



AIR FORCE RESEARCH LABORATORY



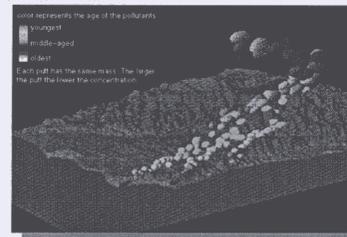
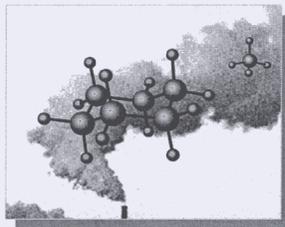
ATMOSPHERIC CHEMISTRY FOR DISPERSION MODELING SUPPORT

Mike Henley
AFRL/MLQL
(850)283-6050
mike.henley@tyndall.af.mil



Introduction

- **Relevance of Atmospheric Chemistry**
 - OH and NO₃ 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

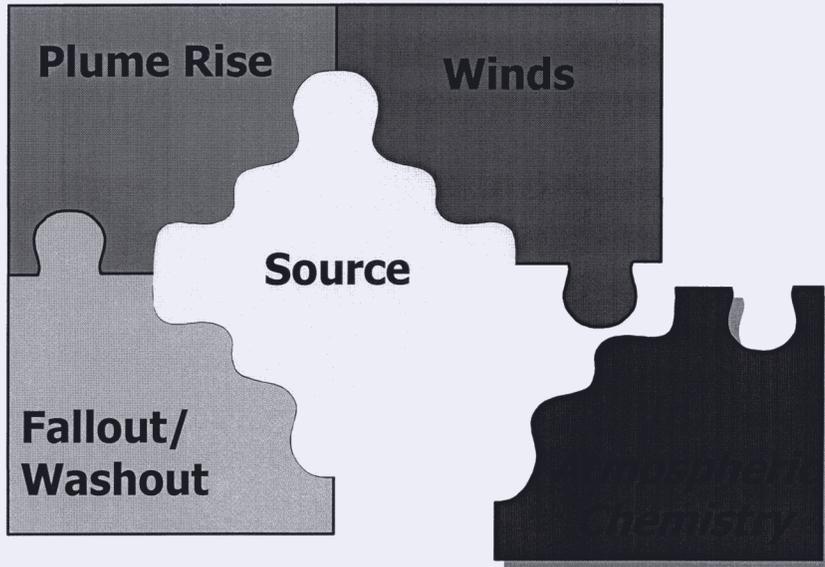




Air Team Helps Complete the Picture

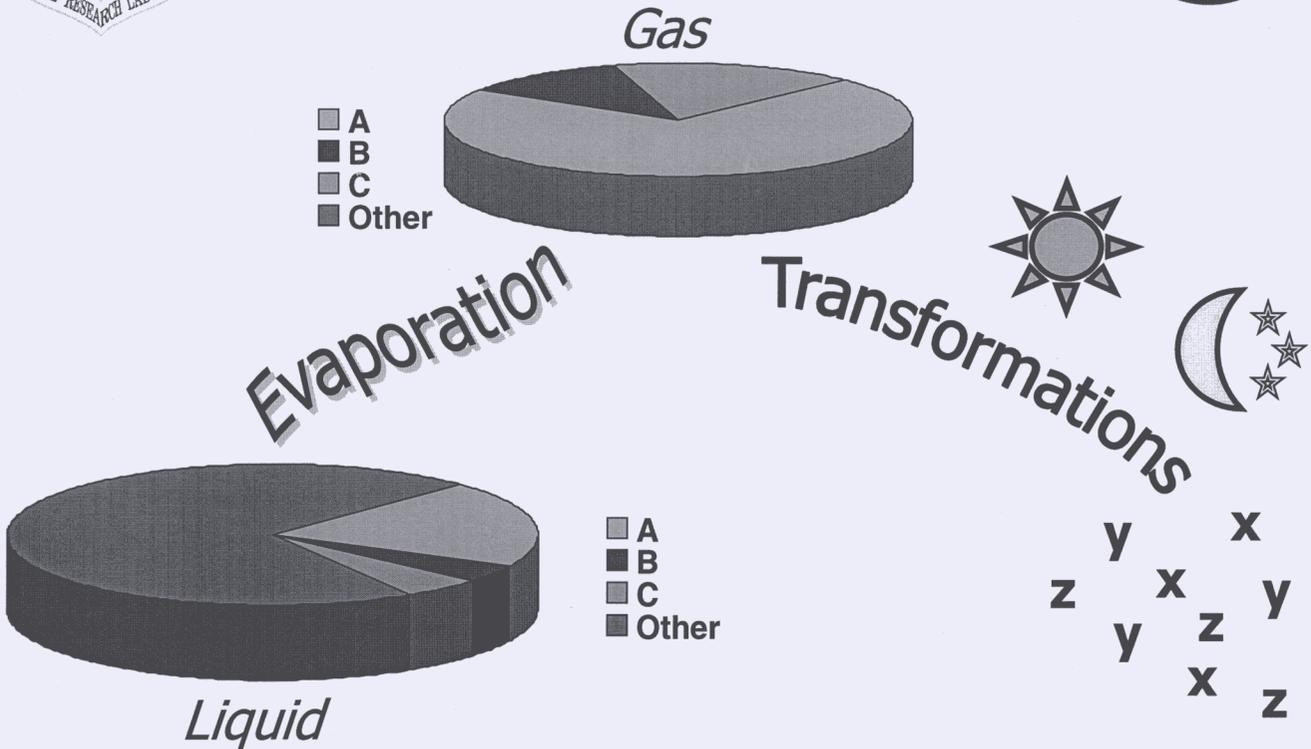


Dispersion Modeling



