State of California
AIR RESOURCES BOARD

Resolution 03-32

December 11, 2003

Agenda Item No.: 03-10-5

WHEREAS, the Air Resources Board has been directed to carry out an effective research program in conjunction with its efforts to combat air pollution, pursuant to Health and Safety Code sections 39700 through 39705;

WHEREAS, a research proposal, number 2542-232, entitled "Updated Chemical Mechanism for Airshed Model Applications," has been submitted by the University of California, Riverside;

WHEREAS, the Research Division staff has reviewed and recommended this proposal for approval; and

WHEREAS, the Research Screening Committee has reviewed and recommends for funding:

> Proposal Number 2542-232 entitled "Updated Chemical Mechanism for Airshed Model Applications," submitted by the University of California, Riverside, for a total amount not to exceed $166,132.

NOW, THEREFORE BE IT RESOLVED, that the Air Resources Board, pursuant to the authority granted by Health and Safety Code section 39703, hereby accepts the recommendation of the Research Screening Committee and approves the following:

> Proposal Number 2542-232 entitled "Updated Chemical Mechanism for Airshed Model Applications," submitted by the University of California, Riverside, for a total amount not to exceed $166,132.

BE IT FURTHER RESOLVED, that the Executive Officer is hereby authorized to initiate administrative procedures and execute all necessary documents and contracts for the research effort proposed herein, and as described in Attachment A, in an amount not to exceed $166,132.

ATTACHMENT A

"Updated Chemical Mechanism for Airshed Model Applications"

Background

Air quality simulation models are used to assess the effectiveness of the control strategies and to develop plans and regulations for achieving air quality standards by regulatory agencies. An example is the use of urban airshed models in the State Implementation Plan (SIP) development. Among many factors that affect the model performance, the gas-phase chemical mechanism that represents the gas-phase chemical reactions involved in the model is a critical component for predictions of pollutants such as ozone, particulate matter, and other secondary pollutants (e.g., air toxics).

Under the sponsorship of the ARB, a detailed version of atmospheric chemical mechanism (referred to as SAPRC-99) was developed in 1999 by Dr. Carter at UCR. This mechanism was peer-reviewed and found to be a state-of-the-science mechanism. It has been widely used in many regulatory and research applications. For example, this mechanism was recently used in updating the reactivity scales for volatile organic compounds (VOCs) for the California's aerosol coatings regulation. Since the chemical information used in the SAPRC99 mechanism is evolving and improving, it is crucial that the mechanism is reviewed and updated periodically to be consistent with the up-to-date atmospheric science.

The most cost-effective and reliable way to test the accuracy of a chemical mechanism is to compare its predictions against results of environmental chamber experiments that simulate the range of conditions in the atmosphere. Due to the experimental limitations, most of the chamber experiments that have been carried out lack measurement data for important intermediate and product species. This limits the level of detail to which the mechanisms can be evaluated, and the types of air quality impact predictions that can be assessed. The U.S. EPA funded Dr. Carter to develop a "next generation" environmental chamber facility to provide an improved capability for more comprehensive mechanism evaluation under more realistic conditions (e.g., low NOx conditions). This project will take advantage of this advanced facility.

Objective

The overall objective of this project is to develop and comprehensively evaluate updated detailed and condensed SAPRC atmospheric mechanisms for use in photochemical airshed models for predicting formation of secondary gas-phase pollutants (e.g., ozone and air toxics).

Methods

Both experimental and model studies are proposed to accomplish the objectives of this project. The proposed project will incorporate the most recent laboratory and environmental chamber data, improve representations for aromatics, develop a capability of representing chlorine chemistry, conduct environmental chamber

experiments, develop a condensed mechanism for model applications requiring computational efficiency, and implement the updated mechanisms into a regional air quality model.

Expected Results
The product from this effort will be updated detailed and condensed versions of SAPRC chemical mechanism for airshed model applications.

Significance to the Board
The results of this project will provide the ARB, other regulatory agencies, and researchers with improved and more up-to-date models for the prediction of secondary pollutants, and lead to more scientifically sound control plans and strategies.

Contractor:
University of California, Riverside

Contract Period:
18 months

Principal Investigator (PI):
William P. L. Carter, Ph.D.

Contract Amount:
$166,132

Cofunding:
The U.S. EPA has funded Dr. Carter to develop the next-generation environmental chamber facility needed for evaluating gas-phase and gas-to-particle atmospheric reaction mechanisms. Specifically, this facility is designed for mechanism evaluation under more realistic conditions (e.g., low NO_x conditions). Considering the significant amount of the U.S. EPA funding allocated for the chamber work, this project is considered significantly cost-effective.

Basis for Indirect Cost Rate:
The State and UC System have agreed to a ten percent indirect cost rate.

Past Experience with this Principal Investigator:
The principal investigator, Dr. William Carter, is one of the pioneers in developing the gas-phase atmospheric chemical mechanism. He has published approximately 75 journal articles and almost 70 technical reports in the areas of atmospheric chemistry, chemical mechanism development, and VOC reactivity assessment. He has completed several projects on the gas-phase chemical mechanism developments and has always delivered a quality product at a very reasonable cost. Currently, the Principal Investigator is conducting two ARB projects on reactivity assessment and low NO_x evaluation, respectively.

BUDGET SUMMARY

The University of California, Riverside

"Updated Chemical Mechanism for Airshed Model Applications"

DIRECT COSTS AND BENEFITS			
1.	Labor and Employee Fringe Benefits	$ 112,546	
2.	Subcontractors	$ 0	
3.	Equipment	$ 0	
4.	Travel and Subsistence	$ 0	
5.	Electronic Data Processing	$ 825	
6.	Reproduction/Publication	$ 0	
7.	Mail and Phone	$ 0	
8.	Supplies	$ 13,544	
9.	Analyses	$ 0	
10.	Miscellaneous*	$ 26,525	
	Total Direct Costs		$ 153,440
INDIRECT COSTS			
1.	Overhead	$ 12,692	
2.	General and Administrative Expenses	$ 0	
3.	Other Indirect Costs	$ 0	
4.	Fee or Profit	$ 0	
	Total Indirect Costs		$ 12,692
TOTAL PROJECT COSTS			**$ 166,132**

*** CE-CERT is a permanent off-campus facility, federal regulations require us to account for facilities rental as a direct cost. Facilities rental is charged based on 20.9% of Modified Total Direct Costs (MTDC). MTDC consists of total direct costs minus equipment, facilities rental, graduate student partial fee remission/health insurance (included benefits), and subcontracts over $25,000.**