Numerical Simulations of Atmospheric Chemistry and Its Impacts on Air Quality, Weather, and Climate

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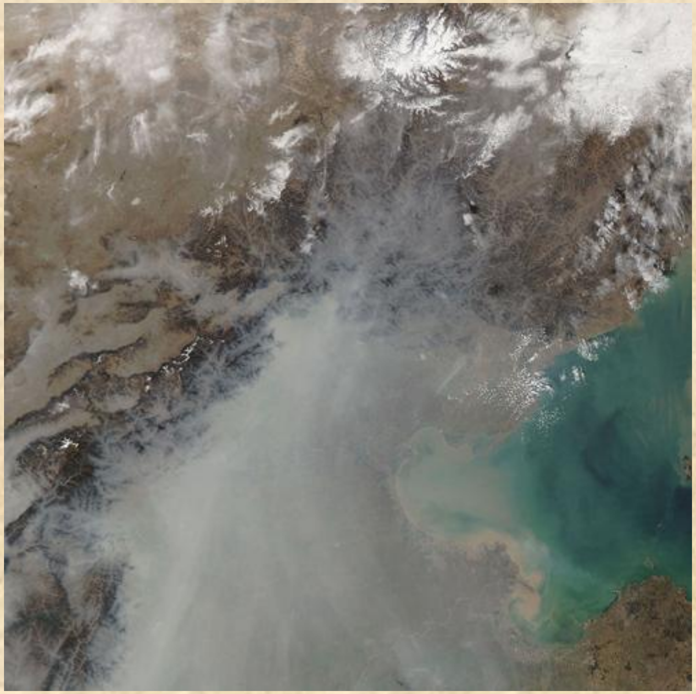
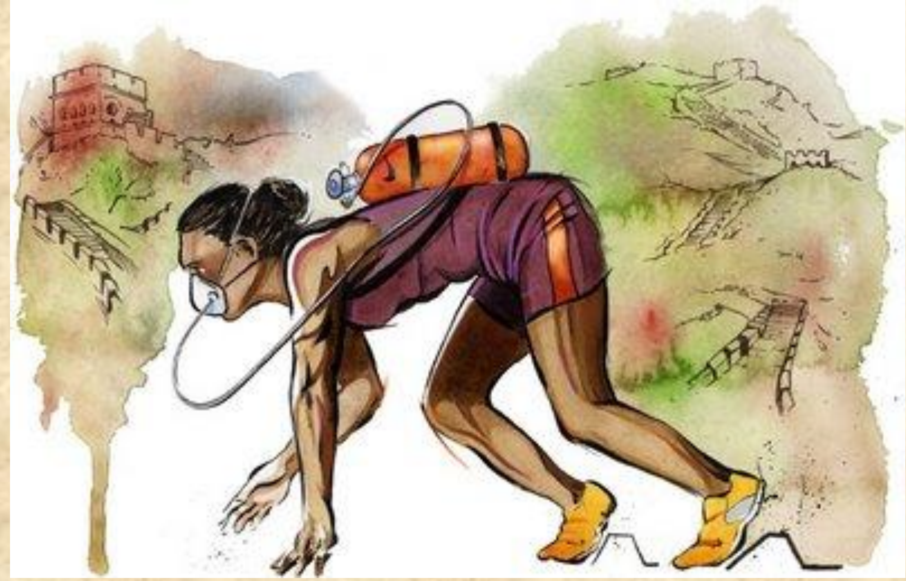
Troposphere 0-7 miles from the earth's surface
The COMET Program

Effects of Asian Air Pollution





A&M studies Beijing's air

By HOLLY HUFFMAN

Eagle Staff Writer

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Eagle Staff Writer

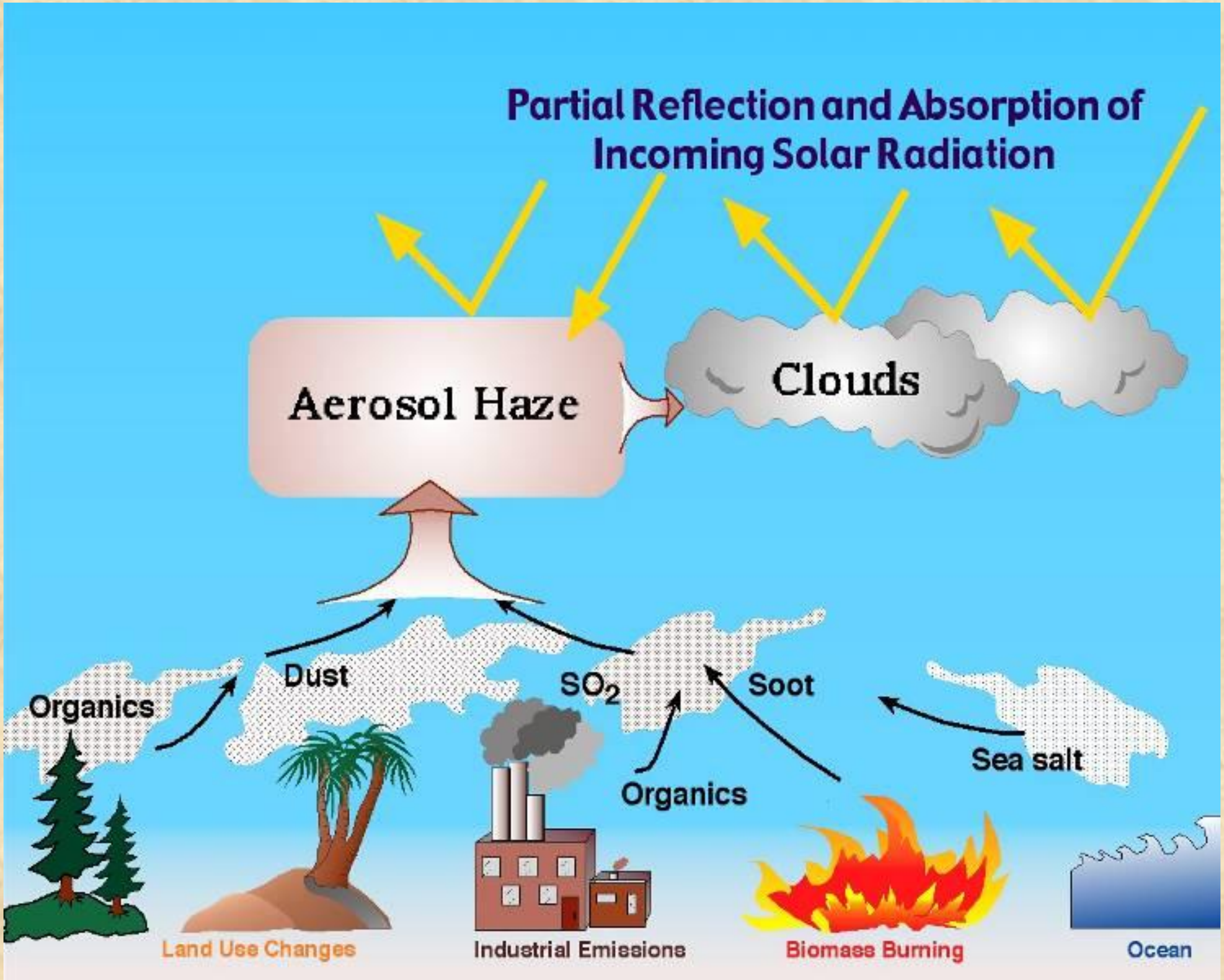
Millions of people around the globe are focusing on Beijing, and Texas A&M University professor Renyi Zhang is no exception.

But while most people have set their sights on China because it is home to the 2008 Olympic Games, Zhang is concentrating on the country's second-largest city because of its air pollution.

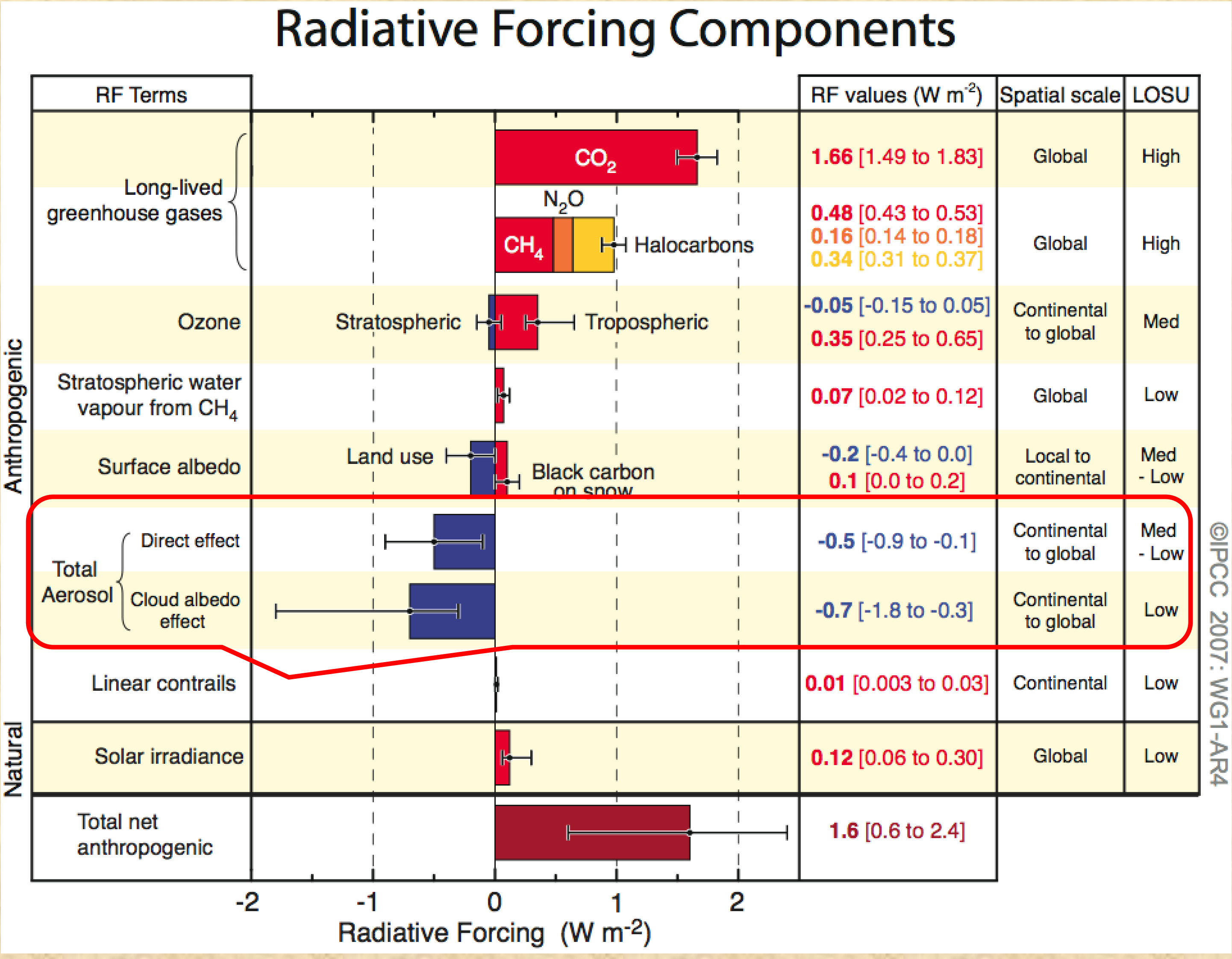
"There are a lot of places which are heavily polluted, so we've been doing this kind of research for a while," said Zhang, a professor in the department of atmospheric sciences. "We've studied air quality in Houston and Mexico City. Recently, we're working on Beijing."

