Atmospheric Chemistry Program Facilities:
Gulfstream 159 Research Aircraft
and
W. R. Wiley Environmental Molecular Sciences Laboratory

W.R. Barchet

Pacific Northwest National Laboratory

June 23, 1999

DOE Research Aircraft Facility

Grumman Gulfstream 159 (G-1) twin turboprop aircraft

DOE Research Aircraft Facility

- **A DOE/OBER/ESD resource for atmospheric chemistry research**
- **Instrument development, testing, and application; field study support**
- **Up to 250 flight hours per year**
- **Requests for access reviewed and recommended by Advisory Panel**

Attributes of the G-1 Research Aircraft

imensions: Length 20 m, Wingspan 24 m, Height 21 m,
Veight 16,330 kg max
ominal operation: Altitude 0.5-7.5 km, Cruise speed 80-200 r
mpling speed 100 m/s, Climb 160-330 m/min
ndurance with maximum fuel: 6 hr
ower: 4,000 VA @ 115&230 VAC, 28 VDC
rew: 2 pilots, 1-4 scientists
abin payload: 1,300 kg

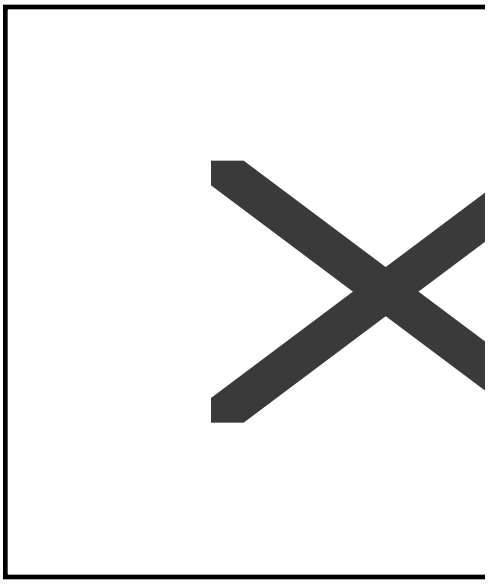
Instrumentation on G-1

Meteorological sensors

- **Temperature, pressure, dew point temperature**
- **Gust probe vector winds**

Chemical sensors

- **Real-time: O_3, CO, SO_2, NO/NO_2, H_2O, H_2O_2**
- **Integrating: filter pack (SO_2, SO_4, NO_3, HNO_3, NH_4), PAN, VOC**



Gust Probe Ports

Instrumentation on G-1

(continued)

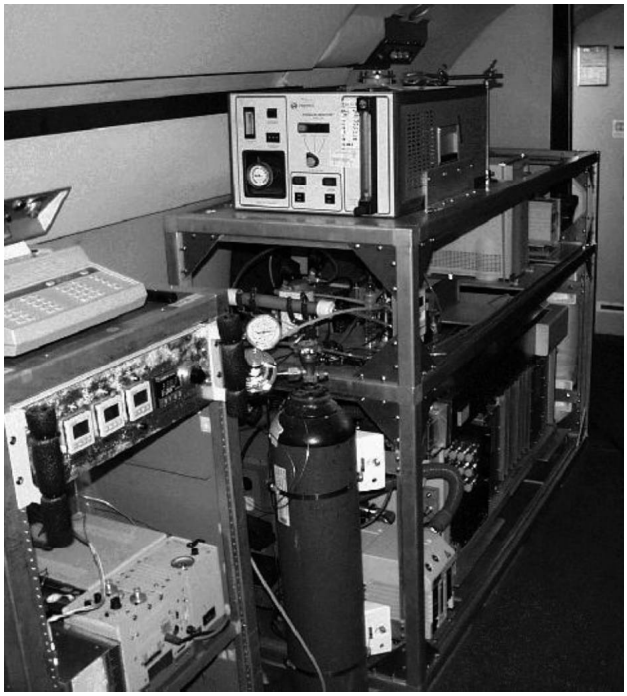
- **Cloud & Aerosol Microphysic**
  - **PMS PCASP, FSSP, 2D aerosol/cloud size spectra**
  - **Total scatter/back scatter nephelometers**
  - **Condensation particle coun**
  - **Ultrafine particle counter**
  - **Liquid water content**
- **Radiation**
  - **UV/solar/IR radiometers**
  - **Up/down-looking IR thermometers**

Instrumentation on G-1

(continued)

External instrumentation collaboration

- **BNL: NO_x/NO_y, H_2O_2, Carbonyl**
- **BCO: API-MS, PAN-GC, VOC**
- **ANL: VOC, VOC-GC, NO_2/PAN**
- **U-WA: CFVI, CCN, B_{scat}**
- **U-NV/DRI: CCN spectrometer**
- **PNNL: ITMS, Radionuclide collector**



