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5. Karabaev J.A., Kapustin V.M., Tanashev S.T., SakibaevaS.A.and others. The intensification of the process of vacuum distillation Kumkol oil fuel oil by adjusting the phase transition oil disperse systems.CHEMISTRY AND TECHNOLOGY OF FUELS OILS Volume: 577 Issue: 3 Pages: 33-37 Published: DEC 2013
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NUMERICAL SIMULATION OF THE ELECTRON IRRADIATION IMPACT TO THE KINETICS OF OIL

[1]Kizbayev A.P., [1]Zhakebayev D.B., [2]Cherny S.G.

[1]Al-Farabi Kazakh National University, Almaty, Kazakhstan,
[2]Institute of Computational Technologies SB RAS, Novosibirsk, Russia

Abstract: The purpose of this paper is numerical modeling of low conductive incompressible multicomponent hydrocarbon mixture in a channel under influence of electron irradiation, developing of mechanism of radiation transfer and separation of the mixture's components. The three-dimensional non-stationary Navier-Stokes equation is used for numerical modeling of low conductive incompressible multicomponent hydrocarbon mixture in a channel under influence of electron irradiation. The problem is solved numerically, electron irradiation equation and momentum equation for the mixture are solved by using Crank-Nicolson method, equation of motion is solved by using Adams-Bashforth method in combination with penta - diagonal matrix method and Poisson equation is solved by using the matrix sweep method. On the basis of numerical modeling studied influence of electron irradiation intensity to the kinetics of oil. Suggested the mechanism of radiation transfer and separation of the mixture's components. Chemical reactions kinetics has been studied based on the developed model.

Keywords: kinetics, the rate of chemical reactions, electron irradiation, non-Newtonian fluid,hydrocarbon mixture,numerical simulation, penta-diagonal matrix method.

INTRODUCTION

Development of oil-refining industry in the Republic of Kazakhstan is connected with intensification and improvement of petroleum feedstock's refining processes. Within the framework of the "National Program of forced industrial and innovative development of the Republic of Kazakhstan for 2014 – 2019" and the National plan "100 specific steps towards entry into the top thirty world leaders" it is worth mentioning the importance of creation and development of new technologies for production of high-quality oil products based on the separation of oil into light and heavy fractions. In this connection it should be noted that technologies relating to energy industry and allowing reconstruction of the initial substances' structure without significant energy costs have been actively studied throughout last fifteen years.

Exposure to electron irradiation relates to one of the most advanced technologies, as it outstands with energy efficiency and environmental security. Application of electrical action allows achieving significant destruction of oil associates' structures in a short time period and maintaining this level over the long term. Conversion of the raw materials into active state provides a possibility for wider use of the raw materials' potentials, increase of the end products yield or improvement of their quality parameters.

Electron irradiation was for the first time ever studied in the scientific paper [1] at the beginning of the sixties of the last century.The major part of the fifty-year period was spent on the study of regularities and mechanisms of electron irradiation based on the examples of various model hydrocarbons.Since the beginning of 1990s these researches have been applied to heavy hydrocarbon mixtures with complex composition. Among scientific researches devoted to experimental studies of electron irradiation it is worth mentioning publications of famous scientists Nadirov N.K. [2] and Zaikin Y.A. [3]. Experimental work of Nadirov N.K. allow us to understand the nature of the electron irradation, and gives an idea of the effect of various parameters such as dose, power, intensity of electron irradiation on the kinetics of chemical reactions. At work Galimbekova A.D. presented mathematical model of the influence of electromagnetic fields on the multicomponent medium.On the basis of the constructed theory by Galimbekova A.D. revealed mechanisms of impact of the electromagnetic field to the constant of chemical equilibrium and rate of chemical reactions.

The present scientific paper contains results of the numerical modeling of low conductive incompressible multicomponent hydrocarbon mixture in a channel when exposed to electron irradiation. Moreover, we have developed and realized three-dimensional case of hydrodynamic constituent of a model and suggested the mechanism of radiation transfer and separation of the mixture's components. Chemical reactions kinetics has been studied based on the developed model.