Zhang and his research team are collaborating with scientists from Peking University in Beijing. Zhang and his team are studying measurements and data collected by researchers in Beijing.

Effects of Atmospheric Aerosols on Climate

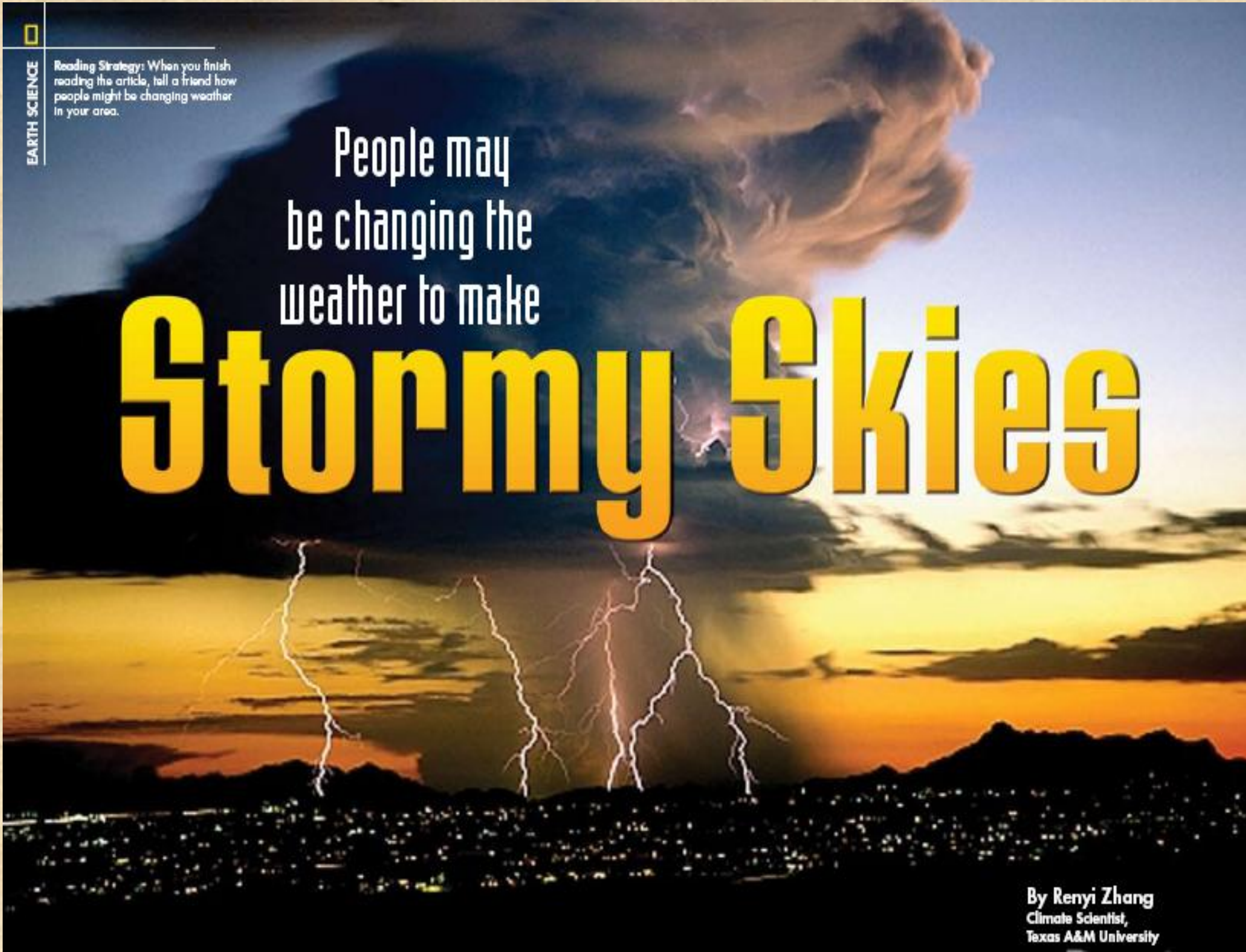


Global-average Radiative Forcing Estimates and Ranges in 2005 by Inter-Government Panel on Climate Change (*IPCC*), 2007



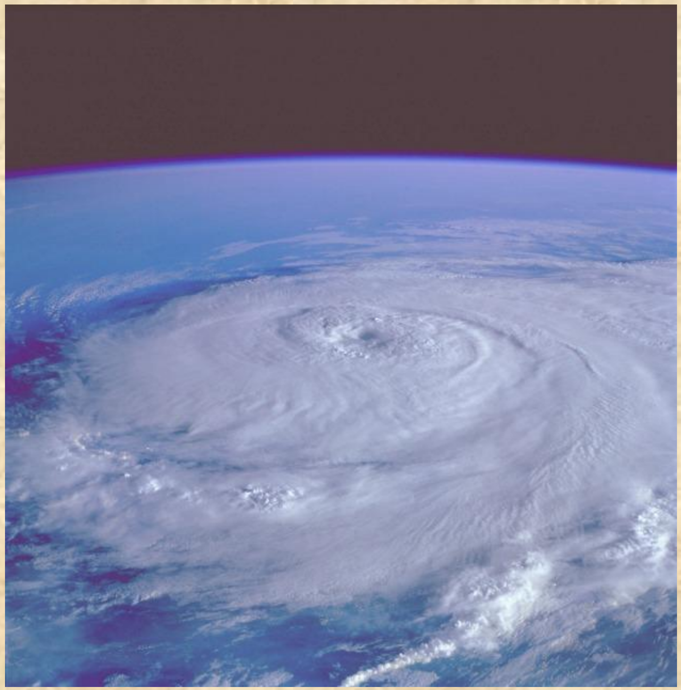
EARTH SCIENCE

Reading Strategy: When you finish reading the article, tell a friend how people might be changing weather in your area.



People may be changing the weather to make Stormy Skies

By Renyi Zhang
Climate Scientist,
Texas A&M University

Scientific American, May, 2001

Retallack's earthly rocks, which record the history of Permian river basins, reveal an intense spike of light carbon values—a telltale sign of a greenhouse warming crisis—during the extinction. More specifically, the carbon values indicate that the atmosphere was loaded with methane. Tons of this potent greenhouse gas could have been released instantly if the offending space rock slammed into a deposit of methane hydrate, Retallack says.

In the end, scientists may be forced to rely on tracers such as fullerenes to prove whether an impact prompted the world's worst mass extinction. "I have a feeling we're either going to go down in flames," Becker says, "or we're going to be heroes."

METEOROLOGY

Bright Sky, Dirty City?

HOUSTON, WE HAVE GROUND STRIKES. LOTS OF THEM BY STEPHEN COLE

To look at the false-colored U.S. map of cloud-to-ground lightning flashes over the past decade, you would think that someone had planted a huge lightning rod in the middle of Houston. During peak thunderstorm season (June to August), the city is hit by an average of 1,700 ground flashes a month—only areas in Florida are hit worse. And there are twice as many ground strikes over and immediately downwind of Houston as there are upwind just 80 kilometers away.

"Somehow 4.5 million people are having a major effect on the meteorology of Houston," says Richard Orville of Texas A&M University, lead author of a paper to be published in *Geophysical Research Letters*. The researchers relied on the National Lightning Detection Network, a database that pinpoints ground flashes with unprecedented accuracy. A 1995 study of 16 Midwestern U.S. cities used these data and found a correlation between city size, air pollution and lightning, but it could not single out one factor responsible for the extra lightning, which was generally much less than in Houston.

The new research seeks to narrow the possibilities. Local meteorological conditions produced by nearby Galveston Bay, which enhances convective activity and thunderstorm development, can be counted out, Orville believes. The researchers simulated the meteorology of the region with and without Houston's urban elements and found that the strong patterns of convergence over the city were not caused by the bay but by the "heat island effect" of the city itself.

But urban heat may not be the whole story. Orville's analysis also found a lightning hot spot over Lake Charles, La., just east of Houston. Ground flashes over this small city reached levels as high as Houston's, but there is no urban landscape to fuel them.

One thing the two cities share is major air pollution sources, including petroleum refineries. Renyi Zhang, an atmospheric chemist at Texas A&M, says that air pollution particles, or aerosols, could boost lightning by helping more cloud water get into the upper reaches of a deep convective cloud, where supercooled water droplets collide with ice crystals. "The particle collisions act just like rubbing your hand through your hair to separate electric charge," Zhang says.

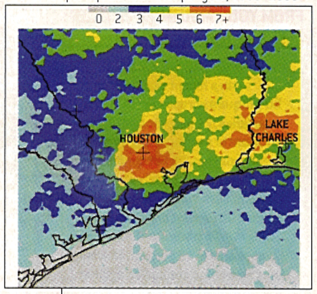
Daniel Rosenfeld of the Hebrew University of Jerusalem recently reported observations in the Brazilian Amazon of how aerosols can boost lightning: smoke particles from biomass burning create many small cloud droplets that carry more water high into the cloud.

Here, too, separating the effect of aerosols from other related factors isn't easy. "This supercooled water can get high in the clouds by stronger updrafts or with the help of aerosols," Rosenfeld explains. "Usually the stronger updrafts are also in the more polluted air."

Orville plans to take a closer look at both Houston and Lake Charles. With the wealth of high-resolution lightning data in hand, he hopes to pinpoint the reasons why Houston's skies are so often bright.

Stephen Cole is a science writer and editor based in Washington, D.C.

Flashes per square kilometer per year, 1989–1999



LIGHTNING-FLASH DENSITY is high over Houston and Lake Charles, La.

COURTESY OF THE LIGHTNING PROJECT, TEXAS A&M UNIVERSITY

NEED TO KNOW:
CHARGED UP

Last year the Environmental Protection Agency funded a **"supersite" monitoring program** in Houston to study the sources and composition of its particulate pollution.

The National Lightning Detection Network records **ground flashes every microsecond** and locates the strikes to within less than a kilometer.

Rather than pollution or the heat island effect, Florida experiences a lot of lightning because of its **peninsular geography and subtropical climate**, which help to make it the undisputed lightning champ from coast to coast.

