time, data were mainly based on operating readings obtained in field conditions. They included such parameters as a volume flowrate, thermophysical properties of each phase, pressure inside a pipeline, an internal diameter and an inclination angle. Based on this humble set of information, the first scientific studies appeared [1,2]. Further studies also infiltrated a field of refining of crude oil and natural gas [3,4] and were accompanied by developing a large class of mathematical methods [5–10]. Up to now, the petrochemical industry uses advanced technologies of computer simulation, which are realized in such well-known software packages as HYSIM, HYSYS, Pro II, ProVision, Pipeface, Protiss, Aspen Plus, Speed UP, Dyna Plus, CHEMCAD, PROSIM, etc. In a modern situation, many of them are unavailable for use in the domestic petrochemical industry, which requires their import substitution. However, a more important aspect is to develop new simulation technologies and to create digital platforms for the oil and gas industry.

The present study deals with one of specific tasks of oil refining, which is related to production of freeze-thaw-resistant diesel fuels. An object of research was a technology of hexadecane isomer production in a laboratory setup, which is based on thermal stimulation of a catalytic reaction in presence of hydrogen. A catalyst material was porous aluminium phosphate.

Unlike a purely thermal method of refining, in which feedstock is cleaved by thermal energy only, a basis of the considered production process is a multi-stage catalyst-stimulated diagram of chemical transformations. The final production cycle is more cost-effective, since a product with required properties is generated at lower temperatures and with a higher rate. The obtained product contains much less unsaturated hydrocarbons and does not require addition of antioxidizers.

Selecting the above-said field of research is related to the following. Liquid hydrocarbons are main components of a modern energy infrastructure. Synthetic gasoline and diesel fuel contain a much higher density of energy than initial natural components: methanol, ethanol, methane and hydrogen. This makes it possible to develop and use transport systems based on producing power from hydrocarbons for a long time yet.

Hydrocarbon streams are theoretically and numerically analyzed so as to provide engineers and technologists with an effective tool of optimizing production processes. In the modern situation, when computers and software simulation means are so commonly used, it is important to develop so-called multiphysical models and high-accuracy numerical algorithms of their implementation. Relevant tasks in the field considered by us include complex models that reflect all stages of a feedstock refining process and take into account heat- and mass-transfer processes and chemical transformations at the same time. It is also important that they should take into account a structure of a catalyst medium, a composition of a hydrocarbon fluid and geometry of the laboratory or production setup. It is still relevant to implement these models both numerically and for computers

The present study is aimed at developing a numerical procedure of computer analysis of processes of hydroisomerization in presence of an aluminium-phosphate-based catalysts. Practically, this analysis is aimed at efficiency of application of a catalyst and monitoring of its state when the setup is operated, which makes it possible to go over to a cycle of catalyst regeneration or its complete replacement in due time.

The present study considers a problem of transmission of a hydrocarbon liquid containing hexadecane and hydrogen through a porous medium that includes glass and catalyst granules. In a catalyst layer, we consider a mechanism of hydro-isomerization, which is described by chemical transformations of feedstock into the product with formation of a side fraction as methane. In case of three-dimensional geometry, for the selected problem formulation we have proposed a complex mathematical model, constructed a mesh option of its discretization based on a finite volume method and developed the algorithm and program for computational experiments. The software program was used to perform a series of numerical calculations.

1. Problem formulation and the mathematical model

Let us consider an active zone of a laboratory chemical reactor of a cylindrical axisymmetric form, which is shown in Fig. 1. It has input and output holes arranged on the left and on the right, respectively. A central region includes the catalyst layer fixed on the left and on the right by glass crumbs. The reactor axis has a cylindrical copper heater arranged, which induces chemical reactions in the catalyst layer. The catalyst material is aluminium phosphate.

