



**AIR FORCE RESEARCH  
LABORATORY**



***ATMOSPHERIC CHEMISTRY  
FOR  
DISPERSION MODELING SUPPORT***

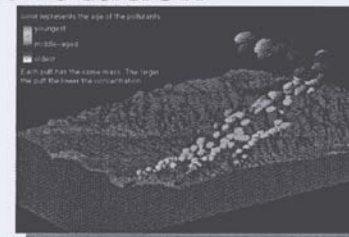
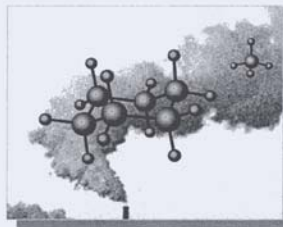
**Mike Henley**  
**AFRL/MLQL**  
**(850)283-6050**  
**[mike.henley@tyndall.af.mil](mailto:mike.henley@tyndall.af.mil)**



# Introduction



- **Relevance of Atmospheric Chemistry**
  - OH and NO<sub>3</sub> radicals
  - Transformations of volatile organic compounds
  - Effects on chemical composition and concentration within a dispersion plume
- **Importance of Laboratory Data**
  - Accurate rate constants & reaction mechanisms
  - Improve or verify dispersion model
  - Improve detection schemes & source location

