

## RSAC Meeting Summary

The ARB's Reactivity Scientific Advisory Committee (RSAC), consisting of John Seinfeld (Chair), Roger Atkinson, Jack Calvert, Harvey Jeffries, Jana Milford, and Ted Russell, met on March 25, 2009. The purpose of this meeting was to formulate recommendations to the ARB on the science related to the SAPRC-07 chemical mechanism and its associated MIR values. After an introduction by the Bart Croes (ARB's Research Division Chief), Bill Carter gave a presentation on his recently developed SAPRC-07 chemical mechanism, and derived MIR tables. This was followed by presentations by four SAPRC-07 peer reviewers (Dick Derwent - rdscientific, UK; Merched Azzi - CSIRO, Australia; Rob Harley - UC Berkeley; and Bill Stockwell - Howard University), as well as Bill Carter's response to the peer reviews.

Dr. Carter's presented an overview of the SAPRC mechanisms, and highlighted the updates made for the latest version, SAPRC-07. He reviewed the anticipated changes in ambient ozone predictions that would result from its application. Subsequently, Dr. Carter reviewed the changes in ozone reactivity (MIR) values that would ensue from the adoption of SAPRC-07. Finally, he presented recommendations for further work.

Dr. Derwent's review compared incremental ozone impacts of 121 compounds calculated using the SAPRC-07 mechanism and version 3.1 of the Master Chemical Mechanism (MCM). Although he found significant differences for certain compounds, he concluded that for most compounds, the ozone impacts calculated using the two mechanisms were consistent. Dr. Carter concluded that this data did not clearly indicate the need to change SAPRC-07.

Dr. Azzi's review compared the ability of the SAPRC-07 mechanism, and also SAPRC-99 and MCM 3.1, to simulate the results of isoprene, toluene, *m*-xylene, and evaporated fuel in environmental chamber experiments carried out in Australia at the Commonwealth Scientific and Industrial Research Organisation (CSIRO). SAPRC-07 performed reasonably well in simulating these data. The results indicated some problems with the toluene mechanism that merit further investigation, but did not clearly indicate the need to change that mechanism.

Dr. Harley's review discussed implementing the mechanism in 3-D modeling, and brought up several important issues. These include the need to develop a version of the mechanism that can be used for sensitivity studies on the uncertain but important OH + NO<sub>2</sub> reaction rate constant, and the need to update the base ROG mixture used to derive the fixed parameter version of the mechanism. Dr. Carter said this work should be given priority for future research.

Dr. Stockwell's review compared the individual chemical reactions and rate constants in the SAPRC-99, RACM2 (Regional Atmospheric Chemistry Mechanism, version 2), and CB05 (Carbon Bond, 2005) mechanisms. Dr. Stockwell also commented on differences among these mechanisms and assessed their chemical reasonableness. He concluded that SAPRC-07 represented the state-of-the-science, but had several criticisms and recommendations. In two cases, his comments lead to Dr. Carter making changes to the SAPRC-07 mechanism.

Dr. Carter revised the SAPRC-07 mechanism as a result of Dr. Stockwell's peer review and his own discovery of some errors. Using the revised mechanism, Dr. Carter re-evaluated the environmental chamber data, and recalculated the MIR and other reactivity scales. He incorporated these into a revised version of the SAPRC-07 mechanism documentation report that is available at the website <http://www.cert.ucr.edu/~carter/SAPRC>. The modifications did not result in any significant changes to the fits to the chamber data and did not justify changes to adjustable parameters for any compounds. These reactivity scale changes were minor in the MIR

scale (less than 4% for all compounds). However, in a few cases, changes of up to 30% were made to the lower NO<sub>x</sub> scales because the affected reactions are more important in low-NO<sub>x</sub> conditions.

After the RSAC discussed the peer reviews and Dr. Carter's response, they found that the use of the SAPRC-07 chemical mechanism represents the state-of-the-science in urban atmospheric chemical reaction mechanisms. In addition, the RSAC found that the updated MIR values were arrived at in an appropriate scientific manner. Following is the letter sent from the RSAC Chair to the ARB's Research Division Chief.

April 14, 2009

Mr. Bart Croes, Chief  
Research Division  
California Air Resources Board  
1001 I Street  
Sacramento, Ca 95814

Re: Reactivity Science Advisory Committee (RSAC)

Dear Bart,

I am writing to report to you that the ARB Reactivity Scientific Advisory Committee has reviewed the peer review reports on the SAPRC-07 chemical mechanism prepared by R.G. Derwent, M.E. Jenkin and M. J. Pilling of the U.K, M. Azzi, S. White and D. Angove of CSIRO in Australia, R. Harley of U.C. Berkley, and W. R. Stockwell of Howard University, response to the peer reviewers' comments prepared by W. P.L. Carter, and the proposed amendments to the table of MIR values prepared by W.P.L. Carter. At its March 25, 2009 meeting, the RSAC accepted the peer review and finds that the use of the SAPRC-07 chemical mechanism as representing the state-of-the-art in urban atmospheric chemical reaction mechanisms. In addition, the RSAC finds that the updated MIR values were arrived at in an appropriate scientific manner.

Sincerely,

John H. Seinfeld

cc: RSAC members  
D. Luo, CARB