Atmospheric Chemistry: The "Vacuum Cleaner" Story

The Atmosphere is an oxidation medium

Tropospheric Ozone Formation

$O + O_2 \rightarrow O_3$

An Example: SO_2 Oxidation

- **Photochemistry**

  $O_3 + hv \rightarrow O(^1D) + O_2$

  $O(^1D) + H_2O \rightarrow 2OH$

- **Gas-Phase Chemistry**

  $SO_2 + OH \rightarrow OHSO_2$

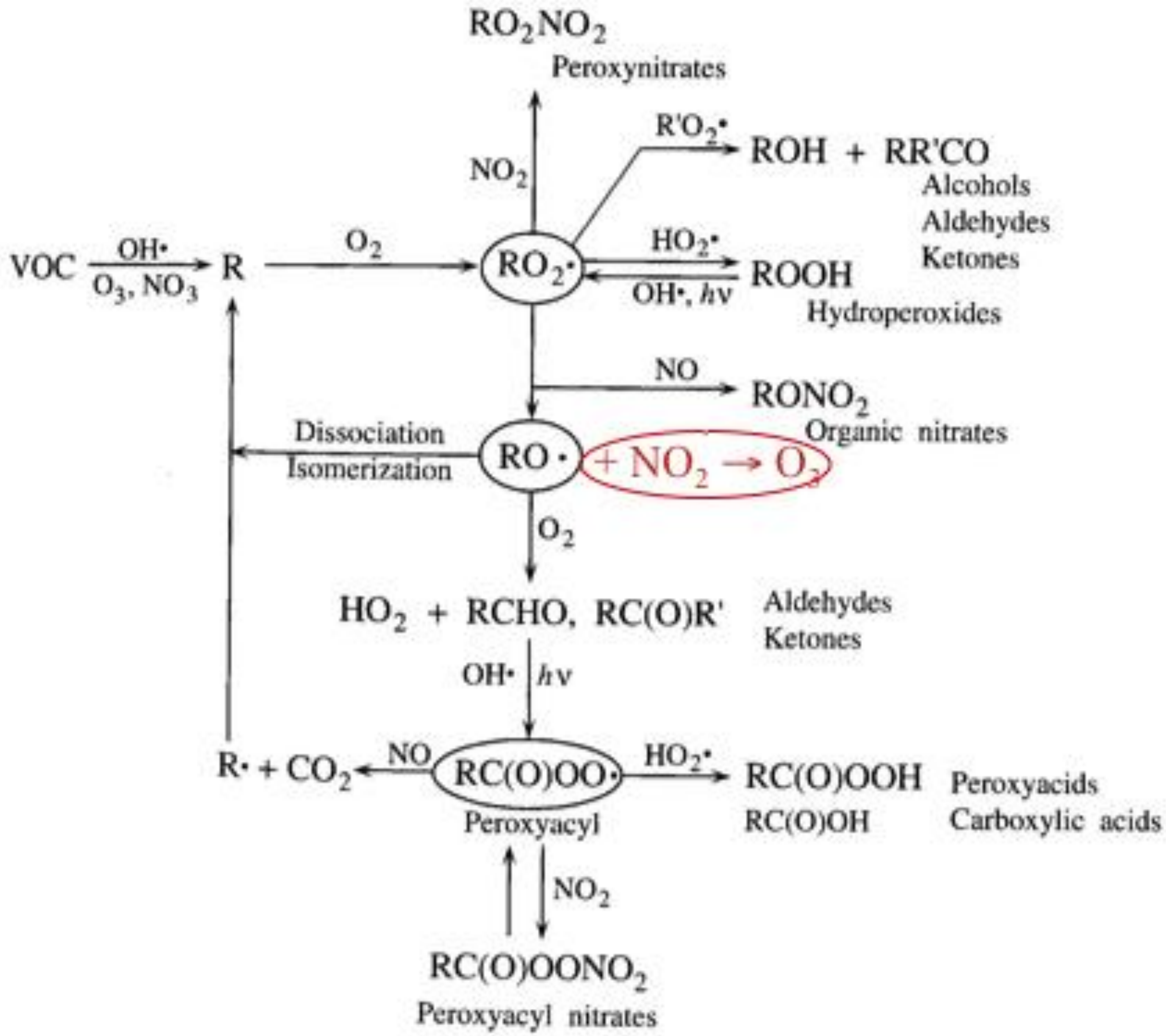
  $OHSO_2 + O_2 \rightarrow SO_3 + OH_2$

  $SO_3 + H_2O \rightarrow H_2SO_4$

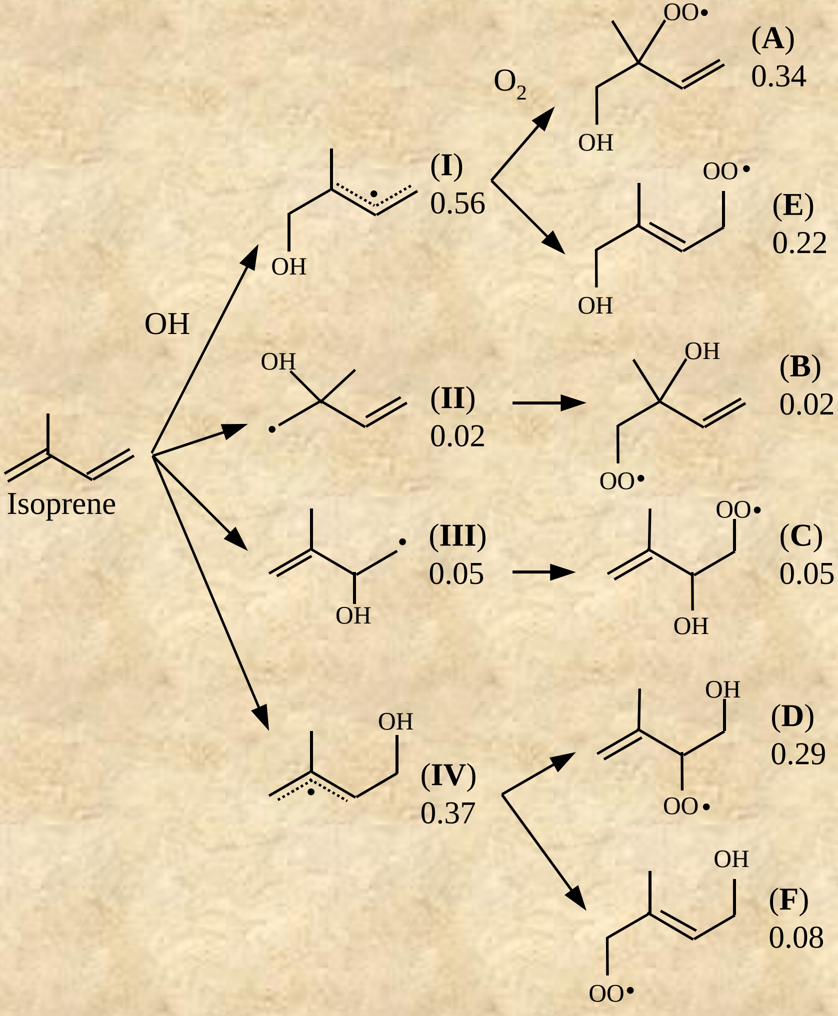
- **Heterogeneous Chemistry**

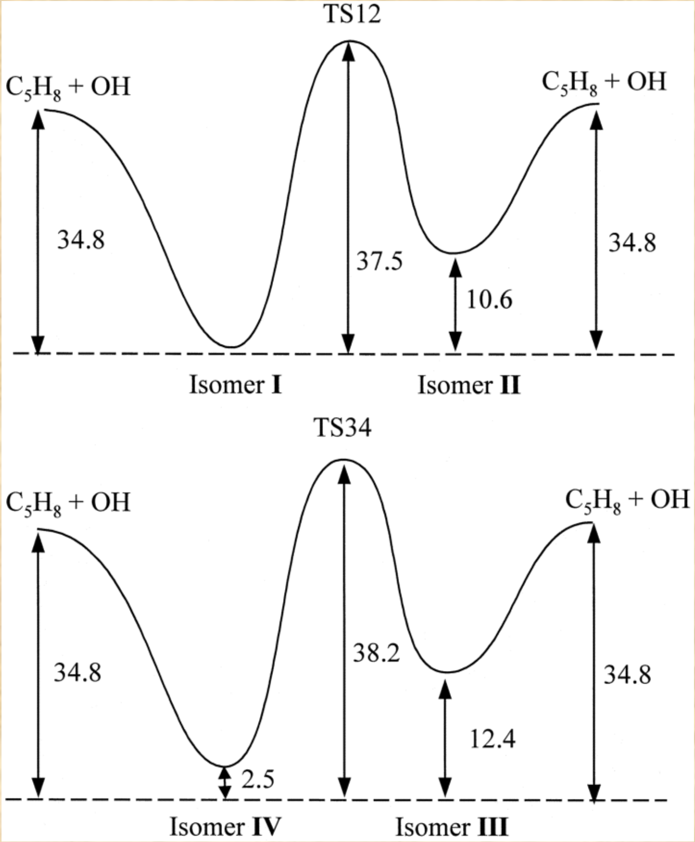
  $H_2SO_4 \rightarrow$ Sulfate Aerosols $\rightarrow$ Removal by wet deposition or precipitation

Tropospheric Oxidation of VOCs by OH, NO_3, Cl



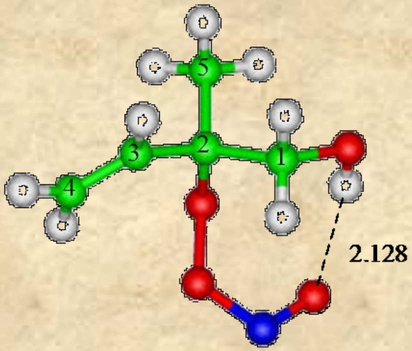
W. Lei *et al*., Theoretical study of OH-O_2-isoprene peroxy radicals, *J. Phys. Chem.*, 105, 471 (2001)



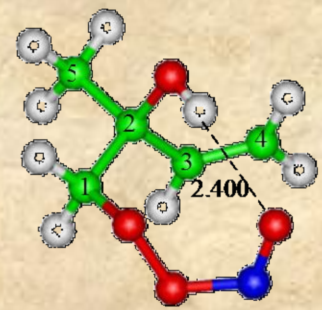


D. Zhang *et al*., Hydroxyperoxy nitrites and nitrates from OH initiated reactions of isoprene, *J. Am. Chem. Soc*., 124, 9600 (2002)