A hydrocarbon mixture is supplied into a reactor volume, whose main component is hexadecane $n\mathrm{C}_{16}$ ($\mathrm{C}_{16}\mathrm{H}_{34}$), and in which a hexadecane isomer $i\mathrm{C}_{16}$ ($\mathrm{C}_{16}\mathrm{H}_{34}$), molecular hydrogen ($\mathrm{H}_2$) and methane ($\mathrm{CH}_4$) are dissolved in small concentrations. This mixture hits the catalyst layer, in which the following chemical reactions proceed: 1) $n\mathrm{C}_{16}i\mathrm{C}_{16} \leftrightarrows i\mathrm{C}_{16}$, 2) $n\mathrm{C}_{16} \xrightarrow{H_2} \mathrm{CH}_4$, 3) $i\mathrm{C}_{16} \xrightarrow{H_2} \mathrm{CH}_4$.

The reactions are stimulated both by presence of the catalyst as well as heating the catalyst layer by means of the heater. The catalyst medium with sealant layers is considered by us as a porous medium with a fixed frame. The liquid going into it is considered to be a single-phase, hardly-compressible and multi-component one. Under these assumptions, in the conditions of the constant fluid temperature it is possible to use the following complex model of the isomerization process.

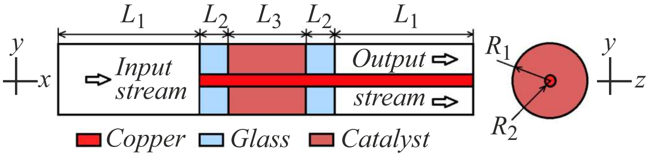

Figure 1. Diagram of the chemical reactor in a longitudinal (on the left) and a transverse (on the right) section.

The first part of the model is based on a VANS approximation for the porous layer [5–10] and a quasi-hydrodynamic approach (QHD) [11,12]. It uniformly describes the flow of the multi-component medium with a total density ρ and a rate $\mathbf{u}$ in free space and in the porous body as (1), (2):

$$\nabla(\mathbf{n} - \mathbf{w}) = 0, \tag{1}$$

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla\Big(\frac{1}{\varepsilon}\rho(\mathbf{u} - \mathbf{w}) \otimes \mathbf{u}\Big) = - \varepsilon\nabla p + \nabla(\mathbf{\Pi}_{NS} + \mathbf{\Pi}_{QHD}) - G\mathbf{u}, \tag{2}$$

Here ∇ and $\otimes$ is a nabla operator and an external product of vectors in the coordinates x, y, z, t is time, $\varepsilon = \varepsilon(x, y, z) = V_l/V$ is porosity, V_L is a volume of the liquid phase, V is a total volume of the medium, $\mathbf{u}$ and $\mathbf{w}$ is a filtration rate vector and a QHD correction for it written as (3):

$$\mathbf{w} = \frac{\tau}{\rho}\Big[\Big(\frac{1}{\varepsilon}\rho\mathbf{u}, \nabla\Big)\mathbf{u} + \varepsilon\nabla p + G\mathbf{u}\Big], \tag{3}$$

τ — a parameter of regularization of the QHD approach (under the low stream rates it is selected for reasons of providing stability of the numerical algorithm, it is assumed to be $\tau \sim \frac{1}{\mathrm{Re}}$), p is pressure, $\mathbf{\Pi}_{NS}$ and $\mathbf{\Pi}_{QHD}$ is a Navier-Stokes tensor and the QHD correction for it, which is determined by expressions (4), (5):

$$\mathbf{\Pi}_{NS} = \{\Pi^{NS}_{\alpha\beta}\},$$

$$\Pi^{NS}_{\alpha\beta} = \mu\Big(\frac{\partial u_\beta}{\partial\alpha} + \frac{\partial u_\alpha}{\partial\beta}\Big) - \delta_{\alpha\beta}\frac{2}{3}\mu\mathrm{div}\mathbf{u}, \ \ \alpha, \beta = x, y, z, \tag{4}$$

$$\mathbf{\Pi}_{QHD} = \frac{1}{\varepsilon}\rho\mathbf{u} \otimes \mathbf{w}. \tag{5}$$

μ — dynamic viscosity, $\delta_{\alpha\beta}$ is a Kronecker symbol, $G = \varepsilon\mu K^{-1} + \rho F(\varepsilon)K^{-1/2}|\mathbf{u}|$ is a momentum drain coefficient related to motion of the liquid through the porous medium, K is permeability of the porous medium, $F(\varepsilon)$ is an empirical Forchheimer coefficient [13], $\mathrm{Re} = \frac{u_0 D_0 \rho}{\mu}$ is a Reynolds number, u_0 is a typical flow rate, D_0 a hydrodynamic diameter of an area under research.