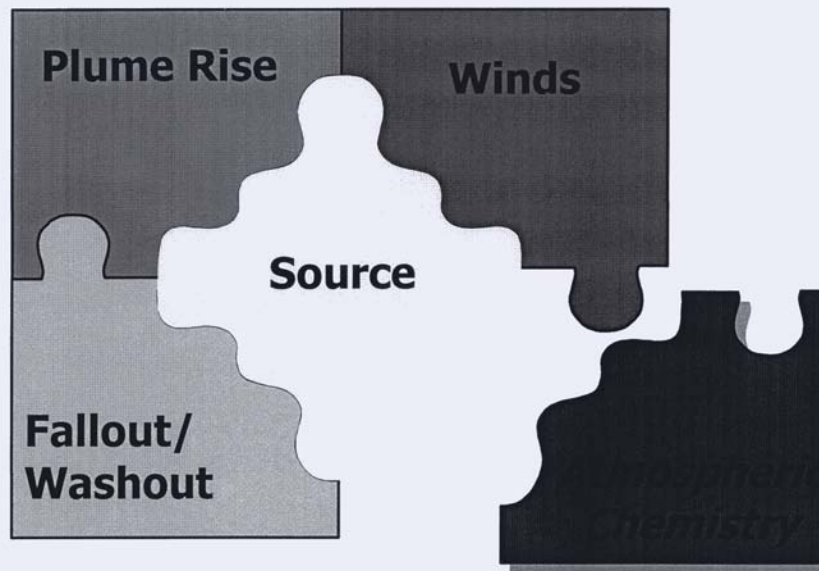




# Air Team Helps Complete the Picture

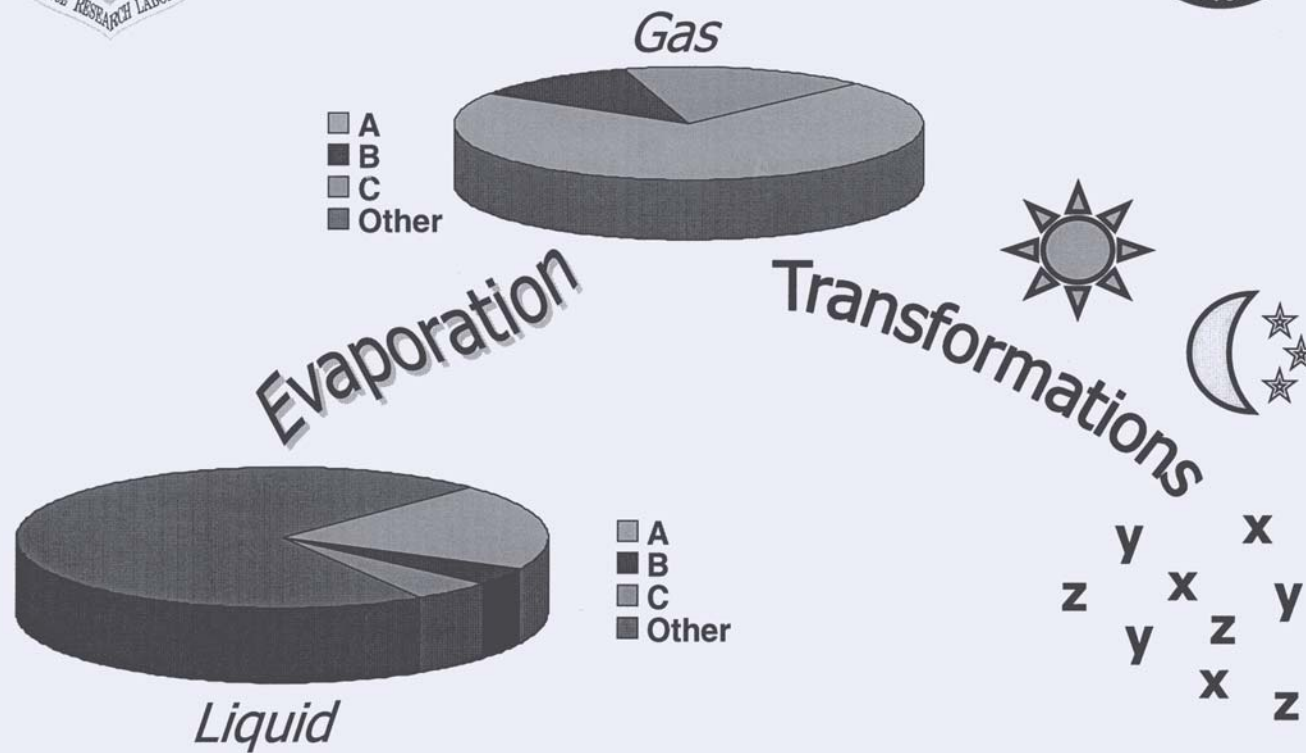


## Dispersion Modeling



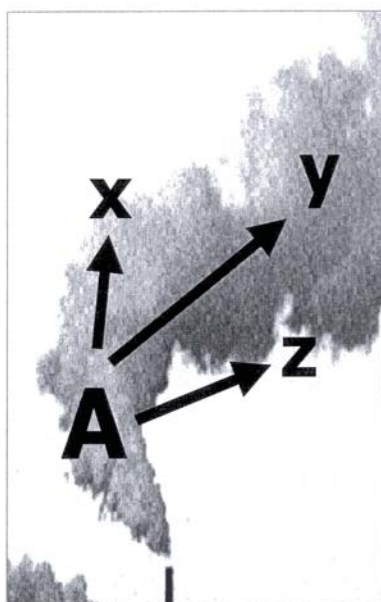


# Emissions Systems





## Understanding Emissions



- How quickly does the concentration of "A" change due to reactions?
- What products does "A" form in these reactions?

***Air Team Answers with expertise in:***  
***Kinetics***  
***Mechanisms***  
***Day and Nighttime Chemistries***





## Applications



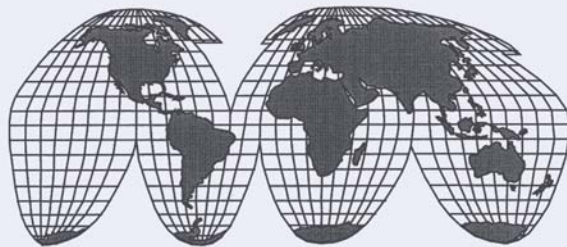
### Modeling Support



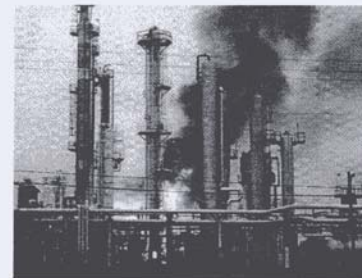
### CBW Defense



### Counterproliferation



### TIMs



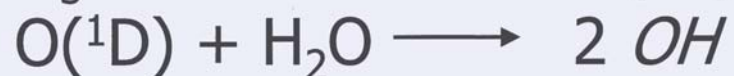


## Pertinent Radical Formation Reactions

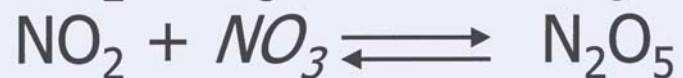
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### OH Radical



### NO<sub>3</sub> Radical





## Reactive Species Data



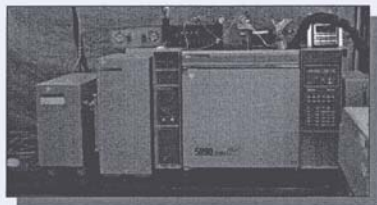
<u>SPECIES</u>	<u>CONC</u> (molc/cm <sup>3</sup> )	<u>DAY/NIGHT</u>	<u>HC RATE</u> (cm <sup>3</sup> /molc sec)
OH	10 <sup>6</sup>	day	10 <sup>-10</sup> to 10 <sup>-15</sup>
NO <sub>3</sub>	10 <sup>9</sup>	night	10 <sup>-11</sup> to 10 <sup>-19</sup>
O <sub>3</sub>	10 <sup>12</sup>	both	10 <sup>-15</sup> to 10 <sup>-20</sup>





