

State of California  
AIR RESOURCES BOARD

**RESEARCH PROPOSAL**

Resolution 12-44

December 6, 2012

Agenda Item No.: 12-9-4

WHEREAS, the Air Resources Board (ARB or 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 2751-275 entitled "Improving Chemical Mechanisms for Ozone and Secondary Organic Carbon," has been submitted by the University of California, Davis;

WHEREAS, in accordance with Health and Safety Code section 39705, the Research Screening Committee has reviewed and recommends for funding:

Proposal Number 2751-275 entitled "Improving Chemical Mechanisms for Ozone and Secondary Organic Carbon," submitted by the University of California, Davis, for a total amount not to exceed \$450,024.

WHEREAS, the Research Division staff has reviewed Proposal Number 2751-275 and finds that in accordance with Health and Safety Code section 39701, the results of this project will improve air quality models so that they more accurately simulate secondary organic aerosol (SOA) formation and its influence on ambient conditions in California, ensuring that ARB's regulatory efforts continue to be based on the most credible air quality models. The results will also advance our understanding of the processes by which chemistry involving  $N_2O_5$  could have important consequences for the production of secondary atmospheric particulate matter (PM). Additionally, assessment of the reactivity of volatile organic compounds on ozone and secondary PM formation will be useful for the development of future ozone and PM control strategies. Research Division staff recommends this proposal for approval.

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 recommendations of the Research Screening Committee and Research Division staff and approves the following:

Proposal Number 2751-275 entitled "Improving Chemical Mechanisms for Ozone and Secondary Organic Carbon," submitted by the University of California, Davis, for a total amount not to exceed \$450,024.

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 \$450,024.

I hereby certify that the above is a true and correct copy of Resolution 12-44, as adopted by the Air Resources Board.

/s/

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Tracy Jensen, Clerk of the Board

## ATTACHMENT A

### “Improving Chemical Mechanisms for Ozone and Secondary Organic Carbon”

#### Background

Despite improvements in urban air quality in recent years, unacceptable levels of ground-level ozone and atmospheric particulate matter (PM) continue to be a persistent problem in both urban and rural areas of California. To meet National Ambient Air Quality Standards, state and local agencies must develop State Implementation Plans and adopt additional regulations to control emissions of these pollutants and their precursors. It is therefore necessary to understand the physical and chemical processes that form these pollutants under various atmospheric conditions. Photochemical air quality models are the primary tool for determining the limiting precursors for various secondary pollutants in California air sheds. Chemical mechanisms are an integral part of these photochemical air quality models and must represent the state-of-the-science understanding of how ozone and other secondary pollutants are formed, as well as their relationships to the primary pollutants emitted from different sources. Statewide Air Pollution Research Center (SAPRC) chemical mechanisms have been developed and updated several times under ARB's sponsorship. Further improvements to the chemical mechanisms will allow ARB regulatory efforts to be based on the most credible air quality models.

#### Objective

The primary objectives of this project are to extend the SAPRC chemical mechanisms to allow for prediction of secondary organic aerosol (SOA), and to assess the reactivity of volatile organic compounds (VOCs) in California's airsheds. Additionally, the latest understanding of nitrogen pentoxide ( $N_2O_5$ ) formation and heterogeneous reactivity, and its impacts on secondary PM, will be incorporated into SAPRC.

#### Methods

This project is a collaboration between the University of California at Davis (UCD) and the California Institute of Technology (Caltech) to extend SAPRC to allow for prediction of SOA through the incorporation of a sequential oxidation model (SOM) into the reaction scheme. Investigators at UCD will combine SAPRC and SOM into one photochemical modeling framework (SAPRC-14). They will use an existing library of results from smog chamber experiments in the development of the SOA component of SAPRC-14, as well as results from new experiments that will be incorporated into the model as they become available. New smog chamber experiments will also be performed at Caltech to help fill gaps in the understanding of biogenic and anthropogenic VOCs that lead to SOA. Furthermore, air quality meteorological scenarios will be updated and combined with recent measurements of background urban reactive organic gases to provide an up-to-date framework for reactivity modeling assessments. Finally, the latest understanding of  $N_2O_5$  formation and heterogeneous reactivity will be incorporated into SAPRC to evaluate its impacts on SOA and inorganic aerosol.

