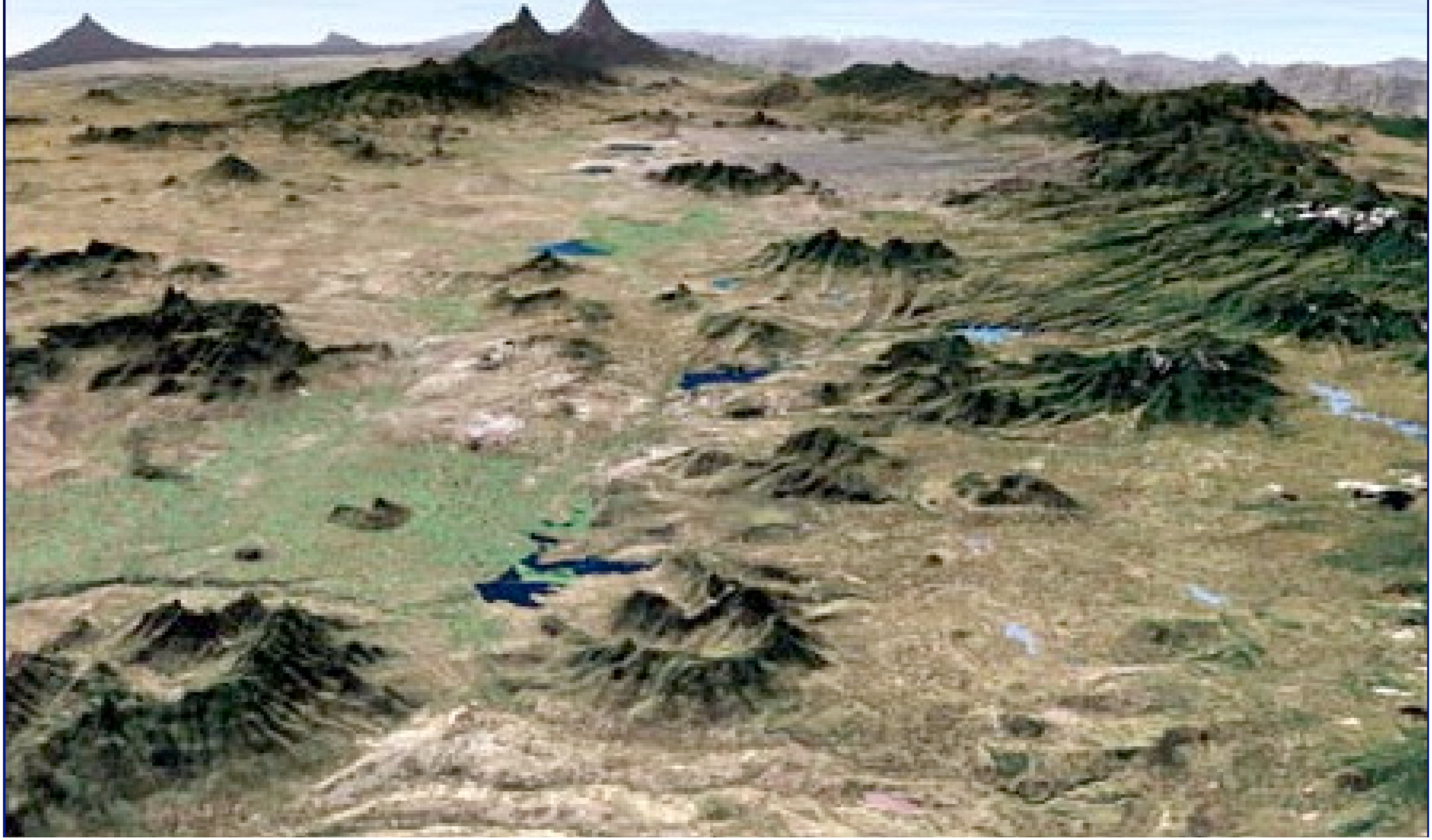
Modeling Meteorology and Atmospheric Chemistry over Central Mexico: A Review

Jerome Fast, Pacific Northwest National Laboratory



Themes

Meteorology:

- Thermally-driven circulations and their effect on pollutant dispersion
- Boundary layer evolution
- Sensitivity studies of parameterizations of land surface and PBL processes
- Effect of land-use change on local circulations and pollutants

Chemistry:

- Performance of chemical transport models and photochemical mechanisms
- Evaluate anthropogenic emission estimates
- Determine the effects of biogenic emissions
- Sensitivity of photolysis rates to aerosols
- Receptor modeling

Particulates:

- Performance of thermodynamic equilibrium models
- Local transport of dust / PM10
- Effect of particulates on local visibility
- Relative contribution of megacity emissions on global sulfate burden

Modeling and Field Campaigns

Mexico City Air Quality Modeling began in the early 1990's

- HOTMAC, Williams et al., *Atmos. Environ*., 1995
- HOTMAC, Sosa and Aguirre, *1st Intl. Conf. On Air Pollution*, 1993
- MEMO, Wellens et al., *2nd Intl. Conf. On Air Pollution*, 1994
- UAM, Greenfield et al., *85th Annual Meeting of AWMA*, 1992
- Photochemical model, Varela et al., *2nd Intl. Conf. On Air Pollution*, 1994
- and other conference proceedings

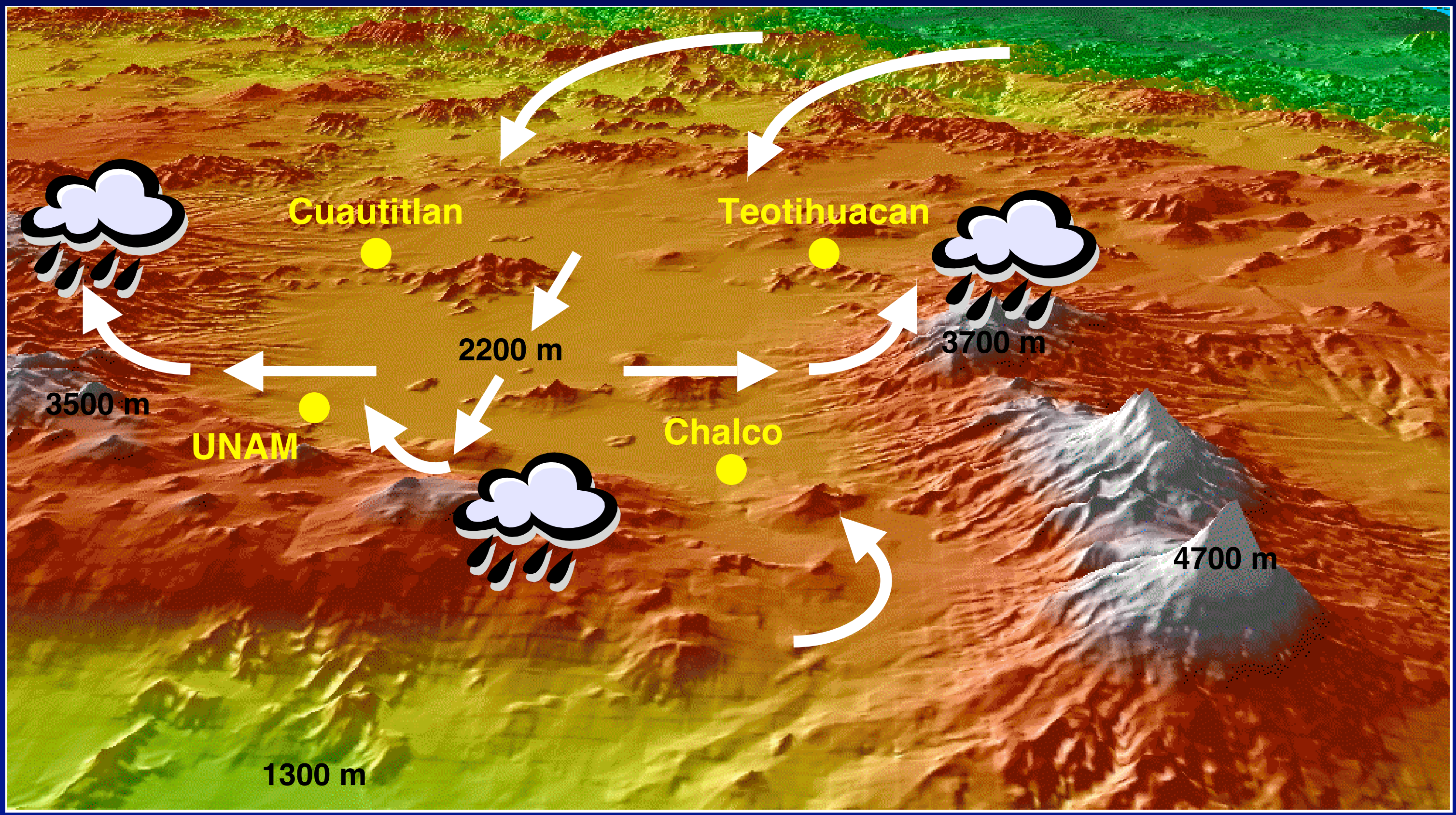
More Recently:

