

# Update of ARB's Reactivity-related Research

RRAC meeting  
August 15, 2001  
Cal/EPA Headquarter, Room 550  
Sacramento, CA 95812

Dongmin Luo, Ph.D.  
Research Division  
ARB

## Outline

- Atmospheric Chemistry
- Mechanism Development
- Reactivity Assessment
- Speciation Profiles

Atmospheric Chemistry (homogeneous)

“Atmospheric chemistry of selected linear, branched, and cyclic C<sub>10</sub> compounds of Mineral Spirits”

Profs. Roger Atkinson and Janet Arey  
University of California, Riverside  
\$84,000

Tasks:

- Selection of three C<sub>10</sub> alkanes of representative constituents of mineral spirits: n-decane, 3,4-diethylhexane, and butylcycloalkane;
- Investigation of the products and initial rates of OH reactions with these compounds.

Status:

The draft final report was approved by the RSC in April 2001 and the final report will be available soon.

Atmospheric Chemistry (homogeneous)

“Yield and reactions of intermediate compounds formed from the initial atmospheric reactions of selected volatile organic compounds”

Profs. Roger Atkinson and Janet Arey  
University of California, Riverside  
\$106,000

Tasks:

- Investigation of ambient  $\text{NO}_3$  radical levels in SCOS97-NARSTO study;
- Review of the mechanism of atmospheric oxidation of the alkenes;
- Reviews of the atmospheric chemistry of VOCs and  $\text{NO}_x$  and chemical oxidation mechanism for air quality modeling.

Status:

The draft final report was approved by the RSC in April 2001 and the final report will be available soon.

Atmospheric Chemistry (homogeneous)

“Studies of the atmospheric chemistry of volatile organic compounds and of their atmospheric reaction products”

Profs. Roger Atkinson and Janet Arey  
University of California, Riverside  
\$300,000

Tasks:

- Quantification of the products of the first- and second-generation reactions of selected VOCs (alkenes, alkanes, and aromatics) with OH, NO<sub>3</sub> radicals, and O<sub>3</sub>.
- Development of atmospheric reaction mechanisms of aromatics and selected carbonyl compounds.

Status:

This project started in July 2000 and will be completed in three years.

Atmospheric Chemistry (heterogeneous)

“The formation of gaseous nitrous acid (HONO): a key determinant of tropospheric ozone and fine particles”

Prof. Barbara Finlayson-Pitts  
University of California, Irvine  
\$300,000

Tasks:

- Method development of HONO measurement;
- Elucidation of the kinetics and mechanism of HONO formation;
- Impact analysis of this new discovered chemistry on ozone and PM.

Status:

The draft final report was approved by the RSC in May 2001 and the final report will be available soon.

Atmospheric Chemistry (heterogeneous)

“Impacts of NO<sub>x</sub> surface reactions on the formation of particles, ozone, and the development of control strategy options”

Prof. Barbara Finlayson-Pitts  
University of California, Irvine  
\$600,000

Tasks:

- Investigation of heterogeneous reactions of HNO<sub>3</sub>, NH<sub>4</sub>NO<sub>3</sub>, and HONO on surfaces;
- Investigation of the kinetics and mechanisms of the heterogeneous hydrolysis of NO<sub>2</sub> in surface;
- Impact assessment of heterogeneous NO<sub>x</sub> chemistry on ozone and particle formation.

Status:

The research proposal was approved by the RSC in July and will be completed in 27 months.

## Mechanism Development

“Development and evaluation of a gas-phase atmospheric reaction mechanism for low NO<sub>x</sub> conditions”

Dr. William Carter  
University of California, Riverside  
\$80,000

### Tasks:

- Completion of development of low NO<sub>x</sub> version of SAPRC-99;
- Mechanism evaluation using available low NO<sub>x</sub> chamber data;
- New chamber experiments for low NO<sub>x</sub> mechanism evaluation;
- Mechanism updates and modifications.

### Status:

The research proposal was approved by the RSC in July 2001 and will be completed in two years.

## Reactivity Assessment (modeling)

“Development of reactivity scales via 3-D grid modeling of California ozone episodes”

Prof. Robert Harley at UC, Berkeley  
Prof. Jana Milford at Univ. of Colorado  
Prof. Ted Russell at Georgia Tech.  
\$240,000

### Tasks:

- Incorporation of SAPRC99 chemical mechanism into two urban airshed models: CIT and MAQSIP;
- Estimates of incremental reactivity for South Coast and San Joaquin Valley;
- Sensitivity and uncertainty analysis associated with emissions, deposition, and chemical mechanism.

### Status:

This project started in February 1999 and will be completed by May 2002.

## Reactivity Assessment (modeling)

“Assessment of the ozone and aerosol forming potentials (reactivities) of organic compounds over the Eastern United States”

Prof. Ted Russell  
Georgia Institute of Technology  
\$15,000

### Tasks:

- Selection of individual organic compounds for study;
- Extension of the chemical mechanism;
- Quantification of VOC reactivity in the Eastern United States;

### Status:

This research project was approved by the RSC in May 2001 and will be completed in 15 months.

Reactivity Assessment (experimental)

“Development and application of improved methods for measurement of ozone formation potentials of volatile organic compounds”

Dr. William Carter  
University of California, Riverside  
\$300,000

Tasks:

- Development and evaluation of a direct reactivity measurement method at lower cost and with greater sensitivity for low volatility compounds or poorly characterized mixtures;
- Development of standard procedures for estimating reactivities and their associated uncertainty ranges.

Status:

This project started in April 1998 and will be completed by May 2002.

Reactivity Assessment (experimental)

“Evaluation of atmospheric impacts of selected coatings VOC emissions”

Dr. William Carter  
University of California, Riverside  
\$60,000

Tasks:

- Reactivity and uncertainty survey of coatings VOCs;
- Environmental chamber studies of Texanol;
- Application of a direct reactivity measurement method to selected architectural coatings constituents;
- Development and evaluation of procedures to quantify reactivity and uncertainty of petroleum distillates.

Status:

This project started in July 2001 and will be completed in three years.

## Speciation Profiles

“Investigation of low reactivity solvents for use in consumer products”

Profs. Albert Censullo, Dane Jones,  
& Max Wills

California Polytechnic State University,  
San Luis Obispo

\$85,000

### Tasks:

- Preparation of a database of solvent properties to facilitate the production of less reactive formulations for consumer products;
- Chemical speciation of selected low reactivity solvents and solvent mixtures.

### Status:

This project started in February 1999 and will be completed by the end of this year.