Final report on activities and findings under DOE grant "Interactive Photochemistry in Earth System Models to Assess Uncertainty in Ozone and Greenhouse Gases"

#DE-SC0007021 (University of California Irvine)

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Summary:

Atmospheric chemistry controls the abundances and hence climate forcing of important greenhouse gases including N2O, CH4, HFCs, CFCs, and O3. Attributing climate change to human activities requires, at a minimum, accurate models of the chemistry and circulation of the atmosphere that relate emissions to abundances. This DOE-funded research provided realistic, yet computationally optimized and affordable, photochemical modules to the Community Earth System Model (CESM) that augment the CESM capability to explore the uncertainty in future stratospheric-tropospheric ozone, stratospheric circulation, and thus the lifetimes of chemically controlled greenhouse gases from climate simulations. To this end, we have successfully implemented Fast-J (radiation algorithm determining key chemical photolysis rates) and Linoz v3.0 (linearized photochemistry for interactive O3, N2O, NOy and CH4) packages in LLNL-CESM and for the first time demonstrated how change in O2 photolysis rate within its uncertainty range can significantly impact on the stratospheric climate and ozone abundances. From the UCI side, this proposal also helped LLNL develop a CAM-Superfast Chemistry model that was implemented for the IPCC AR5 and contributed chemical-climate simulations to CMIP5.

Key Tasks Accomplished:

The team of Earth/climate and computer scientists has succeeded in tasks that have added unique scientific capability to the Community Earth System Model (CESM). These include *inter alia*:

1) Implementation of a new Fortran 90 version of photolysis codes for key atmospheric chemical species (Fast-J codes v7.0+) into the Community Atmosphere Model version 5 (CAM5, the atmospheric component of CESM) at LLNL. The Fast-J photolysis module has been upgraded in two major ways specifically for CESM. For one, the cross-sections and quantum yields (particularly for the Volatile Organic Carbons, VOCs) were fully revised to most recent values assessed by Jet Propulsion Laboratory (JPL Publications 06-2 and 09-31) and the new photolysis of VOCs now incorporate a pressure interpolation (with assumed lapse rate) instead of just a temperature interpolation as has been done for cross sections in most photolysis codes to date. The task is completed in collaboration between the UCI ESS team and the LLNL members.

2) The new numerical scheme (Linearized Ozone, Linoz v3.0) to parameterize the stratospheric photochemistry (interactive O_3, CH_4, N_2O and NO_y), as a drop-in replacement for Linoz v2 code, is already implemented as F90 codes in CAM-LLNL. These are critical to running climate ensembles when the cost of doing fulstratospheric chemistry (as in WACCM) is deemed as not critical. Linoz v3 allows for background evolution of CH_4 and N_2O for projecting future chemistry.

3) Analysis of CAM5-LLNL results examining photolysis uncertainties with updated Fast-J (photolysis code) and Linoz (stratospheric chemistry code) led to the publication (Hsu et al., 2013) from the collaboration between the UCI ESS and LLNL members. In this study, we show the first time how uncertainty in O2 photolysis rate (consistent with known uncertainties) can propagate into the climate dynamics. Changes in O2 photolysis rate at 30 percent level can significantly change the temperature and static stability near the tropopause through change in O3 production. Consequently, the height of tropopause, the route of wave propagation from troposphere, and the high-latitude variability of the polar vortices are significantly affected while the time-mean Brewer-Dobson circulation is not. Moreover, because these simulations were carried out on both CAM4 and CAM5, we found that the degree of changes in high-latitude variability (for the same perturbation in chemistry) also depend on the basic state of the lower stratosphere.

4) UCI computer scientists (Nicolau and Veidenbaum) examined re-writes of the block tri-diagonal solver (identified here as the bottleneck in Fast-J execution) with Nvidia and Fermi GPUs. We have shown on Fermi GPU that, for matrix computations, we improve accuracy by up to a whole digit and increase performance by up to 27%, over and beyond the performance offered by the GPU itself, which can be up to 3x faster for double precision and 6x faster for single precision (likely adequate for Fast-J).

