

July 21, 2008  
NCAR GEO Turbulance

UNIVERSITY of HOUSTON

IMAQS

# Improvement of Meteorological Inputs for Air Quality Study

Fong (Fantine) Ngan

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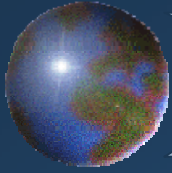
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Web: <http://www.imaqs.uh.edu>



## Ozone Problem in Houston

➤ Ozone: Good up high, bad nearby

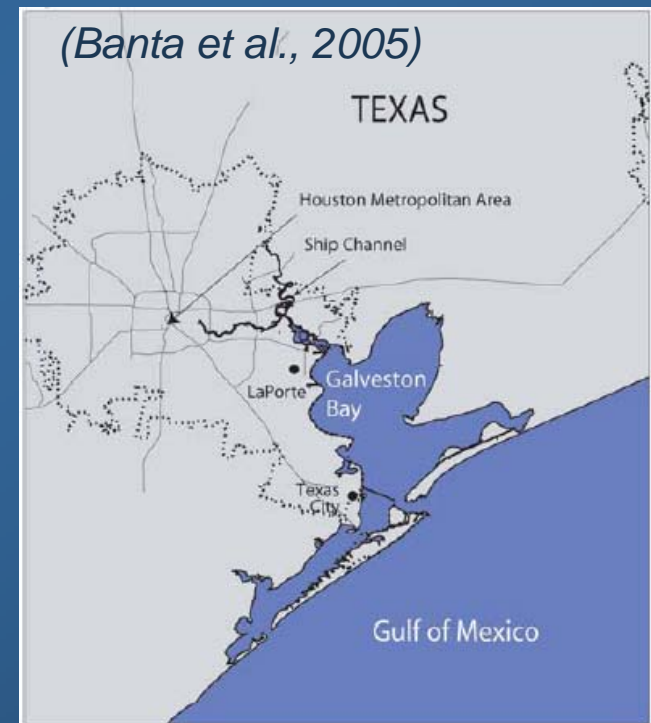
([http://earthguide.ucsd.edu/virtualmuseum/climatechange2/10\\_1.shtml](http://earthguide.ucsd.edu/virtualmuseum/climatechange2/10_1.shtml))

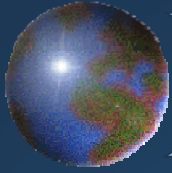
Stratosphere: most abundant (max @ ~25km)  
1000 - 10,000 ppb  
produced naturally  
filter out UV radiation

Troposphere: damage plants & crops  
cause respiratory problems  
greenhouse gas

Natural source – mixing from stratosphere  
reaction of NO<sub>x</sub> from lightning  
reaction of CH<sub>4</sub> from soil ...  
15-25 ppb @ surface globally

Anthropogenic – reactions of nitrogen oxides & organic compounds  
sources from mobiles, industries & power plants  
sunlight & temperature dependent reactions





## Ozone Problem in Houston

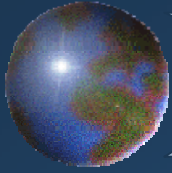
TexAQS 2000 --- An intensive field study in Houston Galveston Area (HGA) for ozone and other pollutant issues during Aug-Sep, 2000 .

Main features of the O<sub>3</sub> problem in Houston (*Olague et al., 2005*):

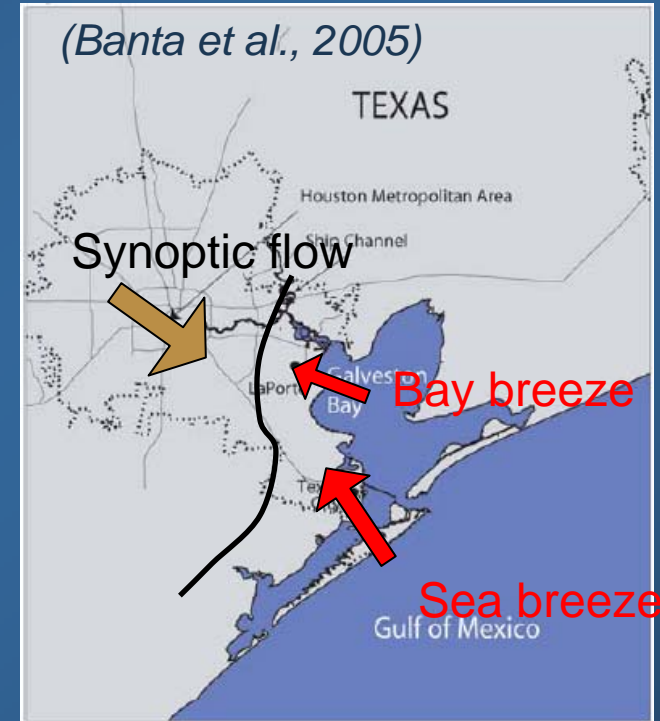
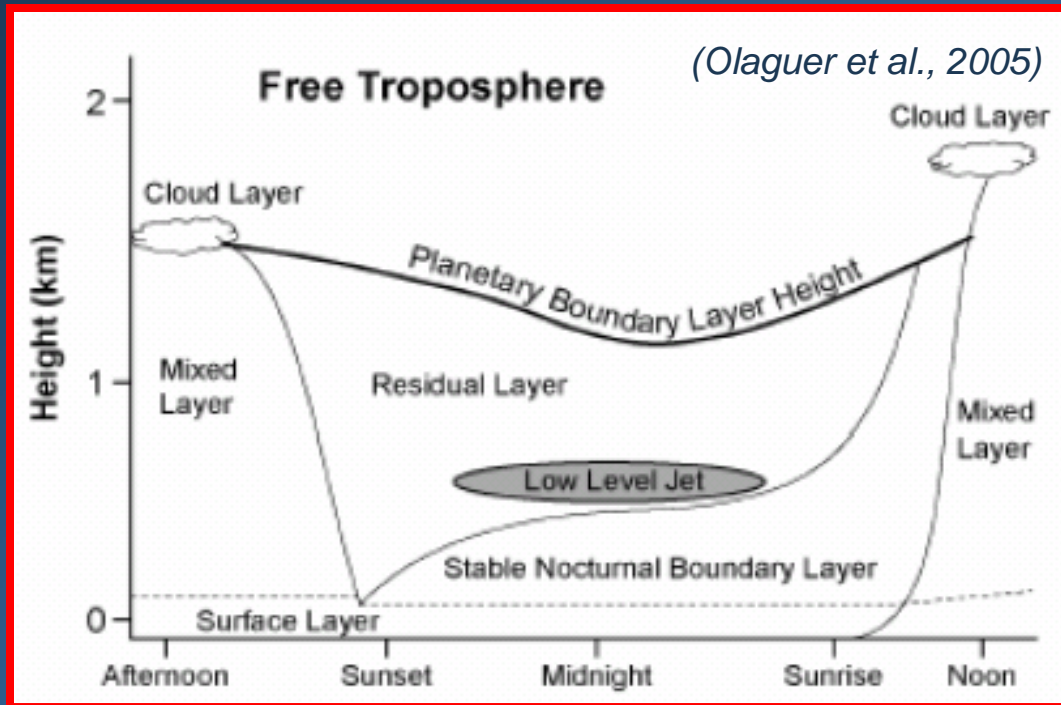
1. Houston (Ship Channel) is a major international port and the largest producer of petroleum products with large amount of Highly Reactive Volatile Organic Compounds (HRVOCs) emissions.
2. Complex interaction between meteorology and chemistry is present. The stagnant condition associated with sea breeze traps the O<sub>3</sub> precursor; high O<sub>3</sub> levels are built up by photochemical reaction.  
→ Frequent & rapid increase of O<sub>3</sub>, > 20 ppb per hr, in HGA