MATERIALS AND METHODS

The given paper examines issues connected with the numerical modeling of low-conductive, incompressible, multicomponent non-Newtonian liquid in a flat channel (Figure 1) with the speed $\mathbf{v} = (0.01; 0; 0)$ m/s and concentration of heavy component $c_{heavy} = 1$ on the left border, while upper and lower borders are walls with adhesion conditions. For a three-dimensional computational domain taken a box with the corresponding dimensional parameters: $x \in [0, 0.2]$ m,

$y \in [0, 0.04]$ m, $z \in [0, 0.05]$ м. The fluid is exposed to ionizing irradiation with electrons with intensity $I = 1$ in the center $(0.07 < x < 0.13$ m, $0.01 < y < 0.03$ m, $z = 0.05$ m$)$ of this channel.Under the influence of the electron irradiation mass transfer processes and chemical transformations occurs in low-conductive, incompressible, multicomponent non-Newtonian fluid. In this paper, we will not take into account the heat transfer and we assume the process is isothermal and any other external body forces are does not have effect to the system. Required to describe this process and establish mechanisms of mass transfer and chemical transformations between reacting components and identify factors that have a dominant influence to this process.

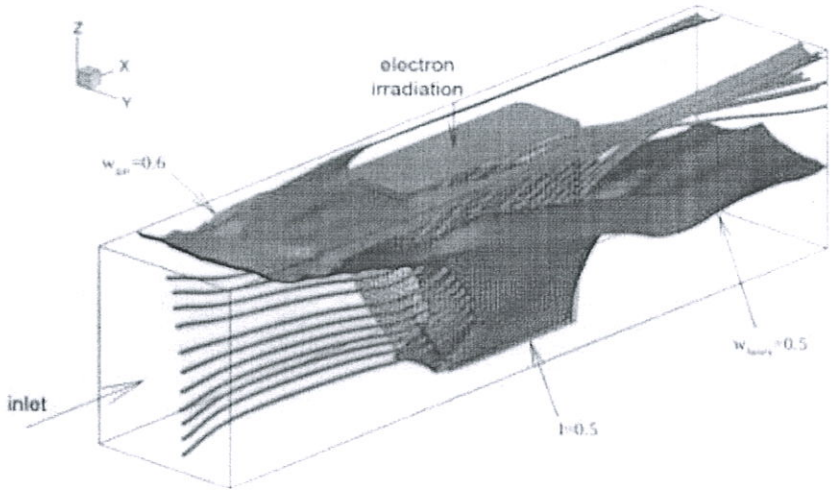

Figure 1. Reaction in the flow under the influence of electron irradiation in a three-dimensionalcase. A general view of the domain with the selected isosurfaces and streamlines.

MATHEMATICAL MODEL

Mathematical model of ionizing radiation's effects on incompressible non-Newtonian fluid is based on the solution of the electron irradiation equation, moment-of-momentum equation, continuity equation and the momentum equation for the mixture:

$$\begin{cases} \dfrac{\partial I}{\partial t} + s \cdot \nabla \cdot I = -\eta(x,t) I, \\ \rho \dfrac{\partial \mathbf{v}}{\partial t} + \rho \nabla \cdot (\mathbf{v}\,\mathbf{v}) = -\nabla p + \nabla \tau + f + \rho Q^V \mathbf{v}, \\ \nabla \cdot \mathbf{v} = Q^V, \\ \dfrac{\partial \rho_k}{\partial t} + \nabla \cdot (\rho_k \mathbf{v}_k) = Q_k^M, k = 1 \ldots N \end{cases} \tag{1}$$

where s - the direction of the flow of electrons; I - the intensity of the electron irradiation (energy): $\eta = \sum_{k=1}^{N} c_k \eta_k$ - electron absorption coefficient for the mixture; η_k - electron absorption coefficient for k-component; $\mathbf{v}_k$ – speed of motion of components; $\mathbf{v}$ – speed of the mixture; τ – stress tensor; $Q^V = \sum_{k=1}^{N} 1/\rho_k^0 \cdot Q_k^M$ – volume source of mixture; ρ_k^0 – true density of k-component; Q_k^M – mass source, which is determined by chemical transformations; $\sum_{k=1}^{N} Q_k^M = 0$; p –pressure; $f = (0, 0, -\rho g)$ – vector of external forces; g – acceleration of gravity.