BCO API 365 MS/MS

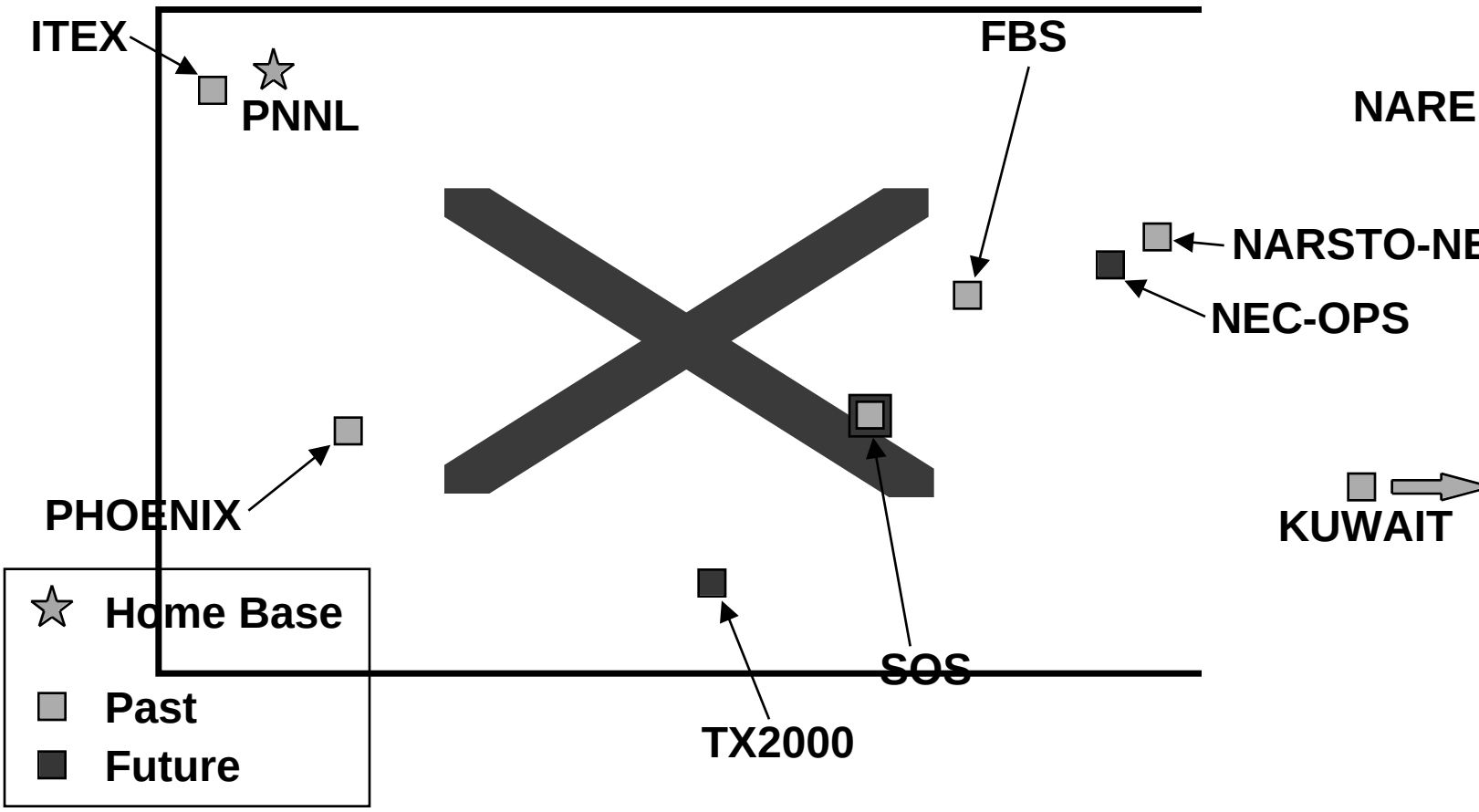
Instrumentation on G-1

(continued)

View aft

View forward

Locations of ACP Projects Using the DOE RAF G-1



Requests for DOE RAF Use

- **Requests are submitted to a review panel for evaluation**
- **DOE authorizes flight time**
- **Priority given to DOE/OBER/ESD projects**
- **Contact W. R. Barchet for more information or application for flight hours:**
  e-mail: rich.barchet@pnl.gov
  phone: 509-372-6158
  fax: 509-372-6168

W. R. Wiley
Environmental Molecular Sciences Laboratory

- **Tour of the EMSL Laboratory**
- **Examples of Research Directed at Atmospheric Sciences Needs**

P Facilities: Gulfstream 159 and Wiley EMSL

Mission

. . . provide the fundamental scientific basis needed to solve the nation's environmental problems.

. . . advance molecular science in support of the long-term missions of the U.S. Department of Energy.

National Scientific User Facility

. . . make unique research resources available to DOE scientists and researchers from academia and industry.

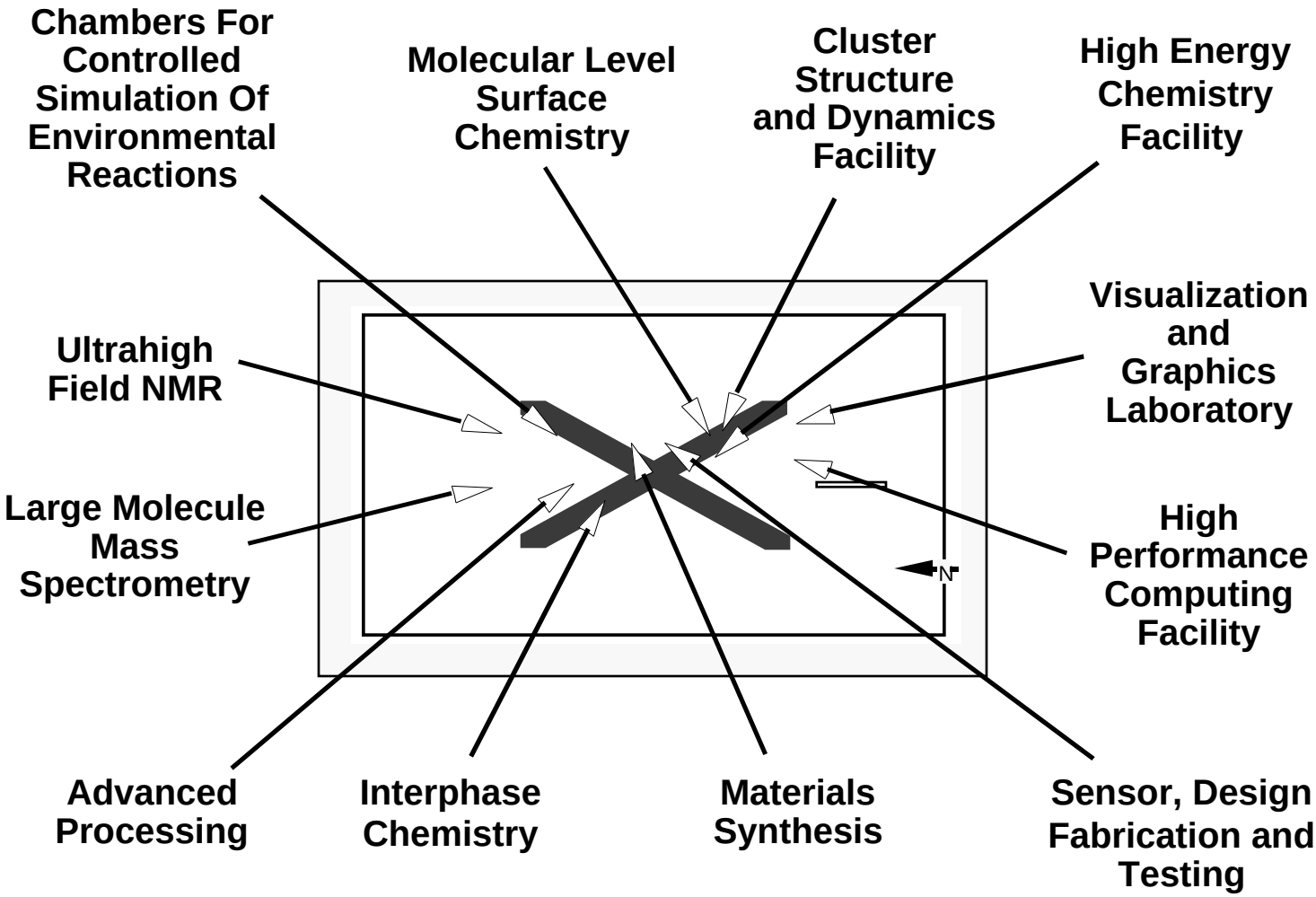
. . . provide opportunities needed to educate and recruit young scientists to meet the demanding environmental challenges of the future.