**The weather parameters (wind, T and PBL Height) are controlling the development of ozone production and the transportation of other pollutants.**

→ A successful meteorological simulation is one of the required steps to predict air quality phenomena realistically under such complex conditions over HGA.



# PBL Development and Land-sea Breeze



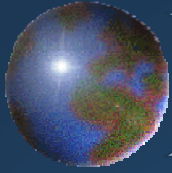
## Planetary Boundary Layer (PBL)

The bottom part of the atmosphere  
Highly influenced by surface  
Parameters well mixed

ex. Low PBL height

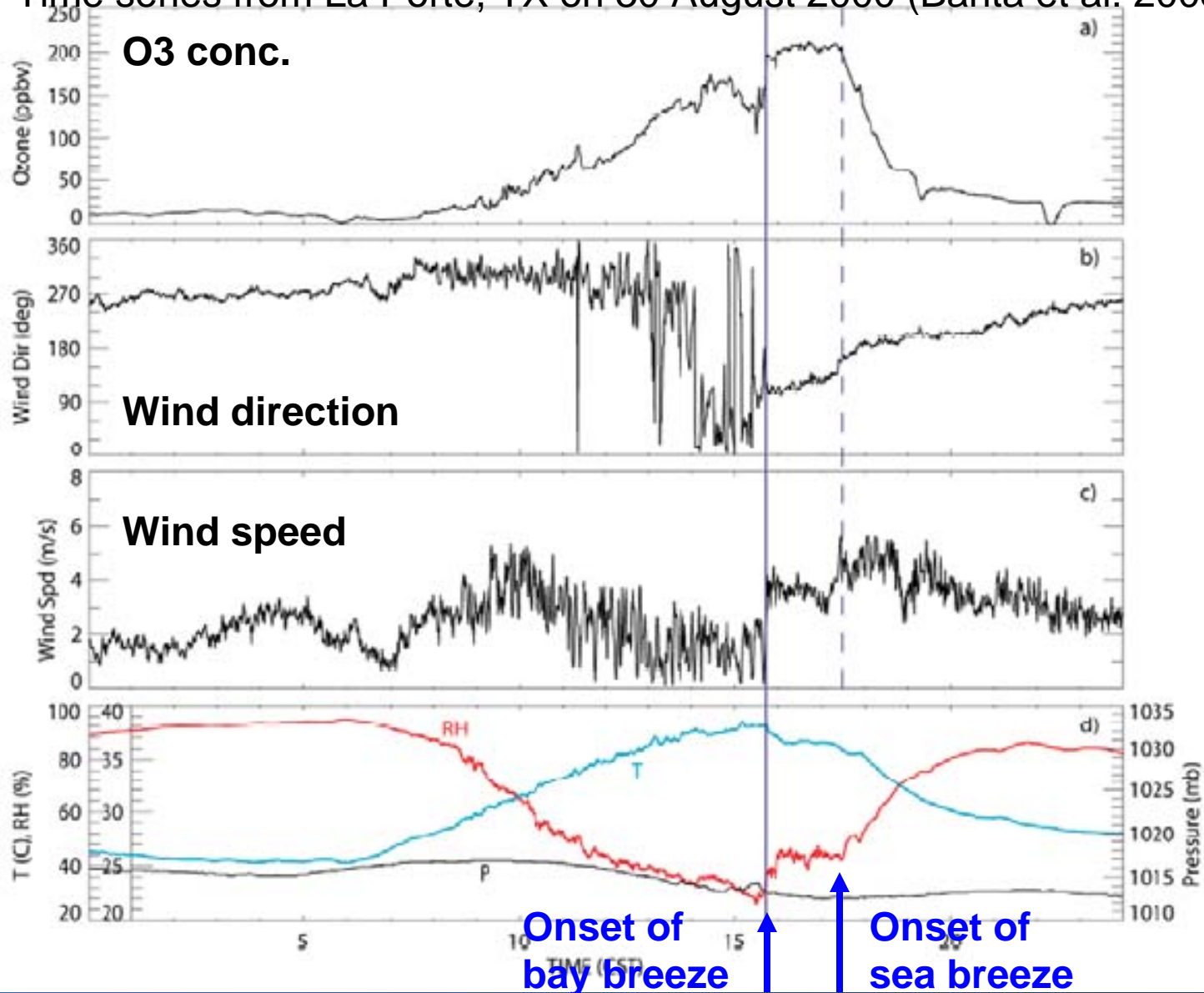
- pollutants trapped near surface
- high concentration of primary (i.e., directly emitted) pollutants