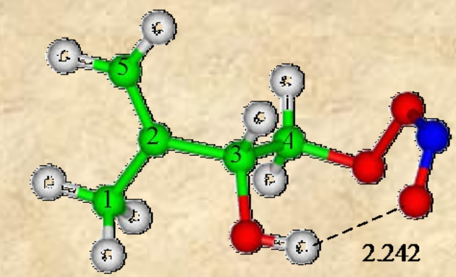
ROONO I



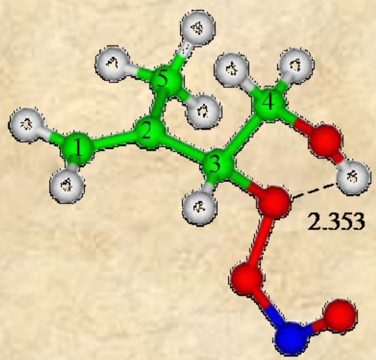
ROONO II



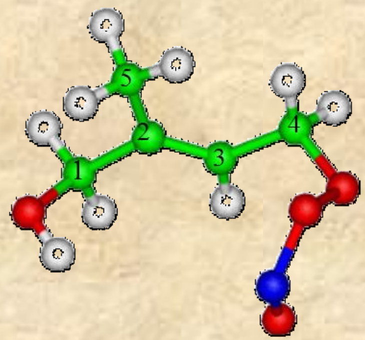
ROONO III



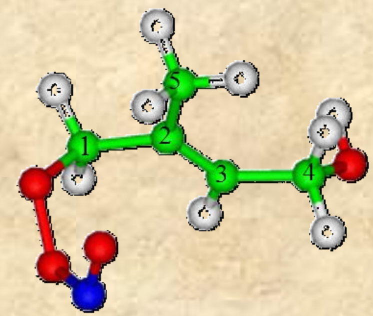
ROONO IV



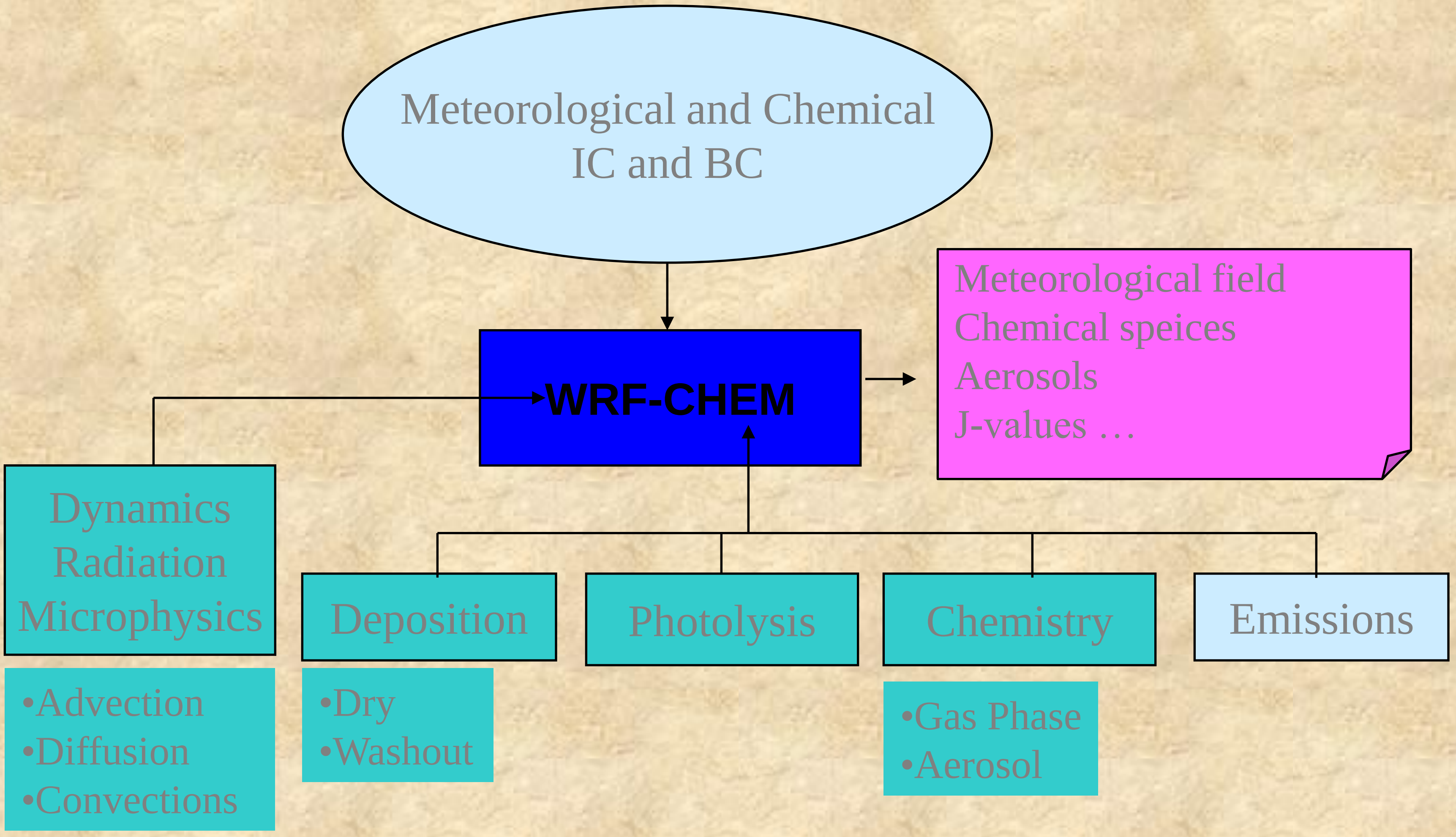
ROONO V



ROONO VI



Chemical Transport Models



6346–6350 | PNAS | April 27, 2004 | vol. 101 | no. 17

Industrial emissions cause extreme urban ozone diurnal variability

Renyi Zhang*†, Wenfang Lei*, Xuexi Tie‡, and Peter Hess‡

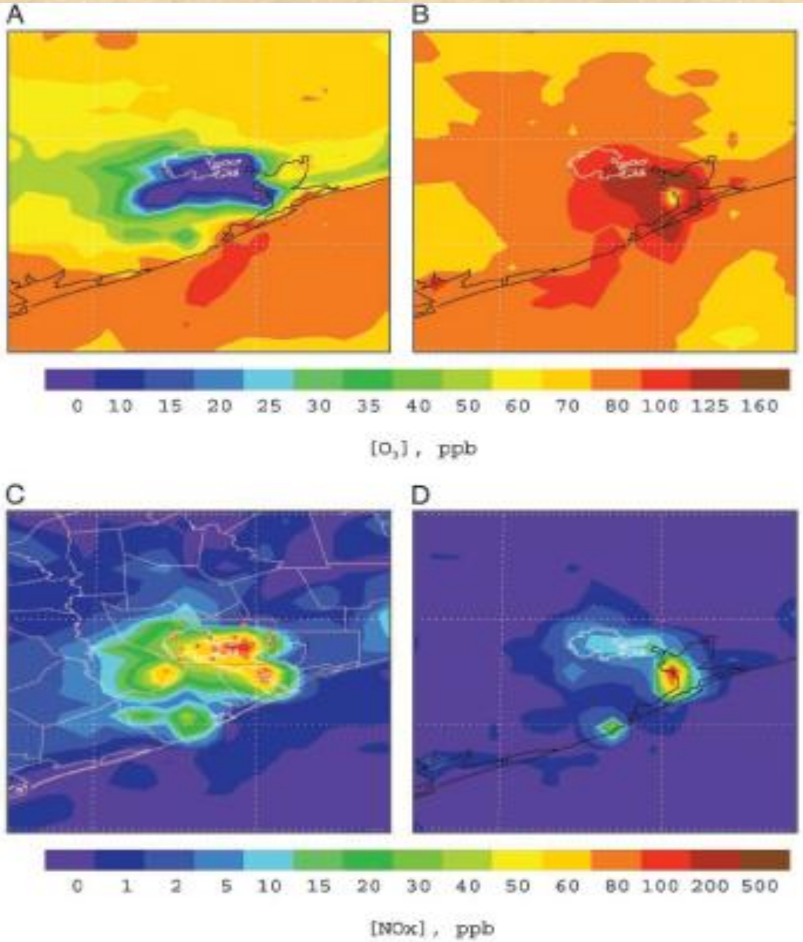
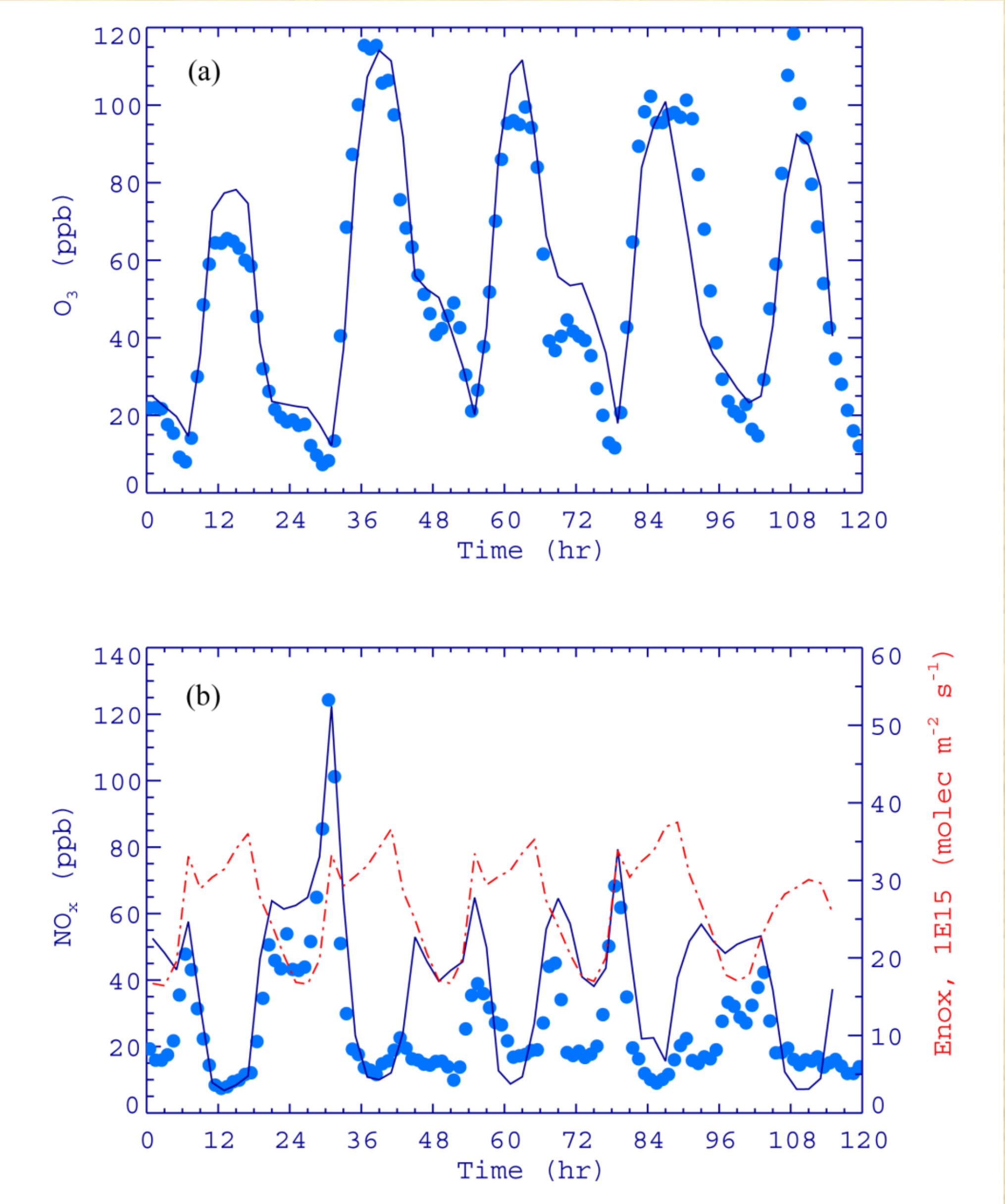
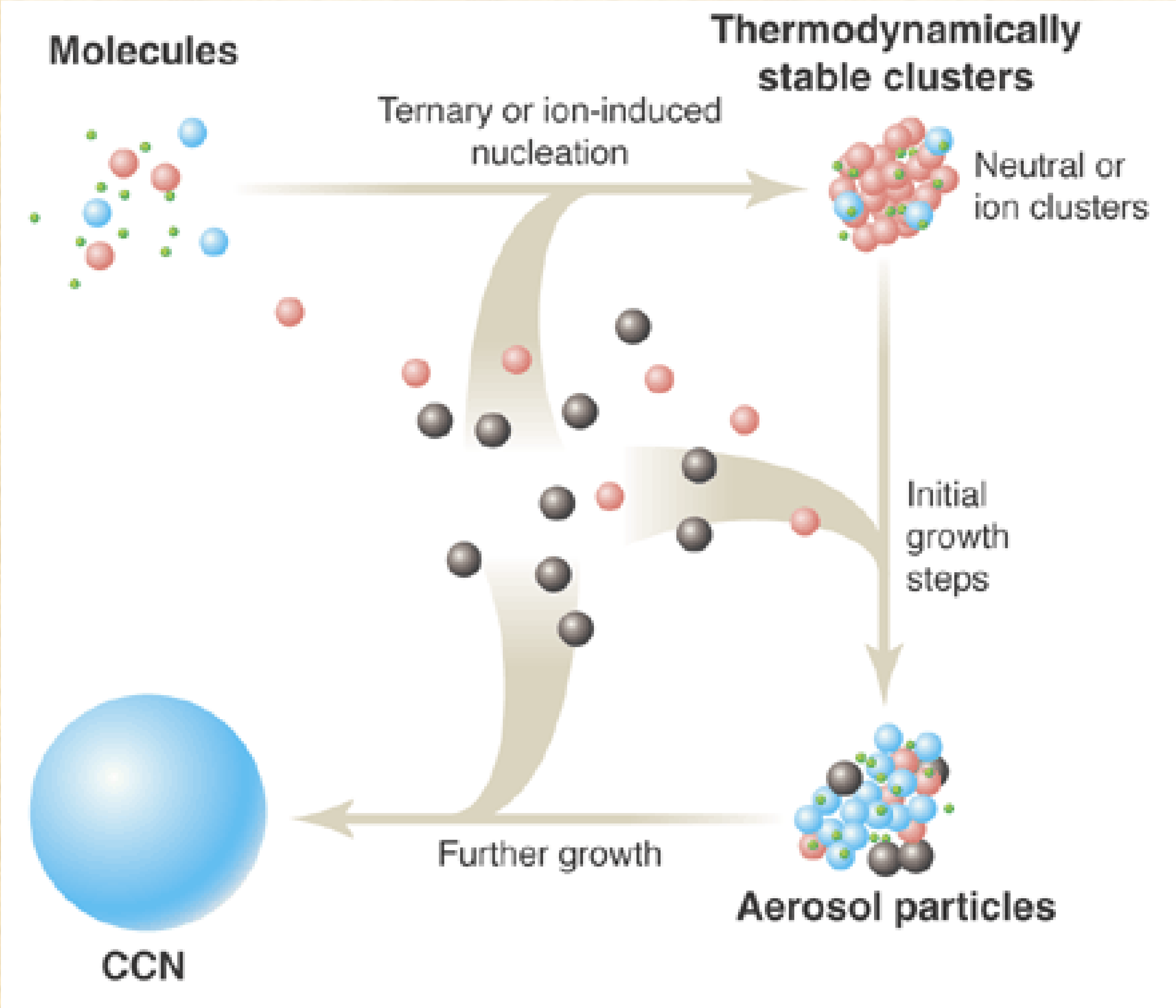


