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O-07. Sergey Smyshlyaev: Chemical solver benchmark testing

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Present Chemistry Transport Models (CTM) involve complex and coupled phenomena including transport, chemistry, radiative, and mass transfer process. The performance of numerical technique in solving differential equations of gas-phase chemistry is the most important factor in determining the overall computational cost for any CTM. Operator splitting technique is the fundamental computational framework of the almost all CTMs. Consequently, chemical transformations may be treated separately and effective chemical solvers may be constructed to use in the atmospheric models of different type.

In this work we explored how the different simplified chemical solvers affect the accuracy and computational cost of the box chemistry model based on comparison to benchmark calculations for the several spatial points. Among the chemical solvers selected, one is fully implicit solver, one chemical solver using quasi-steady state approximation, and two are hybrid solvers. The chemical solver constructed based on Shimazaki scheme has the best overall performance both for stratosphere and troposphere and is pointed to be the most robust in dealing with CTM and Air quality models.

By applying this solver to a global interactive three-dimensional Chemistry-Climate-Model (CCM) we demonstrate that this solver may be effective for sophisticated atmospheric modeling.