The second part of the model describes chemical reactions in the catalyst layer and processes of convection-diffusion of mixture components (6):

$$\frac{\partial(\varepsilon C_k)}{\partial t} = \nabla[\varepsilon D_k \nabla C_k] - \nabla(\mathbf{u}C_k), \ \ k = 1, 2, 3, 4. \tag{6}$$

Here C_k are concentrations of the mixture components, the index $k = 1, 2, 3, 4$ subsequently numbers hexadecane, isohexadecane, hydrogen and methane.

Transformations of the mixture components were calculated using reaction equations as part of a method of splitting by physical processes. Based on concentration fields obtained by means of the equations (6), they are locally recalculated in the catalyst region. In this case, the catalysis process is described by means of the following system of equations (7):

$$\begin{gathered}\frac{\partial C_1}{\partial t}=-w_1-w_2,\ \ \frac{\partial C_2}{\partial t}=w_1-w_3,\\ \frac{\partial C_3}{\partial t}=-w_2-w_3,\ \ \frac{\partial C_4}{\partial t}=2w_2+2w_3,\\ w_1=k_1C_1-k_2C_2,\ \ w_2=k_3C_1C_3,\ \ w_3=k_4C_2C_3,\end{gathered}\tag{7}$$

where $k=1,2,3,4$ are empirically-obtained reaction coefficients. The system (7) reflects the following properties of the reaction in question. Hydrogen is not generated during catalysis. Methane is formed from initial impurity hydrogen, hexadecane and isohexadecane. Besides, when summing the equations of the system (7), one can see that there are not additions sources and, consequently, fulfilment of the mass conservation law during the chemical transformations, i.e.

$$\frac{\partial C_1}{\partial t}+\frac{\partial C_2}{\partial t}+\frac{\partial C_3}{\partial t}+\frac{\partial C_4}{\partial t}=0.$$

The equations (1)–(6) are dedimensionalized and supplemented with necessary boundary and initial conditions [14]. The equation for determining a pressure field is obtained by substituting (3) into (1) and written as (8):

$$\nabla(\varepsilon\nabla p)=\nabla\left[\frac{\rho}{\varepsilon}\,\mathbf{u}-\left(\frac{1}{\varepsilon}\rho\mathbf{u},\nabla\right)\mathbf{u}-G\mathbf{u}\right].\tag{8}$$

The boundary conditions depend on a boundary type of the area under research. For an inlet, we use a steady Poiseuille flow and a known distribution of the concentrations

$$\mathbf{u}=\left\{1-\frac{y^2-z^2}{R_1},0,0\right\},\ \ \frac{\partial p}{\partial n}=\frac{2}{\mathrm{Re}R_1^2},$$

$$C_1=\mathrm{const},\ \ C_2=\mathrm{const},\ \ C_3=\mathrm{const},\ \ C_4=\mathrm{const}.$$

On the wall, we pre-define adhesion conditions and a zero stream for the concentrations:

$$\mathbf{u}=\mathbf{0},\ \ \frac{\partial p}{\partial n}=0,$$

$$\frac{\partial C_1}{\partial n}=\frac{\partial C_2}{\partial n}=\frac{\partial C_3}{\partial n}=\frac{\partial C_4}{\partial n}=0.$$

At an outlet, we pre-define free-output conditions:

$$\frac{\partial \mathbf{u}}{\partial n}=0,\ \ p=0,$$

$$\frac{\partial C_1}{\partial n}=\frac{\partial C_2}{\partial n}=\frac{\partial C_3}{\partial n}=\frac{\partial C_4}{\partial n}=0.$$

A numerical diagram of discretization of the equations (2), (6), (8) on a hexahedral grid was constructed by means of the finite volume method [15]. Cells of a calculation mesh were used as a finite volume when calculating the pressure. Components of the rate vector and the concentrations were calculated by node finite volumes. Derivatives with respect to time are discretized based on an explicit scheme.

