NUMERICAL MODELLING OF INFLUENCE OF THERMOMECHANICAL IMPACT ON MULTICOMPONENT FLUIDS

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Abstract In this work consider the multivariate modeling of impulsive impact on heterogeneous fluid to produce light oil fractions and the degradation of molecular compounds is considered turbulent mixing in a cylindrical area, caused by the rotation of propeller blades, located on the top . The cases when the blades are at an angle to the base of the cylinder. By modeling the problem of hydrodynamic effects on heavy oil based on the filtered solution of unsteady Navier-Stokes equations and the continuity equation in cylindrical coordinates Large eddy regularities of the influence of thermo-mechanical effects on the viscous oil, these data can be used in oil refining.

Interest in the influence of centrifugal and other mechanical fields in multicomponent and heterogeneous objects grew out of work in the field of methods for calculating chemical equilibrium in chemical thermodynamics, whose task is to model chemical systems in equilibrium and steady-state conditions [1]. When considering the more complex mixtures proved that the opposite phenomenon - homogenization of heterogeneous systems can be observed only in systems with more than two components. In binary mixtures can be observed only delamination homogeneous mixtures.

Existing traditional methods of calculation of chemical reactors based on kinetic studies of chemical reactions and hydro models flow patterns using the theory of similarity present difficulties due to the effect of scaling due to incompatibility of the defining criteria of similarity: Damkeller -chemical and hydro-Reynolds. Avoid these difficulties is possible with the joint solution of equations describing the kinetics and structure of flows, heat and mass transfer processes in chemical reactors, using mathematical modeling methods [2].

Oil and oil products are multicomponent continuous mixture of hydrocarbons and heteroatomic compounds, the most common methods of distillation is not possible to separate them into individual compounds with well-defined boiling point at a given pressure. Be divided oil and petroleum products by distillation into separate components, each of which is less complex mixture. Such components are called fractions or distillates.

Multivariate impulsive action on heterogeneous liquid to produce light oil fractions and the degradation of molecular compounds is considered turbulent mixing in a cylindrical region caused by the rotation of propeller blades, located on the top . The cases when the blades are at an angle and to the base of the cylinder.

The process principle of the device is such that the rotation of the propeller blades in a cylindrical region there are large shear stresses, where the fluid velocity is high and the fluctuation. Thus, in this area the intense turbulence, which leads to the destruction of molecular structures.

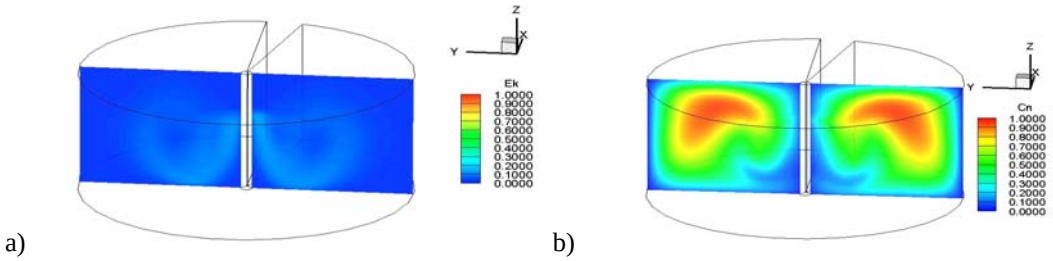
Chemical reactions occur when reactants are mixed at the molecular level at a high enough temperature. In turbulent flow, reagent consumption is highly dependent on the molecular mixing. It is known that the micro-level processes that are critical to the molecular mixing and dissipation of turbulent energy into heat are highly intermittent ie concentrated in certain regions of which the entire amount is a small fraction of the liquid volume. These regions are also fine structures whose dimensions are small in one or two directions, but not in the third. These fine structures are thought to be the vortex tubes, sheets and plates, the characteristic dimensions of the same order as the Kolmogorov microscale. Fine structure are responsible for the dissipation of turbulence in the heat. In these structures, so we can assume that the reagents are mixed at the molecular level. These structures thus create space for reaction evenly distributed agents.