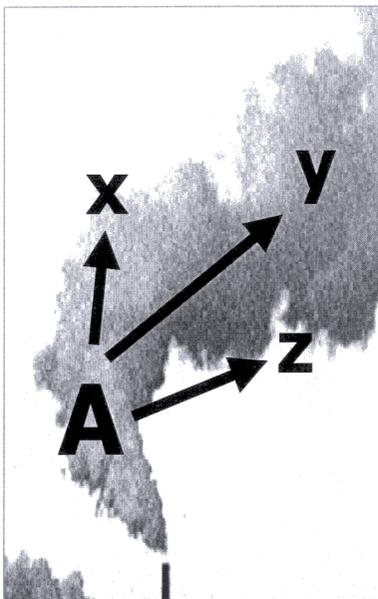


Emissions Systems





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



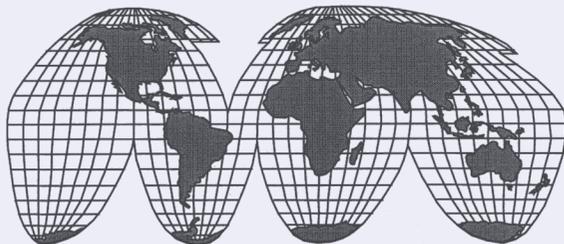
Modeling Support



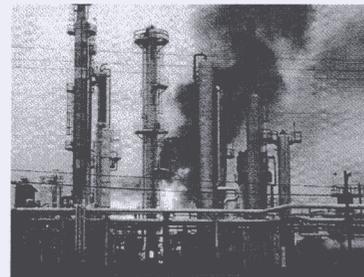
CBW Defense



Counterproliferation



TIMs





Pertinent Radical Formation Reactions



OH Radical



NO₃ Radical





Reactive Species Data



<u>SPECIES</u>	<u>CONC</u> (molc/cm ³)	<u>DAY/NIGHT</u>	<u>HC RATE</u> (cm ³ /molc sec)
----------------	--	------------------	---

