Simulation of the dynamics complex influence on hydrocarbon mixtures

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Abstract

The present research paper examines issues connected with the modeling of mechanoactivation and acoustic effects on the hydrocarbon blends. Modeling of mechanoactivation and acoustic effects on the hydrocarbon blends is carried out based on the three-dimensional Navie-Stockes equation considering equation of continuity and equitation of concentration for the components of hydrocarbon blends in the rotary drum with the rotating disks. Mechanoactivation and acoustic effects on the hydrocarbon blends occurs due to special rotation of disks in the cylindrical domain with equal speed but in different directions. An experiment confirming integrated effect was carried out based on the special equipment developed during the present scientific research. Obtained results may encourage development of new technologies for production, transportation and storage of oil and oil products, and may be also beneficial for crude hydrocarbons processing plants.

Keywords: hydrocarbon blends, integrated effects, mechanoactivation effects, acoustic effects, Navier-Stokes equations, hydrodynamic activator, rotating disks.

Implementation of the "State Program on Forced Industrial-Innovative Development of Kazakhstan for 2014-2019" and "100 specific steps towards entry into the top thirty countries worldwide" [1, 2] reveled necessity in accumulation of local scientific developments, which results may be used for creation of new technologies for production of light and heavy fractions of oils. Such scientific researches include low-energy effects on the hydrocarbon blends. It is worth mentioning that such effects allow reconstruction of the mother substance without significant external energy costs (and sometimes by using internal reserves of the substance). The specified effects shave been studied throughout last fifteen years and include – electromagnetic, electric, magnetic, acoustic and vibrational fields, as well as mechanoactivation and thermomechanical effects. Energy technologies (such as acoustic, vibrational, magnetic, etc) relate to the most perspective developments, especially considering their efficient performance, effectiveness and affordability. These researches have been included into scientific papers of many famous researchers [3-12].

The specified effects on oil are finding ever-widening applications in oil industry. The use of the specified techniques allows achieving significant levels of oil associates structure's destruction within the short period of time and maintaining these levels in the course of time. Transformation of the hydrocarbon blend into active condition enables complete realization of potentials of such hydrocarbon blend, increasing the product yield and ensuring obtainment of required physical and chemical parameters.

Among factors limiting widespread application of effective technological processes connected with effects on the hydrocarbon blends it is worth mentioning absence of the required and state-of-the art equipment in real working environment.

This problem may be solved due to creation of necessary technological equipment based on the mathematical modeling, considering physical parameters of the process and determination of the most optimal area of influence on hydrocarbon blends with obtainment of desired physical and chemical parameters.

Pilot version of the hydrodynamic activator (see Fig. 1) has been developed, produced and successfully tested based on the previous scientific researches directed on the development of technology for preparation of hydrocarbon liquids to pipeline transportation [13].

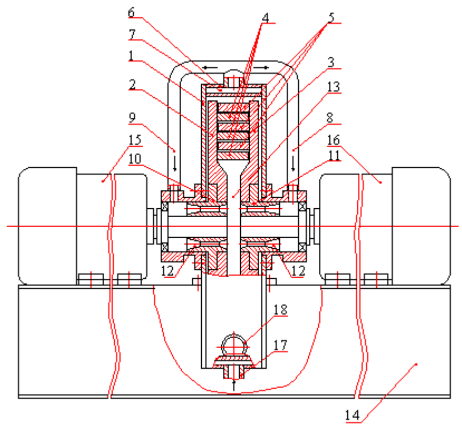

Figure 1: Diagram of the pilot version of the hydrodynamic activator.

Pilot version of the hydrodynamic activator consists of a housing 1, in which the rotors in the form of the disks 2 and 3 are placed against each other on the rollers. Fingers 4 and 5 are placed in concentric rows on the specified rotors. The shell 6 of the housing 1 is equipped the pressure-tight cavity 7, which is

*Footnotes may appear on the first page only to indicate research grant, sponsoring agency, etc. These should not be numbered but referred to by symbols, e.g. *,+. The footnote text may be produced in a small font. Delete this sentence and leave the space empty if not used.

placed in a circumferential direction, which outlet is equipped with the separating nozzles 8 and 9. Rotor hubs 10 and 11 have concentrically placed holes 12 connected with separating nozzles 8 and 9 on the one side and with the wheel space 13 on the other side. Meanwhile total area of all holes 12 shall be lesser than the area of holes of the separating nozzles 8 and 9. The hydrodynamic activator's housing 1 is installed on the frame 14. Electric motors 15 and 16 are also installed on the frame. Liquid flow enters the activator through feeding pipe 17, while discharge liquid is drained through the discharge outlet 18.

Conduction of the experimental researches required significant improvement of the pilot version of the activator and production of the experimental version of the hydrodynamic activator (see Fig. 2), considering all of the identified shortages and structural modifications in course of previous experimental researches.