- IMADA 1997 obtained a good meteorological data set; however, …
- missing certain chemistry and particulate data needed to fully evaluate chemical transport models and a lack of a common data base poses problems for modelers
- MCMA 2002 / 2003 obtained more detailed chemistry and particulate measurements to evaluate models; however, …
- meteorological data is more limited than IMADA 1997 and modeling studies using data form MCMA 2003 have yet to be published or are currently being performed

Meteorology

Thermally-Driven Circulations

- Mountain valley circulations [Lauer and Klaus, *Arch. Met. Geoph. Biokl.*, 1975]
- IMADA field campaign: 4 boundary layer sites, February - March 1997



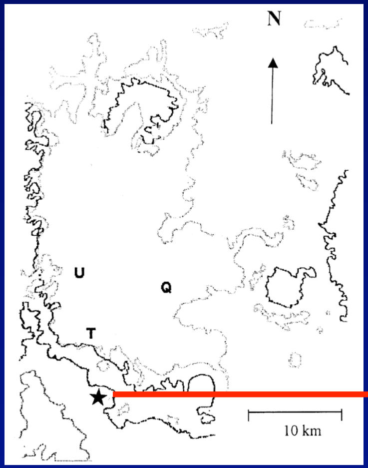
1: slope flows
[Jauregui, *Atmosfera*, 1988]

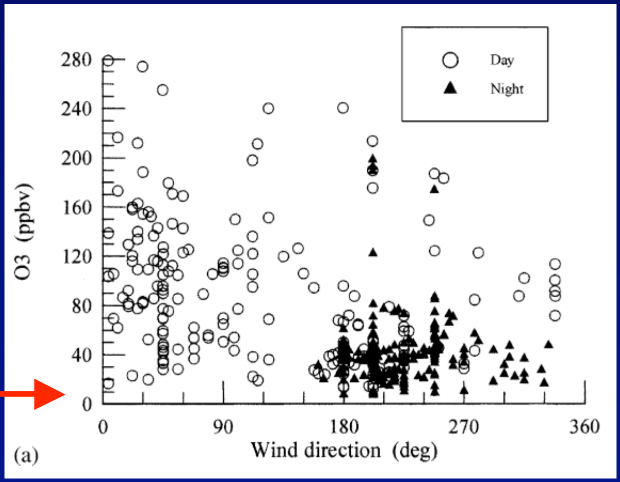
2: density current
[Bossert, *JAM*,1997]

3: gap wind
[Doran and Zhong, *JAM*, 2000]

Upslope flows

- Long history of measurements and analyses of flows with the valley that affect pollutant transport [e.g. Jauregui, *Atmosfera* 1988]
- Most wind measurement sites located over valley floor
- Usually no direct data of slope flow, except for AZTECA 1997 that found pollutants transported into the mountains south of Mexico City during the afternoon [Raga et al., *Atmos. Environ*., 1999]



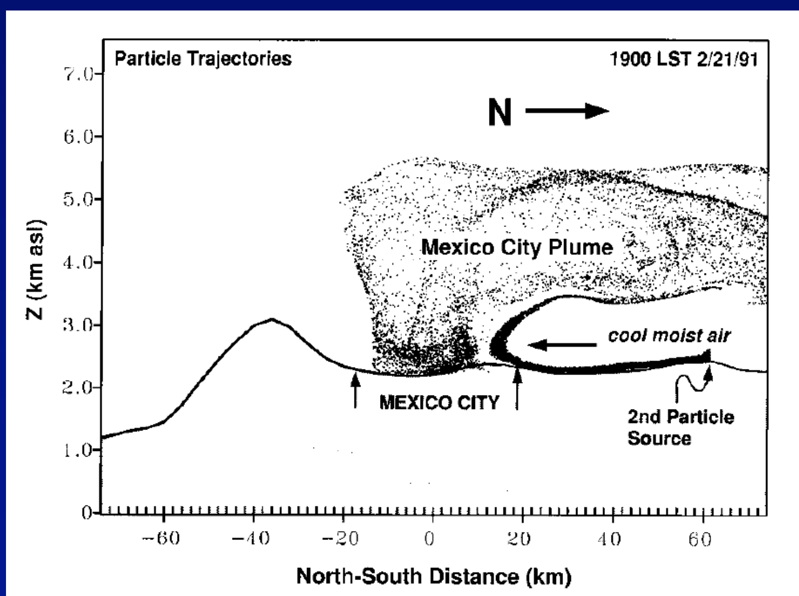


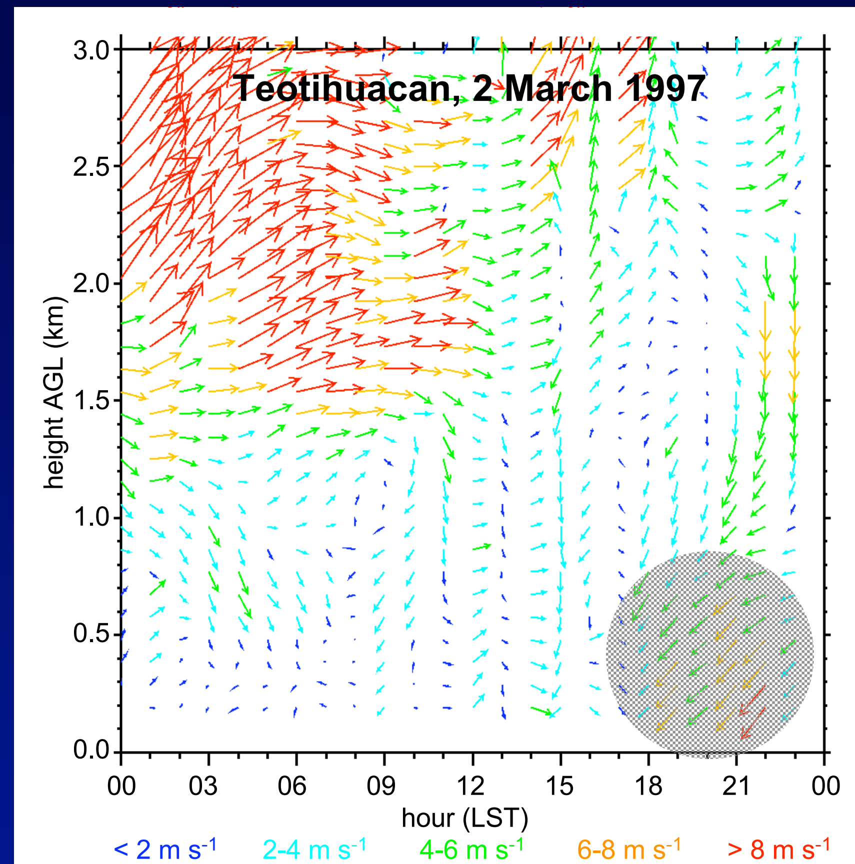
- No modeling studies that focus on slope flows; modeling studies usually coupled to other winds in valley

Propagating Density Current

Bossert, *JAM*, 1997:

- RAMS mesoscale model (Δx = 16, 4 km) and particle dispersion model simulations of MARI 1991
- Propagating density current was a regular feature in the model predictions



