

Distributed Software System for Data Evaluation and Numerical Simulations of Atmospheric Processes

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A distributed software system for numerical simulations of atmospheric physicochemical processes is presented. It is a multi-layer Java based system for theoretical investigation of complex interactions of atmospheric trace gases and ice particles. The simulations are based on the fundamental theory of Langmuir adsorption and second Ficks law applied for adsorption, desorption and diffusion processes. The system consists of three basic layers: (1) input/output interface layer, (2) dispatcher layer, (3) grid-based layer for simulations distributed over multiple machines. The core software module used in level (3) is based on previously published by us software prototype for simulations of adsorption, desorption and diffusion in a closed system and Flow Tube Reactor. The main task of the current distributed system is to derive numerical estimations of several significant constants: adsorption/desorption rates, ice entry rate, ice bulk diffusion coefficient and etc. The constants are estimated by comparison of experimental signals from a Flow Tube Reactor and simulations results from the system described in this paper. The difference between both curve profiles is minimized by an exhaustive search in a multi-dimensional parameter space which represents all possible values of the physicochemical constants. The dispatcher layer of the system defines several regions of the multi-dimensional parameter space. For each region, a separate task is configured and dispatched to a node from a computer GRID or cluster. The entire parameter space is searched in a parallel manner and after that all results are united in order to find the global minimum of the difference between experimental and simulated curves. The results are printed via the input/output software layer. Example kinetic simulations performed by the software system are presented and discussed.