# Air Team Products

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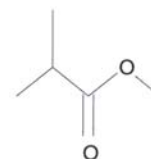
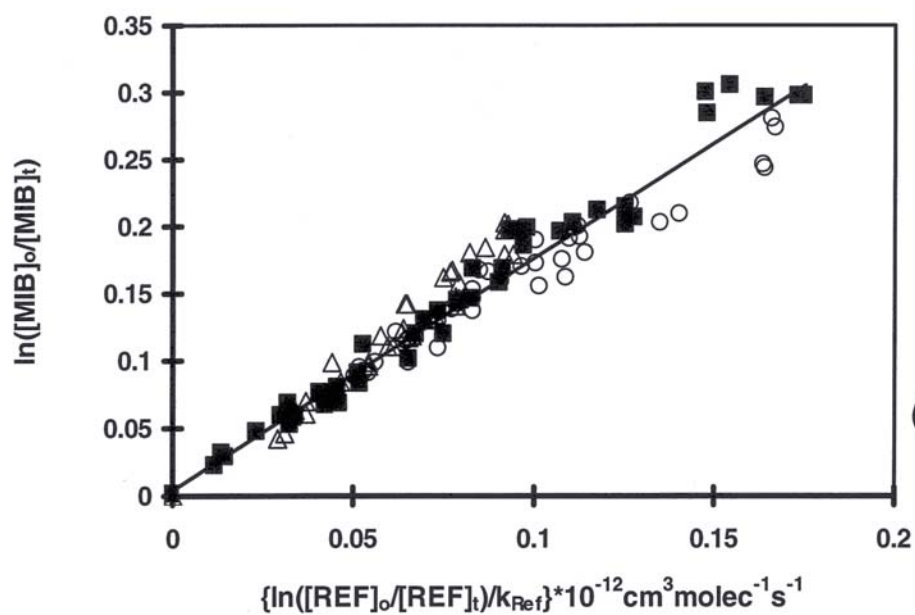


## Experts in...

- Determining OH and NO<sub>3</sub> reaction rate constants
- Identifying products and yield
- Elucidating reaction mechanisms



## Hydroxyl Radical Rate Constant for Methyl Isobutyrate

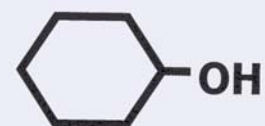
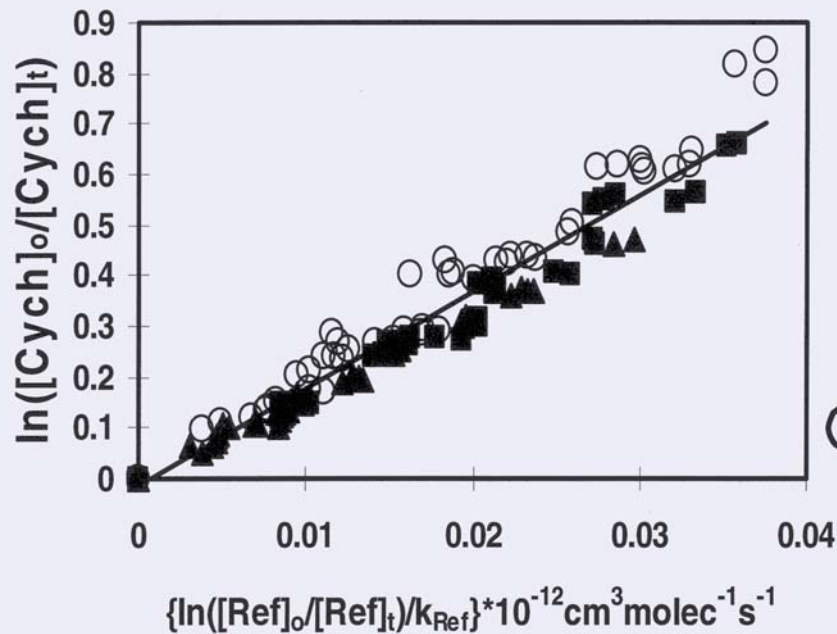


•  $k_{OH} = 1.70 \times 10^{-12}$   
( $\text{cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ )