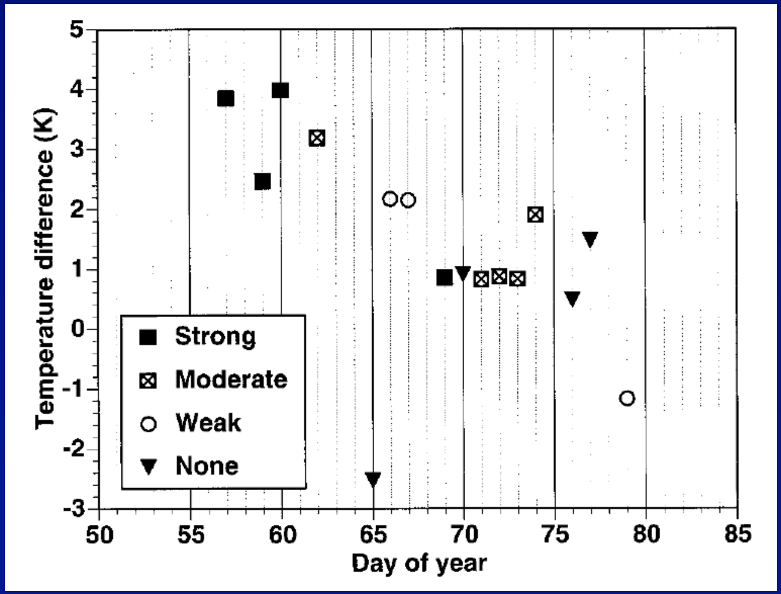


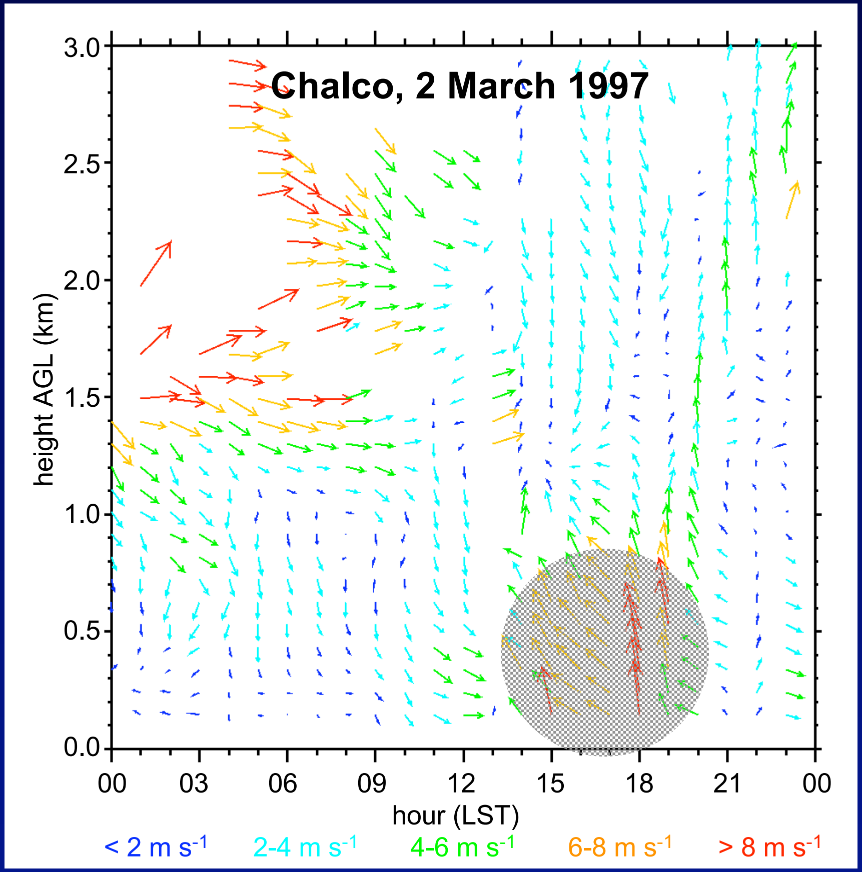
- Radar wind profiler data from IMADA 1997 confirm model predictions
- northerly flow occurred 8 out of 22 days during IMADA 1997

Gap Winds

Doran and Zhong, *JAM*, 2000:

- RAMS mesoscale model (Δx = 36, 9, 2.25 km) simulations of IMADA 1997
- Observations and predictions showed dependence of gap wind on horizontal temperature gradient
- Gap winds were important in producing convergence in valley

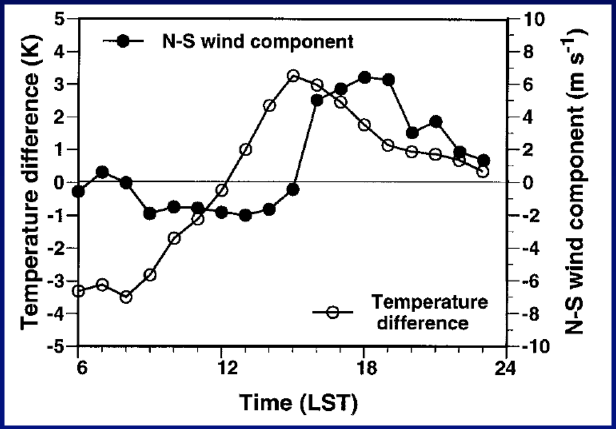


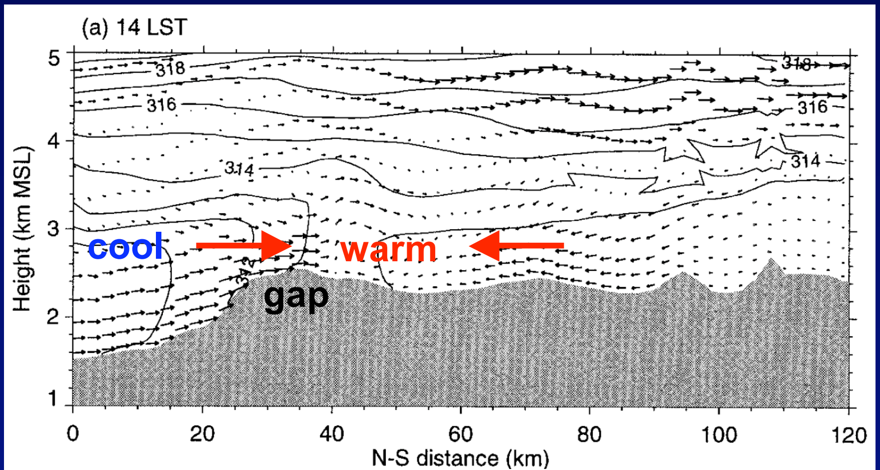


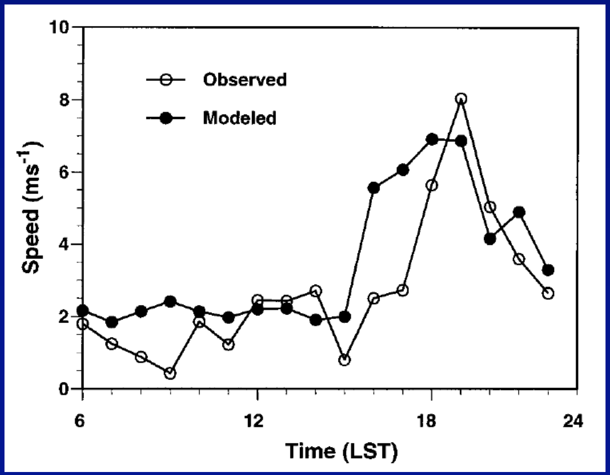
- gap flow occurred 12 out of 22 days during IMADA 1997

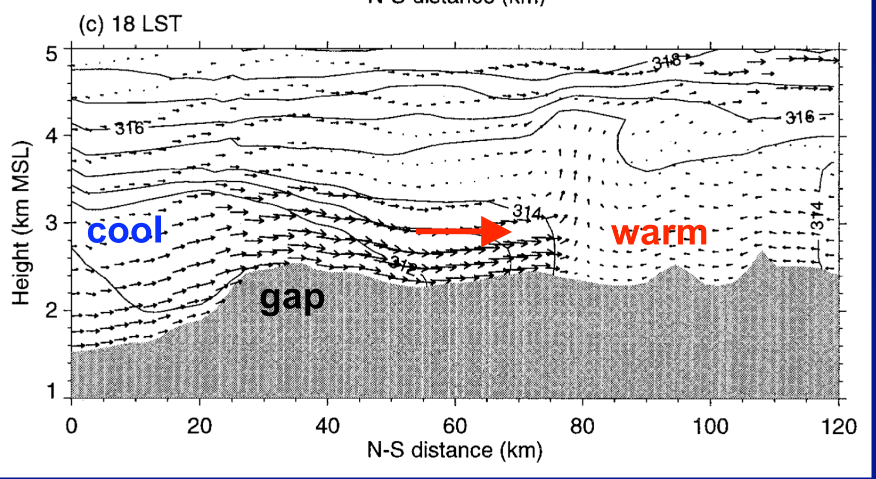
Gap Winds (2)

- Maximum jet speed occurs several hours after the maximum temperature difference between the valley and the region to the south
- Simulated jet similar to observed jet, except for timing of the initial onset





