Studying Atmospheric Chemistry with MCMC

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A model describing chemical reactions in the stratosphere ([1]) is studied with MCMC methods. The model is a large ODE system consisting of 33 components, roughly 150 reactions and 150 reaction rate parameters. Thus, it is a good case study for adaptive MCMC methods designed for high-dimensional problems. In this case, the Delayed Rejection Adaptive Metropolis (DRAM, [2]) is succesfully applied.

Three types of MCMC analyses are considered. First of all, the dynamics of the system are studied with accurate simulated data to reveal the governing reactions in different circumstances (temperature, day/night, pressure). The results may be used as basis for model reductions - this is a new potential application are for MCMC methods.

Secondly, the system is considered from the point of view of data assimilation and design of experiments: the goal is to find out which components of the system are identified with certain measurements.

In addition, a current issue in atmospheric chemistry is studied with MCMC. New lab experiments suggest that one of the reaction rates would be *"almost an order of magnitude smaller than previously thought"* ([3]). The effect of uncertainty in model parameters can be determined using MCMC.

References

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[3] Quirin Schiermeier. Chemists Poke Holes in Ozone Theory. *Nature News*, published online 26.9.2007.