• 163 hour lifetime



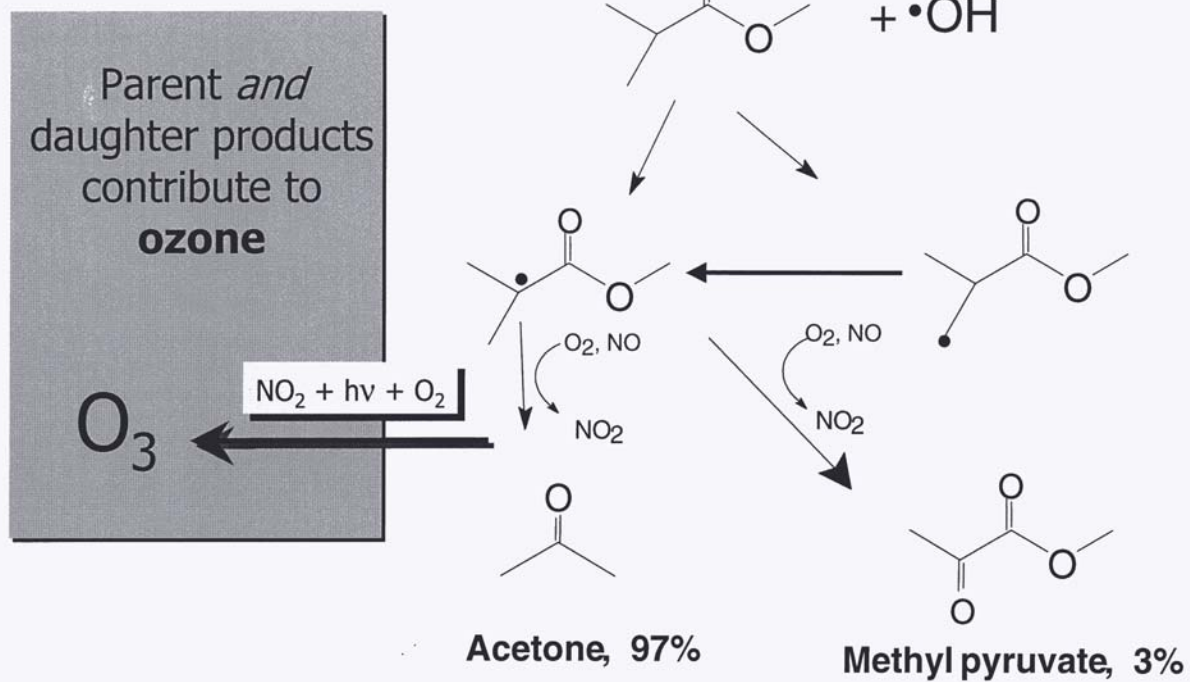
## Hydroxyl Radical Rate Constant for Cyclohexanol



- Three References
- $k_{OH} = 19.0 \times 10^{-12} \text{ (cm}^3 \text{ molec}^{-1} \text{ s}^{-1})$
- 15 hr lifetime



## Atmospheric Transformation Mechanism for MIB



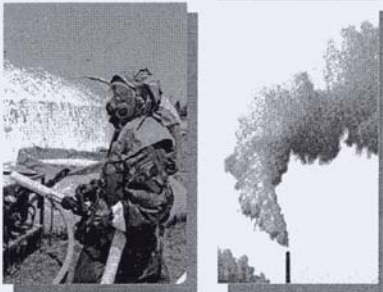
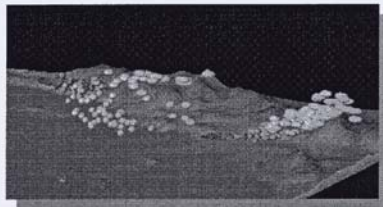


# SUMMARY

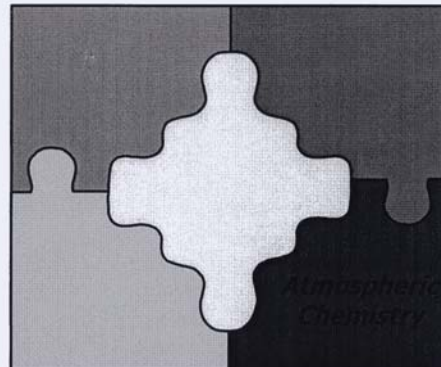
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**Air Team has unique capabilities that:**



- **Improve atmospheric dispersion model inputs**
- **Result in more accurate source location and identification**
- **Lead to more effective detection, response and decontamination**



**Completing the picture  
with Atmospheric Chemistry**