

# Reactivity Estimates for Selected Consumer Product Compounds

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## Outline

- Objectives
- Approach
- Progress to date
- Remaining work

# Objectives

- Reduce uncertainties in reactivity estimates for VOCs in consumer products for which insufficient reactivity data are available.
- Uncertainties in reactivities of amino-2-methyl-1-propanol (AMP) and other amines are a particular concern
- After discussions with CARB staff and examining consumer products inventory, compounds chosen for study are as follows (in order of priority):
  - AMP:  $\text{HOCH}_2\text{C}(\text{CH}_3)(\text{CH}_3)(\text{NH}_2)$
  - Ethanolamine:  $\text{HOCH}_2\text{CH}_2\text{NH}_2$
  - D-Limonene
  - Dipropylene glycol monomethyl ether

# Approach

- Conduct environmental chamber incremental reactivity experiments for selected compounds
- Utilize the UCR EPA Chamber
- Measure impacts of compounds on PM formation as well as ozone reactivity
- Evaluate estimated mechanisms for selected compounds against chamber experiments and revise as needed. Use the SAPRC-07 mechanism as the starting point
- Calculate reactivities in MIR and other reactivity scales.

# Progress to Date

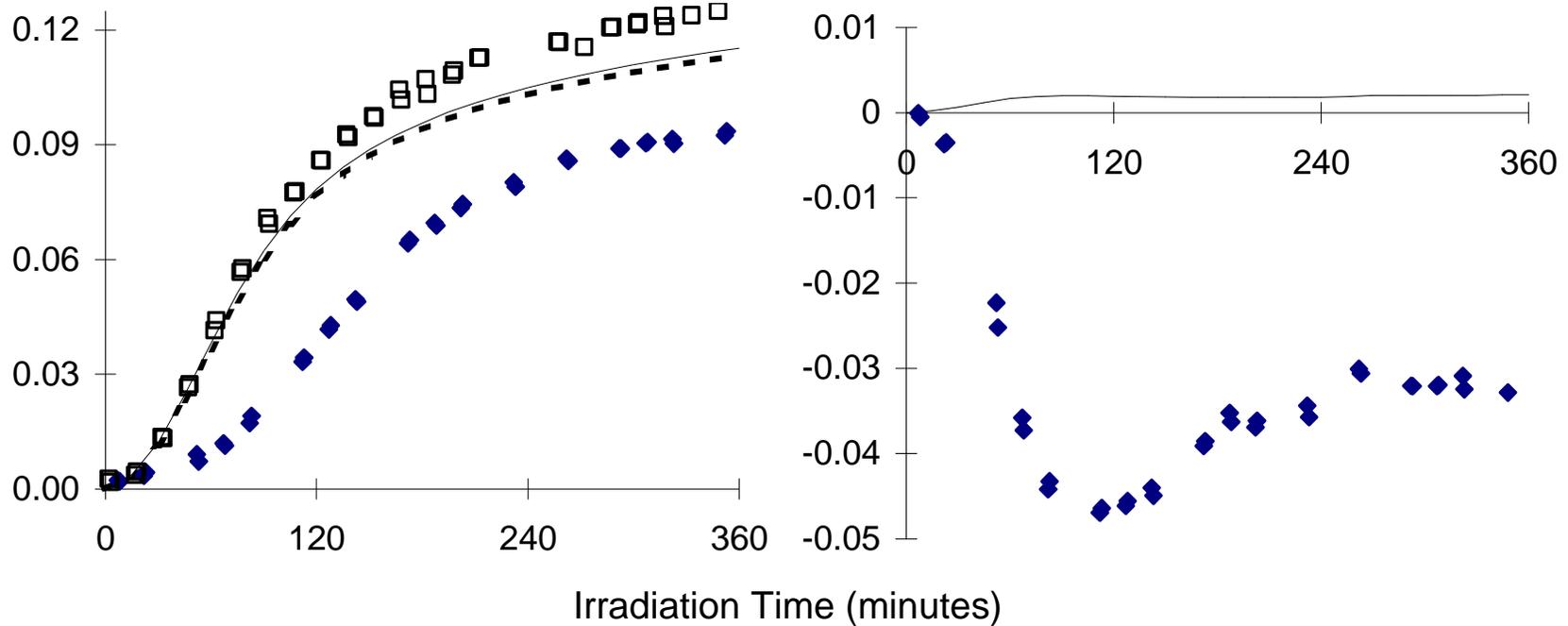
- All experiments and initial data processing for this program have been completed. Mechanism development and modeling now underway
- Experiments conducted with AMP, Ethanolamine, and d-Limonene. Insufficient resources to study other compounds
- Unable to develop a satisfactory gas-phase analysis for the amines, and evidence exists that not all injected amines available for gas-phase reactions. Therefore, mechanism evaluation for amines will be qualitative at best.
- Nevertheless, data indicate that amine mechanisms used in draft SAPRC-07 report are incorrect
- Existing mechanism for d-limonene appears to be satisfactory
- All three compounds found to large PM impacts