Nature of the EMSL as a User Facility:

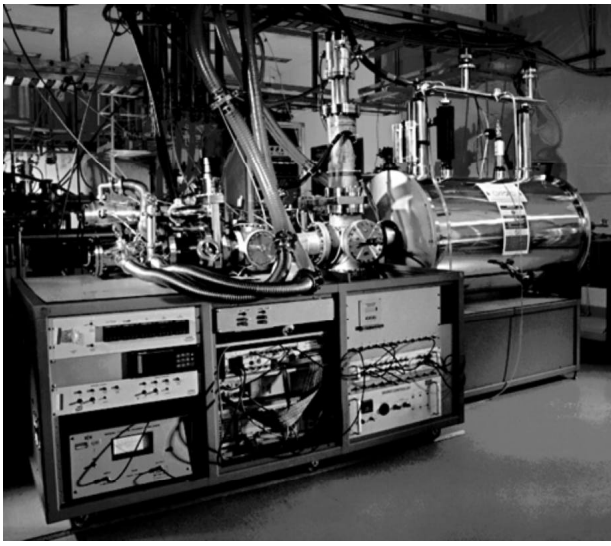
- **Primary Mission is Environmental Molecular Science**
- **Equipment Available for Both Collaborative and Independent Use**
- **Wide Range of Capabilities Available Within One Facility**
- **Web Based Applications Judged by**
  - **Scientific Merit**
  - **Applicability of Proposed Use**
  - **Equipment/Staff Availability**

P Facilities: Gulfstream 159 and Wiley EMSL

vanced Research Capabilities for Environmental Molecular Scien



ne High Field Mass Spectrometry Facility



World's first 11.5-tesla Fourier transform ion cyclotron resonance mass spectrometer

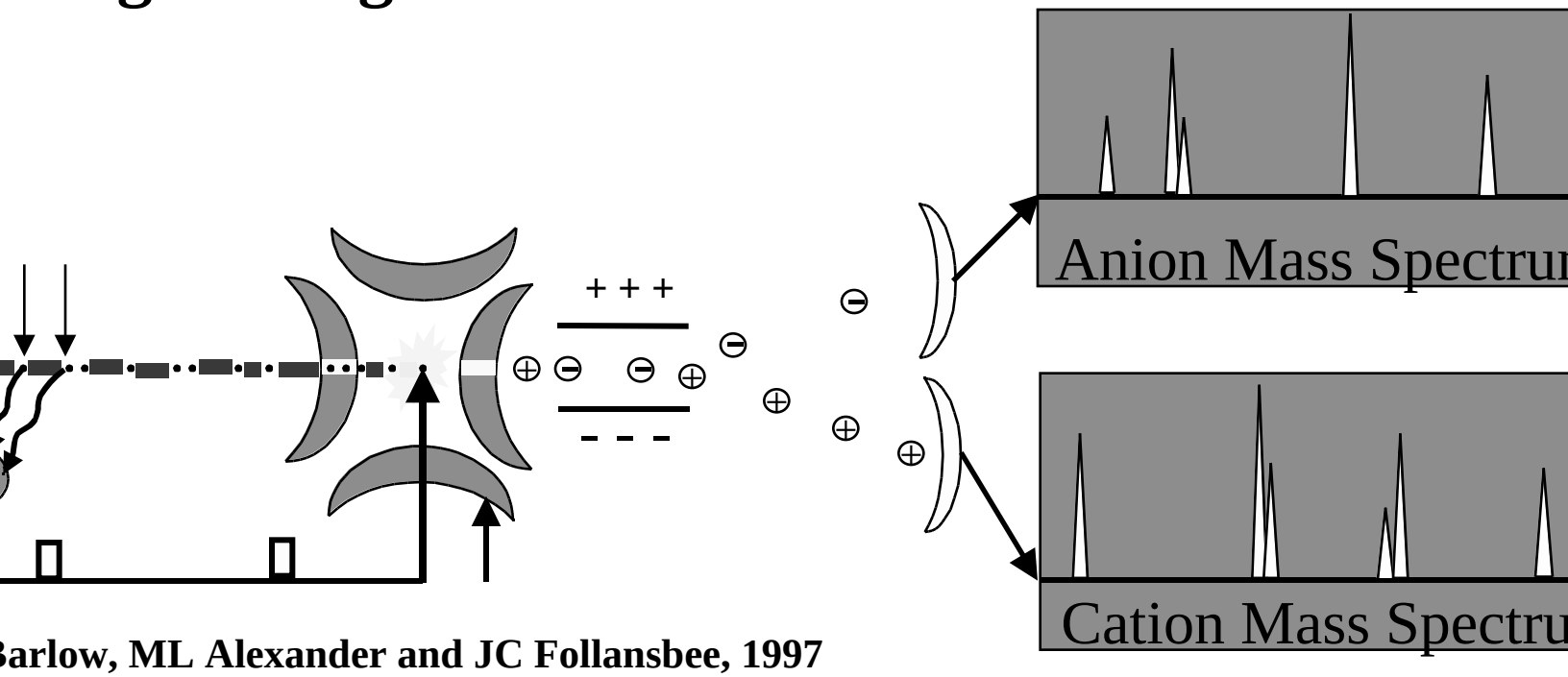
State-of-the-art 7- tesla FTICR mass spectrometer