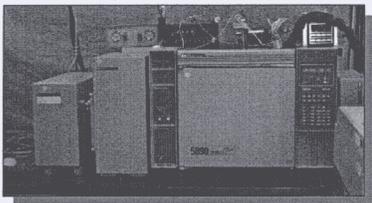
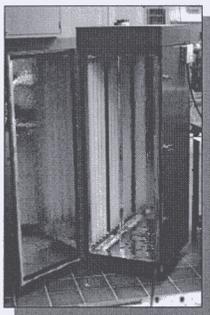
OH	10⁶	day	10⁻¹⁰ to 10⁻¹⁵
-----------	-----------------------	------------	---

NO₃	10⁹	night	10⁻¹¹ to 10⁻¹⁹
-----------------------	-----------------------	--------------	---

O₃	10¹²	both	10⁻¹⁵ to 10⁻²⁰
----------------------	------------------------	-------------	---



Air Team Products

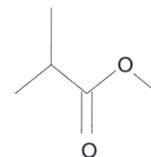
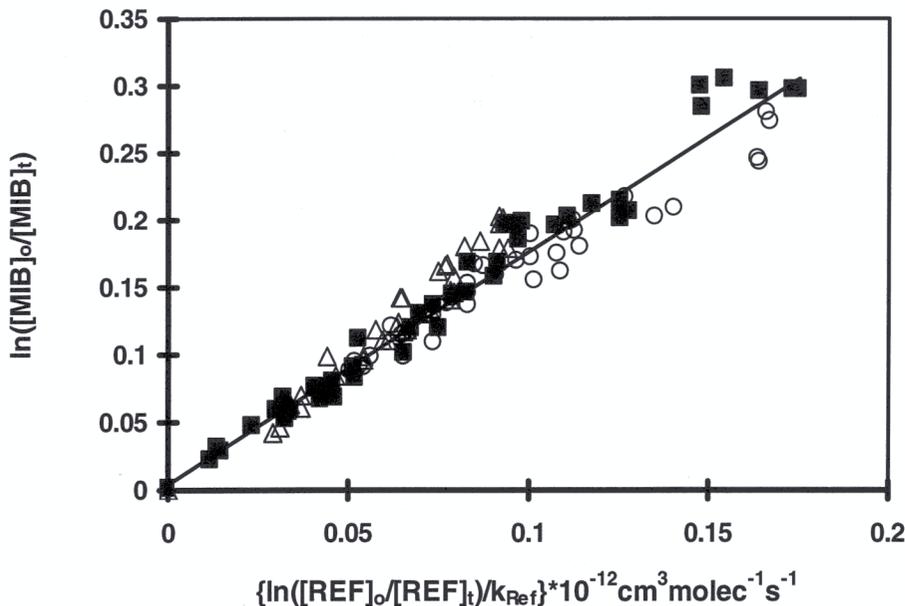


Experts in...

- Determining OH and NO₃ reaction rate constants
- Identifying products and yield
- Elucidating reaction mechanisms



Hydroxyl Radical Rate Constant for Methyl Isobutyrate

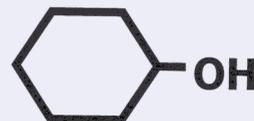
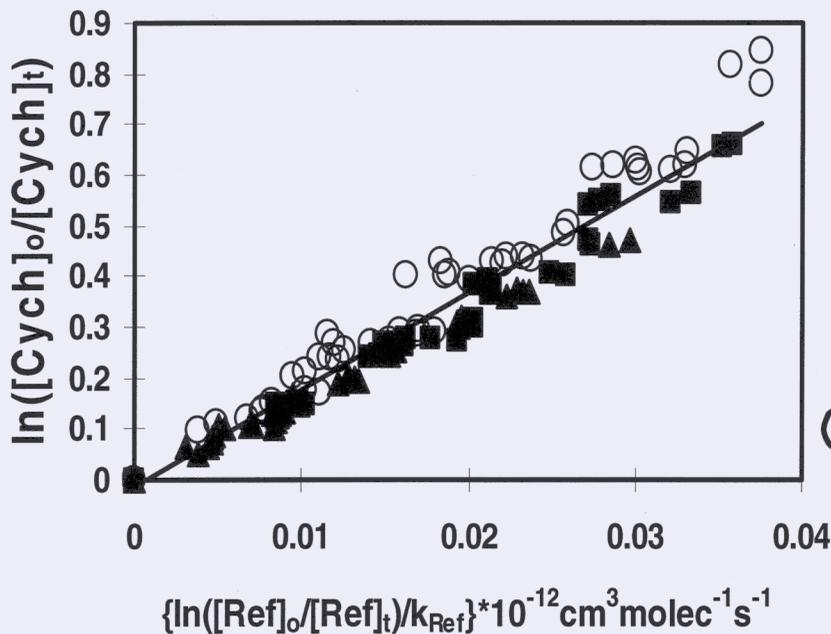