The Latitude of Houston is 30N where the sea-breeze cycle is at maximum amplitude.



# Sea Breeze & Bay Breeze in Houston

Time series from La Porte, TX on 30 August 2000 (Banta et al. 2005)



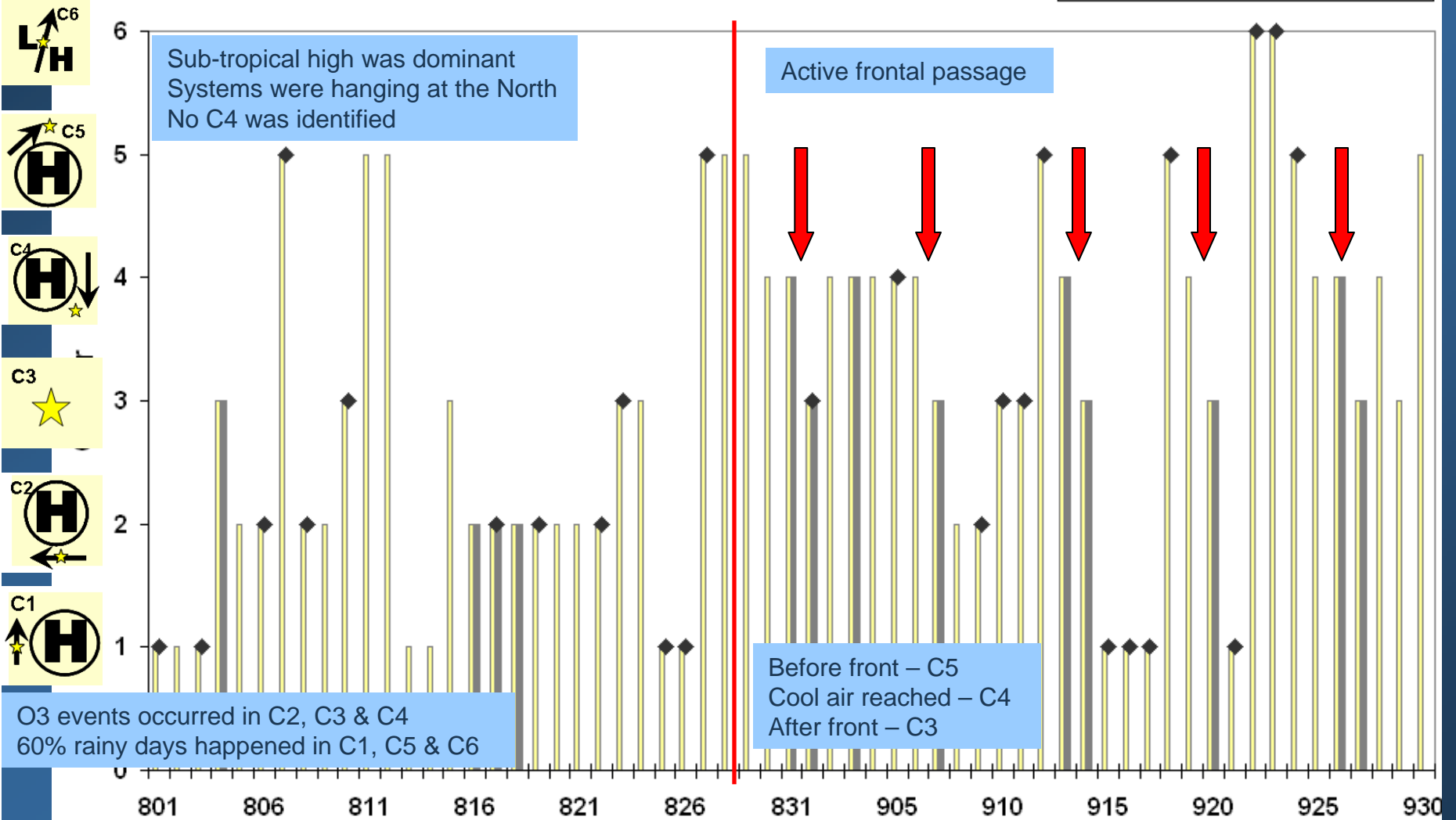


# Cluster Characteristics during TexAQS-II intensive period (Texas Air Quality Study II – May 2005 through September 2006)

850mb flow pattern

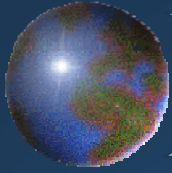
TexAQS II period (August - September, 2006)

clusters O3ep Rainfall



Precip. prevents O3 events in C2 & C3

Day



## Met. Modeling for TexAQS-II Intensive Period

UH-AQF successfully used for the planning of various measurement but systematic problems were shown in the evaluations.