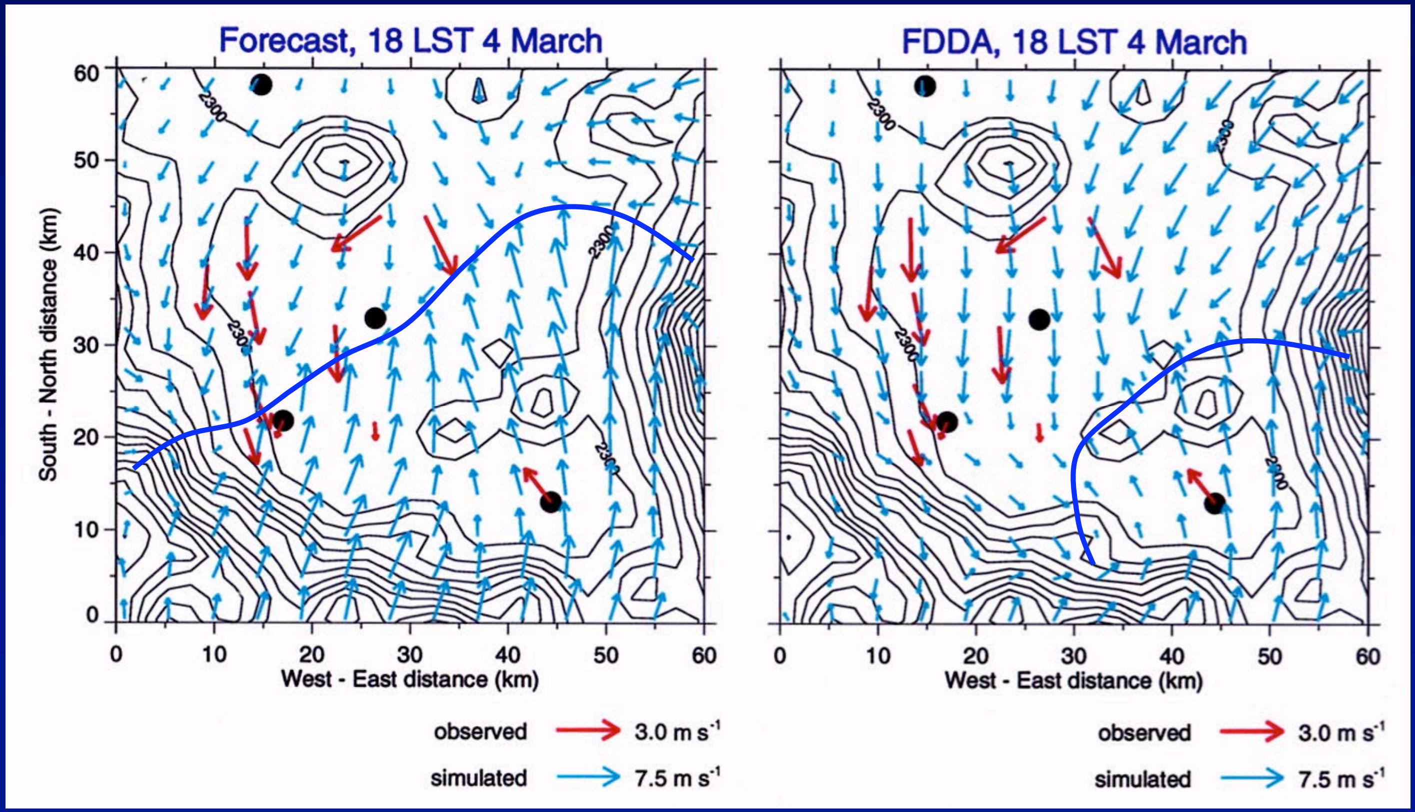




Dispersion

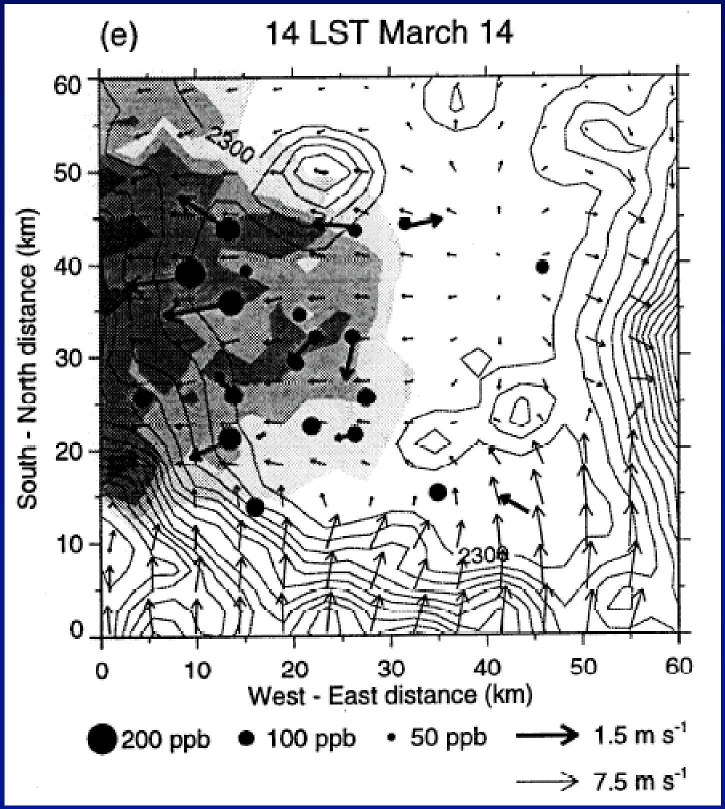
Fast and Zhong, *JGR*, 1998:

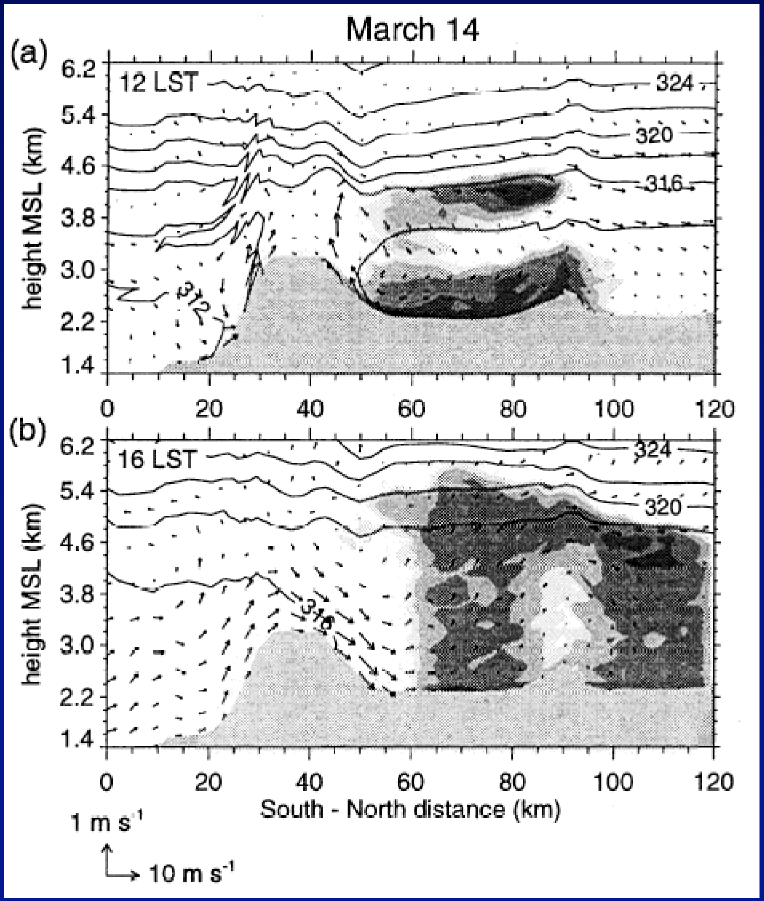
- RAMS mesoscale model (Δx = 36, 9, 2.25 km) and particle dispersion model simulations of IMADA 1997
- Four-dimensional data assimilation (FDDA) using the radar wind profiler data



Dispersion (2)

- Day-to-day variations of peak tracer concentrations demonstrated the importance of interaction of synoptic and local circulations
- Upslope flows, mountain venting, and vertical wind shears often produced same-day recirculation of tracer
- Little multi-day accumulation of tracer





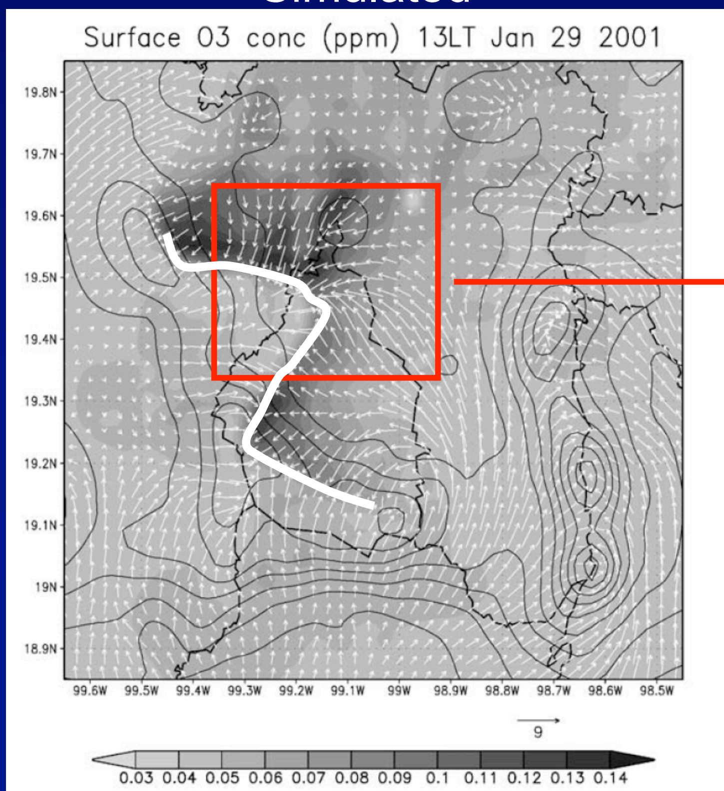
Convergence in the Valley

Jazcilevich et al., *Atmos. Environ.*, 2005:

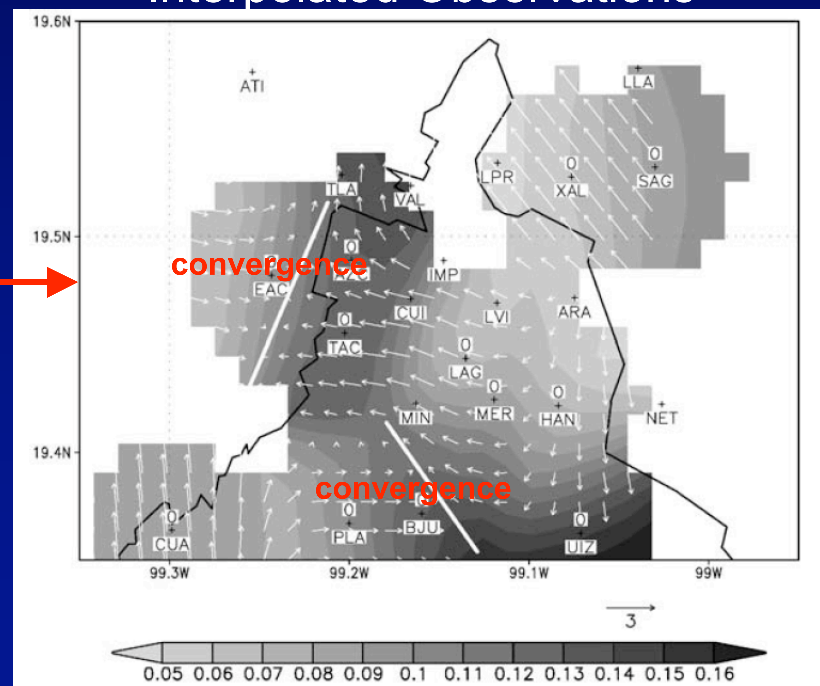
- MM5 (Δx = 27, 9, 3 km) coupled to a photochemical model, MCCM
- Examined predicted ozone and ozone precursor distributions during two events when convergence was strong