A general algorithm consists of integrating the equations (2) and (6) by time at each step. At the same time, within a time step a difference analogue of the equation (8) is solved by an iteration method of conjugate gradients with a diagonal preconditioner. Since the equations (2), (8) are independent on the concentrations of the mixture components, the genera algorithm is divided into two stages. The first stage includes a quasi-steady-state fluid flow through the reactor. At the second stage, the equations (6) are integrated. When the equations (6) are integrated, the concentrations locally in nodes of the catalyst region are recalculated at each time step according to the equations of the chemical reactions (7).

For the computational algorithm, we have developed parallel software implementation in the language C++ using libraries Eigen, OpenMPI, GMSH and VTK. The calculations were performed in a hybrid supercomputer K60 installed in a Supercomputer Collective Use Center of KIAM RAS.

2. Numerical simulation results

The object of research was a fragment of the laboratory chemical reactor for catalytic reforming [16]. Parameters of the subsequent calculations were selected taking into account experimental data of the study [17]. The calculations were performed in a three-dimensional region (Fig. 2, *1*) on a non-structured tetrahedron mesh (Fig. 2, *2*). According to the designations in Fig. 1 the geometry parameters have the following values: $L_1=3$, $L_2=0.5$, $L_3=2$ and were normalized to a radius of the inlet of the setup $R_0=10^{-2}$ m. The calculation mesh was constructed using the GMSH software complex and contained 1 940 377 volume elements, 368 446 dots. With the parallel calculations, the mesh is divided into 28 subregions (Fig. 2, 3).

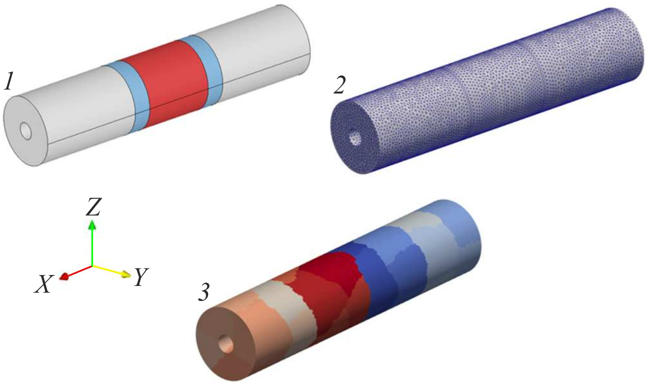

Figure 2. Geometry of a computational region (*1*), a tetrahedron mesh (*2*), division of the mesh into parallel count domains (*3*).

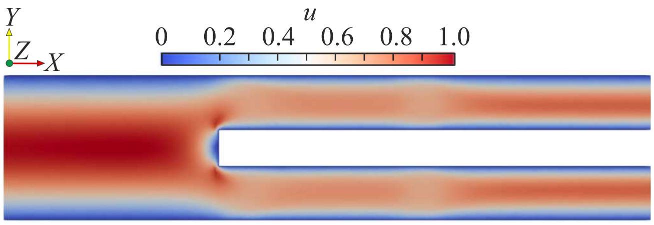

Figure 3. Distribution of the rate modulus in a central part of the calculation region (XY). Normalization of the rate $u_0 = 0.043$ m/s.