\* MM5, SOMKE, CMAQ

Over-prediction of northerly wind, too strong southerly, discrepancies in max & min temperature, precipitation & clouds not simulated well

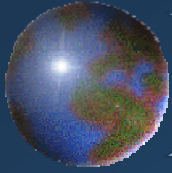
MUltiscale Nest-down Data Assimilation System (MUNDAS):

Utilize existing objective analysis and nudging tools in the MM5 system  
Incorporate extensive OBS available in the simulated domain for the retrospective simulation of the TexAQS-II period.

With MUNDAS, we intend to

**Generate better initial and boundary conditions using the objective analysis with observations**

**Use the recursive nudging procedure to maximize the correcting capabilities of FDDA.**



# MULTIscale Nest-down Data Assimilation System (MUNDAS)

AQF: grid nudging with ETA in D36 & D12, no nudging in D04.

Simulations of TexAQS 2000: grid nudging with EDAS in D36 & D12, OBS nudging with profiler/sounding in D04.

## LITTLE\_R (objective analysis)

Use Cressman successive correction methods to **modify first guess** fields (NCEP analyses or coarse domain nest-down) by ingesting information from **observations**.

Generate updated **IC/BC** for MM5 and **analyzed fields** (3D & surface) for grid nudging.

## Nudging

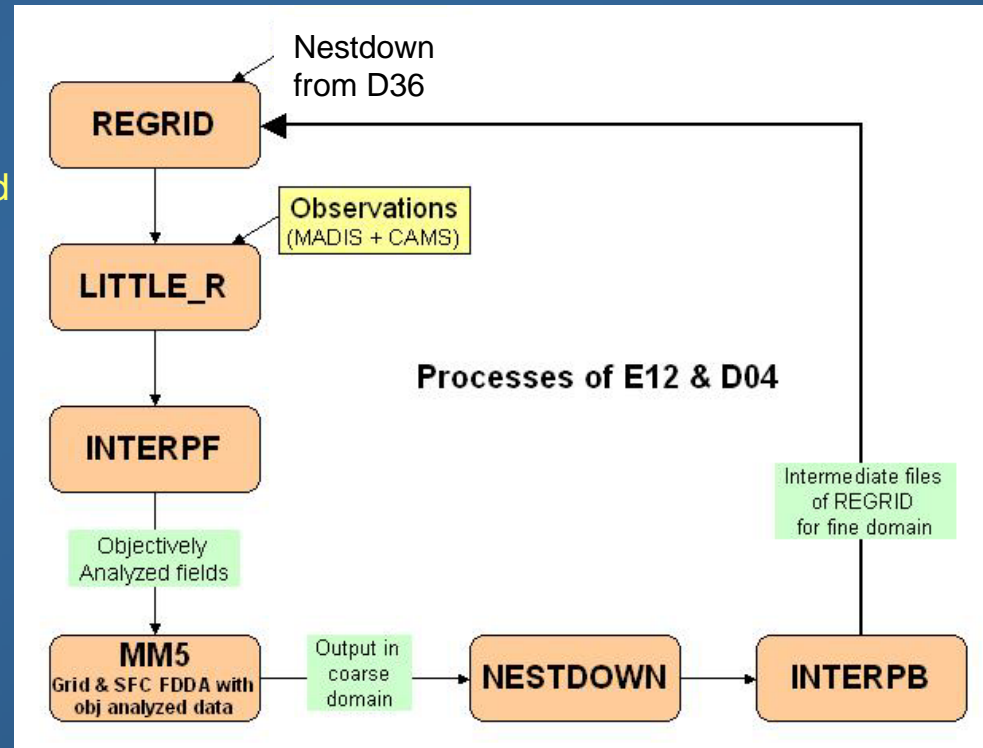
Adjust model state based on the difference between model and observed value continuously that help on **minimize error's growth** during the simulation.

Use grid (analysis) nudging **both 3D and surface** with objectively analyzed fields from LITTLE\_R.

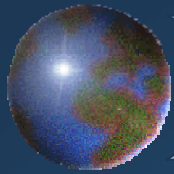
CAMS: surface met., only in TX, concentrating in big city

MADIS: surface – METARS & Buoy etc.