**Expected Results**

Final deliverables will include a version of SAPRC that integrates the code and concepts of the SOM, giving SAPRC a framework for including SOA-forming reactions along with identification of key uncertainties in the integrated SAPRC-SOM, and a detailed description of SAPRC-SOM.

At the conclusion of the project, a draft final report and text files of all relevant data used in this study will be submitted to ARB. The updated version of the SAPRC mechanisms will also be delivered to ARB along with associated data files from the environmental chamber experiment.

**Significance to the Board**

The results of this project will improve air quality models so that they more accurately simulate SOA formation and its influence on ambient conditions in California, ensuring that ARB's regulatory efforts continue to be based on the most credible air quality models. The results will also advance our understanding of the processes by which chemistry involving  $N_2O_5$  could have important consequences for the production of secondary PM. Additionally, assessment of the reactivity of volatile organic compounds on ozone and secondary PM formation will be useful for the development of future ozone and PM control strategies.

**Contractor:**

University of California, Davis

**Contract Period:**

36 months

**Principal Investigator (PI):**

Anthony Wexler, Ph.D.

**Contract Amount:**

\$450,024

**Basis for Indirect Cost Rate:**

The State and the UC system have agreed to a ten percent indirect cost rate.

**Past Experience with this Principal Investigator:**

Professor Anthony Wexler will serve as the principal investigator coordinating and synthesizing the effort for the overall project. He has managed many multi-investigator research projects, and his extensive research experience in aerosol science and strong publication record make him ideal to fulfill this role.

**Prior Research Division Funding to University of California, Davis:**

Year	2012	2011	2010
Funding	\$ 4,949,363	\$ 1,394,560	\$ 508,267

# BUDGET SUMMARY

University of California, Davis

“Improving Chemical Mechanisms for Ozone and Secondary Organic Carbon”

## **DIRECT COSTS AND BENEFITS**

1.	Labor and Employee Fringe Benefits	\$ 308,764
2.	Subcontractors	\$ 80,000
3.	Equipment	\$ 0
4.	Travel and Subsistence	\$ 4,000
5.	Electronic Data Processing	\$ 20,000
6.	Reproduction/Publication	\$ 0
7.	Mail and Phone	\$ 0
8.	Supplies	\$ 0
9.	Analyses	\$ 0
10.	Miscellaneous	<u>\$ 1,349</u>

Total Direct Costs \$ 414,113

## **INDIRECT COSTS**

1.	Overhead	\$ 35,911
2.	General and Administrative Expenses	\$ 0
3.	Other Indirect Costs	\$ 0
4.	Fee or Profit	<u>\$ 0</u>

Total Indirect Costs \$ 35,911

## **TOTAL PROJECT COSTS**

**\$ 450,024**

Attachment 1

**SUBCONTRACTORS' BUDGET SUMMARY**

Subcontractor: California Institute of technology (Caltech)

The Caltech chamber facility contains a broad suite of instrumentation that will be used by Caltech investigators to measure both gas- and particle-phase species. Chamber data will be analyzed to parameterize the statistical oxidation model within SAPRC.

**DIRECT COSTS AND BENEFITS**

1.	Labor and Employee Fringe Benefits	\$	43,243
2.	Subcontractors	\$	0
3.	Equipment	\$	0
4.	Travel and Subsistence	\$	0
5.	Electronic Data Processing	\$	0
6.	Reproduction/Publication	\$	0
7.	Mail and Phone	\$	0
8.	Supplies	\$	0
9.	Analyses	\$	0
10.	Miscellaneous	\$	<u>32,433<sup>1</sup></u>
	Total Direct Costs		\$ 75,676

**INDIRECT COSTS**

1.	Overhead	\$	4,324
2.	General and Administrative Expenses	\$	0
3.	Other Indirect Costs	\$	0
4.	Fee or Profit	\$	<u>0</u>
	Total Indirect Costs		\$ <u>4,324</u>

**TOTAL PROJECT COSTS** **\$ 80,000**

<sup>1</sup> Miscellaneous item includes graduate student tuition that is charged at a rate of 75 percent of the student's stipend.