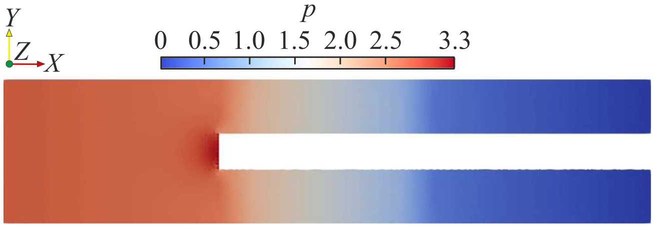

Figure 4. Distribution of overpressure in a central part of the calculation region (XY). Normalization of pressure $p_0 = 1.4237$ Pa.

The flow was calculated for the following parameters of a moving medium: $\rho_0 = 770\,\mathrm{kg/m^3}$, $\mu_0 = 3.3 \cdot 10^{-3}$ Pa·s, $u_0 = 0.043$ m/s. The presented parameters correspond to the main mixture components — hexadecane and isohexadecane. These values correspond to the Reynolds number $\mathrm{Re} = 100$. The parameters of the porous regions have the same values: $\mathrm{Da}_g = 0.1$, $\mathrm{Da}_c = 0.2$, $\varepsilon_g = 0.28$, $\varepsilon_c = 0.6$, here g is glass crumbs, c is a catalyst. It was calculated up to the value $t_{\max} = 10$ with a time step $\tau_t = 2.4 \cdot 10^{-4}$ and a regularization parameter $\tau = 5 \cdot 10^{-3}$. The parameter of time normalization was $t_0 = 0.233$ s. The calculation is performed from a state of the resting medium with boundary conditions: at the inlet — the Poiseuille flow, at the walls — adhesion conditions, at the outlet — the free-output conditions. Steady-state distributions of the main flow parameters — the rate and overpressure — are shown in Fig. 3, 4.

The presented computational algorithm for flow calculation and its software implementation for the two-dimensional formulations were compared with the Ansys Fluent software complex in the study [14]. The results obtained herein make it possible to conclude that the three-dimensional implementation is correct. A free region of the inlet has a parabolic profile of the rate and a linear pressure drop formed. Then, according to geometric 92specific features of the calculation region, the Poiseuille profile is restructured. At the same time, according to the Bernoulli law, deceleration of an oncoming stream near a butt-end of the copper heater results in an increase of pressure. Besides, a difference of porosities and permeabilities of the glass crumbs and the catalyst is adequately reflected. We note that the flowrate of the liquid medium at the inlet and the outlet of the setup is the same. It makes it possible to conclude on correctness and approximation of the flow model.

The obtained rate fields were used for subsequently calculating evolution of the concentrations of the mixture components. The following parameters of the model were pre-defined in the calculation: $D_1 = 0.01$, $D_2 = 0.01$, $D_3 = 0.1$, $D_4 = 0.08$. Reaction coefficients: $k_1 = 1.0$, $k_2 = 0.1$, $k_3 = 0.05$ and $k_4 = 0.05$. These values are obtained when averaging tabular temperature data from the range 300 °C–360 °C. The following values of the concentrations of the mixture components were pre-defined as initial conditions within the entire region and at the setup inlet: $C_1 = 0.948$, $C_2 = 0.001$, $C_3 = 0.05$, $C_4 = 0.001$. The calculations were performed up to the value $t_{\max} = 12.7$, when a steady-state mode of isohexadecane catalysis was set. The distributions of the concentrations, which are obtained at this moment of time, are shown in Fig. 5. They show that in the steady-state mode the catalyst region has a distribution of sources and reaction products formed, which corresponds to theoretical estimates as well as experimental data about product output from the study [17] (Table 1, the Pt/SAPO-11 catalyst).