upper level – NPN, aircraft sounding & radiosonde

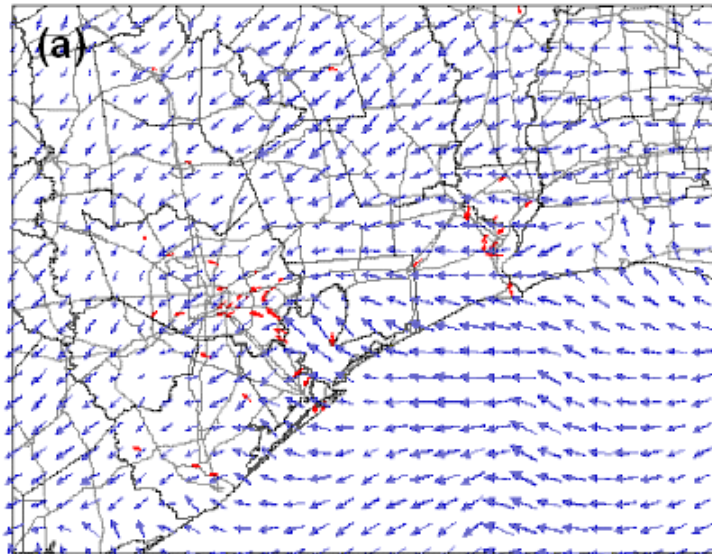






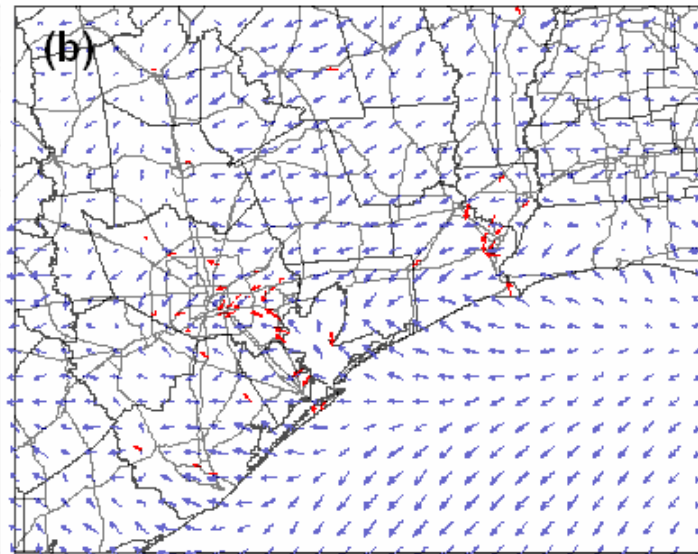
# Improvement of Ozone simulation

Model & Obs. Wind : 20060817:15cst [AQF]



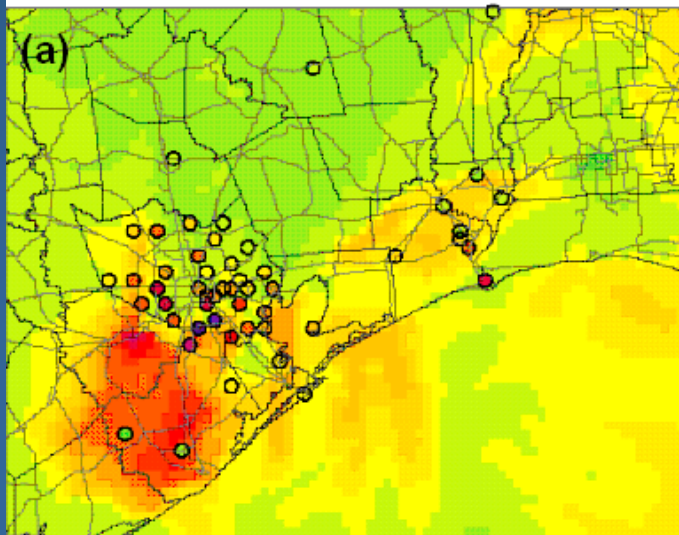
Model=Blue, Obs=Red, 10(m/s) →

Wind Field at 20060817:15cst [T11]

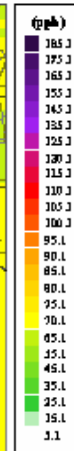
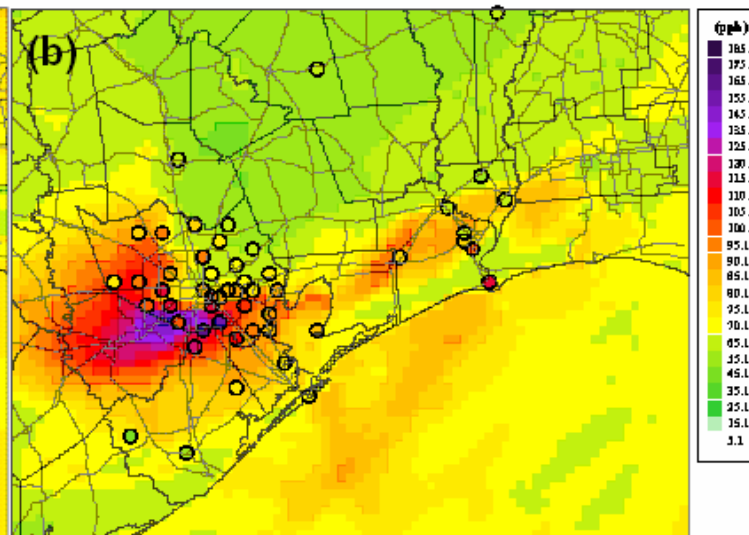


Model=Blue, Obs=Red, 10(m/s) →

Ozone Conc. at 20060817:15cst [AQF]

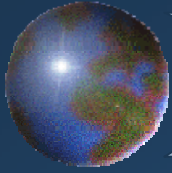


Ozone Conc. at 20060817:15cst [T11]



In T11, Wind was slow down that convergence ozone could be formed at the afternoon