In the hydrodynamic activator the joint, mechanoactivation and acoustic effects on the hydrocarbon blends occur due to separation of initial flow of the hydrocarbon blend into two separate flows, which are supplied into the housing of the hydrodynamic activator, where separated flows are put into vortex rotation in the opposite directions. Acoustic effects occur due to periodical passages of blends between blades of two rotating disks. Then, counter-current flows encounter at the periphery of the shell and create conditions for occurrence of mechanoactivation effect, while the treated hydrocarbon blend is simultaneously exposed to the effect of acoustic vibrations, generated by actuator's operating devices, being the precursors of intense turbulence, which lead to destruction of molecular structures. Then the treated hydrocarbon liquid shall be discharged from the housing of the hydrodynamic activator.

Figure 2: General view of the experimental hydrodynamic activator

It is worth mentioning that joint, mechanoactivation and acoustic effects on the hydrocarbon blend results in it's heating up to 70^{0}C and higher, and thus, for the avoidance of any possible influence that may be rendered by the gas, accumulating as a result of chemical transformations, on the studied process, conditions for creation of excess pressure inside the housing of the hydrodynamic activator have been excluded.

Development and practical application of two-dimensional and three-dimensional mathematical models of integrated effects on the hydrocarbon blend, as well as calculation of algorithms for realization of constructed mathematical models relate to one of the most important tasks at the subsequent design and development of the main technical equipment for joint, mechanoactivation and acoustic effects on the hydrocarbon blends and will effectively promote development and creation of advanced and efficient devices depending on the assigned specific technical tasks.

Mechanoactivation and acoustic effects on the hydrocarbon blends are described by averaged Navie-Stockes equations, equations of continuity and equitation of concentration and temperature considering chemical reactions kinetics, recorded in cylindrical coordinates system with corresponding boundary and initial conditions [14-15].

Consideration of chemical reactions kinetics is essential primarily because chemical reactions occur when reagents are blending at the molecular level. It is known that at the level of microprocesses, having crucial importance for molecular blending, the dissipation of the turbulent energy represents strongly discontinuous operation, i.e., observable in separate regions – small, relatively to the general volume, areas, sizes of which re small in one or two directions (but not in three directions simultaneously). These regions occupy fine structures, which may be vortex tubes, sheets and plates, which characteristic dimensions coincide with the order of Kolmogorov's microscales. Fine structures are responsible for the dissipation of turbulence. Thus, it can be assumed that reagents in these regions will be blended on the molecular level, thereby creating a space for reaction of nonuniform reagents.

Dissipative vortex model is used for realization of mathematical description of the specified process. Originally this model was developed by B.F. Magnussen in 1976. This model describes turbulence-chemistry interaction, which is considered as single-step irreversible reaction with terminal velocity. In the reaction of the following type: $Y_A \to sY_B + (1+s)Y_C$, the speed of formation i, R_i of blends, shall be determined using the minimal speed of the turbulent decomposition: $R_i = A\rho l \frac{\varepsilon}{k} \min\left(Y_A, Y_B, B\frac{Y_C}{1+s}\right)$, where A – is the constant, having its value equal to 4, B is equal to 0.5, ε – dissipation of energy,– k turbulent kinetic energy. Modified version of the specified vortex decomposition model was developed .F. Magnussen in 2005 [16].

Solution of problems considering aforementioned models of the turbulent motion of incompressible liquids in the cylindrical domain is based on the splitting scheme with respect to physical parameters. At the first 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 with the fractional steps method, in radial and axial directions when using five-point elimination method, and in tangential direction when using the cyclic five-point elimination method. The second 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 Fourier's method in combination with the method of matrix elimination, which is also used for determination of Fourier coefficient. Obtained pressure field shall be used for recalculation of final velocity field at the third stage. The fourth stage provides determination of energy and turbulent kinetic energy dissipation based on the calculated velocity field, which also allows determination of the chemical reaction rate. The fifth stage provides solution of equation of concentration of hydrocarbon blend's components in accordance with known velocity field and considering chemical kinetics. Determined concentrations of the hydrocarbon blend's components shall be used for calculation of density and viscosity of the blend. Temperature field shall be determined at the sixth stage in accordance with obtained velocity field.

Numerical model allows us to describe hydrocarbon blend's turbulent motion in the rotor device equipped with the disks rotating in opposite directions. Calculations shall be made for the different angular speed of rotation of disks: – $\omega_1 = 314$ rad/s revolutions per second and $\omega_2 = 377$ rad/s revolutions per second, – installed on the rollers. Diameter of each hydrodynamic activator's disk is equal to 46 cm. Computational grid having 128*256*64 elements shall be used.