Broad array of other mass spectrometers available for use

Aerosol Mass Spectrometer

symmetric Ion Trap: Single Particle MS

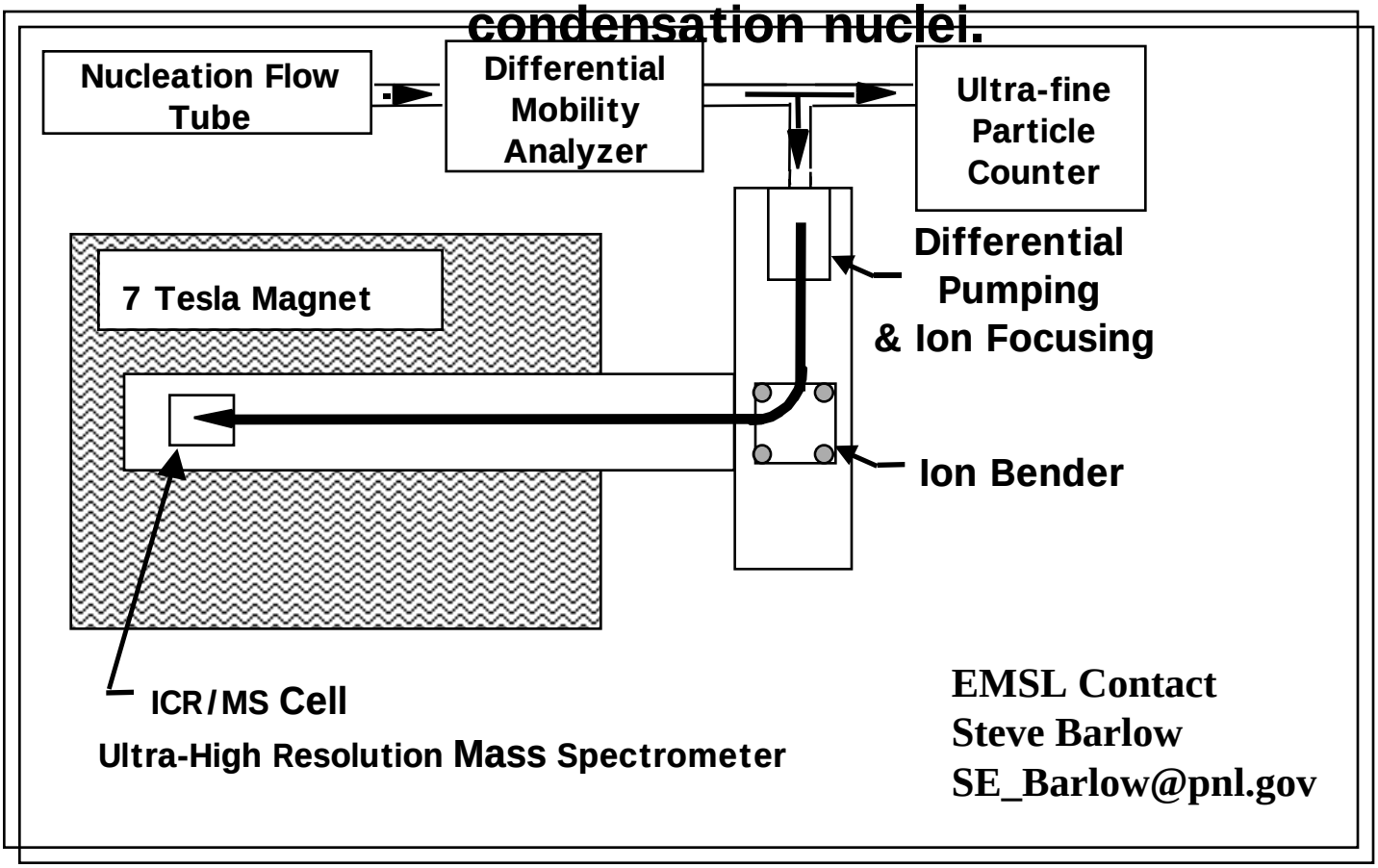
- Mass M/Z of 10 amu to 650 amu with unit resolut
- Simultaneous Anion/Cation Detection
- Light Weight/Low Power - Portable



Barlow, ML Alexander and JC Follansbee, 1997

chematic of Aerosol Nucleation Experime

Research to determine critical concentrations of trace gases e.g., ammonia and/or nitric acid, that promote formation o condensation nuclei.



EMSL Contact
Steve Barlow
SE_Barlow@pnl.gov

The Molecular Science Computing Facility MSCF

512-processor IBM RISC System/6000 Scalable POWER parallel (IBM SP) computer system

- **67 gigabytes of memory**
- **2.9 terabytes of online disk**
- **20 terabyte EMASS storage**

Graphics and visualization system

- **High-performance Silicon Graphics**
- **Integrated digital video and audio editing system**

A new generation of molecular modeling software

- **Electronic structure and molecular dynamics calculation**

Molecular Science Computing Facility

Supports:

- **benchmark calculations on small molecules**
- **reliable calculations on large molecules and solids**
- **simulations of large biomolecules**
- **reactive chemical transport modeling.**

Includes: Hardware, software, associated support staff, and a user-support staff (2 to 3 consultants).

Access: Centered around the concept of "Computational Grand Challenge" teams.

MSL Contact: Dave Dixon
A_Dixon @pnl.gov

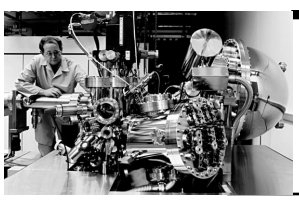
www.emsl.pnl.gov

Molecular Theory and Modelin

- **Nucleation of Tropospheric Aeros**
- **Molecular Dynamics Simulation of Uptake by Water Droplets**

- **Potential of Mean Force**
- **Water Density**
- **Ethanol Density**

EMSL Contact: Bruce Garrett
BC_Garrett@pnl.gov



One Hundred Research Stations for Environmental Molecular Sciences Research

Nanostructural Materials - Design and synthesis of model materials.

Interfacial Structures and Compositions - Characterization of atomic and molecular structures, defect structures, and compositional variations across and through interfaces.

Reactions and Interfaces - Studies of chemical and physical processes at model and natural interfaces.

Gas-Phase Monitoring and Detection - Research in detection and monitoring of trace chemicals.