Ozone and Winds 13 LST 29 January 2001

Simulated



Interpolated Observations

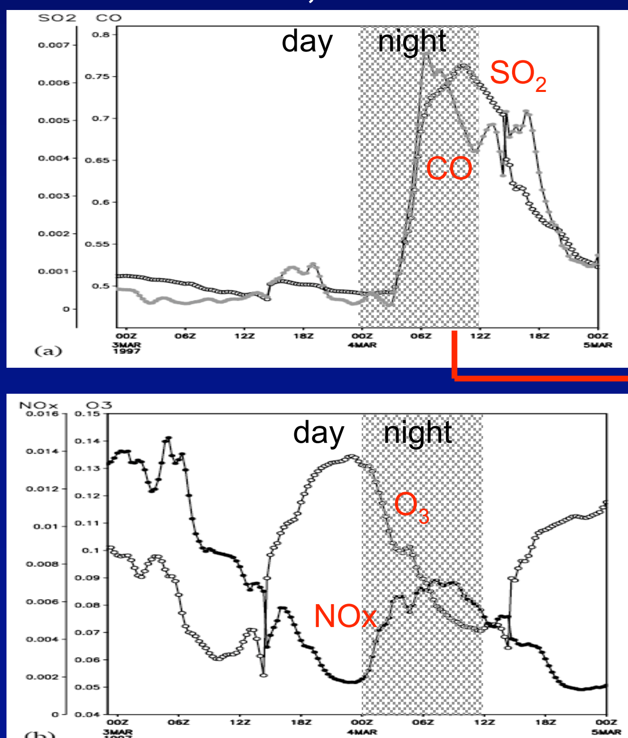


Nocturnal Transport

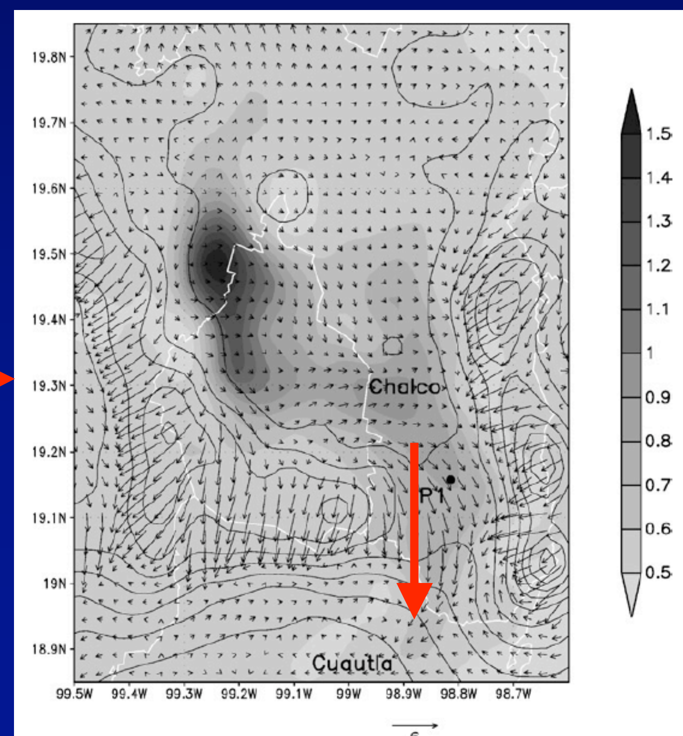
Jazcilevich et al., *Atmos. Environ.*, 2003:

- MM5 (Δx = 27, 9, 3 km) coupled to a photochemical model, MCCM
- During an El Norte event, conditions favorable for transport of pollutants from the Valley of Mexico to the Valley of Cuautla

Simulated Trace Gases at Chalco, 3-5 March



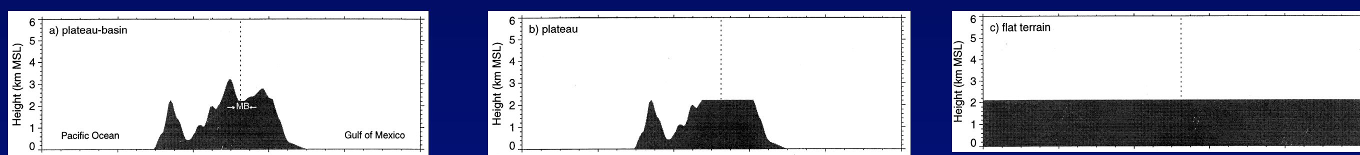
Simulated Surface Winds and CO 09 UTC 4 March

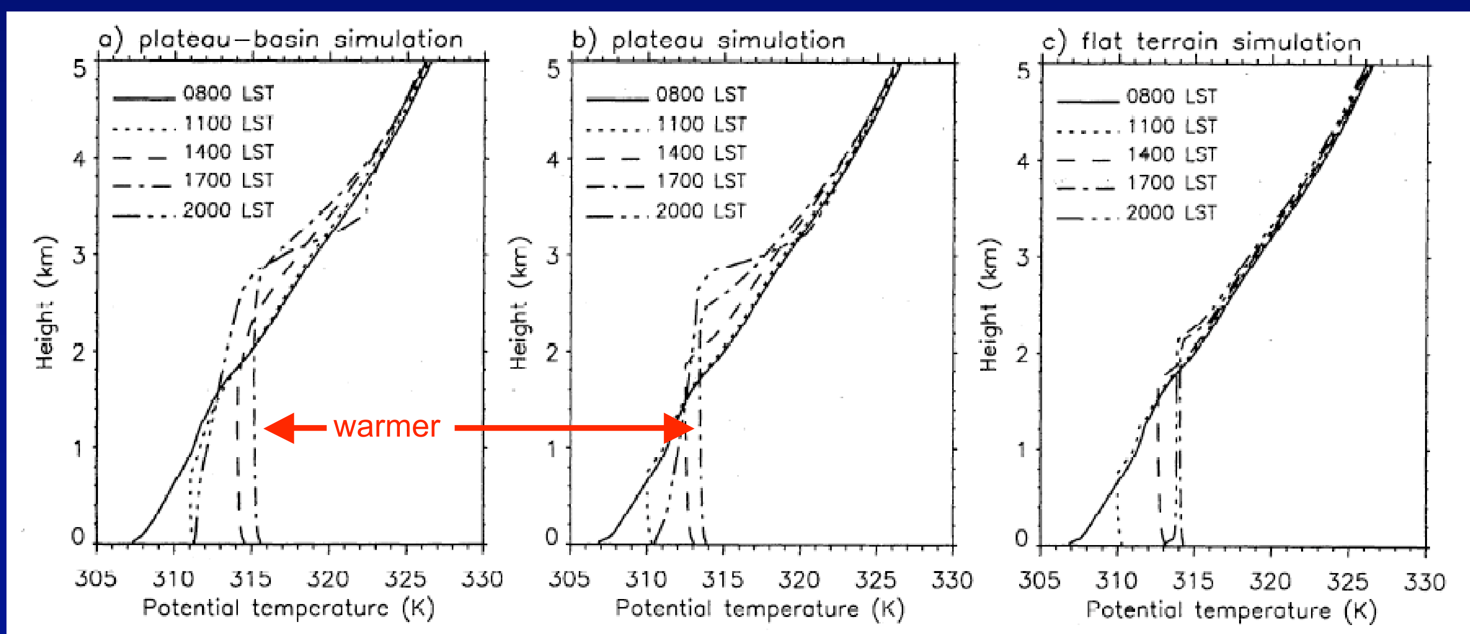


Boundary Layer Energetics

Whiteman et al., *JGR*, 2000:

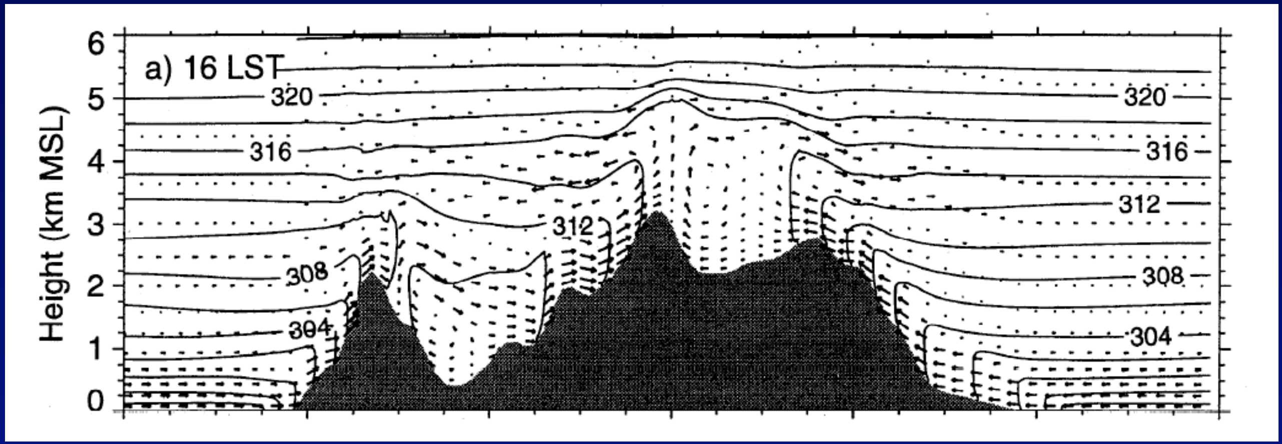
- RAMS, idealized 2-D simulations and 3-D simulations
- Examine rapid growth of PBL
- Valley topography has an effect on local heating: terrain amplification factor

