Atmospheric Chemistry and Physics
An Interactive Open Access Journal of the European Geosciences Union

Atmos. Chem. Phys., 6, 187-195, 2006
www.atmos-chem-phys.net/6/187/2006/

Technical note: Simulating chemical systems in Fortran90 and Matlab with the Kinetic PreProcessor KPP-2.1

A. Sandu[1] and R. Sander[2]
[1]Department of Computer Science, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24060, USA
[2]Air Chemistry Department, Max-Planck Institute for Chemistry, Mainz, Germany

Abstract. This paper presents the new version 2.1 of the Kinetic PreProcessor (KPP). Taking a set of chemical reactions and their rate coefficients as input, KPP generates Fortran90, Fortran77, Matlab, or C code for the temporal integration of the kinetic system. Efficiency is obtained by carefully exploiting the sparsity structures of the Jacobian and of the Hessian. A comprehensive suite of stiff numerical integrators is also provided. Moreover, KPP can be used to generate the tangent linear model, as well as the continuous and discrete adjoint models of the chemical system.

Final Revised Paper (PDF, 209 KB) Supplement (1069 KB) Discussion Paper (ACPD)

Citation: Sandu, A. and Sander, R.: Technical note: Simulating chemical systems in Fortran90 and Matlab with the Kinetic PreProcessor KPP-2.1, Atmos. Chem. Phys., 6, 187-195, 2006. Bibtex EndNote Reference Manager