# Examples of Results: Reactivity Experiment with AMP

EPA789: MOIR/2 Surrogate + 0.05 ppm AMP

$\Delta([\text{O}_3]-[\text{NO}])$  (ppm)

$\Delta([\text{O}_3]-[\text{NO}])$  Change (ppm)



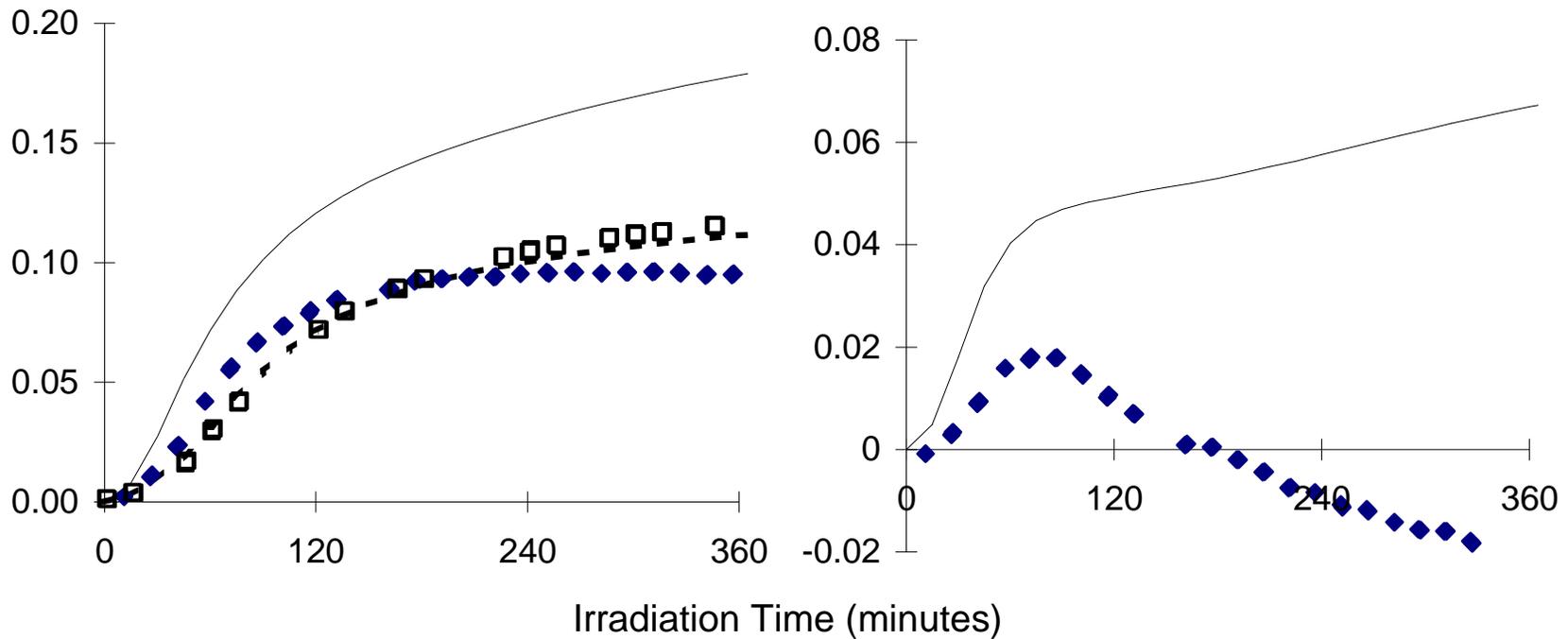
◆ Test Experiment    □ Base Experiment    — Test Model    - - - Base Model