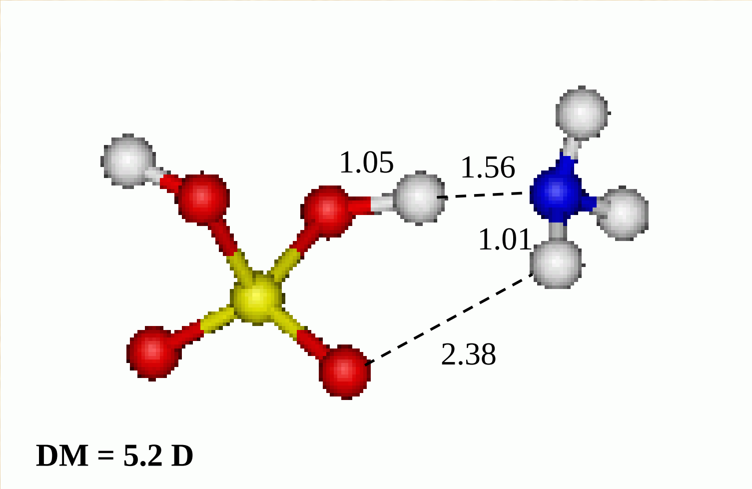
Fig. 2. Simulated surface O_3 (*A* and *B*) and NO_x (*C* and *D*) distributions at 11 p.m. (*A* and *C*) and 3 p.m. (*B* and *D*) CDT during the time period of September 7–8, 1993. The Houston City limit is marked by thin white lines, and the other white lines in *C* label the county limits near Houston. Also shown in *C* are the locations of surface air quality monitoring stations marked by the brown dots. The brown frame encompassing all of the stations is defined as the Houston domain in the text.

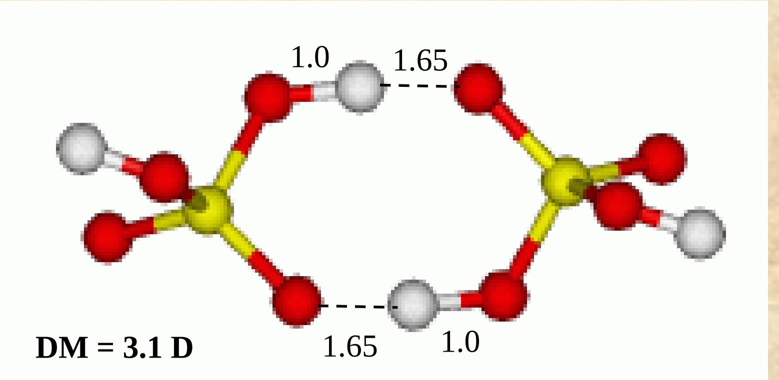


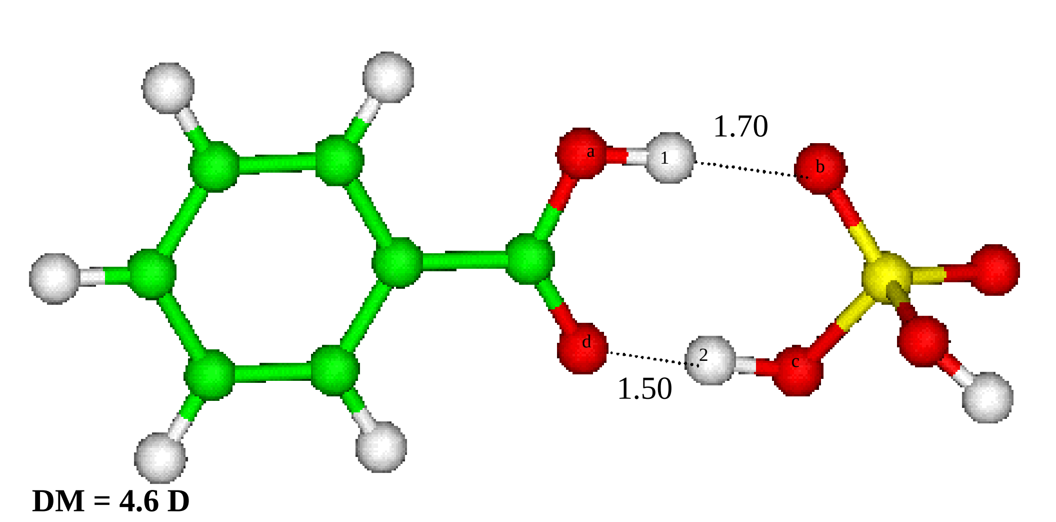
(a)
O_3 (ppb)
0
20
40
60
80
100
120
0 12 24 36 48 60 72 84 96 108 120
Time (hr)
(b)
NO_x (ppb)
0
20
40
60
80
100
120
140
Enox, 1E15 (molec m^{-2} s^{-1})
0
10
20
30
40
50
60
0 12 24 36 48 60 72 84 96 108 120
Time (hr)