Further development of the proposed mathematical model will be related to more exact determination of diffusion constants and reaction constants based on experimental data

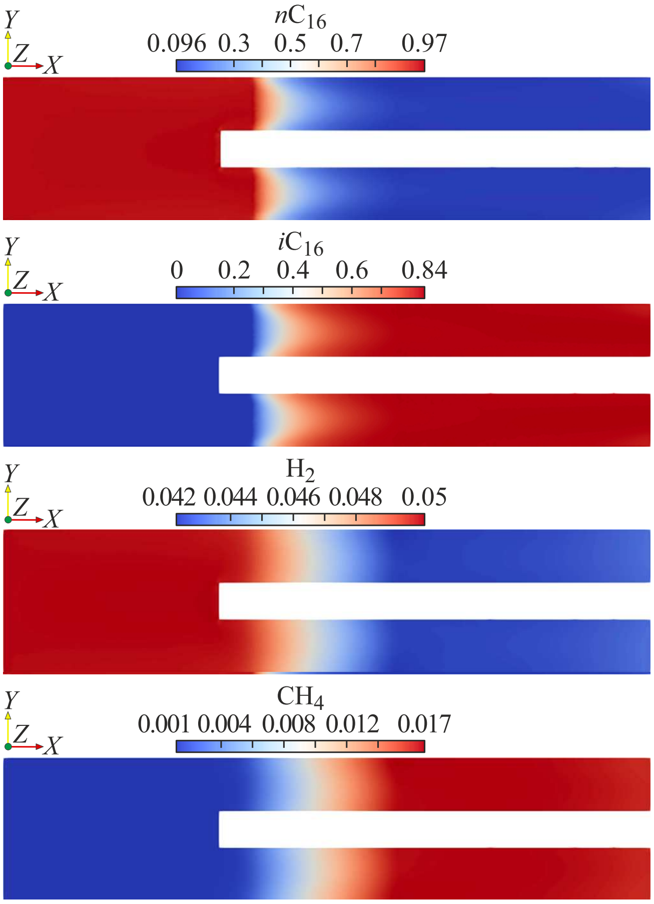

Figure 5. Distribution of the concentration of $n\mathrm{C}_{16}$, $i\mathrm{C}_{16}$, H_2 and CH_4 in the central part of the calculation region (XY).

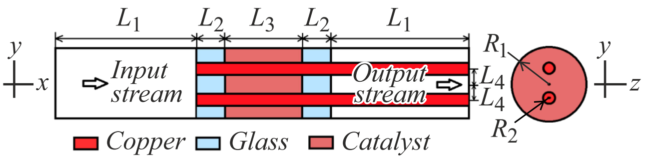

Figure 6. Diagram of the chemical reactor with two heaters in the longitudinal (on the left) and the transverse (on the right) section.

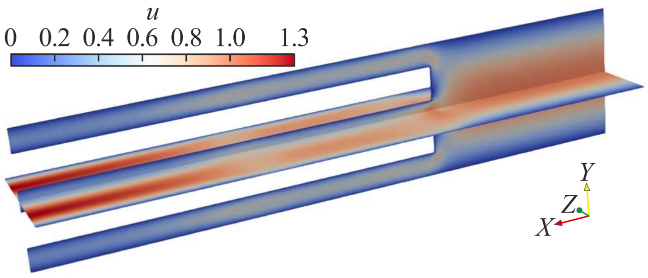

Figure 7. Distribution of the rate modulus in the sections XY and XZ.

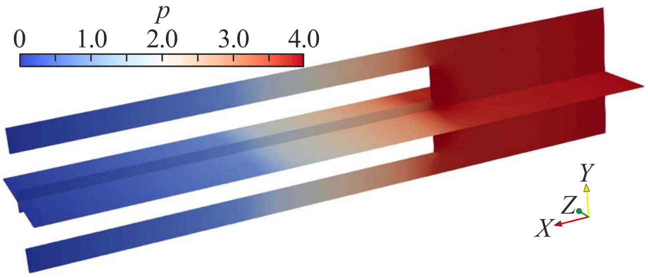

Figure 8. Distribution of overpressure in the sections XY and XZ.

and molecular simulation. Dependences of these parameters on the temperature will also be taken into account.