# Examples of Results: Reactivity Experiment with Ethanolamine

EPA805: MOIR/2 Surrogate + 0.25 ppm Ethanolamine

$\Delta([\text{O}_3]-[\text{NO}])$  (ppm)

$\Delta([\text{O}_3]-[\text{NO}])$  Change (ppm)

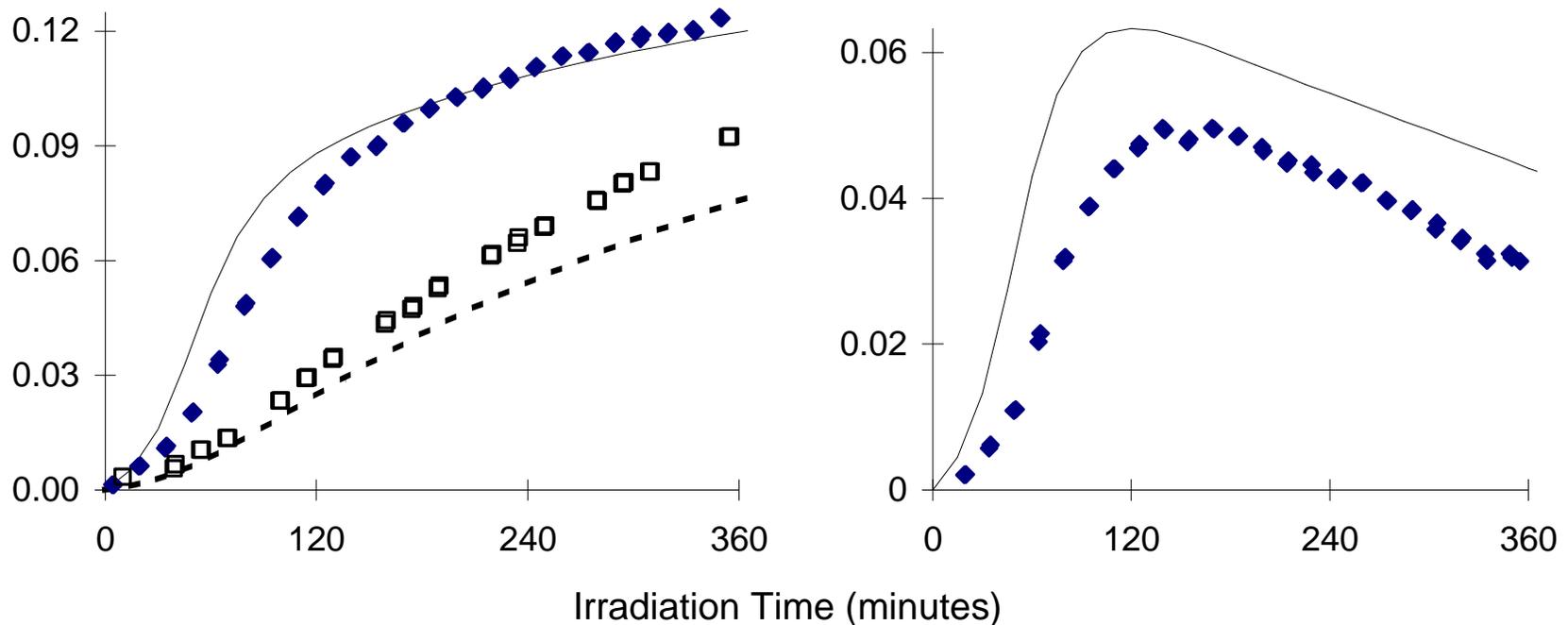


# Examples of Results: Reactivity Experiment with D-Limonene

EPA793: MIR Surrogate + 35 ppb D-Limonene

$\Delta([\text{O}_3]-[\text{NO}])$  (ppm)