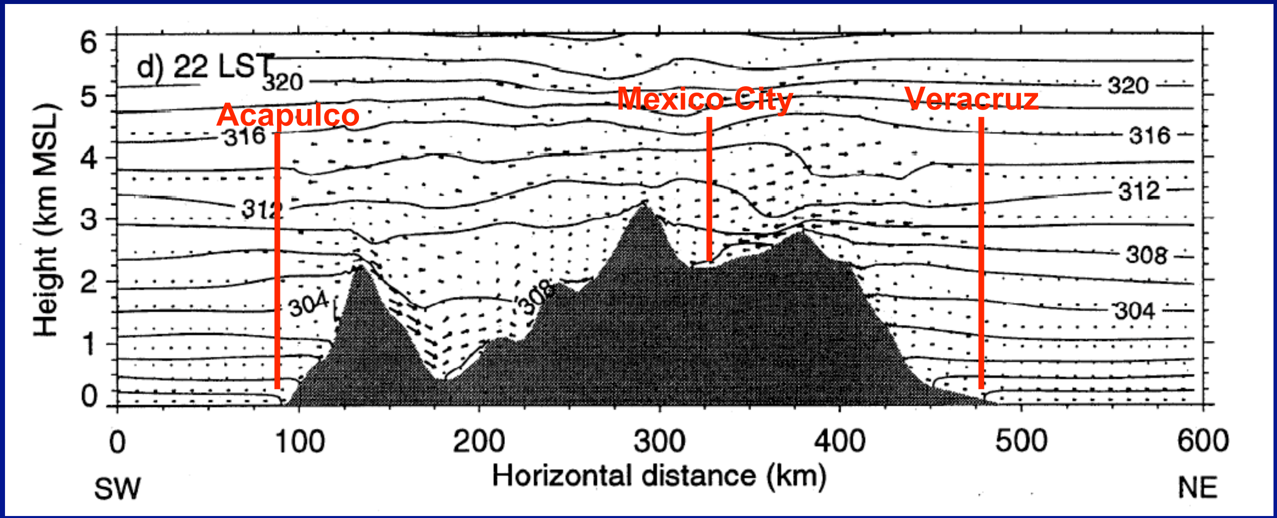




Boundary Layer Energetics (2)

- Topography produces daytime elevated source
- Rapid equilibration between plateau atmosphere and its surroundings after heating of the boundary layer ceases



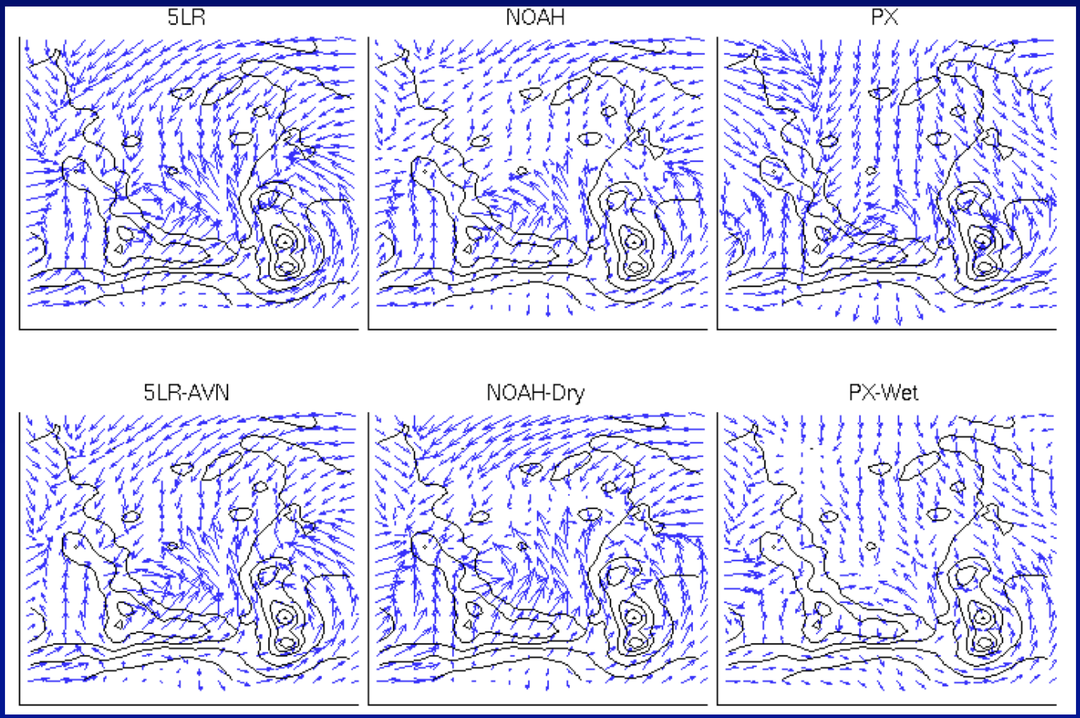


Model Parameterizations

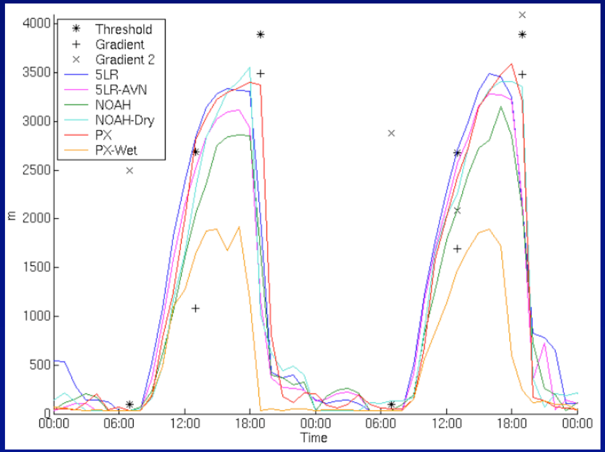
de Foy et al., *5th MM5/WRF Workshop*, 2004:

- MM5 (Δx = 27, 9, 3 km) applied to episode during MCMA 2003
- Six simulations: 3 land use schemes each with 2 soil moisture distributions
- Large differences among 3 land use parameterizations

surface winds



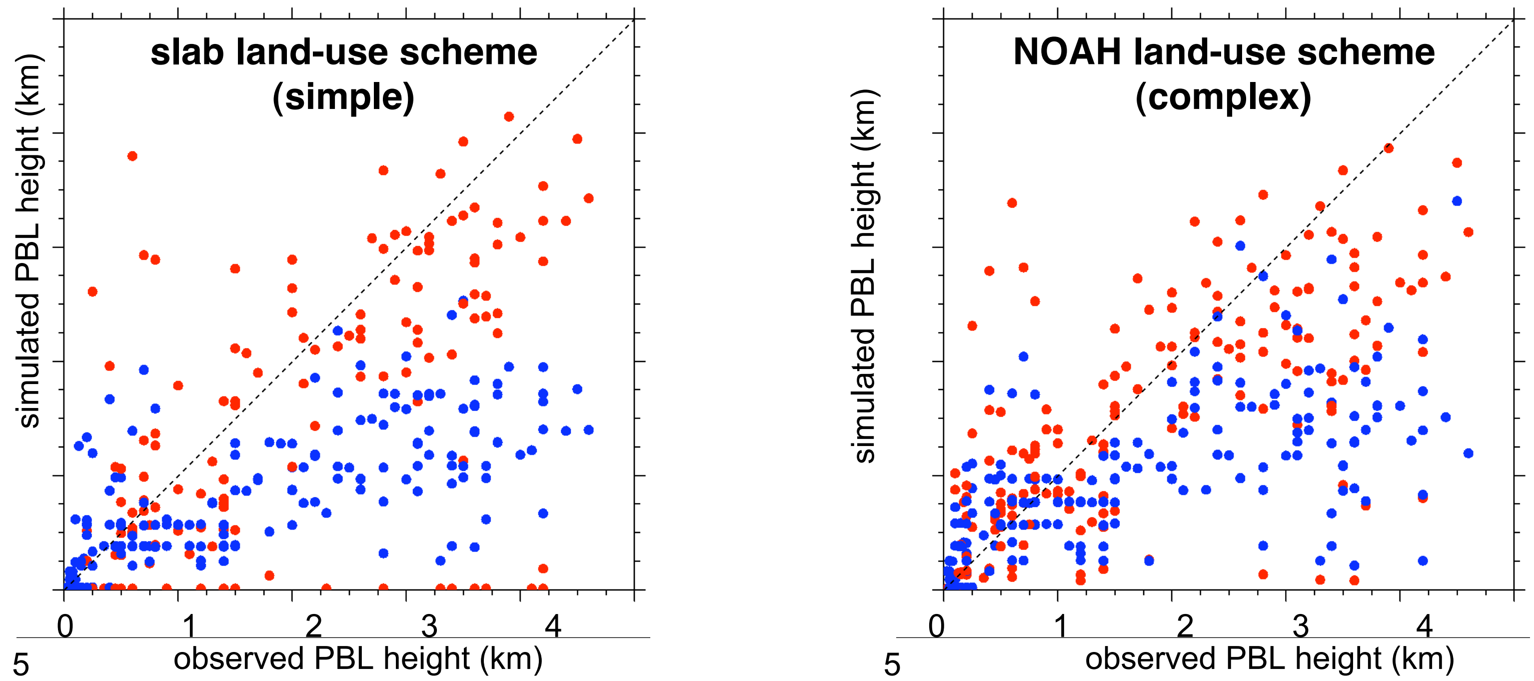
boundary layer height



Model Parameterizations (2)

