Trip report, Atmospheric Chemical Mechanisms Conference, December 8-11, 2010, University of California, Davis, attended by Mark Estes.

Atmospheric chemical mechanisms are models of the chemistry occurring in the atmosphere. Chemical mechanisms can be nearly complete summaries of the current state of knowledge about atmospheric chemistry (e.g., the Master Chemical Mechanism), or they can be condensed versions of the chemistry that are simple enough to use operationally in photochemical grid modeling and air quality control strategy modeling (e.g. the Carbon Bond or SAPRC mechanisms). The purpose of this conference was to discuss the latest research on the greatest uncertainties that currently exist in atmospheric chemical mechanisms. In total, there were 53 presentations and 54 posters presented at the conference.

Summary of important findings:

- The new, more accurate OH+NO2 reaction rate observed by Mollner is likely to have a large effect upon ozone sensitivity to VOC and NOx emissions in urban areas. The new rate constant is smaller, indicating that NOx will persist longer in the urban environment. In modeling experiments for Los Angeles using the new rate, the size of the VOC-sensitive areas increased substantially when the new reaction rate replaced the old one. (Cai, Cohan)
- HOx radicals are regenerated during the oxidation of isoprene and its products. Previously, it was thought that isoprene oxidation was primarily a radical sink, but the new findings indicate it can be a radical source. There are several newly-proposed mechanisms; none can fully explain the radical observations. The current chemical mechanisms do not make enough radicals, so adding a new source of radicals will be very useful. (Dillon, Archibald, Stevens, Orlando)
- HONO is being formed in urban conditions, and acts as another important source of radicals. There are several newly-proposed mechanisms for HONO formation, some of which appear valid, but none can fully explain the HONO observations. (Bejan, Kleffman, Stutz, Pilling, Rappenglück, Czader)
- Aromatic oxidation is exceedingly complex, and is not well depicted by current mechanisms. Ring-opening reactions can create highly reactive multifunctional products, but current experiments haven't fully identified all of the products. Aromatic nitrates appear to form easily, and photolyze easily to create HONO, but alone cannot explain the discrepancies in HONO concentrations. (Atkinson, Elrod, Bejan)
- Organic nitrate formation can apparently affect ozone formation substantially, especially isoprene-derived nitrates. Alkyl nitrates could play a role as a radical and NOx sink, like HNO3, and could also play a role in recycling NOx. (Pratt, E. Brown, Xie, Orlando)
- In spite of the chemical mechanisms' inability to simulate some processes, our state of knowledge is apparently good enough to formulate policies that have greatly improved air quality throughout the United States. (Magliano, Wallington)

- Modeling of secondary organic aerosols has improved dramatically. Eventually, particulate matter modeling will need to be included even in ozone modeling, because ozone formation reactions occur in both the gas phase and the aerosol phase. (Pilling, Ziemann)
- The Carbon Bond mechanism is still recommended by EPA for SIP development, due to its ease of use and ability to predict ozone concentrations. The SAPRC mechanism is not oriented solely toward simulating ozone, but it requires separate and more elaborate processing of the emissions inventory than the Carbon Bond mechanism. The Master Chemical Mechanism is the most accurate summary of the state of knowledge, but it is also incomplete, and would require an even more meticulously speciated emissions inventory than SAPRC. MCM also would require huge computer resources if used on a routine basis. (Luecken, K. Baker, Carter, Pilling, Q. Ying, Volkamer)
- Chemical mechanism research operates on a shoestring budget, but billion dollar decisions are based upon it. Perhaps industry could be persuaded to help advance smog chamber and laboratory experimental research, since it can have a large effect upon our understanding of ozone and particulate matter pollution. (Carter, Jeffries)