The true density ρ_k^0 of the component is defined as the ratio of the weight k-th component per unit volume of the component. In turn, the density (partial density) of the component ρ_k - is the ratio of the mass of k-th component per unit volume of the whole mixture. The volume fraction of the components c_k is determined as the ratio of k-th component to the total volume of the mixture:

$$\sum_{k=1}^{N} c_k = 1,$$

$$\rho_k = c_k \rho_k^0, \quad k = 1 \ldots N, \tag{2}$$

and the mixture density ρ is determined by the law

$$\rho = \sum_{k=1}^{N} \rho_k$$

Using the relation (2), continuity equation can be obtained from the first equation (1) in terms of volume fraction

$$\frac{\partial c_k}{\partial t} + \nabla(c_k \mathbf{v}_k) = \frac{1}{\rho_k^0} Q_k^M, \quad k = 1 \ldots N, \tag{3}$$

We obtain equation of continuity of the mixture by summarizing the equation (3).

The viscous stress tensor τ for non-Newtonian fluids is given by

$$\tau = \mu_e D,$$

$$\mu_e = \mu_e(\dot{\gamma}), \quad \dot{\gamma} = \sqrt{\frac{1}{2} D \cdot D}, \quad D = D_{i,j} = \left(\frac{\partial \mathrm{v}}{\partial \mathrm{x}}\right) + \left(\frac{\partial \mathrm{v}}{\partial \mathrm{x}}\right)^*$$

For non-Newtonian fluids effective molecular viscosity is described by:

$$\mu_e = (\tau_0 + k\dot{\gamma})\dot{\gamma}^{-1} \qquad \text{–Bingham fluid}$$

where τ_0 –visco-plastic fluid yield strength; $\dot{\gamma}$ – shear rate; n, k – parameters of rheological models.

Distribution of electrons is described in the medium approximation with a small scattering - the electrons are distributed in a straight line. During the spread of the electron, the energy is absorbed by the environment, which is described by the equation

$$s \cdot \nabla I = -\eta(x,t) I,$$

Speed of the mixture and values of the volume fractions of all components are defined on the front edge. Adhesion condition is defined on solid walls - velocity of the mixture is equal to the velocity of the wall

$$x = 0\,\mathrm{m}: \; u = (0.01; 0; 0)\,\mathrm{m/s}, \; c_{heavy} = 1, \; c_{light} = 0, \; c_{gas} = 0,$$

$$x = 0.2\,\mathrm{m}: \frac{\partial u}{\partial x} = 0, \; \frac{\partial c_k}{\partial x} = 0,$$

$$y = 0\,\mathrm{m}, \; y = 0.05\,\mathrm{m}: u = (0; 0; 0)\,\mathrm{m/s}, \; \frac{\partial c_k}{\partial x} = 0,$$

$$z = \pm 0.02\,\mathrm{m}: u = (0; 0; 0)\,\mathrm{m/s}, \; \frac{\partial c_k}{\partial x} = 0$$

The mechanism of separation of dispersed component

Components such as gas bubbles or solid particles considered disperse ($k \in K_{dispersed}$), and the other - carrier ($k \in K_{carrier}$). The carrier phase moves with the same rate $\mathrm{v}^{\text{carrier}}$

$$\mathrm{v}_k = \mathrm{v}^{\text{carrier}}, \quad k \in K_{carrier} \tag{4}$$

The velocity difference between the dispersed and carrier phases is determined by Stokes' law

$$\mathrm{v}_k = \mathrm{v}^{\text{carrier}} + u_k^{settling}, \quad k \in K_{carrier} \tag{5}$$

$$u_k^{settling} = \frac{(\rho_k^0 - \rho) \cdot d_k^2}{18\mu} g,$$

where d_k –particle diameter of the$k$-th dispersed phase.