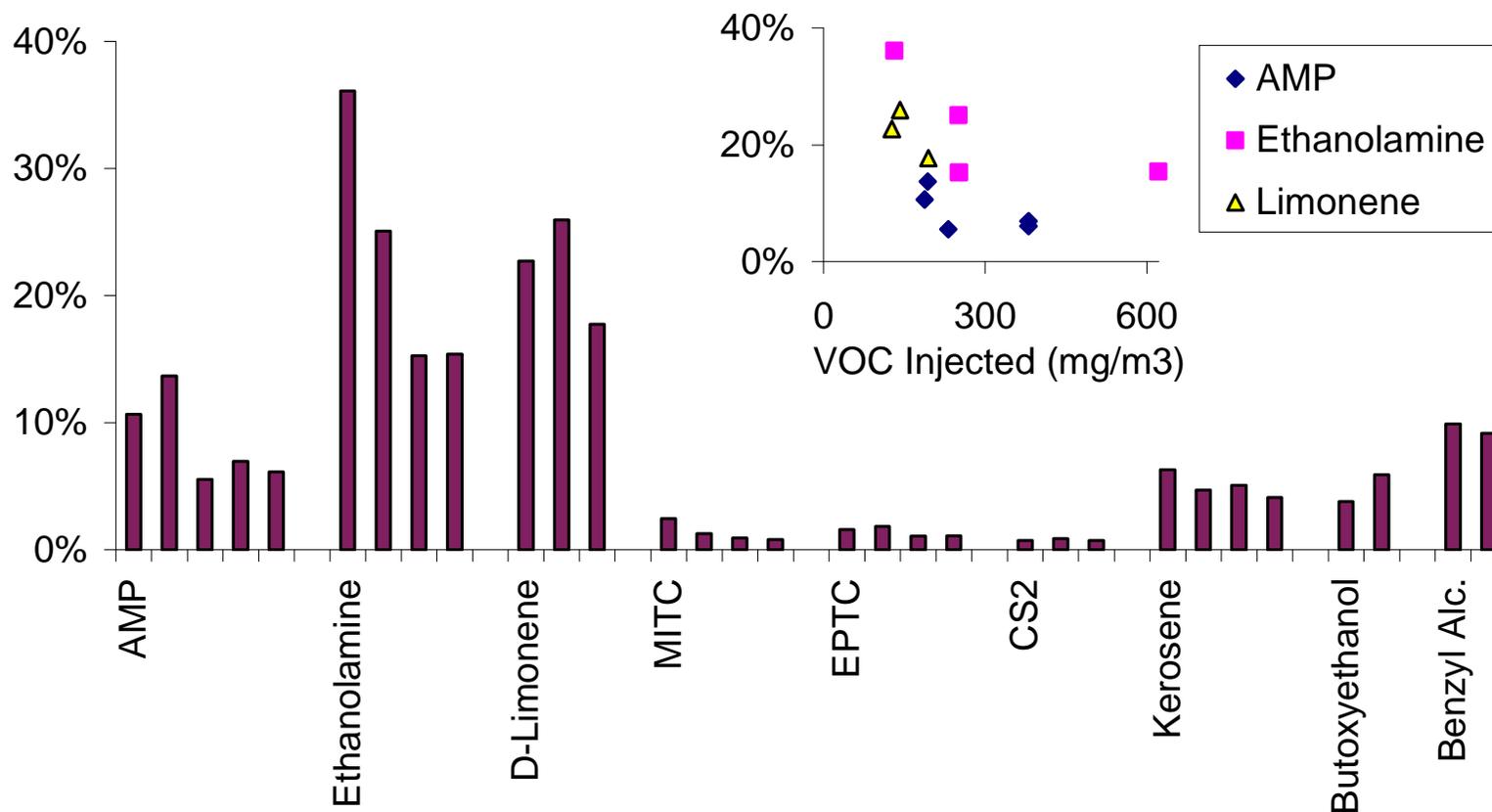
$\Delta([\text{O}_3]-[\text{NO}])$  Change (ppm)



# Representative PM Results

(Data from pesticide and coatings projects shown for comparison)

**Ratio of 5-Hour PM mass to Initial VOC Mass Injected  
(uncorrected for PM wall losses)**



# Remaining Work

- Mechanisms for amines need to be revised to be more consistent with the available data
  - Revised structure-reactivity estimates for initial OH reactions have already been developed
  - Preliminary mechanisms have been developed that give better simulations of the data but further work is needed.
- Mechanisms for other amines will be estimated based on those developed for AMP and ethanolamine.
- Reactivities for amines will be calculated and added to the SAPRC-07 reactivity tabulations.
- Mechanism for d-limonene will probably not need to be revised.
- Hope to submit draft final report before end of September