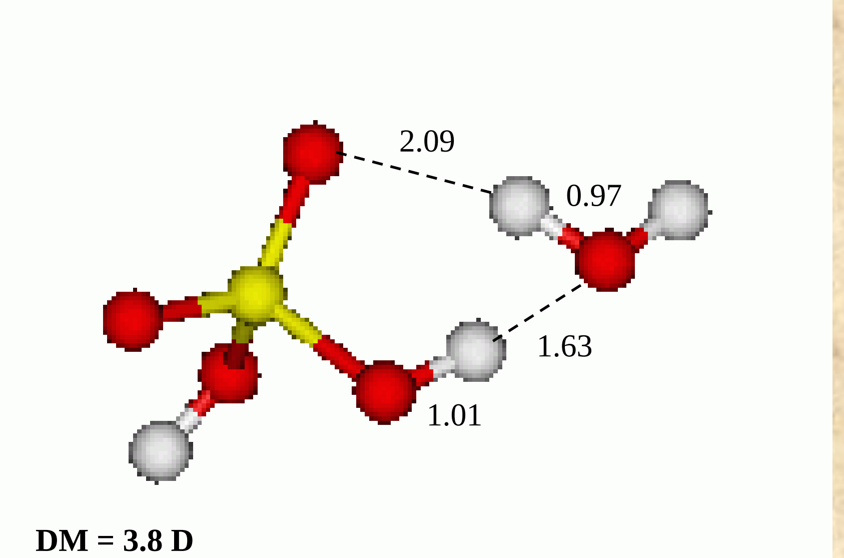


M. Kulmala, How Particles Nucleate and Grow
Science, 302, 1000 (2003)



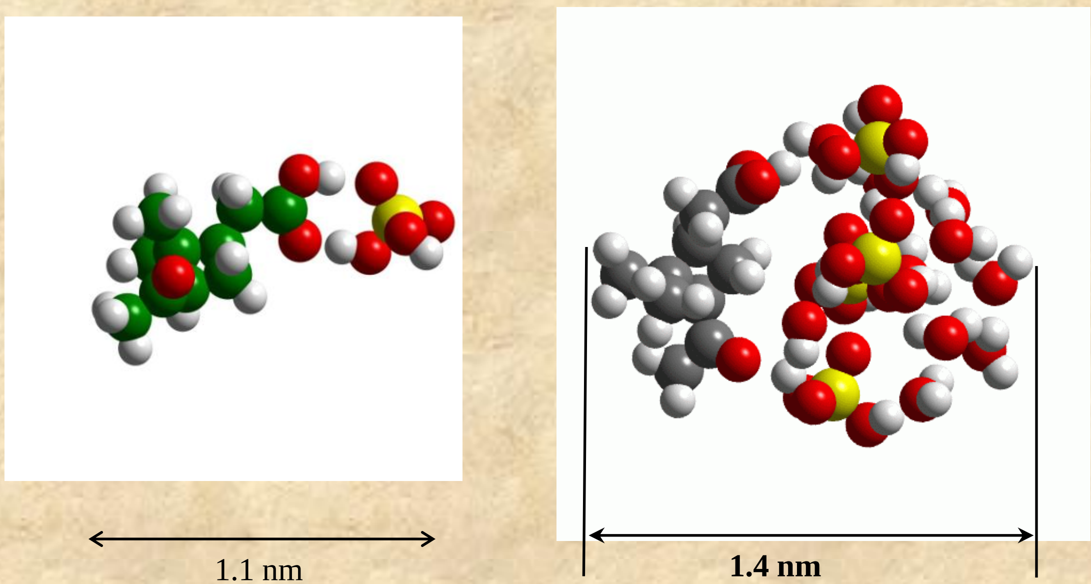






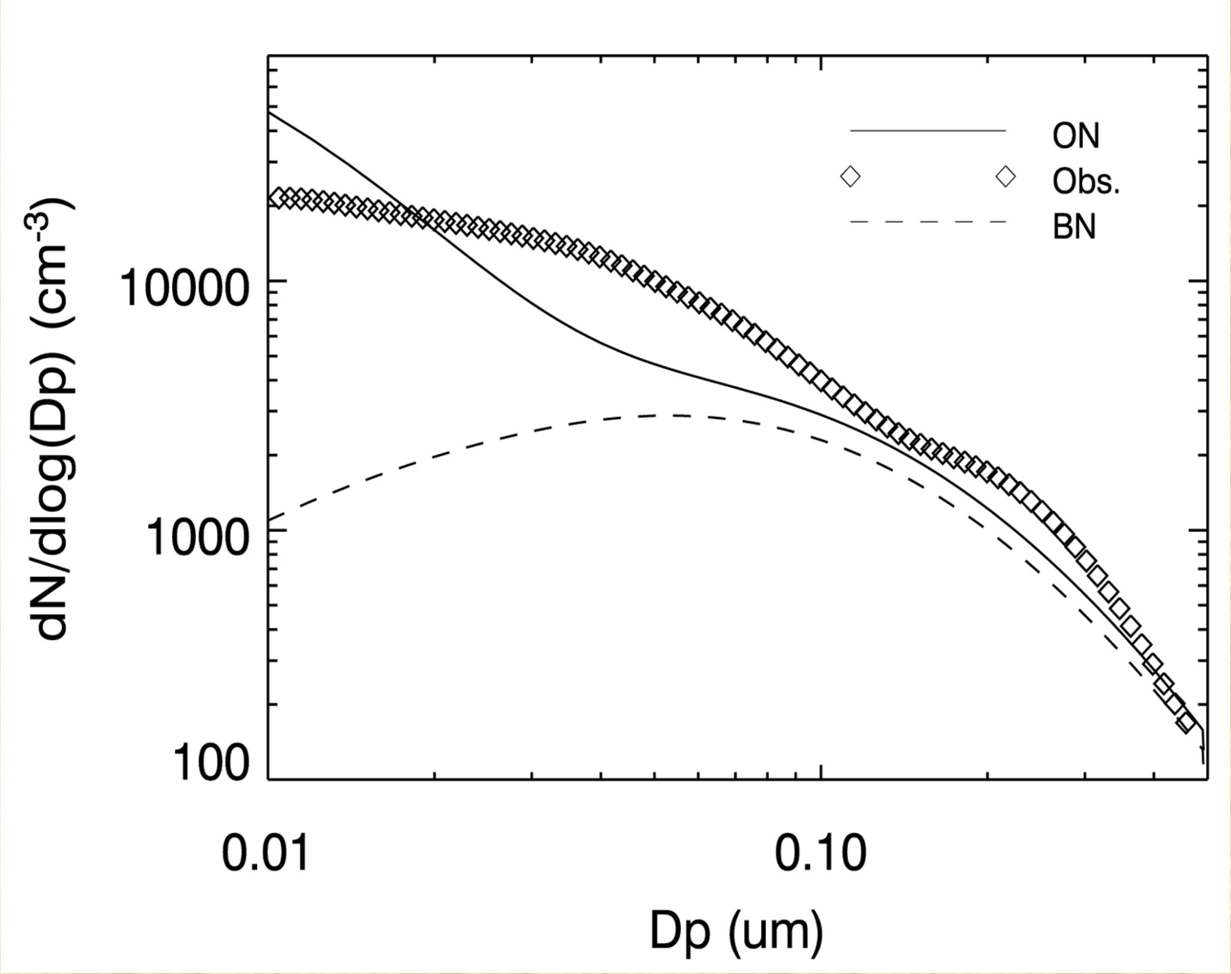
Comparison of Molecular Complexes (Zhang *et al.*, Science, 2004)

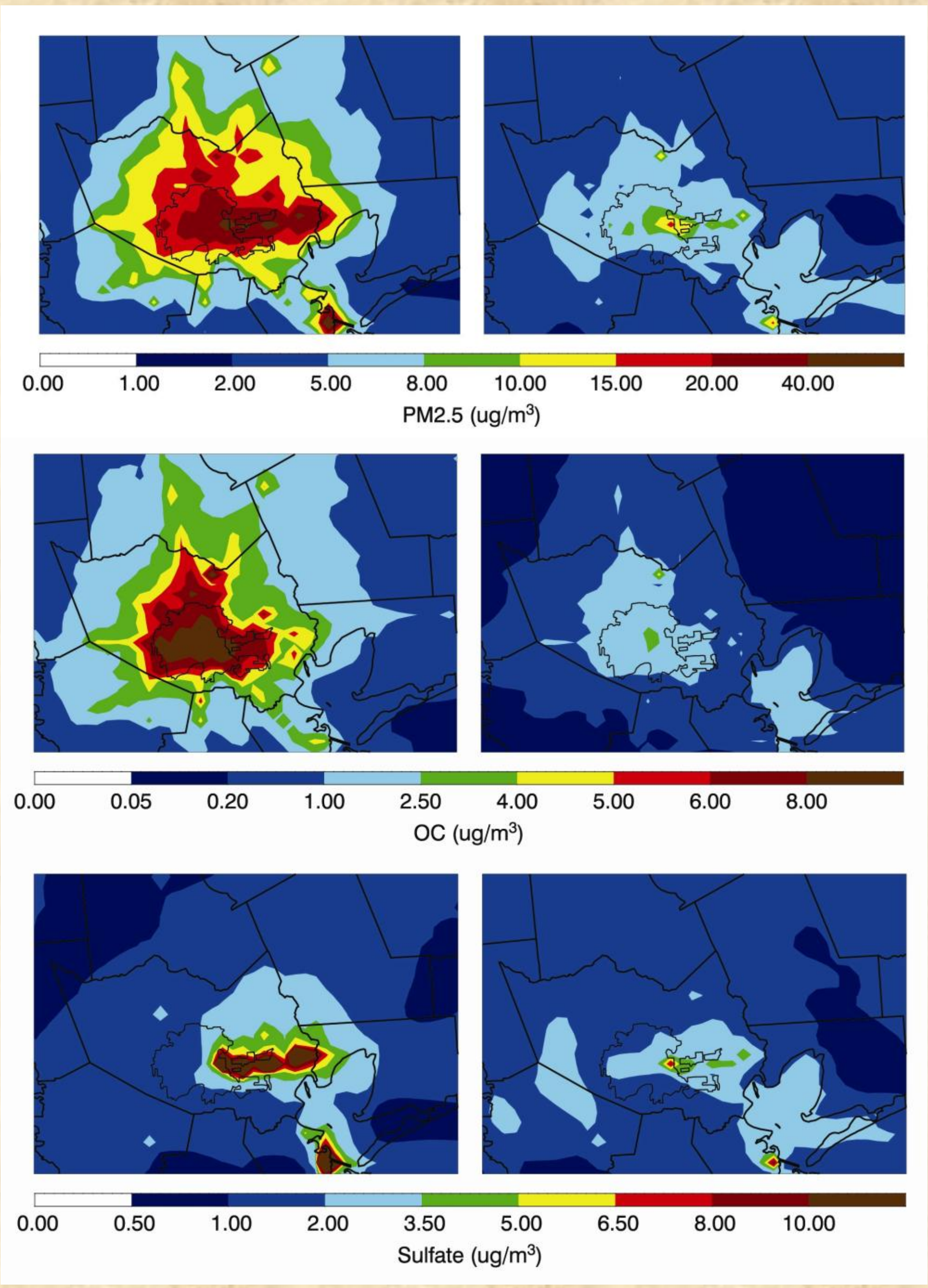
A B



Quantum Chemical and Molecular Dynamic Calculations of Cis-pinonic-Sulfuric Acid Complex and Critical Nucleus

J. Fan *et al*., Contribution of Secondary Condensable Organics to New Particle Formation: A Case Study in Houston, Texas, *Geophys. Res. Lett*., 33, L15802, doi:10.1029/2006GL026295 (2006)





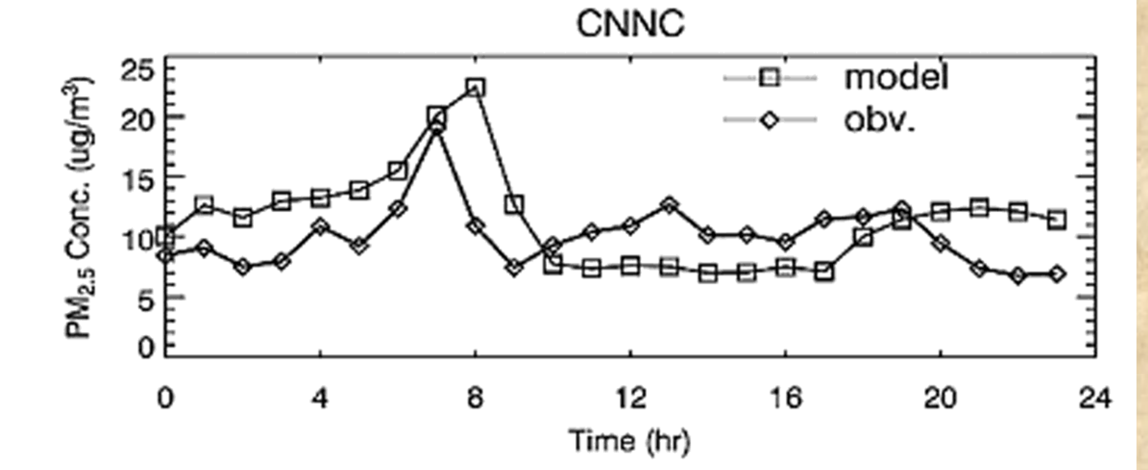
$PM_{2.5}$ concentrations at 8am (left) and 3pm (Right)