Fast, *6th MM5/WRF Workshop*, 2005:

- WRF (Δx = 18, 6, 2 km) applied to episodes during IMADA 1997
- Four simulations: 2 land use schemes each with 2 PBL schemes
- Large differences in local PBL heights, but winds similar

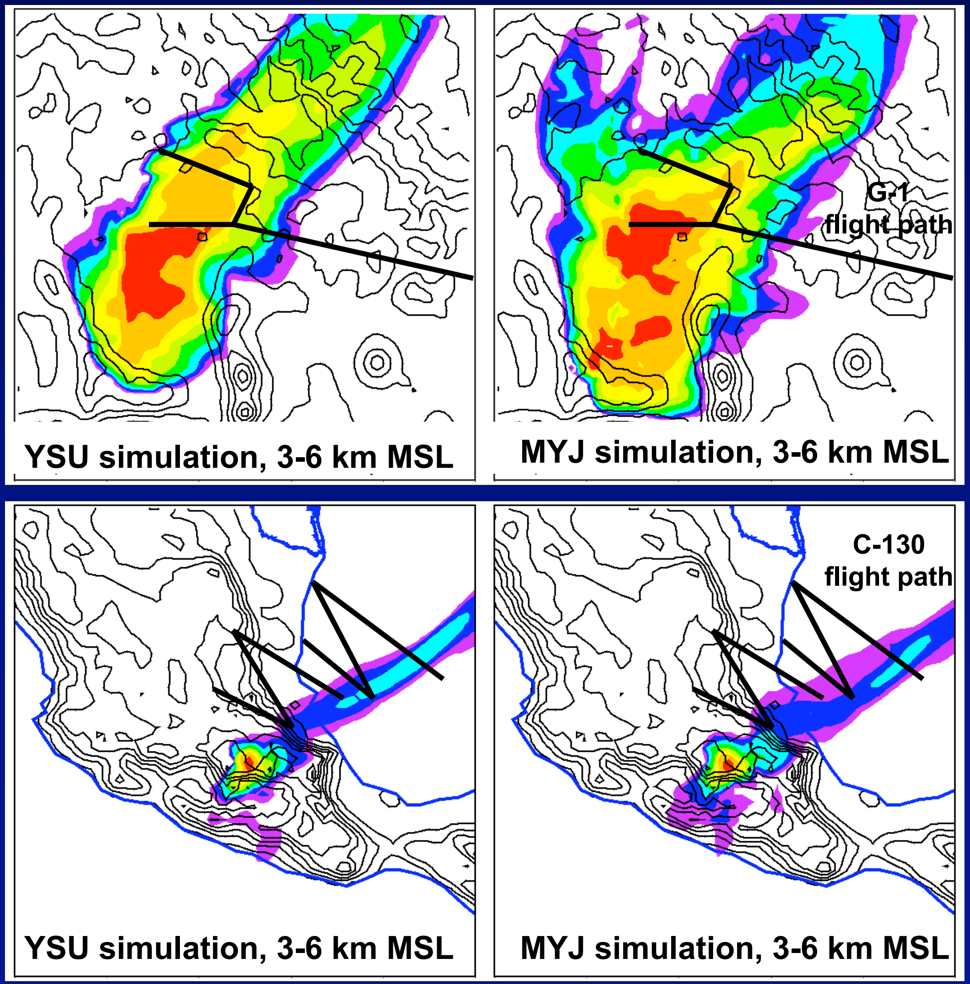


YSU PBLsimulations: bias = -411 m, r =0.71
MYJ PBL simulations: bias = -833 m, r = 0.77

YSU PBL simulations: bias = -279 m, r =0.78
MYJ PBL simulations: bias = -715 m, r = 0.70

Model Parameterizations (3)

- Tracer concentration fields using YSU scheme smoother than MYJ scheme
- Large differences in the vicinity of Mexico City, but not so much downwind



Day 1 Forecast
23 UTC (05 LST) 1 March
CO Footprint

southerly ambient winds

Day 2 Forecast
23 UTC (05 LST) 2 March
CO Footprint

westerly ambient winds

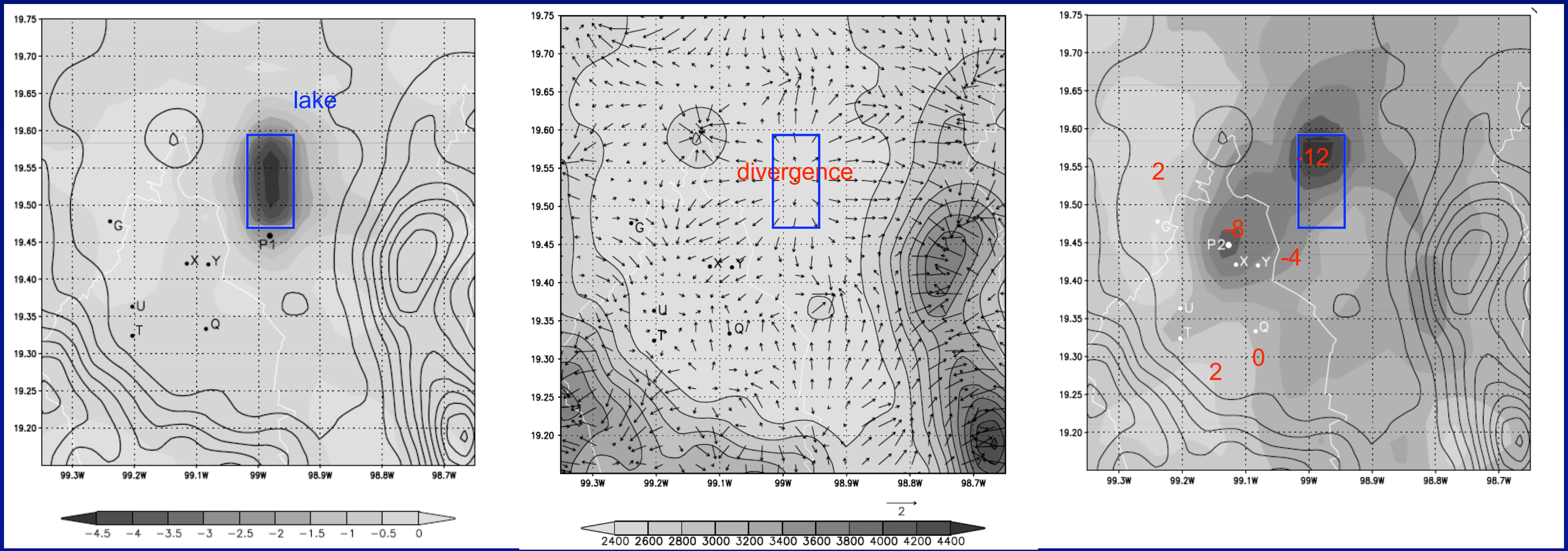
Land Use Change

Jazcilevich et al., *Atmos. Environ*., 2002:

- MM5 (Δx = 27, 9, 3 km) coupled to a photochemical model, MCCM
- Examined the effect of partial recovery of Lake Texcoco
- Lake surface reduced temperatures and produced divergence that lead to lower ozone concentrations over the northeastern valley