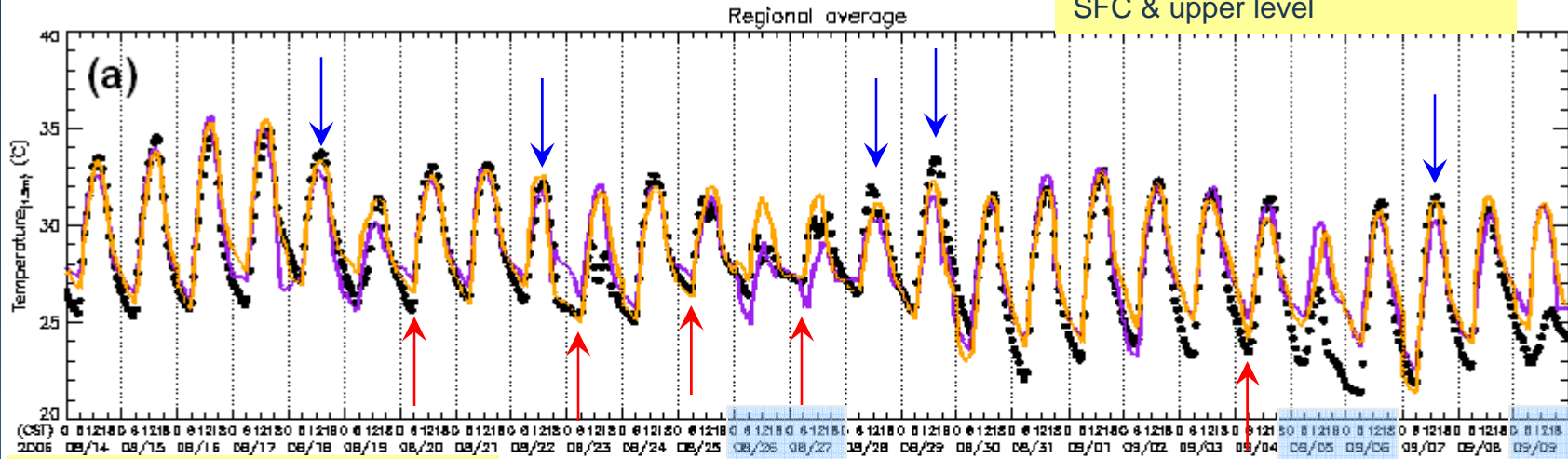
With T11 met., O3 was able to build up & location of peak stayed south of downtown.



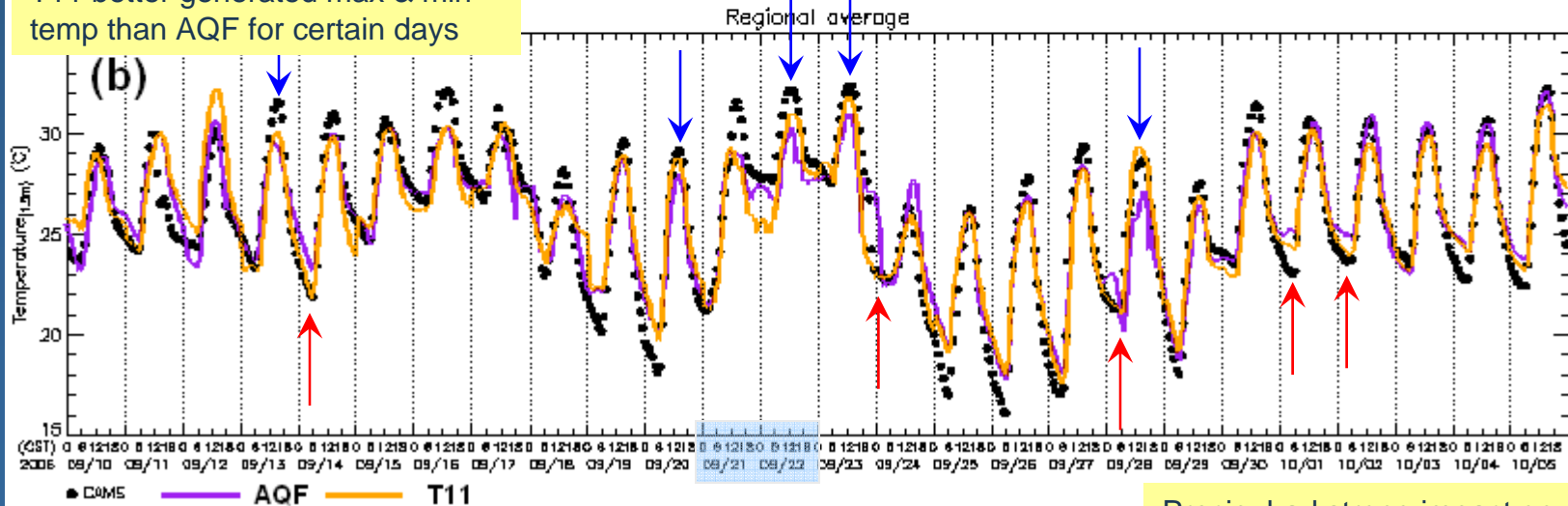
# 1.5 m temperature 8/14 – 10/5 (54 days)

Regional average of observed and model 1.5 m temperature

NO T & RH nudging at both SFC & upper level

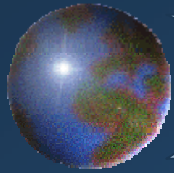


T11 better generated max & min temp than AQF for certain days



Precip. had strong impact on variation of SFC temp.





## Coupling of Met. & AQ model

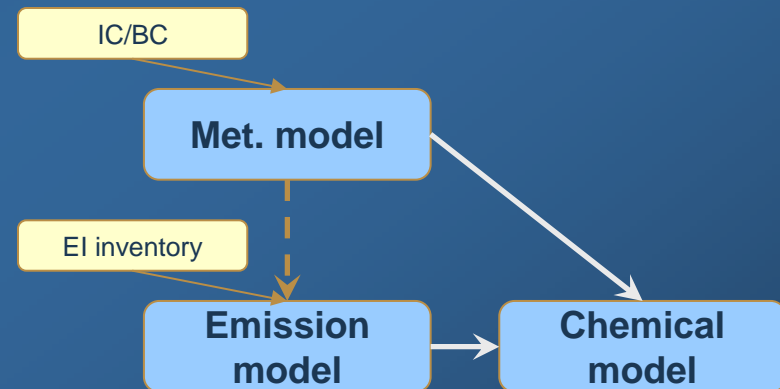
### Two ways to couple met. and chemical models

#### On-line coupling: Chemical process is implemented in meteorological model.

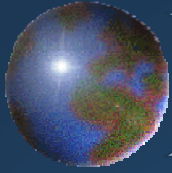
- ❖ The information loss in data transfer & numeric disparities can be minimized.

