Revisions to the Final Report
"Development of the SAPRC-07 Chemical Mechanism and Updated Ozone Reactivity Scales",
by William P. L. Carter

CARB Contract 03-318
Date of 2nd Draft: June 15, 2007
Date of Revised Final Report: August 31, 2007.

Comment	Response
CARB Requests: Change the title from "Documentation of the SAPRC-07 Chemical Mechanism and Updated Ozone Reactivity Scales" to "Development of the SAPRC-07 Chemical Mechanism and Updated Ozone Reactivity Scales",	Report renamed
Prioritize recommended research	A final sub-section to the "Recommendations" section at the end of the report was added discussing how I see priorities.
Consider addressing ACC's request to add MIR's for unspeciated mixtures.	Unspeciated alkane and aromatic mixture categories were added to the reactivity tabulation. No recommendations are made for mixtures where the aromatic fraction is unknown.
Revise MIR values for amines based on the ongoing consumer products project if time permits.	Time does not permit adding estimated reactivities for amines based on the results of this project, which is still ongoing. However, results to date indicate that the draft report had incorrect mechanisms for the amines, so all amine mechanisms and reactivities given in this report have been deleted. The report states that these will be updated later once the consumer products project is completed.
Other Corrections and Revisions: Table 1, which showed changes in rate constants in the base mechanism, had several errors	Errors in this table, which included some duplicated reactions and an incorrect computation of the percent change, were corrected. No changes were made to the actual mechanism, and most of the qualitative information in the original table was correct.
The reactions of the peroxy radical operators do not represent the loss of HO_2 when peroxy radicals react with HO_2.	The error is in Reactions BR08 and BR13, which should be changed from "RO2C + HO2 = HO2" and "RO2XC + HO2 = HO2" to "RO2C + HO2 =" and "RO2XC + HO2 =", respectively. This error will have a substantial effect on simulations of HO_2 under low NO_x conditions, but should generally have a negligible effect on O_3. This error was corrected and the mechanism listing and all reactivity scales have been corrected. The figures showing ozone or ozone changes in the reactivity scenarios were also replaced. The changes in reactivity values were less than 3% in all cases. All the chamber runs were also re-simulated, and the change in $\Delta([O_3]-[NO])$, which was used as the primary metric in the mechanism evaluation, was found to be less than 5% in all cases,

Comment	Response
	with no significant changes in biases. Therefore, the tabulations and figures in the section describing the mechanism evaluation against chamber data were not replaced. The amount of work required to do this would have been considerable, and the result would be hardly noticeable.
New chamber data for the ongoing consumer project indicate that the amines mechanisms in the draft report is incorrect.	See discussion of "MIR values for amines", above.
The comparisons of O_3 in the base case MIR, MOIR, and EBIR scales in Figure 16 are not done on an equal NO_x basis, because the NO_x is adjusted separately for each mechanism to yield MIR, MOIR, or EBIR conditions.	Figure 16 was revised to show only the maximum O_3 concentrations in the scenario and a new Figure 17 was added showing the O_3 changes caused by the mechanism update when the NO_x was adjusted separately and also when the NO_x was held constant at the levels used in the SAPRC-99 scenarios. The results for the MIR and EBIR scenarios were quite different, and the discussion was modified accordingly. The results are more consistent when the NO_x is not adjusted, and the change is much greater for the MIR scenarios.
The reference list indicated that the updates to the emissions speciation database files are in preparation.	The emissions speciation database files at http://www.cert.ucr.edu/~carter/emitdb have now been updated to the new mechanism, and the reference list now references this as the August 31 version.