OC concentrations at 8am (left) and 3pm (Right)

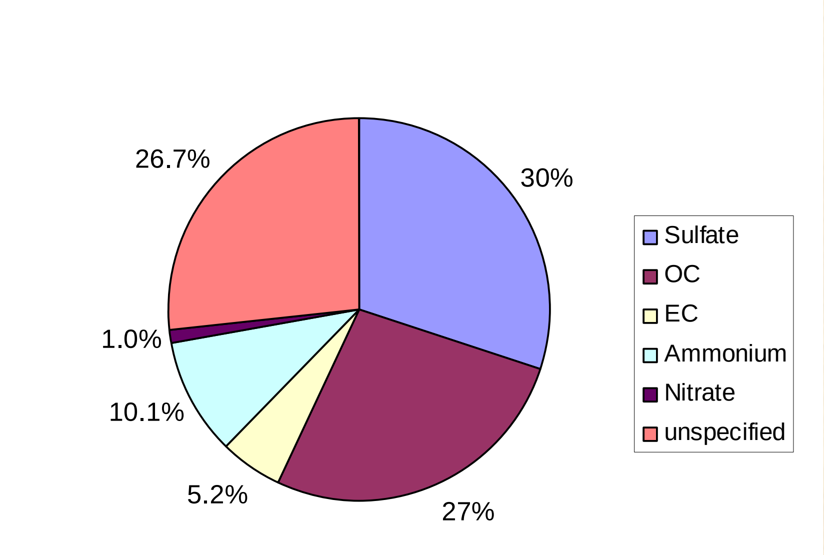
Sulfate concentrations at 8am (left) and 3pm (Right)

(Fan et al., JGR, 2005)

■ Aerosol mass and composition



- The predicted aerosol mass conc. are consistent with the obs.
- The overestimation of $PM_{2.5}$ during night is because of much lower simulated PBL heights.



- **Obv: Sulfate: ~ 30%**
  Organics: ~ 30%

Fan et al., J. Geophys. Res., 110, D16203, 2005

Cloud Simulations using WRF with Two-moment Bulk Microphysics

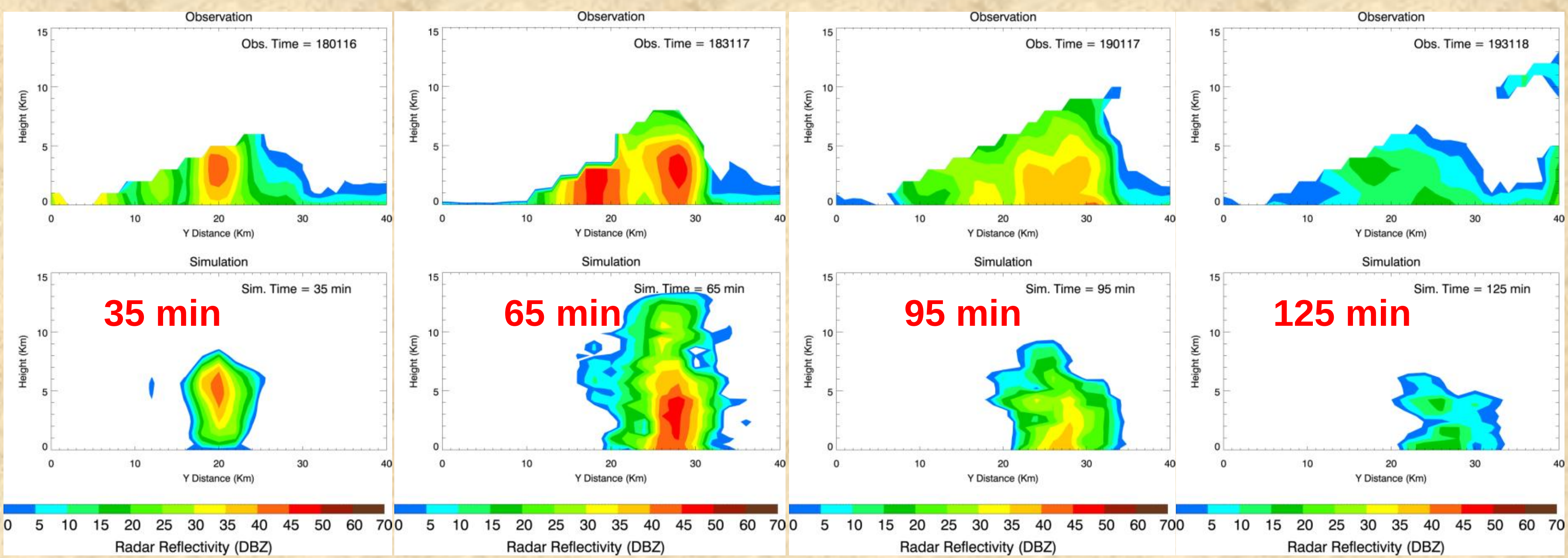
- **Weather Research and Forecasting (WRF) model**

- **Mass mixing ratios of water vapor, cloud droplets, raindrops, ice crystals, snow flakes and graupels and number concentrations of cloud droplets, raindrops, ice crystals, snow flakes and graupels. The size distributions of the five types of hydrometeors are represented by gamma functions;**

- **Third-two microphysical processes: autoconversion of cloud water to rain and graupel, ice to snow, and snow to graupel; freezing of cloud water and rain; melting of ice, snow and graupel; nucleation of CCN and ice; accretion of cloud water by rain, graupel and snow; accretion of ice by rain, graupel, and snow; accretion of rain by ice, snow, and graupel; accretion of snow by rain and graupel; self-accretion of ice, snow, and rain; condensation/evaporation of cloud water and rain; and sublimation of ice, snow and graupel;**

- **Three-moment aerosol representation. For CCN nucleation, the aerosol spectrum is divided into 92 sections from 0.002 mm to 2.5 mm and critical radius of dry aerosols is calculated from the Köhler theory.**

Comparison with Measurements



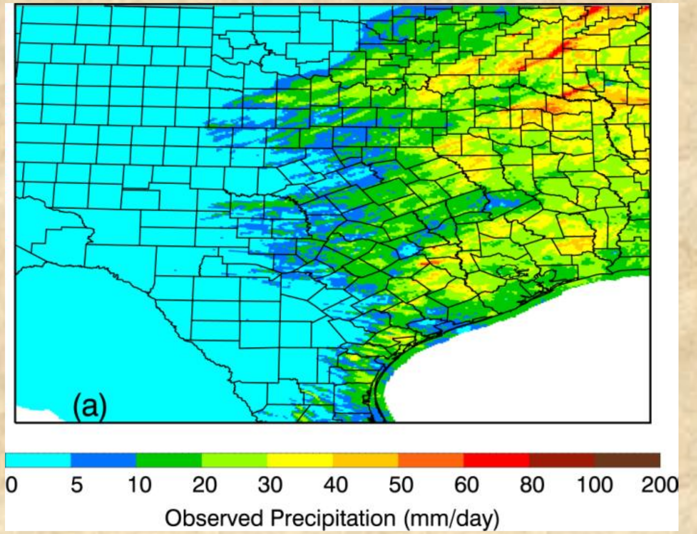
The simulated maximal radar reflectivity is 60.2 dBz, close to the observed 57.8 dBz;

The lifetime of the simulated cumulus is about 110 min, comparable to the 120-min cell lifetime determined from the radar observations;

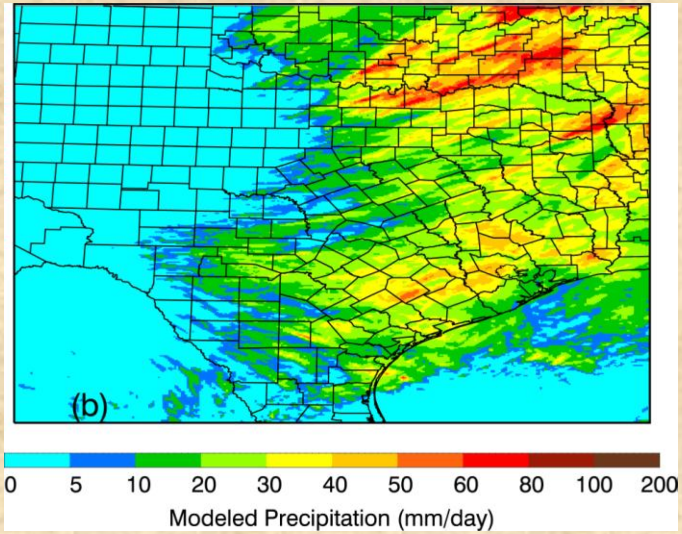
The averaged precipitation of 10.4 mm observed in the area where the deep convection occurs from 1800 to 2100 UTC agrees with the modeled value of 9.6 mm.

