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Atmospheric Chemistry and Physics Discussions

Interactive comment on "A comparison of chemical mechanisms using Tagged Ozone Production Potential (TOPP) analysis" *by* J. Coates and T. M. Butler

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Coates and Butler have produced a very interesting and valuable research paper. Detailed process based studies like this are especially valuable to mechanism developers and air quality modelers.

The comparison of the RADM2 (mislabeled in the paper as RADM, an earlier mechanism), RACM and RACM2 mechanisms was particularly interesting to me. The available laboratory has vastly increased from what was available in 1990 and 1997 when the RADM2 and RACM mechanisms were published. Now RADM2 and RACM are

relics of the past. RACM2 is based on much more recent data especially for aromatic compounds. We only use RACM2 for air quality simulations in my research group. Likewise the US EPA has implemented RACM2 in its most recent version of the Community Multi-scale Air Quality Model (CMAQ) and does not include the earlier obsolete versions. Much the same could be said about the other series of mechanisms.

The authors compare the reduced mechanisms with the explicit MCM. The extra detail does not greatly change the estimated TOPP from VOC on the first day. In line with the simplifications the degradation paths in the reduced mechanisms are shorter and that affects ozone production on subsequent days.

One problem with the paper is that the authors appear to assume that the MCM is "correct". There is a vast difference between being more explicit and having a greater content of laboratory based information. Actually the authors are comparing three different approaches to developing air quality mechanisms: explicit, aggregation by functional group and aggregation by molecule (or reactivity). The most recent versions of all these mechanisms were developed from the same laboratory databases. Even though the MCM has thousands of reactions, its information content is not much more than the reduced mechanisms; my guess is that MCM's information advantage is probably not much more information than 10 to 20%.

This raises and interesting discussion question: Have highly explicit mechanisms taught us anything new and important about the production of air pollutants? For ozone the answer is a resounding "NO" while for secondary organic aerosols its probably "Maybe".

Interactive comment on Atmos. Chem. Phys. Discuss., 15, 12389, 2015.