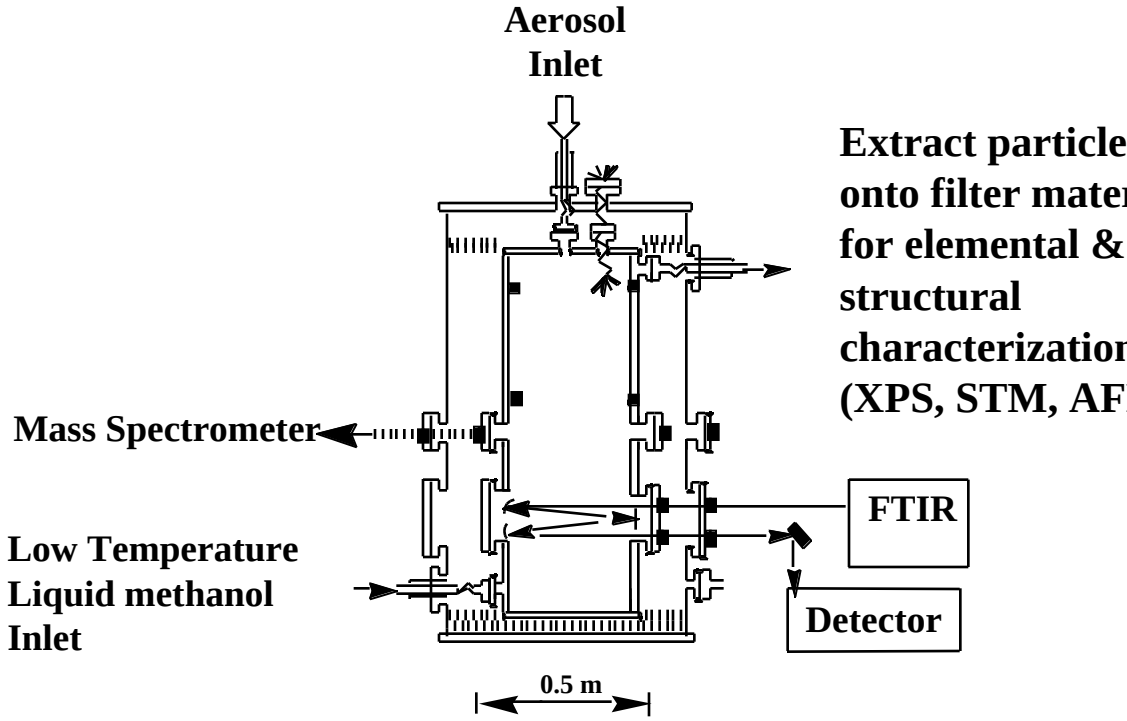
Laboratory Studies of Atmospheric Heterogeneous Chemistry

Typical Research

btain heterogeneous osol reaction efficiencies rbonaceous soot, sea-, etc.) for use in nospheric models.

entify interactions ong trace gas species of nospheric interest.

ucidate chemical chanisms/rate processes.



Aerosol Reactions Chamber

1. Temperature controlled from 300 to 185 K.
2. Teflon coated inner surfaces.

MSL Contact
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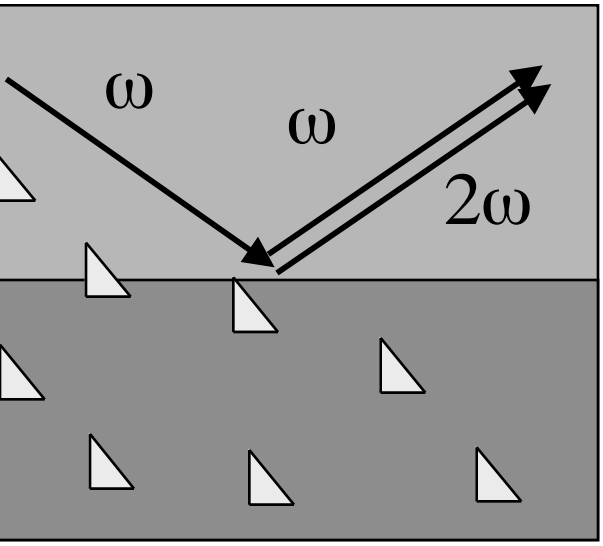
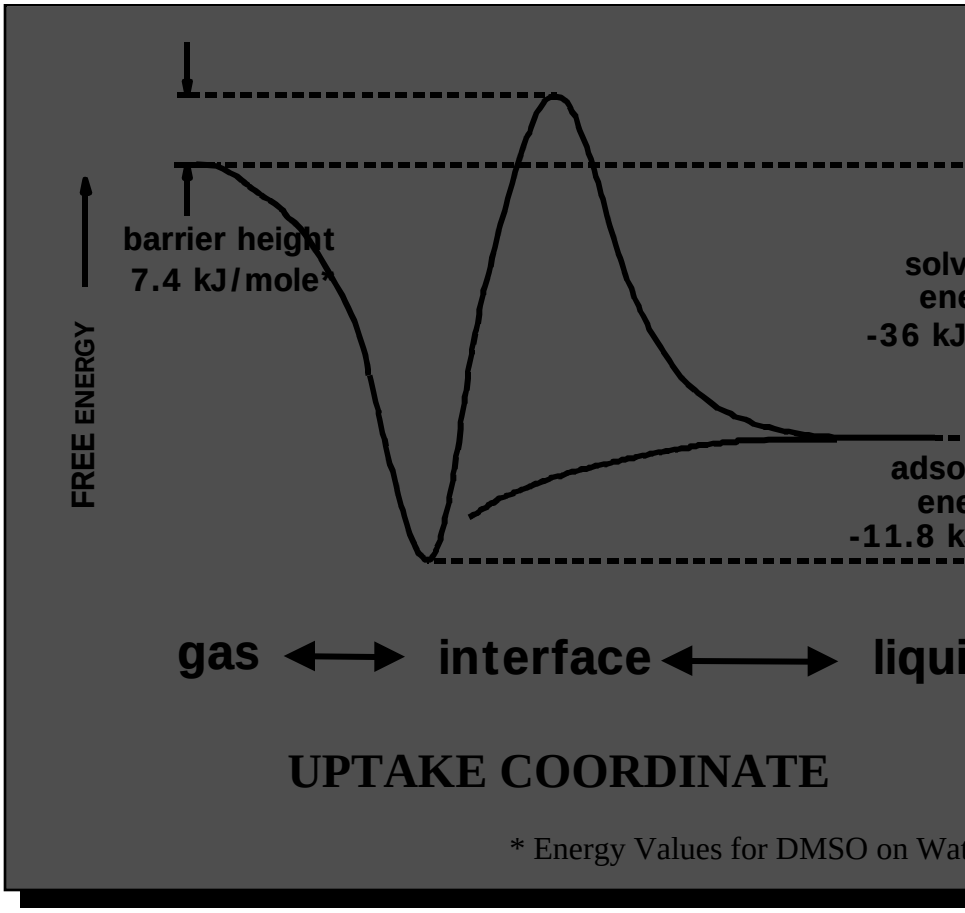
S_Disselkamp@pnl.gov