Generally, the obtained results reflect an axisymmetric nature of the studied geometry. However, today, no less interesting is a task of modernizing reactor unit structures based on preliminary numerical calculations [18]. In this case, use of the three-dimensional model and the non-structured meshes will make it possible to study regions with nonsymmetrical branch pipes (feedstock supply inlets and outlets of the reaction products), additional filters as well as narrowings and widenings of a main tank of the reactor. It is exemplified by the reactor with two heaters, whose diagram is shown in Fig. 6. The calculation parameters as well as the boundary and initial conditions correspond to used ones in the axisymmetric case. A distance between the central axis and the heaters was accepted to be $L_4 = 0.4$. The flow parameters obtained as a result of these calculations are shown in Fig. 7 and 8. The distributions of the mixture components are shown in Fig. 9. Thus, the developed three-dimensional computational algorithm makes it possible to study the catalysis processes in nonsymmetrical geometrical formulations. The obtained software implementation can be a useful tool when designing new reactors and optimizing existing reactors.

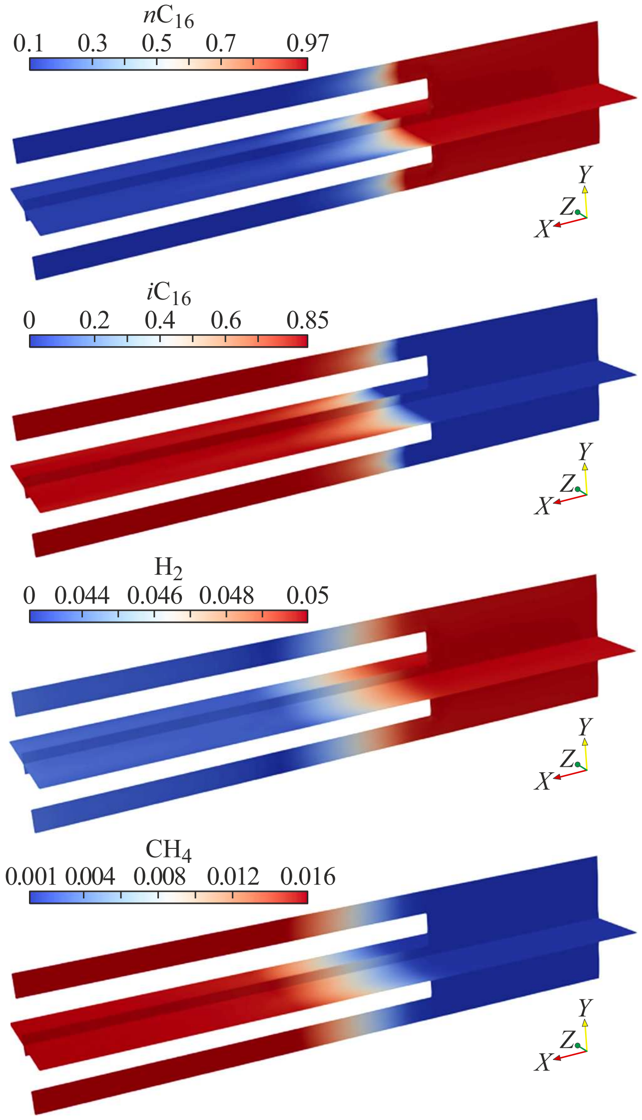

Figure 9. Distribution of the concentration of nC_{16}, iC_{16}, H_2 and CH_4 in the sections XY and XZ.

Conclusion

This study considers a relevant problem of computer simulation of the processes of hydrocarbon feedstock refining. It is exemplified by the technology of hexadecane isomerization in the laboratory setup designed to produce diesel fuel with pre-defined properties. An original complex three-dimensional mathematical model has been proposed for the physico-chemical problem. The model makes it possible to make a through calculation of the hydrocarbon liquid flow across the entire volume of the setup, including free zones, porous seals and the catalyst. The model is based on the promising quasi-hydrodynamic approach as well as diffusion-convection-reaction equations. The numerical implementation of this approach is based on a method of dividing by the physical processes and a mesh finite-volume method on the irregular tetrahedron mesh. The parallel calculations have been applied for software implementation of the developed algorithm. The numerical experiments have confirmed that the developed computational procedure is operable and it can be applied for solving industrial tasks of oil and gas refining.