- $k_{OH} = 1.70 \times 10^{-12}$
($\text{cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$)

• 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



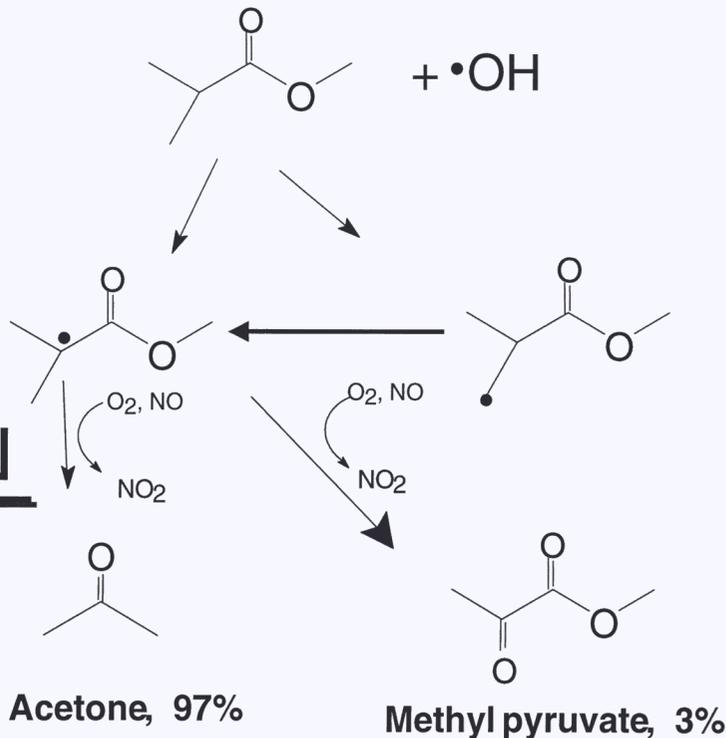
Atmospheric Transformation Mechanism for MIB



Parent *and* daughter products contribute to **ozone**

O_3

$NO_2 + hv + O_2$

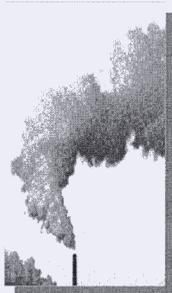
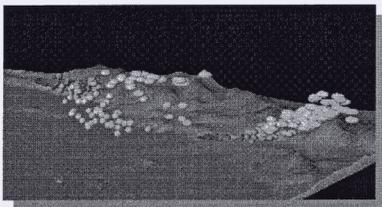




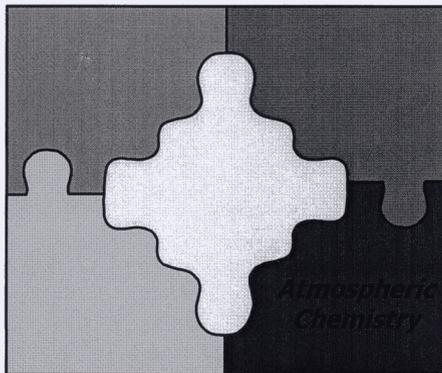
SUMMARY



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**