#### Off-line coupling: Meteorology, emissions and chemistry are processed individually.

- ❖ Changes in one of them produce different chemical simulation
- ❖ Less consumption of computational resources



Interface processor is need for transforming necessary input for air quality modeling. Ex. Meteorology-Chemistry Interface Processor (MCIP) in CMAQ



## Coupling of Met. & AQ model

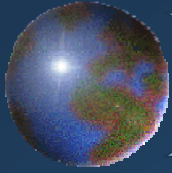
How to transfer the meteorological information effectively into the chemical model is very important to establish a reliable air quality modeling system for use in applications studies to relate emissions sources and air quality problems.

→ Mass inconsistency problem is a possibility during the transition of the data or the computation inside air quality model because of the discrepancies of two modeling system in dynamics, numerical algorithms and grid coordinates.

**In air quality modeling, the mass-consistent simulation of trace gas species is a necessary property. (Byun, 1999a,b)**

→ Wind and density must be consistent to satisfy the continuity equation

If met. Inputs are not transferred or used properly in air quality models, the mass inconsistency will act as a source of spurious emissions in air quality simulations, resulting in inaccurate estimations of pollutant concentrations.



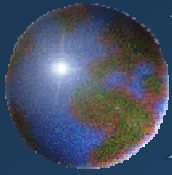
## Off-line coupling paradigm: WRF-CMAQ

### Off-line CMAQ primarily relies on the MM5 system as meteorological driver.

- ❖ MM5 design was focused on energy conservation.  
Equations were cast in an advective form.  
Prognostic thermodynamic variables are temperature and pressure.
- ❖ Nonhydrostatic MM5 simulation produced approximately 6 times larger mass inconsistent error than the hydrostatic MM5 during a 24-h simulation. (*Lee et al, 2004*)

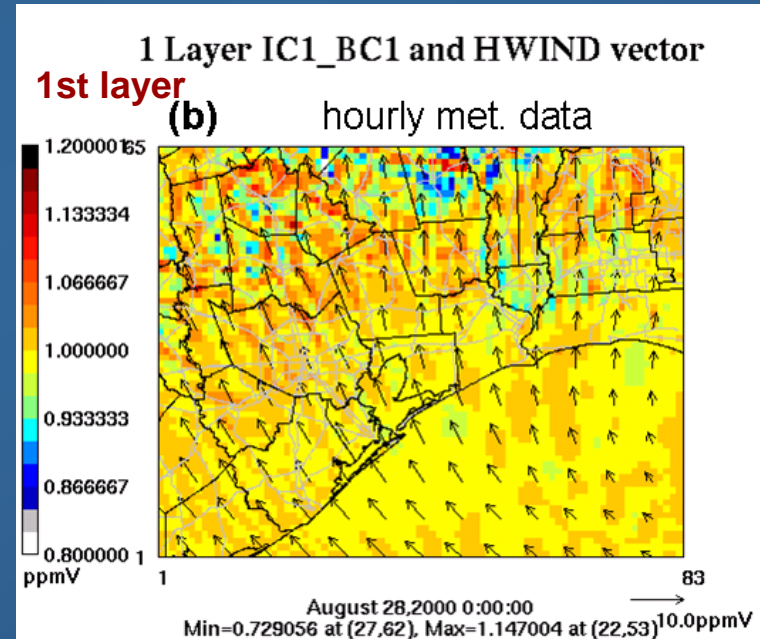
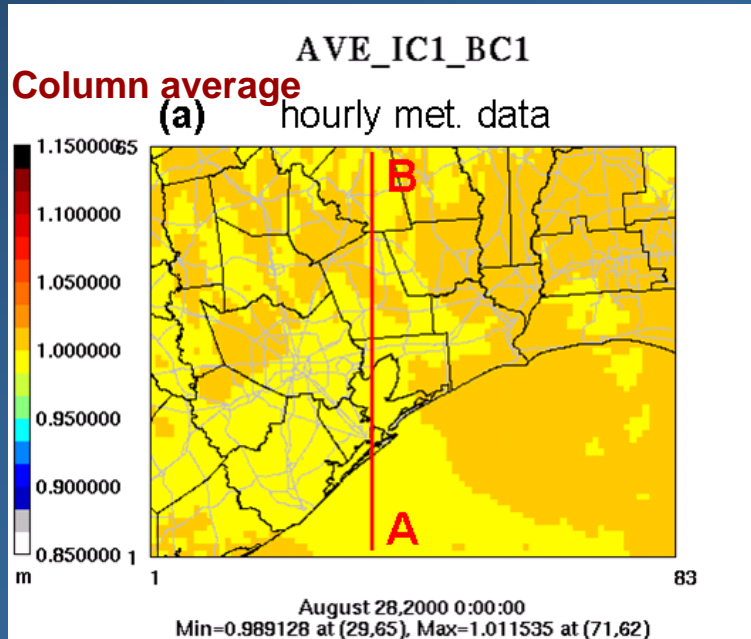
### Off-line modeling for air quality assessment with WRF-CMAQ

- ❖ WRF-ARW was demonstrated to have accurate numerics and high quality mass conservation characteristics.
- ❖ The governing set of equations, coordinate system, numerical algorithms, and computational framework of WRF-ARW are closer to CMAQ than MM5.