Funding

The studies were financed from the federal budget for implementation of the state assignment of Keldysh Institute of Applied Mathematics of the Russian Academy of Sciences.

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] F.H. Poettman, P.G. Carpenter. *The Multiphase Flow of Gas, Oil, and Water through Vertical Flow Strings with Application to the Design of Gas-Lift Instal-lations* (Drilling and Production Practice, NY., 1952, Document ID: API-52-257)

[2] P.B. Baxendell, R. Tomas. J. Pet. Technol., **13** (10), 1023 (1961). DOI: 10.2118/2-PA

[3] R.C. Reid, J.M. Prausnitz, T.K. Sherwood. *The Properties of Gases and Liquids* (McGraw Hill Book Company, 1981)

[4] O.Yu. Batalin, A.I. Brusilovskii, M.Yu. Zakharov. *Fazovye ravnovesiya v sistemakh prirodnykh uglevodorodov* (Nedra, M., 1992) (in Russian).

[5] D.B. Ingham, I. Pop. *Transport Phenomena in Porous Media* (Pergamon Press, Elsevier Science, Oxford, 2002), v. 2.

[6] M.K. Das, P.P. Mukherjee, K. Muralidhar. *Modeling Transport Phenomena in Porous Media with Applications* (Springer, NY., 2018)

[7] S. Whitaker. *Volume averaging of transport equations*, Chapter 1. In J.P. Du Plessis (editor). *Flow in Porous Media* (Computational Mechanics Publications, Southampton, UK., 1997)

[8] I. Rybak, C. Schwarzmeier, E. Eggenweiler, U. Rude. Comput. Geosci, **25**, 621 (2021).

[9] Yu Qi, Ch.-F. Cai, P. Sun, D.-W. Wang, H.-J. Zhu. Petroleum Sci., **20**, 1978 (2023).

[10] V.A.F. Costa, L.A. Oliveira, B.R. Baliga, A.C.M. Sousa. Numerical Heat Transfer, Part A: Applications, **45**, 675 (2004).

[11] T.G. Elizarova. *Quasi-Gas Dynamic Equations* (Springer-Verlag, NY., 2009)

[12] Yu.V. Sheretov. *Matematicheskie modeli gidrodinamiki.* Uchebnoe posobie (Tverskoi gos. un-t, Tver', 2004) (in Russian).

[13] S.V. Polyakov, M.A. Trapeznikova, A.G. Churbanov, N.G. Churbanov. № Preprint 71 (Preprinty IPM im. M.V. Keldysha, M., 2021) (in Russian).

[14] S.V. Polyakov, V.O. Podryga, N.I. Tarasov, K.F. Koledina. Theor. Foundations Chem. Eng., **58** (6), 1900 (2024). DOI: 10.1134/S0040579525600950

[15] R. Eymard, Th. Gallouët, R. Herbin. *Handbook of Numerical Analysis* (North Holland, Amsterdam, 2000), v. 7. DOI: 10.1016/S1570-8659(00)07005-8

[16] R.Z. Zainullin, K.F. Koledina, A.F. Akhmetov, I.M. Gubaidullin. Elektronnyi nauchnyi zhurnal „Neftegazovoe delo“, **6**, 78 (2018) (in Russian). DOI: 10.17122/ogbus-2018-6-78-97

[17] Z.R. Khairullina, M.R. Agliullin, I.E. Alekhina, B.I. Kutepov. Vestnik Bashkirskogo un-ta, **25** (3), 495 (2020) (in Russian).

[18] S.V. Zazhigalov, V.A. Shilov, V.N. Rogozhnikov, D.I. Potemkin, V.A. Sobyanin, A.N. Zagoruiko, P.V. Snytnikov. Chem. Eng. J., **442** (1), 136160 (2022). DOI: 10.1016/j.cej.2022.136160

Translated by M.Shevelev