Comparison of Precipitation

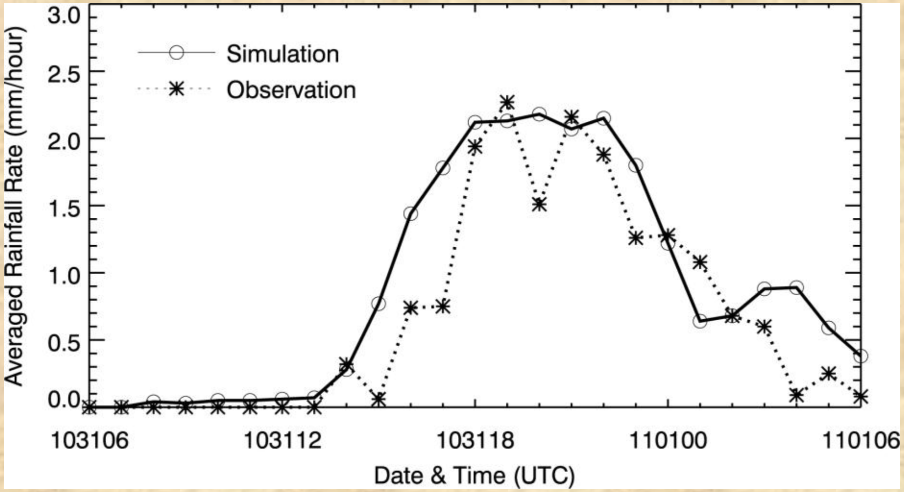
Observed Precipitation



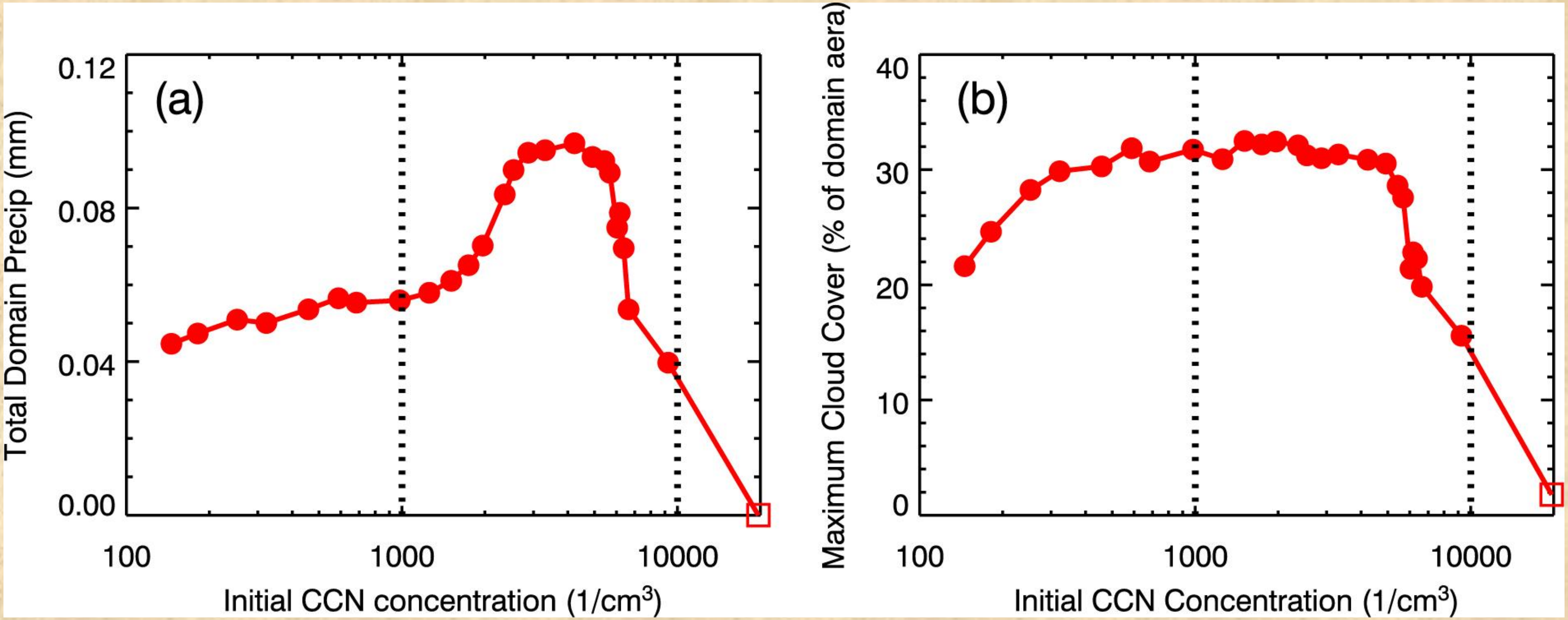
Modeled Precipitation



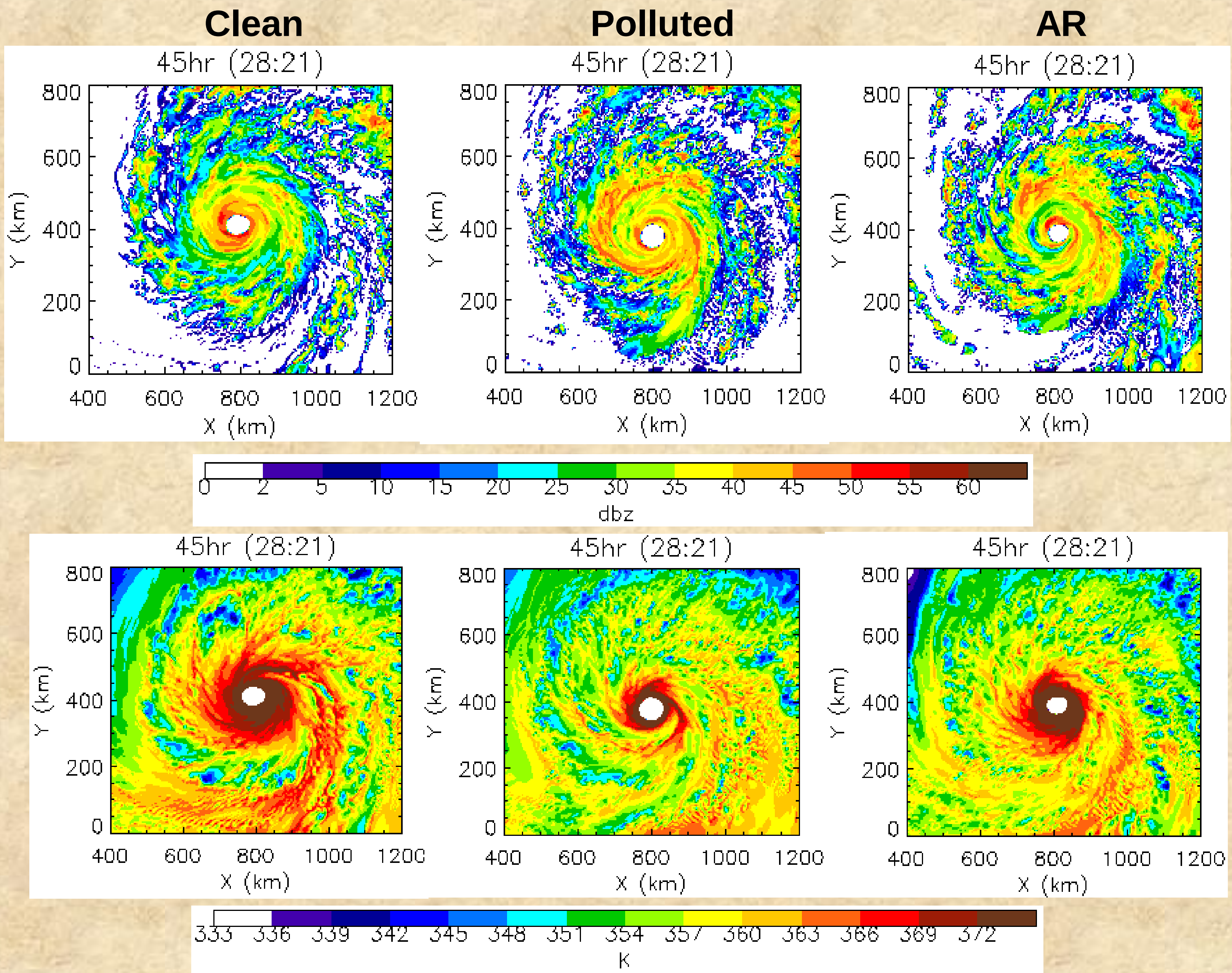
Rainfall Rate Comparison



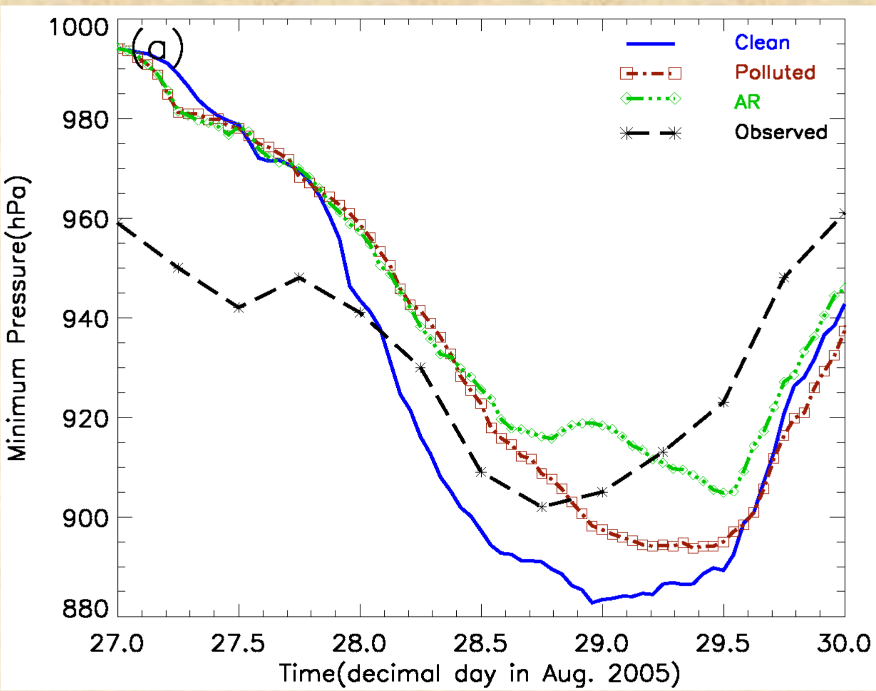
Li et al., Response of Precipitation and Cloud Coverage to Changes in Aerosols, *JGR* (2008)

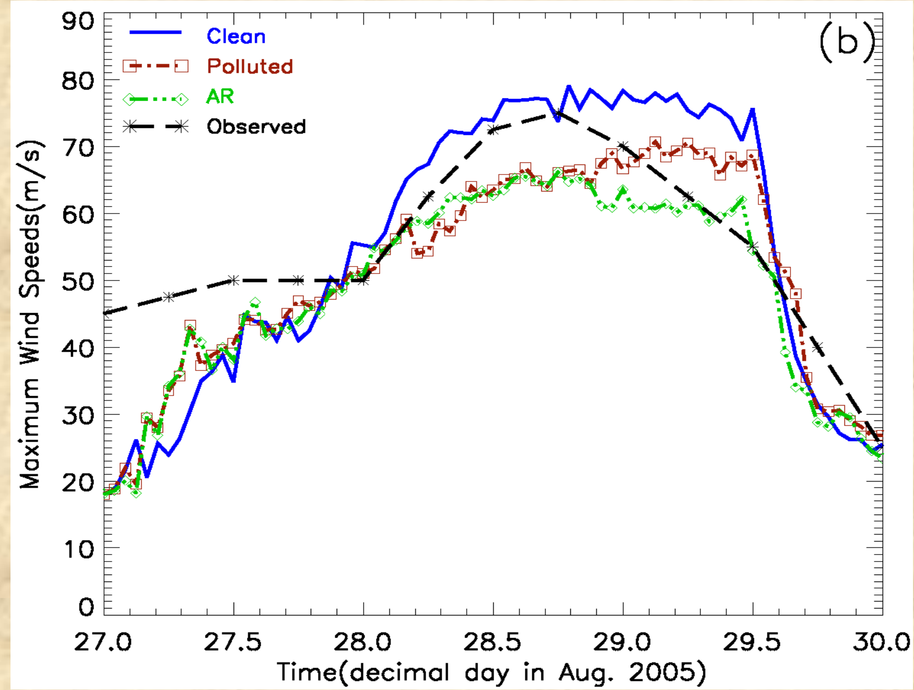


Radar reflectivity (dBZ) and Equivalent potential temperature (K) at 925 hPa



Min. surface pressure (hPa) & Max. surface wind speeds (m/s)





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