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OPTIMIZATION OF PARALLEL COMPUTATIONS FOR SIMULATING WATER PURIFICATION PROCESSES BY ELECTROMAGNETIC METHOD

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Abstract: The problems of computer simulating of technological processes are currently relevant and demanded practice. Computer and supercomputer simulating allows you to explore the details of complex technological processes with the necessary degree of detailing. However, the effective use of high performance equipment is not a trivial matter. In the present paper, the problem of implementing parallel computations for simulating the process of water purification by an electromagnetic method is discussed. The problem of water purification is actual in many areas of the economy, including the food and the medical industry. To solve it, natural experiments and mathematical modeling based on hydrodynamic models are applied. In our study, the electromagnetic purification process is described by a complex hydrodynamic model. The model includes the dynamics of charged ions of iron and its salts that move in the water flow of the purification system. The task is solved in a complete three-dimensional non-stationary formulation for real geometry conditions. The resulting system of equations (obtained from the system of Navier-Stokes equations) is formulated in terms of the vector potential of flow, the vortex, the concentration of impurity particles, and the potential of the electric field. As the main numerical approach, an explicit scheme on time and a finite volume method are used. The main numerical approach is realized on non-uniform triangular-prismatic grid. A discrete model has a large volume of spatial mesh (several million cells and more), as well as the complexity of real geometry. Therefore, the use of parallel computations on high-performance multiprocessor systems becomes relevant. For parallel realization of the developed numerical approach, the domain decomposition technique for area and load balancing for calculators are used. As parallel programming technologies, MPI and OpenMP libraries were used. Approbation of the parallel code was carried out on systems with central and vector processors Intel Xeon and Intel Xeon Phi. Studies of efficiency and acceleration during parallel processing helped to determine the optimum calculated configurations. The large volume of calculations of the simulated process was carried out for several characteristic geometric forms of the purification system, and also for several values of the water flow velocity and constant magnetic field. Within the framework of the computer experiments, the flow features in the purification system were obtained and also the final value of impurity concentration in a purified aqueous medium.