face Second Harmonic eration Studies of Gas/ uid Uptake Energetics





MSL Contact
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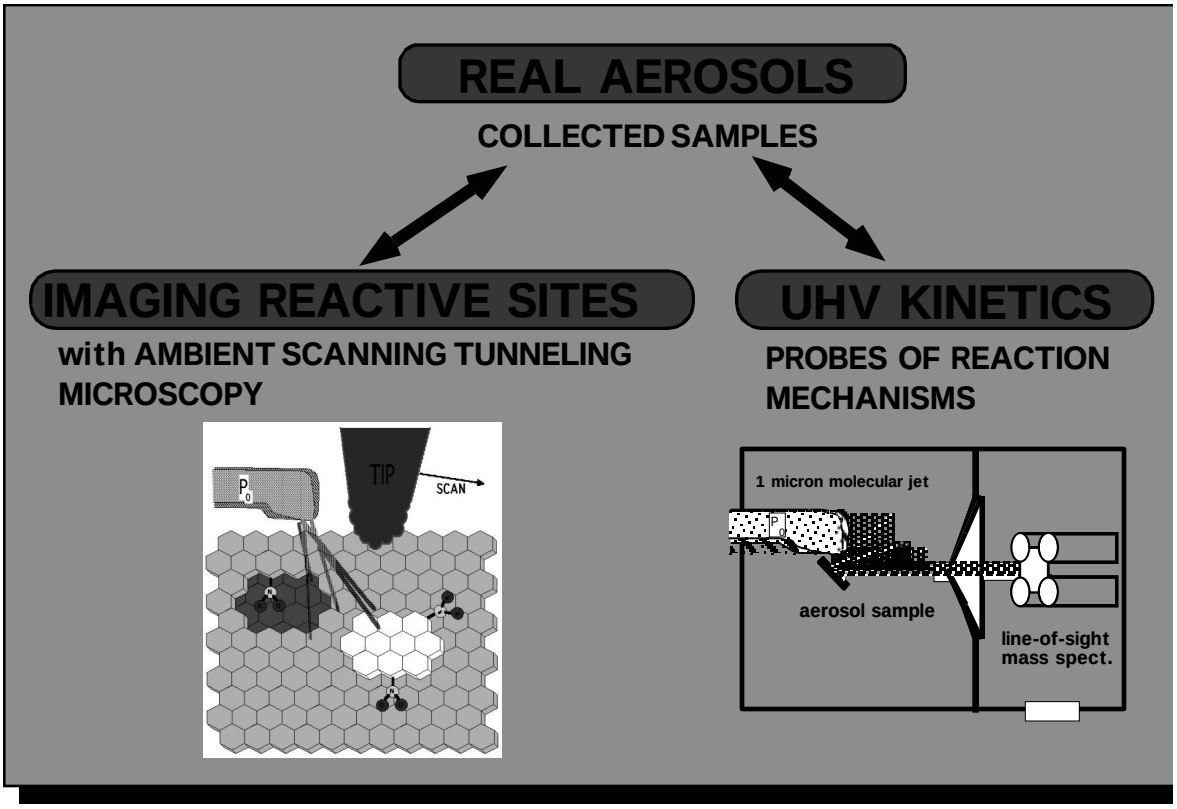
P Facilities: Gulfstream 159 and Wiley EMSL

Combining Surface Characterization (AFM, STM, XPS, …. With Molecular Jet Sources and Mass Spectroscopy to Determine Reaction Mechanisms and Rates.



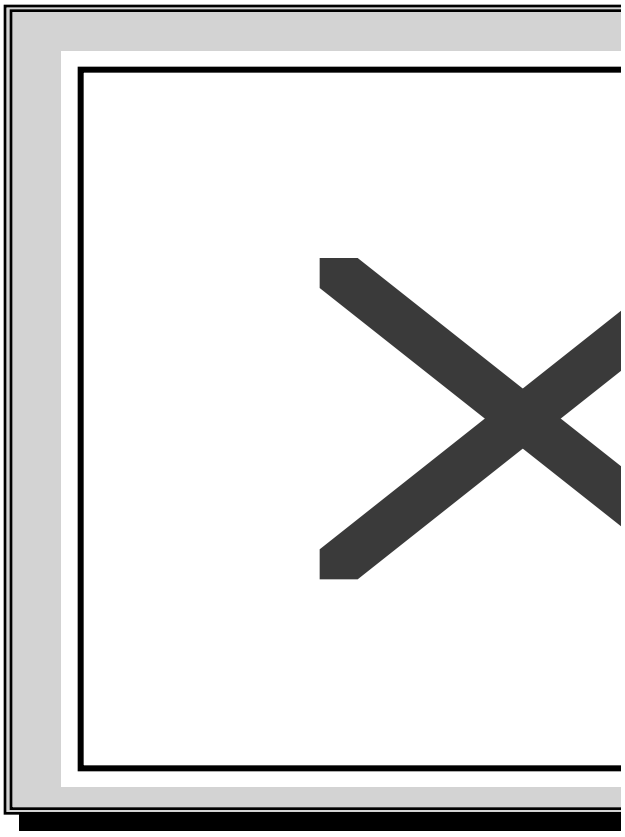
EMSL C
Jim
JP_Cowin@p

P Facilities: Gulfstream 159 and Wiley EMSL

Infrared Spectroscopy: In Cells, Jets & the Field

urrent Research

- **Laboratory measurements of he "atmospheric continuum"**
- **Development of laser-based ensors for trace atmospheric asses**
- **Development of high resolution pectral database**
- **Ultra-cold molecular pectroscopy (5-10K)**



Ultra-cold gas phase spectroscopy

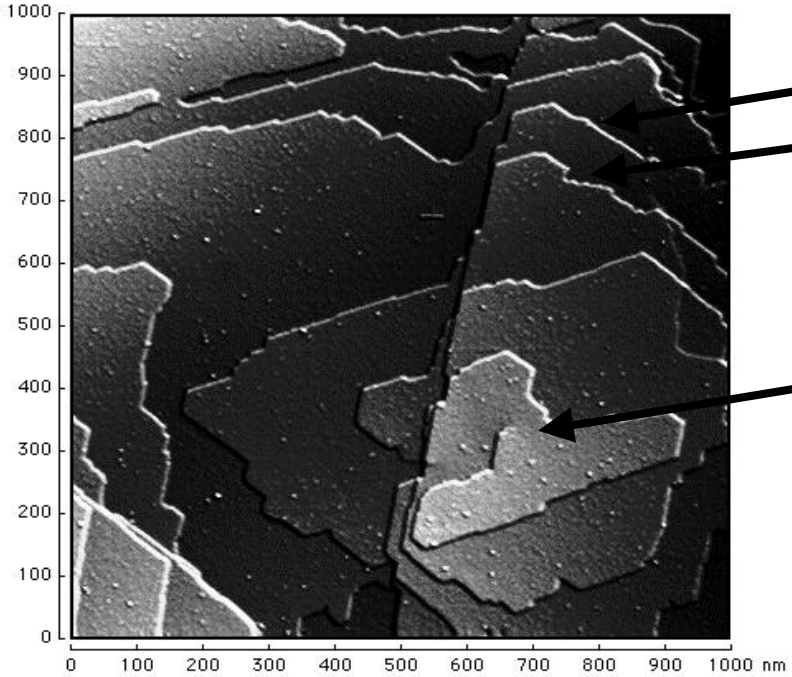
L Contact: Steve Sharpe, SW_Sharpe@pnl.gov