Eddy dissipation model is used to simulate the chemical kinetics. For the first time this model has been developed B.F. Magnussen in 1976, the model offers a chemical-turbulence interaction, where the reaction is considered as a one-step irreversible reaction with a finite velocity. A modified version of the decomposition of the vortex was developed B.F. Magnussen in 2005 [3].

For the numerical solution of the Navier-Stokes splitting scheme is used by physical parameters, which consists of three phases. In the first phase is solved the Navier-Stokes equations without pressure. To approximate the convection and diffusion terms of the equation used compact scheme of high order. In the second stage solved the Poisson equation derived from the continuity equation with the velocity field of the first phase. To solve the three-dimensional Poisson equation algorithm of solutions - spectral transform in combination with matrix factorization. The resulting pressure field in the third stage is used to convert the final velocity field.

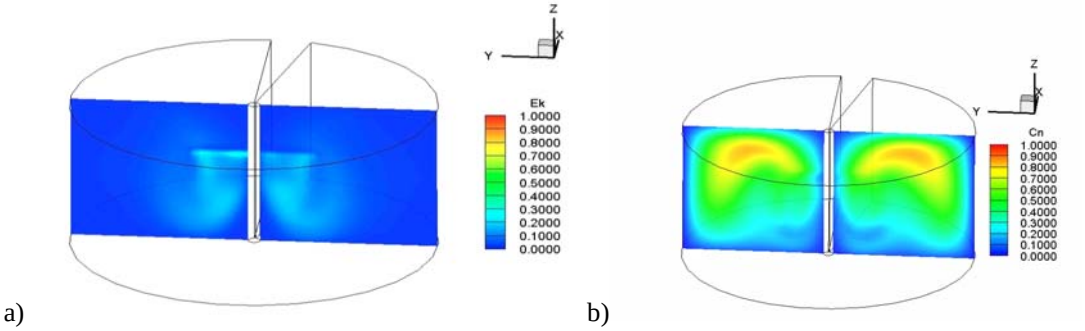
The built model allows to model non-stationary processes in the chemical reactor, with different input mode parameters, and allows to control the course of the reaction process by controlling environmental factors, which are the raw material consumption, pressure, and temperature. Based on modeling of the influence of thermomechanical established effects on viscous oil, these data can be used in oil refining.

Thus, the numerical modeling of the hydrodynamic effect of heavy oil fractions by the unsteady filtered Navier-Stokes equations and the continuity equation in cylindrical coordinates by LES.



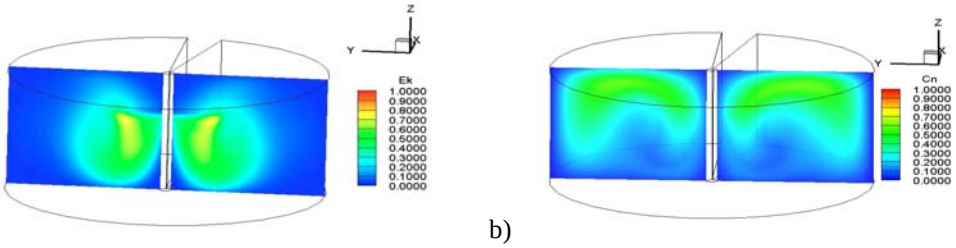
a) b)

Figure 1. Dynamics of change of kinetic energy (and) and change of concentration of heavy fraction (b) at t=0.6 and the angular speed of the propeller =1.



a) b)

Figure 2. Dynamics of change of kinetic energy (a) and change of concentration of heavy fraction (b) at t=0.6 and the angular speed of the propeller =2.



a) b)

Figure 3. Dynamics of change of kinetic energy (a) and change of concentration of heavy fraction (b) at t=0.6 and the angular speed of the propeller =10

References

[1] Abakumov G.A., Fedoseev V.B. Physico-cgemicalprocesses in centrifugal and gravitational fields. Chemistry Reviews. V.24.Pp.41-86, 2001.

[2] 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). – P. 2383–2393. 2004.

[3] Magnussen B. F. “The eddy dissipation concept: a bridge between science and technology” // in Proceedings of the ECCOMAS Thematic Conference on Computational Combustion, 2005.