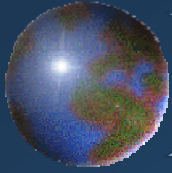
# Tracer simulation of WRF-CMAQ

- ❖ Turning off sources, removal processes, chemical reactions and turbulent diffusion.
- ❖ IC/BC values of the trace species were set at a uniform distribution of 1 ppm.
- ❖ Turning off mass correction process in CMAQ, no layer collapsing.
- ❖ Simulation period: 27 – 28 August 2000 (48 hour)
- ❖ Weather condition: Wind was S to SE.



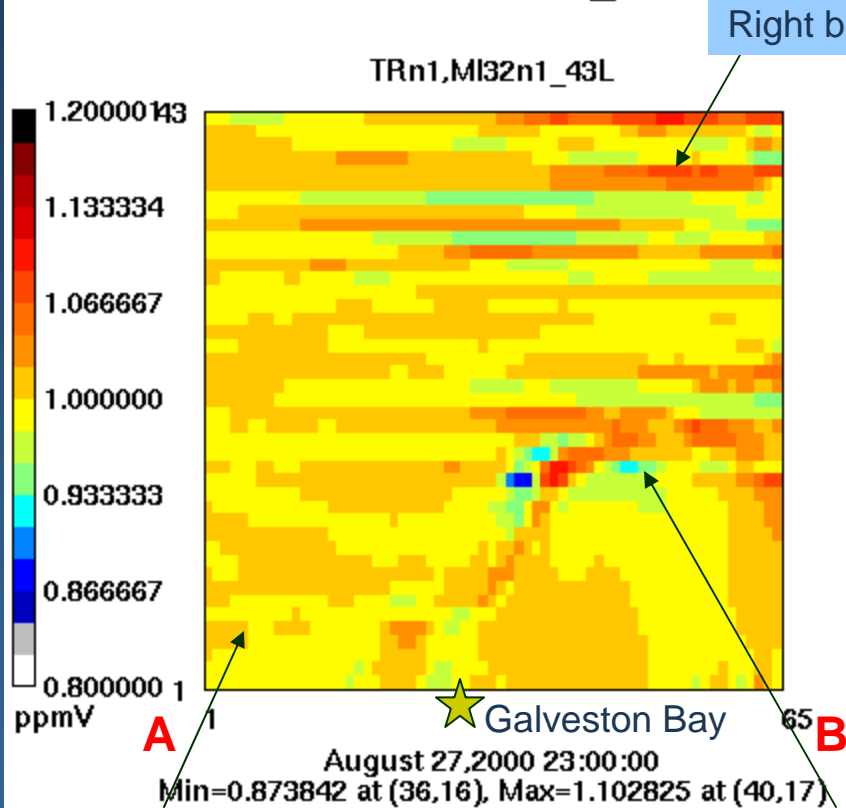
IC1\_BC1 field represents how much mass error is generated during the simulation. If the ratio equals to 1, the air density is perfectly consistent with wind field that no mass adjustment is needed.

- Column average of IC1\_BC1 was close to 1 ppm, range between 0.99 – 1.01.
- Much more variations of IC1\_BC1 happened over the land because of the active mixing during daytime.



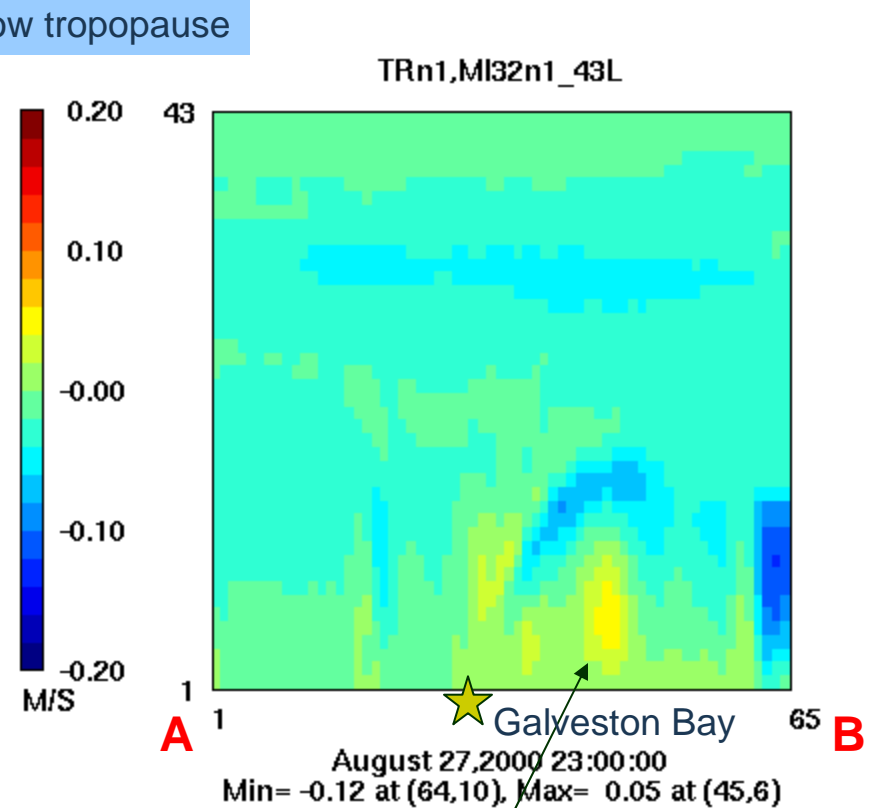
## Vertical cross section of trace specie & vertical wind

### Column 38 IC1\_BC1a



PBL over the ocean during nighttime

### Column 38 WWINDa



Development of PBL during daytime

Most of the mass errors happened near tropopause because of the dynamic instability induced by upper level jet (wind shear) and at top of PBL caused by strong vertical motion.