P Facilities: Gulfstream 159 and Wiley EMSL

Atomic Resolution Surface Analysis of Aerosols

Surface Topology Mapping

Surface Chemical Analyses



Atomic Height

Steps

Screw Dislocation

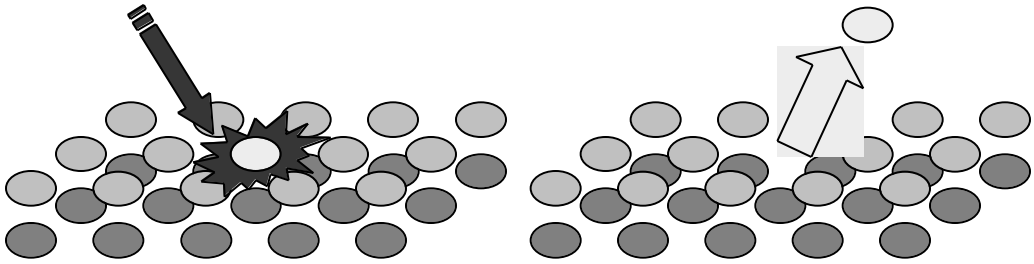
Scanning Tunneling Microscope Image of Natural α–Fe_2O_3 (001) Surface

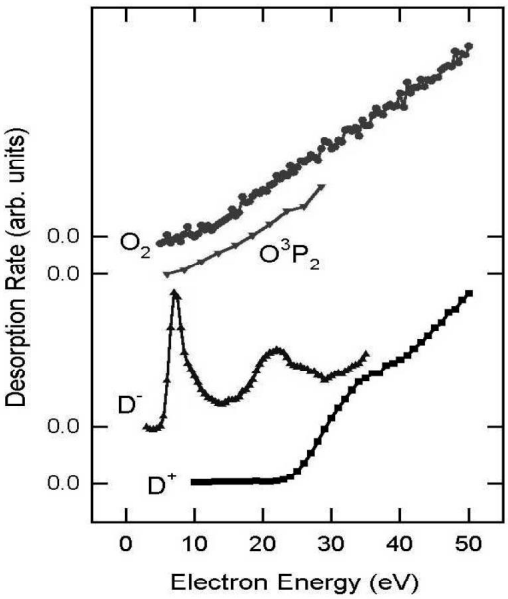
P Facilities: Gulfstream 159 and Wiley EMSL

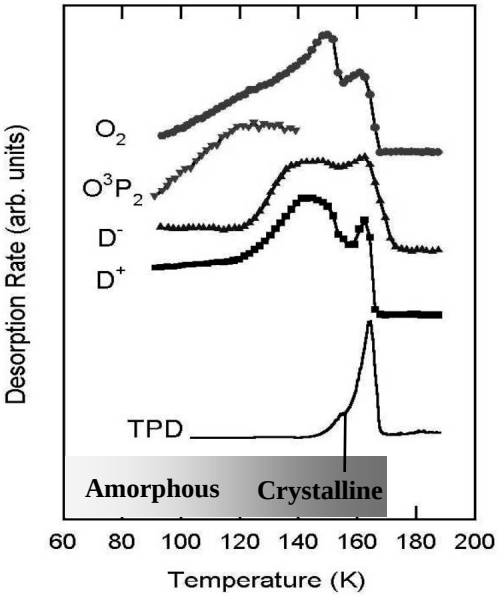
Electron beam, 5-
00 eV

nderstanding Radiochemistry and Plasma Chemistry:

lectron-Stimulated Desorption from D_2O Ice

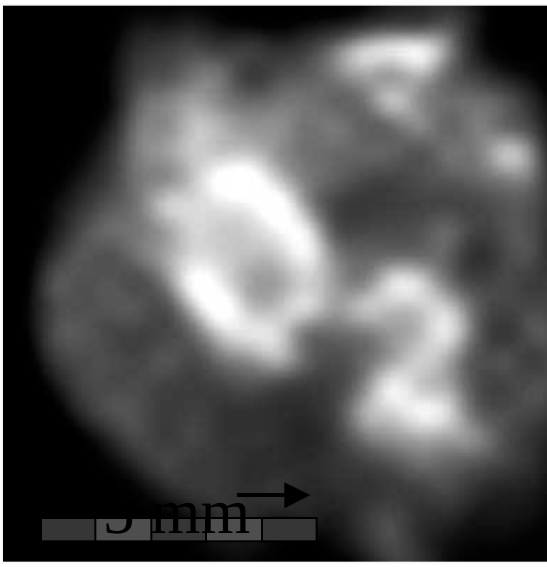


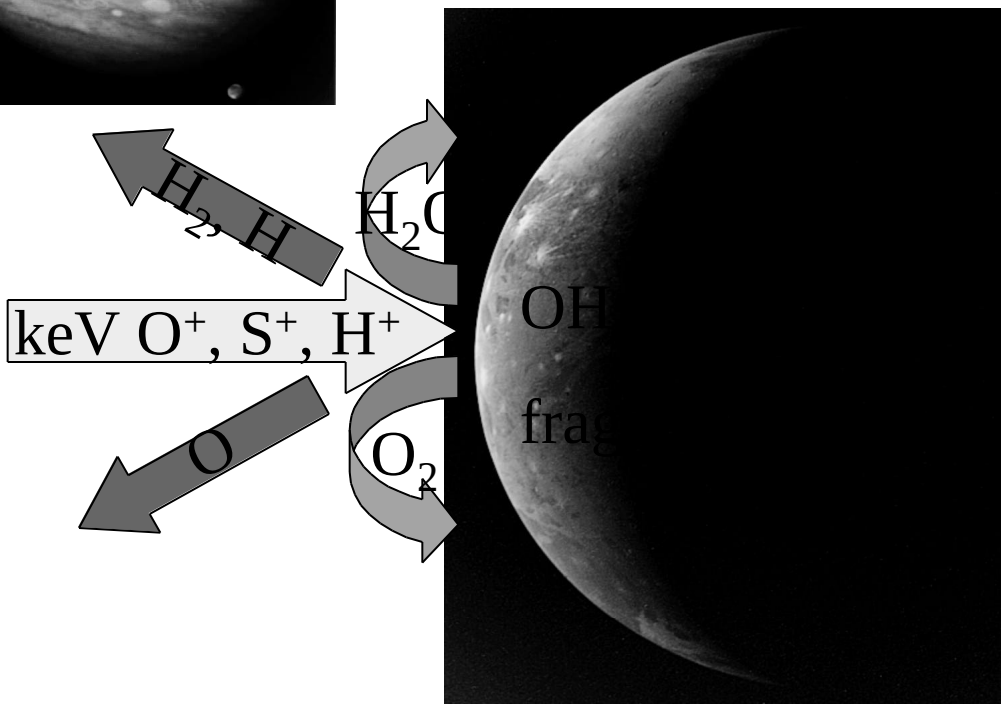




Products chang with electron energy and water mobility

Thin O_2 atmospheres have been reported on the Jovian moons Ganymede and Europa.





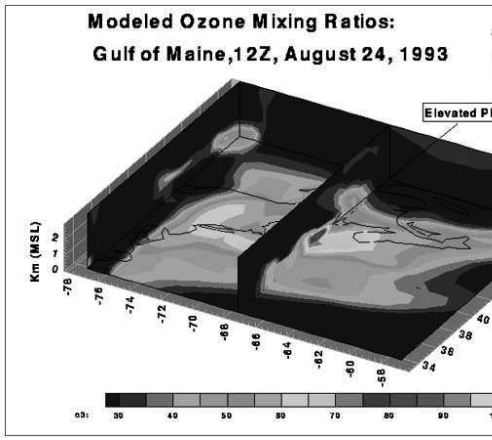
M. T. Sieger, W. C. Simpson, and T. M. Orlando, Nature, in press

Conducting Atmospheric Sciences Research

- **Team Effort Involving Many Disciplines**
- **Focused on National Needs**
  - ***Air Quality: Oxidants, Particles***
  - ***Understanding Global Change***
- **Model Based**
- **Requires Close Coupling of Programs**
  - ***Operational Sensitivity Analysis***

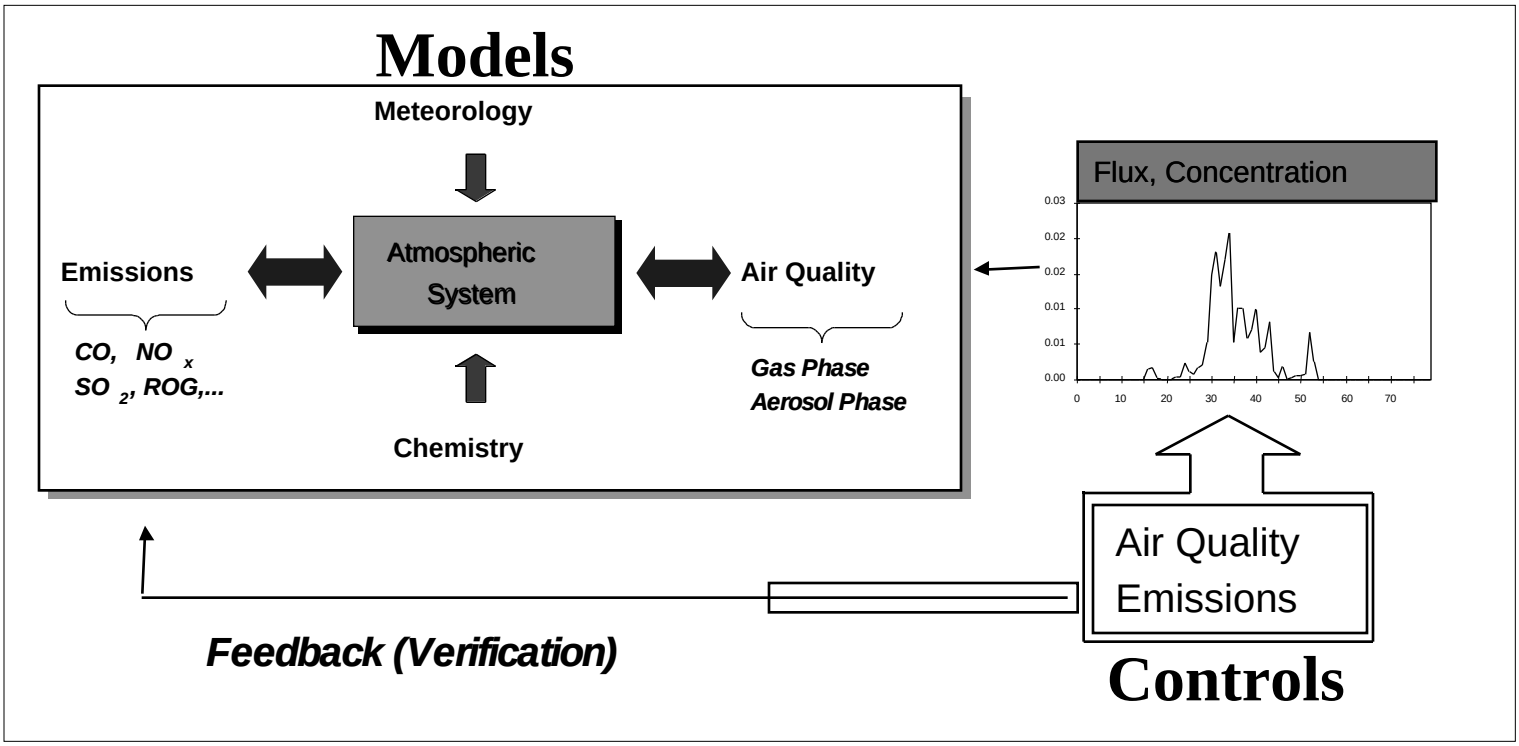
Operational Sensitivity Analysis

•Data Requests
• Results
•Surprises



Models

- **Relationship Between Controls and Air Quality**
- **Basis for Laboratory and Field Experiments**



Gaining Access to the EMSL

- **Use The Web Based Information Resources and User Application: www.emsl.pnl.gov**

- **Contact an EMSL Staff Member (optional)**
  i.e. Steve Colson at
  email: SD_Colson@pnl.gov
  phone: (509) 376-4598
  FAX: (509) 376-0846