Numerical modeling of chemical kinetics with using of supercomputers*

I.G. Chernykh[1], M.S. Antonova[2]

Institute of Computational Mathematics and Mathematical Geophysics SBRAS[1],
Novosibirsk State University[2]

Modeling of detailed chemical kinetics impossible without supercomputers due to the large (more than thousand) size of the chemical reaction system. Modern hybrid (CPU + GPU) supercomputers give possibility to research very large problems efficiently.

1. Introduction

Complex numerical modeling of fluid flows and chemical processes in chemical reactors plays important role in development of new and upgrading of existing chemical processes and chemical reactors [1]

2. Application of CHEMPAK GPU based solvers

There are many solvers for modeling of chemical kinetics tasks was written and a lot of articles with new efforts in supercomputer modeling in chemical engineering journals appear. New solver for CHEMPAK [2] software package was developed by authors. Table 1 shows the tests results of CHEMPAK GPU based solver.

Table 1. Comparison of Intel ODE solver and CHEMPAK GPU solver performance

Solver		Time, s	
		1000 chemical reactions with 500 species synthetic test	Propane conversion test
Intel_ODE [9]	dodesol	2.121614	0.2964019
	Rkm9st	0.9516060	19.12572
CHEMPAK GPU solver		0.15	0.0004

Literature

1. Snytnikov V.N., Mischenko T.I., Snytnikov Vl.N., Chernykh I.G. A reactor for the study of homogeneous processes using laser radiation energy // Chemical Engineering Journal. 2009. Vol. 150. P. 231-236.
2. Chernykh I.G., Stoyanovskaya O.P., Zasypkina O.A.. ChemPAK Software Package as an Environment for Kinetics Scheme Evaluation // Chemical Product and Process Modeling. 2008. Vol. 4 (4,3). P. 1-14.

* This work was partially supported by Federal Program Research and development on priority directions of scientific-technological complex of Russia in 2007-2013" of the Federal Agency for Science and Innovation, Russian Ministry Education and Science. Also this work was partially supported by Integration SB RAS project No. 130.