State of California
AIR RESOURCES BOARD

Resolution 02-12

March 21, 2002

Agenda Item No.: 02-2-2

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 2514-224, entitled "Quantitative Analysis of Aerosol Time-of-Flight Mass Spectrometry Data using YAADA," has been submitted by Arizona State University;

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 2514-224 entitled "Quantitative Analysis of Aerosol Time-of-Flight Mass Spectrometry Data using YAADA," submitted by Arizona State University, for a total amount not to exceed $50,281.

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 2514-224 entitled "Quantitative Analysis of Aerosol Time-of-Flight Mass Spectrometry Data using YAADA," submitted by Arizona State University, for a total amount not to exceed $50,281.

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 $50,281.

I hereby certify that the above is a true and correct copy of Resolution 02-12, as adopted by the Air Resources Board.

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Marie Kavan, Clerk of the Board

ATTACHMENT A

"Quantitative Analysis of Aerosol Time-of-Flight Mass Spectrometry Data using YAADA"

Background

Epidemiological studies have shown that the concentration of very small airborne particles (aerodynamic diameter less than 2.5 μm) is correlated with excess human mortality in cities across the United States. Further studies have shown that some airborne particles contain toxic substances such as carcinogens suggesting that health effects may be associated with a small subset of toxic particles within atmospheric aerosols. One approach taken to understand the cause of these observed health effects is to measure atmospheric aerosol composition in detail and relate this to observations of acute or chronic health effects.

Researchers are now able to measure the size and composition of single aerosol particles using instruments like the Aerosol Time-of-Flight Mass Spectrometry (ATOFMS) instruments developed by Prof. Kimberly Prather and others. Complete mass spectra are collected on individual particles at a rate of approximately one per second. Thus, very large data sets (approximately 200 MB/day) can be collected during a multi-day, multi-instrument experiment. These data sets are too large for *ad hoc* data analysis techniques. YAADA is a software package of data management and analysis that can be used to process these large data sets. YAADA includes functions to import, plot, and quantitatively analyze ATOFMS data. The import module rapidly converts data from the common ATOFMS data acquisition software and performs quality control checks on the data.

Objective

The objectives of this research project are to compare quantitatively ATOFMS data and collocated impactor measurements of aerosol mass to investigate particle detection efficiencies for the modified ATOFMS design, to determine chemical sensitivity of ATOFMS instruments for organic and elemental carbon in the Bakersfield Instrument Intercomparison and other studies, and to develop, test, and distribute the quantification package for YAADA so that other users can perform quantitative comparisons of ATOFMS and reference sampler data.

Methods

The proposed work is based on the hypothesis that ATOFMS data can be scaled to account for nonlinear particle and ion detection efficiencies to yield quantitative aerosol composition. The initial approach will be to develop scaling functions for particle transmission efficiency which have parameters fitted by nonlinear regression of scaled ATOFMS data with reference measurements. ATOFMS data to be used for in this research project are available from several recent field studies. The investigator will also develop scaling functions for carbonaceous species detection efficiency by comparison with quantitative size-segregated aerosol carbonaceous aerosol measurements. In order to perform the complex analyses proposed in this research

project, the investigator will use YAADA software toolkit. Several general functional modules will be written to improve the current proprietary codes. In addition to improved documentation and ease-of-use, the new functions will allow complex mass spectral responses to be compared with reference data.

Expected Results
The deliverables from the proposed research will include a final report summarizing the research methods, results, and conclusions, and the YAADA quantification module. The investigator will release to the public the programs used in this work. The programs will include those used to quantitatively compare ATOFMS data to reference sampler data and those used to scale up ATOFMS data collected to determine continuous aerosol mass, elemental carbon, and organic carbon concentrations.

Significance to the Board
The resulting software will allow for a much wider analysis of the ATOFMS data (very large data sets of approximately 200 MB/day) collected under other ARB contracts. Quantitative aerosol measurements are needed to better understand the sources, transformations, and fate of ambient particles in order to understand the effects of particulate matter on global climate, human health, and regional visibility.

Contractor:
Arizona State University (ASU)

Contract Period:
18 months

Principal Investigator (PI):
Dr. Jonathan O. Allen

Contract Amount:
$50,281

Cofunding:
None

Basis for Indirect Cost Rate:
Indirect cost is calculated per ASU office of research and creative activities guidelines.

Past Experience with this Principal Investigator:
Dr. Allen's research work to analyze large aerosol data sets follows from his long-standing and mutually productive collaboration with other investigators. This collaboration began in 1996 when the PI was a postdoctoral with Prof. Glen Cass at the California Institute of Technology. Numerous peer-reviewed research papers and the YAADA software toolkit are the result of this collaboration.

Prior Research Division Funding to Arizona State University:

Year	2001	2000	1999
Funding	$0	$0	$0

B U D G E T S U M M A R Y

Arizona State University
Quantitative Analysis of Aerosol Time-of-Flight Mass Spectrometry
Data using YAADA

DIRECT COSTS AND BENEFITS			
1.	Labor and Employee Fringe Benefits	$28,054	
2.	Subcontractors	$ -0-	
3.	Equipment	$ 4,000 [1]	
4.	Travel and Subsistence	$ 1,800	
5.	Electronic Data Processing	$ -0-	
6.	Reproduction/Publication	$ 1,000	
7.	Mail and Phone	$ -0-	
8.	Supplies	$ -0-	
9.	Analyses	$ -0-	
10.	Miscellaneous	$ -0-	
	Total Direct Costs		$34,854
INDIRECT COSTS			
1.	Overhead	$ 15,427	
2.	General and Administrative Expenses	$ -0-	
3.	Other Indirect Costs	$ -0-	
4.	Fee or Profit	$ -0-	
	Total Indirect Costs		$15,427
TOTAL PROJECT COSTS			**$50,281**

(notes)

[1] Funding is requested for a data analysis workstation running Linux to be purchased for $4,000. Based on a recent quote, a Dell Precision Workstation 340 computer purchased for this amount would be equipped with a 2 GHz Pentium 4 processor, 1 GB RAM, two 40 GB disks, and a DD3 tape drive.