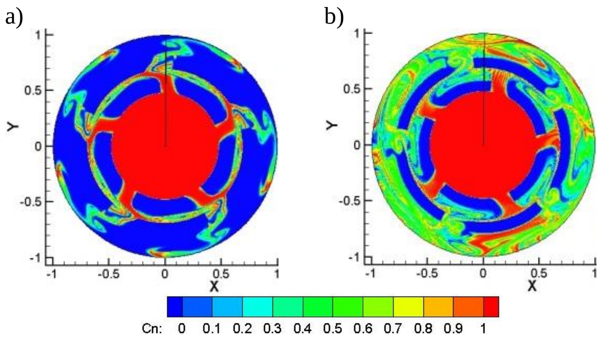

Figure 3: Dynamics of changes in concentration of the hydrocarbon blend's components at angular speed $\omega_1 =$ 314 rad/s revolutions per second at a time $a) t = 0.25,\ b) t = 1.5$

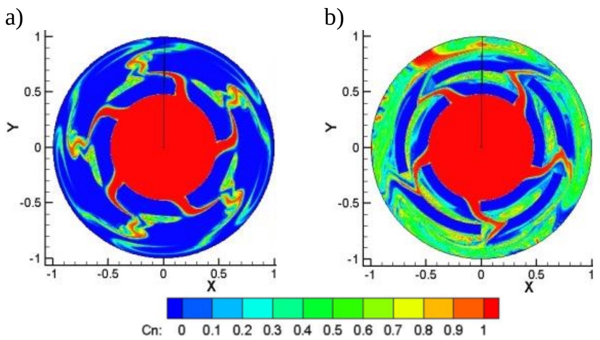

Figure 4: Dynamics of changes in concentration of the hydrocarbon blend's components at angular speed $\omega_2 =$ 377 rad/s revolutions per second at a time $a) t = 0.25,\ b) t = 1.5$

Results obtained from numerical implementation of the problem are illustrated on the Fig. 3 and Fig. 4 above and demonstrate dynamics of changes in concentration of the hydrocarbon blend's components at different angular speeds of rotation – $\omega_1 =$ 314 rad/s revolutions per second and $\omega_2 =$ 377 rad/s revolutions per second.

Solution of the aforementioned problem, relating to simulation of mechanoactivation and acoustic effects on the hydrocarbon blends, has demonstrated effective changes in physical and chemical parameters, such as reduction of density, viscosity and temperature of solidification, as well as vortex formation at the following angular speed of rotation of disks ($\omega_2 =$ 377 rad/s revolutions per second), which result in changes of hydrocarbon blend's allocation inside the observable area, which is confirmed with the results of conducted experimental researches. Implementation of the developed mathematical model for integrated effect on hydrocarbon blend affords an opportunity for studying effects on conditions of setting various angular speeds of rotation of disks and search for the optimal angular speed, which allows capturing of the vortex formation process.

As it was mentioned above, the extent of mechanoactivation and acoustic effects on the treated hydrocarbon blends was determined within the frameworks of experimental researches conducted with samples of Kumkol oil from "Ashisay" oil field. Results of experimental and computational researches are reflected in the Table 1 above. As is evident from the specified table, joint, mechanoactivation and acoustic effects on the treated hydrocarbon blends result in reduction of density, viscosity and temperature of solidification. In this context it is worth mentioning efficiency of the second treatment regime, when the angular speed of rotation makes $\omega_2 =$ 377 rad/s revolutions per second. This regime differs with higher specific intensity of mechanoactivation and acoustic effects caused by increased angular speed of rotation of disks, comparatively to the first regime, which provides angular speed equal to $\omega_1 =$ 314 rad/s revolutions per second.

Analysis of obtained results, illustrated on the figures and in the Table 1 above, has shown that the angular speed of rotation of disks equal to $\omega_1 =$ 314 rad/s revolutions per second results in the change of density by 1%, kinematic viscosity by 56% and solidification temperature by 14%. Angular speed of rotation equal to makes $\omega_2 =$ 377 rad/s revolutions per second changes the density by 3%, kinematic viscosity by 66% and solidification temperature by 60%.

Conducted scientific researches on the mathematical modeling have greater industrial and applied significance, as far as the developed and realized mathematical model has confirmed that integrated mechanoactivation and acoustic effects on the hydrocarbon blends effectively change its properties.

It is worth mentioning that results of mathematical modeling have been confirmed with the experiment conducted within the frameworks of the present scientific research, which also confirms changes of physical and chemical characteristics of the hydrocarbon liquid, thus proving adequacy of the mathematical model and algorithm of its realization.

It should be noted that modification of mathematical model's parameters and change of the processing unit's geometric parameters and design considering desired favorable physical and chemical parameters of the hydrocarbon blend, enable development of the technical design specifications with indication of specific areas of technological processing conditions for creation of sophisticated and effective specimens of processing equipment, which is especially important at the development of new equipment, as it allows to save time and reduce costs connected with the development of new technological equipment.