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C. D. Holmes, M. J. Prather, and G. C. M. Vinken (2014) The climate impact of ship NOx emissions: an improved estimate accounting for plume chemistry, Atmos. Chem. Phys., 14, 6801–6812, doi:10.5194/acp-14-6801-2014

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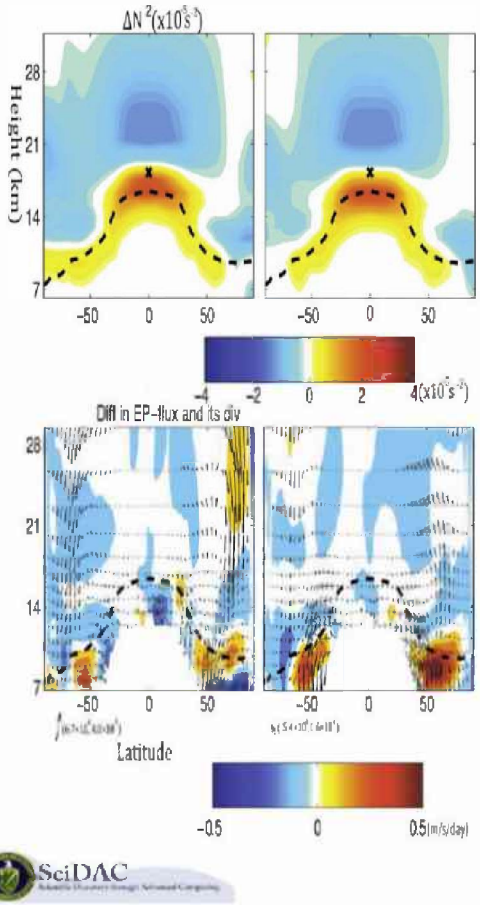
J. Hsu, M.J. Prather, D. Bergmann, P. Cameron-Smith (2013), Sensitivity of stratospheric dynamics to uncertainty in O3 production, J. Geophys. Res. Atmos., 118, 8984–8999, doi:10.1002/jgrd.50689.

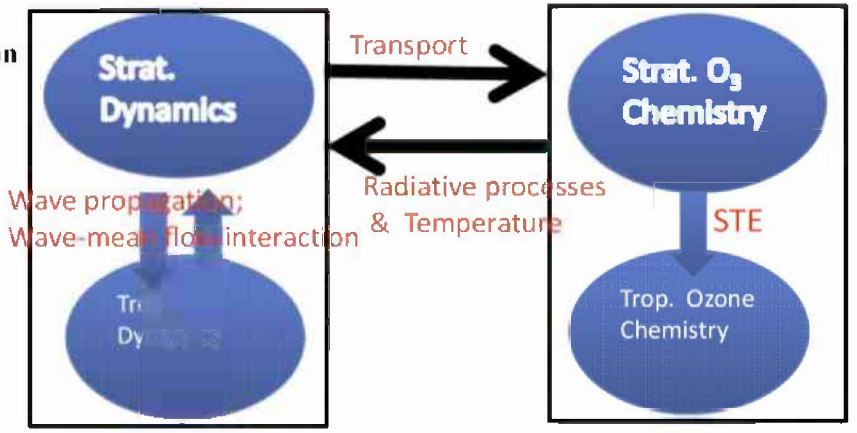
C. D. Holmes, M. J. Prather, A.O. Søvde, G. Myhre (2013) Future methane, hydroxyl, and their uncertainties: key climate and emission parameters for future predictions, Atmos. Chem. Phys., 13, 285–302, doi:10.5194/acp-13-285-2013

M.J. Prather, C.D. Holmes, J. Hsu (2012), Reactive greenhouse gas scenarios: Systematic exploration of uncertainties and the role of atmospheric chemistry, Geophys. Res. Lett., 39, L09803, 5 pp., doi:10.1029/2012GL051440.

Sensitivity of stratospheric dynamics to O_3 production

J.Hsu (UCI), M.Prather (UCI), D.Bergmann (LLNL), P. Cameron-Smith (LLNL), *J. Geophys. Res. Atmos., 118*: 8984–8999, doi:10.1002/jgrd.50689 (2013)





This research is the first to examine how O_3 production perturbed within its uncertainty range through O_2 cross sections in Hertzberg Continuum can change the behavior of stratospheric temperature and circulation on time scales from the annual cycle to interannual variability. For the lower range of O_2 cross sections (-30%), we find increased static stability or stratification near the tropopause (left figure, top panels). As a consequence, it changes the dynamical coupling between the stratosphere and troposphere (left figure, bottom panels). The static stability, which is sensitive to the O_3 just above the tropical tropopause, is a barrier for not only wave propagation but also the exchange of greenhouse gases between stratosphere and troposphere. In addition to basic chemical uncertainties, other factors affecting the tropopause O_3 include the cross-tropopause flux of very short lived bromine or iodine compounds from anthropogenic or oceanic sources.

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