### State of California AIR RESOURCES BOARD

### **RESEARCH PROPOSAL**

Resolution 09-29

April 23, 2009

Agenda Item No.: 09-4-2

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 2671-264, entitled "SOA Formation: Chamber Study and Model Development," 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 2671-264 entitled "SOA Formation: Chamber Study and Model Development," submitted by the University of California, Riverside, for a total amount not to exceed \$474,229.

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 2671-264 entitled "SOA Formation: Chamber Study and Model Development," submitted by the University of California, Riverside, for a total amount not to exceed \$474,229.

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 \$474,229.

I hereby certify that the above is a true and correct copy of Resolution 09-29, as adopted by the Air Resources Board.

/s/

# ATTACHMENT A

# "SOA Formation: Chamber Study and Model Development"

### Background

Secondary organic aerosol (SOA) accounts for an important portion of total fine particulate matter (PM) in urban cities such as Los Angeles especially in summertime, when photochemistry is most intensive. However, the photochemical mechanisms in air quality models involve highly uncertain assumptions to predict SOA concentration owing to the deficiency in the available information on molecular characterization.

Thousands of smog chamber experiments have been conducted to study gas-phase photochemistry relevant to ozone formation. In contrast, SOA has rarely been speciated in smog chamber studies. SOA formation depends on several factors including concentrations of precursors such as oxides of nitrogen (NO<sub>X</sub>) and volatile organic compounds (VOC) compounds, light spectrum and intensity, relative humidity, and temperature. In order to test and improve theories and models for predicting SOA compounds in the atmosphere, it is essential to obtain data on SOA formation in well-characterized experiments representing a range of atmospheric conditions. Since SOA compounds can exceed 70 percent of the fine PM concentration on highly impacted days, accurately predicting its formation is essential to developing cost-effective control strategies for fine PM, and assessing how proposed ozone control strategies may also impact fine PM.

SAPRC-07 and PM-SAPRC were developed recently under funding from the Air Resources Board (ARB) to represent gas-phase processes and reactivity estimates with preliminary molecular representation of PM based on chamber data. The PM-SAPRC showed promise for tracing NO<sub>X</sub> effects on SOA concentration, but needs improvement on its sensitivity to organic compounds.

# Objective

This contract will develop a predictive PM-SAPRC chemical mechanism based on existing and additional chamber data to be collected from the University of California, Riverside – Environmental Protection Agency (UCR-EPA) chamber.

# Methods

Additional chamber experiments will be designed and conducted in the UCR-EPA chamber facility with recent addition of analytical instruments, to improve the predictive capability of the SAPRC-SOA mechanism in California conditions. Over 120 chamber experiments will be designed and conducted with on-line chemical analysis at precursor levels and meteorological conditions in California. The focus will be on the ozone and SOA formation from m-xylene and possibly toluene and corresponding second generation compounds under different conditions.

### **Expected Results**

A final report that contains descriptions and supporting materials for a predictive PM-SAPRC chemical mechanism will be provided to ARB.

### Significance to the Board

Together with other relevant chamber data, a hybrid SOA chemical mechanism based on the well-known SAPRC gas-phase chemical mechanism will be developed and evaluated. The outcome of this project is expected to contribute significantly to the informed decision of developing feasible and cost-effective emission regulations.

### Contractor:

University of California, Riverside

**Contract Period:** 36 months

Principal Investigator (PI): William P.L. Carter

# **Contract Amount:**

\$474,229.

### **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:

The principal investigator, Dr. William Carter, will be responsible for the overall management of the project and also will work on the development of the PM-SAPRC mechanism. Dr. Carter pioneered the development of the gas-phase mechanism and recently developed SAPRC-07, an update to his SAPRC-99 chemical mechanism, which has been widely used in different applications throughout the world. He has completed several studies on VOC reactivity for ARB, and has always delivered a high-quality product at a very reasonable cost. Dr. David Cocker III will be the key researcher directing the chamber experiments and data analysis for the mechanism development. Dr. Robert Griffin at Rice University has extensive expertise in air quality models and developed the Caltech Atmospheric Chemistry Model, which is invaluable in aiding in implementing the mechanism into air quality models.

# Prior Research Division Funding to the University of California, Riverside:

Year	2008	2007	2006
Funding	\$64,942	\$215,898	\$363,372

# **BUDGET SUMMARY**

University of California, Riverside

# SOA Formation: Chamber Study and Model Development

DIRECT COSTS AND BENEFITS						
1.	Labor and Employee Fringe Benefits		244,425			
2.	Subcontractors	\$	25,343			
3.	Equipment	\$\$\$\$\$	0			
4.	Travel and Subsistence	\$	500			
5.	6	\$	0			
6.	Reproduction/Publication	\$	0			
7.		\$	0			
8.	Supplies	\$	66,662 <sup>1</sup>			
9.	Analyses		0			
10.	Miscellaneous	<u>\$</u>	<u>103,772<sup>2</sup></u>			
	Total Direct Costs		\$440,702			
	RECT COSTS					
1.	Overhead	\$	33,527			
2.		\$ \$ \$				
3.		\$				
4.	Fee or Profit	<u>\$</u>				
	Total Indirect Costs		<u>\$33,527</u>			
TOTAL PROJECT COSTS			<u>\$474,229</u>			

<sup>&</sup>lt;sup>1</sup> Includes supplies for office (\$225), laboratory (\$19,773), lamp (\$7909), PM instrument (\$9,491), general analyzer repair (\$11,864), and FEP Teflon (\$17,400). <sup>2</sup> Includes graduate student health insurance and non-resident tuition fee (\$23,307) and facility rental fee

<sup>(\$80,465).</sup> 

### Attachment 1

# SUBCONTRACTORS' BUDGET SUMMARY

### Subcontractor: Rice University

Description of subcontractor's responsibility: The subcontractor will be responsible for optimizing the full version of PM-SAPRC chemical mechanism evaluated with existing and additional chamber experiments with molecular characterizations, to build condensed versions of PM-SAPRC for being implemented into a regulatory model, such as CMAQ5, for urban, costal, and national park conditions in California during summer and winter.

#### DIRECT COSTS AND BENEFITS

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1.	Labor and Employee Fringe Benefits	\$	16,619	
2.	Subcontractors	\$	0	
3.	Equipment	\$	0	
4.	Travel and Subsistence	\$	0	
5.	Electronic Data Processing	\$	0	
6.	Reproduction/Publication	\$	0	
7.	Mail and Phone	Ŝ	0	
8.	Supplies	Ŝ	0	
9.	Analyses	\$ \$ \$ \$ \$ \$ \$ \$ \$ \$	Õ	
10.	Miscellaneous	φ ¢	0 0	
10.	Miscellaneous	$\Psi$	0	
	Total Direct Costs		\$16,	619
INDI	RECT COSTS			
1.	Overhead	\$	4,362*	
2.		\$	4,362*	
3.		\$	0	
4.	Fee or Profit	↓ \$	0	
4.		$\overline{\mathbf{v}}$	0	
	Total Indirect Costs		<u>\$8,</u>	<u>724</u>
TOTAL PROJECT COSTS			<u>\$25,</u>	<u>343</u>

\*Items 1 and 2 are evenly split from the total overhead and administrative expenses, calculated as 52.5% of the total direct cost.