MODELLING OF STRUCTURED DISPERSE SYSTEMS BEHAVIOR UNDER DYNAMIC CONDITIONS

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This investigation was devoted to modelling of dispersions properties under dynamic conditions. The behavior of disperse systems under dynamic nonequilibrium conditions is of considerable interest for both theory and practical applications, because it is characteristic of diverse chemical technological processes. Problems related to the behavior of dispersions under dynamic conditions are considered within the framework of the physicochemical dynamics of disperse systems [1], a new direction that extends the traditional approach to studying the properties of disperse systems predominantly under static conditions.

The existing numerical methods were adapted for solution of equations of the particles motion in viscous liquid [2, 3]. The computer program for simulation of the monodisperse and polydisperse systems flow was developed. These dispersions can contain the nanodisperse components in Newtonian viscous medium. The surface forces (the forces of the dispersion attraction and electrostatic repulsion) acting between particles, the hydrodynamic and inertia forces, as well as Brownian forces which cause the thermal motion of particles were accounted for in the model. The physical-chemical non-uniformity of the particles surface (the lyophobic- lyophilic patchiness) was taken into account while calculations.

The computer program which realizes this approach and allows to carry out the numerical experiments on the investigated systems behavior under indicated conditions in the wide range of the shear rates and the vibration parameters variation.

It has been demonstrated the laws of formation of internal microstructure in dispersions; the thixotropic properties of dispersions have been simulated. It was shown a process of the particle coagulation with formation of the large and dense aggregates (clasters) which can be later precipitated, so dispersion losses both aggregative and also sedimentation stability. The influence of physical-chemical heterogeneity of the particles surface (its lyophilic-lyophobic patchiness) on the character of dispersion flow as well as the influence of the dispersion composition on structure formation processes have been simulated. It has been shown a mechanism of the layered structure formation in dispersion under conditions of shear and orthogonal vibration. These layers were revealed earlier experimentally [1, 4] and investigated theoretically [5]. The conditions of possible destruction of such structures were indicated that allows to reach the isotropic dynamical state with significant diminution of the dispersion apparent viscosity.

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References

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