Experimental researches have confirmed that the present technology of integrated, mechanoactivation and acoustic treatment of the hydrocarbon blend effectively influences on the outcome physical and chemical parameters and creates opportunities for industrial application of this technological line. Besides, it may also promote successful solution of problems connected with production, transportation, processing and storage of oil.

Table 1: Results of experimental and numerical research

№	Indicator/unit. measurement	Initial oil	Processing modes			
			№1, $\omega_1 =$ 314 rad/s		**№2,** $\omega_2 =$ 377 rad/s	
			Experimental data	**Numerical data**	**Experimental data**	**Numerical data**
1	Density at 20^0C/ кg/m^3	863,0	860,0	859	843,0	842,5
2	Kinematical viscosity / mm^2/s	40,4	18,0	17,8	13,9	13,7
3	Freezing temperature / ^{0}C	15	13	13	6	6

Thus, development of the mathematical model of the aforesaid technological process rendering influence on the hydrocarbon blends based on the physical peculiarities of the process and desired outcome physical and chemical parameters of the treated hydrocarbon blend, allows optimizing treatment regimes and revealing essential areas of technological influence in course of design and development of the required processing equipment. Besides, it may also positively influence on creation of more sophisticated equipment, and in general, may ensure significant reduction of time and costs connected with the development of new processing equipment and its subsequent industrial application.

References

[1] Nazarbayev, N.A., State program of industrial-innovative development of Kazakhstan for 2015-2019, *Meeting of the legislation of RK*, №89, 2015.

[2] Nazarbayev, N.A., Plan of Nazarbayev: 100 concrete steps to the Thirty world's leaders, *News of Kazakhstan*, [Electronic resource]. Access: http://www.zakon.kz , 2015

[3] Zaykin, Yu.A., Zaykina, R.F., Nadirov, N.K., Deep conversion of hydrocarbons by radiation-induced cracking, *Oil and gas*, № 4,. pp. 152-159, 2004

[4] Kalybai, A.A., Theory and practice of cold cracking, *Herald of Engineering academy of the RK*, 2003.– № 2 (10) ,. pp. 132-137.

[5] Loskutov, Y., The influence of magnetic field on the rheological properties of the oils, 2003.

[6] Nadirov, N.K., Heavy oil and natural bitumen, pp. 269, 2001.

[7] Buchachenko, A.L., Magnetic effects in chemical reactions *Russian Chemical Reviews*, Vol. 45, pp. 761 -793,1977.

[8] Lesin, V.I., The mechanism of influence of the magnetic fields, *Oil industry*, № 6, pp. 24-27, 1994.

[9] Borsutsky, Z.R., Studies of the magnetic handling mechanism oil based on the results of laboratory and field tests, *Petroleum Engineering*, pp. 28-37, 2002.

[10] Yakovlev, V.A., Zavarukhin, S.G., Kuzavov, V.T., Stebnovskii, S.V., Malykh, N.V., Mal'tsev, L.I., Parmon, V.N., A study of chemical transformations of organic compounds under the action of cavitation, *Effect of external factors on physicochemical transformations*, Vol.4, pp. 227-234, 2010.

[11] Adamowski, J. C., Buiochi, F., Simon, C., Silva, E. C. N. and Sigelmann, R. Ultrasonic Measurement of Density of Liquids, *The Journal of the Acoustical Society of America*, Vol. 97, pp. 354-361,1995.

[12] Kamyanov, V.F., Research in the field of macromolecular chemistry of oil, *Problems and achievements in the study of oil*, pp. 65-99, 1990.

[13] The provisional patent (KZ) №17791 "Method and apparatus for the preparation of a hydrocarbon liquid for transportation". 15.09.2006.

[14] Abdibekov, U.S., Zhakebayev, D.B., Zhumagulov, B.T., Simulation of turbulent mixing of a homogeneous liquid in the presence of an external source force, Turbulence, *Heat and Mass Transfer 6. Proceedings of the Sixth International Sym-posium on Turbulence, Heat and Mass Transfer, Rome, Italy, September 14-18 2009/ K. Hanjalić, Y. Nagano and S. Jakirlić (Editors);* Begell House Inc., pp. 629-632, 2009.

[15] Hartmann, H., Derksen, J.J., Van den Akker, H.E.A., Macro - instability uncovered in a Rushton turbine stirred tank, *A.I.Ch.E. Journal*, № 50 (10) , pp. 2383-2393, 2004.

[16] Magnussen B. F., The eddy dissipation concept: a bridge between science and technology, *In Proceedings of the ECCOMAS Thematic Conference on Computational Combustion*, 2005.