Substituting (4) and (5) equations to the definition of the speed of mixture gives

$$\mathrm{v} = \mathrm{v}^{\text{carrier}} + \sum_{k \in K_{dispersed}} c_k u_k^{settling}.$$

This yields an expression for the speed of the carrier phase through average speed mixture

$$\mathrm{v}^{\text{carrier}} = \mathrm{v} - \sum_{k \in K_{dispersed}} c_k u_k^{settling}.$$

Speed of the dispersed phase is explicitly calculated from (5).

Type of sources of chemical kinetics

Let the equation of chemical kinetics will be in the next form

$$\frac{dN_k}{dt} = R_k(N_1,\ldots,N_N), \quad k = 1\ldots N \tag{6}$$

wherefunction $R_k(N_1,\ldots,N_N)$ satisfies the property of homogeneity

$$R_k(\gamma N_1,\ldots,\gamma N_N) = \gamma R_k(N_1,\ldots,N_N), \quad \forall\gamma$$

Amount of substance N_k is given in a certain volume $\omega(t)$. Amount of substance N_k in volume ω related with density of components and molar mass M_k as follows:

$$N_k = \int_{\omega} \frac{\rho_k}{M_k} dx.$$

Then the the equation of chemical kinetics (6) can be rewritten as

$$\frac{d}{dt}\int_{\omega_k(t)} \frac{\rho_k}{M_k} dx = \int_{\omega_k(t)} R_k\left(\frac{\rho_1}{M_1},\ldots,\frac{\rho_N}{M_N}\right) dx, \quad k = 1\ldots N,$$

where $\omega_k(t)$ –arbitrary moving with speed v_k. This corresponds to the differential equations in the following form

$$\frac{\partial \rho_k}{\partial t} + \nabla(\rho_k \mathrm{v}_k) = M_k R_k\left(\frac{\rho_1}{M_1},\ldots,\frac{\rho_N}{M_N}\right), \quad k = 1\ldots N.$$

Therefore, the bulk sources should be of the form

$$Q_k^M = M_k R_k\left(\frac{\rho_1}{M_1},\ldots,\frac{\rho_N}{M_N}\right), \quad k = 1\ldots N.$$

where $R_k = k_0 \cdot I$, k_0 – coefficient,*I*–electron irradiation intensity.

NUMERICAL METHOD

Solution of the problem connected with the ionizing radiation's effects on incompressible non-Newtonian fluid is based on the splitting scheme with respect to physical parameters. In the *first* stage assumes solution of equation of radiation transfer using the Crank-Nicolson method. At the *second* stage it is assumed that the quantity of motion is transferred due to convection and diffusion only. Approximation of convectional and diffusive members of equation is based on the scheme of the fourth accuracy order. Intermediate velocity field is determined using five-point elimination method [4] with the use of Adams-Bashforth scheme. The *third* stage provides determination of the pressure field based on the previously determined intermediate velocity field. Poisson's equation for the pressure field is to be solved using the method of matrix elimination [5]. Obtained pressure field shall be used for recalculation of final velocity field at the *fourth* stage. The *fifth* stage assumes calculation of the components' density considering chemical transformations using the Crank-Nicolson method.

RESULTS AND DISCUSSION

For studying influence of irradiation on the flow of multicomponent mixture we have performed computations of three-dimensional problem within the area with $L = 0.2\times0.04\times0.05$ m. Computations have been performed on the equally spaced orthogonal grid with the following number of nodes $120\times30\times30$ and along x, y, z axes accordingly. The time step is chosen equal to 0.001.

Boundary conditions assume vanishing of speed on the upper and lower boundaries. The left boundary is considered as input $\mathbf{v} = (0.01, 0, 0)$ m/s and $c_{\text{heavy}} = 1$, and the right boundary as output. Electron irradiation occurs in the center of the channel.

Gas component is the disperse phase with the following particles diameter $d_{gas} = 1\,\text{mm}$.

Intensity of electron radiation $I = 1$ is defined on the upper part of the boundary $(0.07 < x < 0.13\ \text{m}, 0.01 < y < 0.03\ \text{m}, z = 0.05\ \text{m})$, flow of electrons is spread downwards ($s = (0, 0, -1)$).

Conversions of the component across the whole area occur in accordance with chemical kinetics equations

OIL DEEP REFINING AND OIL CHEMISTRY

CHEMISTRY AND PHYSICS OF POLYMERS