Difference Between Simulations With and Without Lake, 10-15 LST Average

Temperature | Winds | Ozone

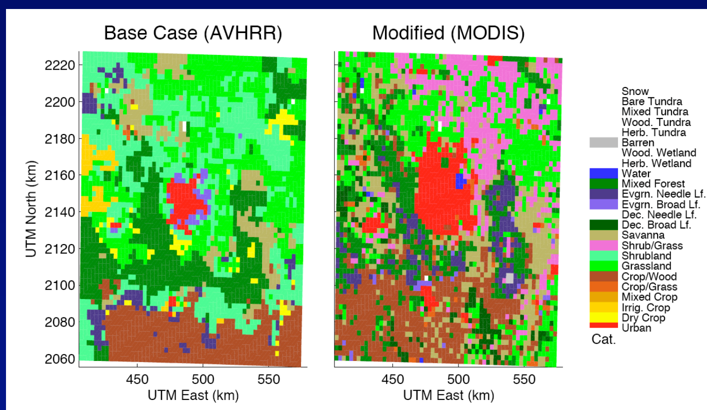


Use of Satellite Data

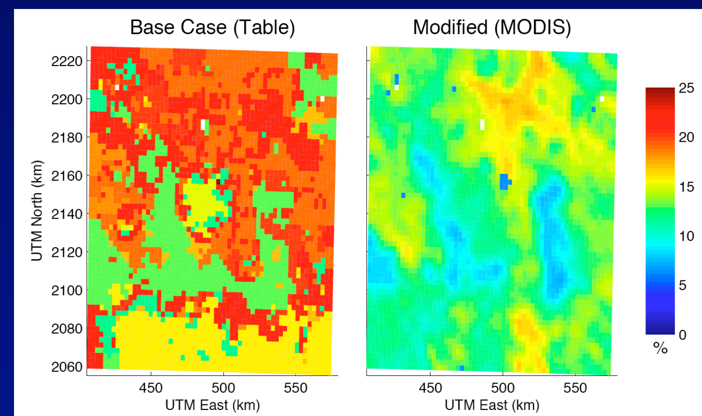
de Foy et al., *ACPD*, 2005:

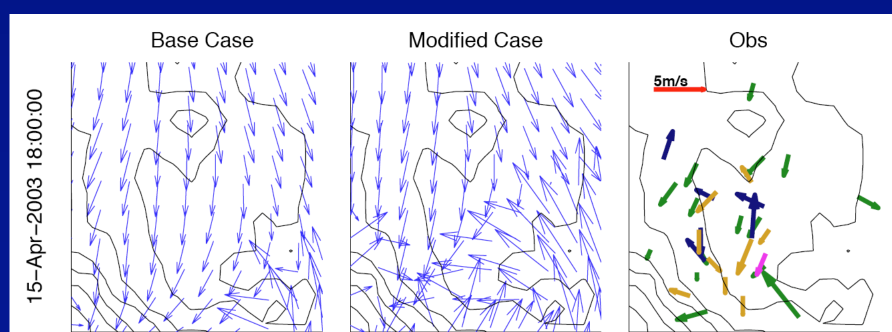
- MM5 (Δx = 36, 12, 3 km), simulations with surface quantities based on default values and derived from satellite measurements
- Sensitivity of boundary layer structure and circulations within the valley

land use



albedo

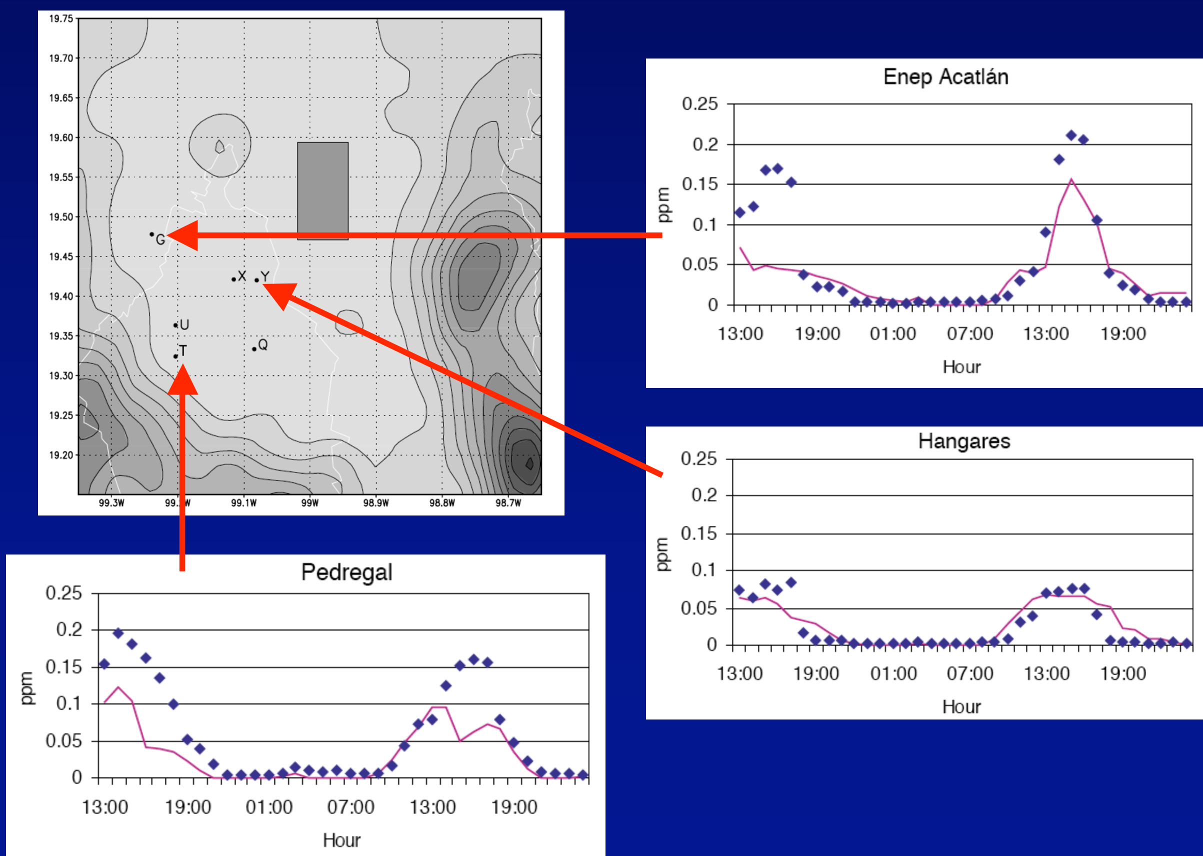




Chemistry

Local Photochemical Modeling

- **Fast, *7th Intl. Conf. on Air Pollution*, 1999:** RAM + PEGASUS
- **Junier et al., *Atmos. Environ*., 2005:** TOPOM
- **West et al., *JGR*, 2004:** RAMS + CIT
- **Jazcilevich et al., *Atmos. Environ*., 2002, 2003, 2005:** MM5 + MCCM



Statistics for Ozone

Correlation: 0.60 - 0.87

RMSE: 10 - 60 ppb

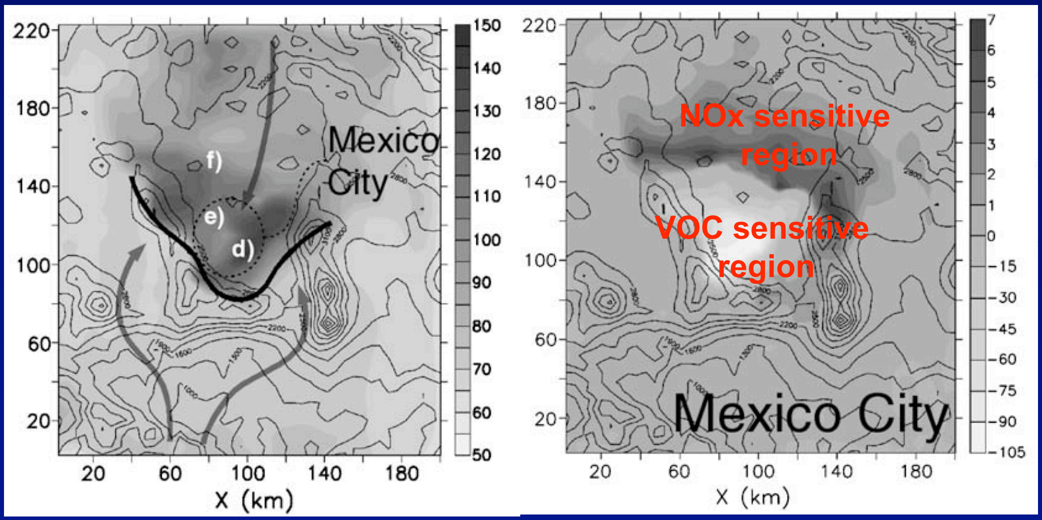
Chemical Mechanism

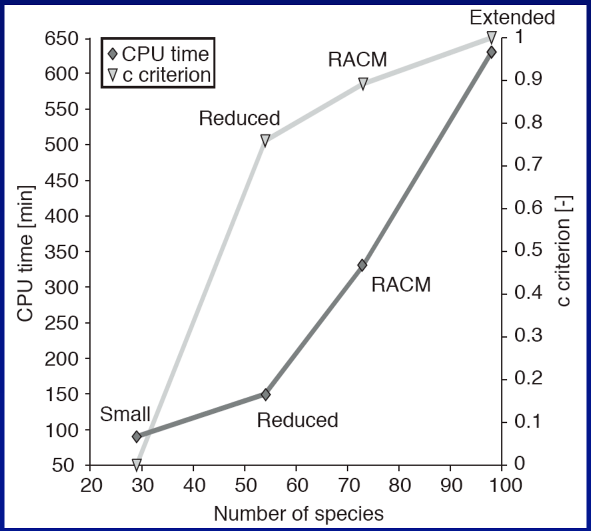
Ruiz-Suarez., *Atmos. Environ.*, 1993: TAPOM

Young et al., *Atmosfera*, 1997: TAPOM

Junier et al., *Atmos. Environ.*, 2005: TAPOM

- Compare RACM, CHEMATA
- Find optimum between calculation speed and mechanism detail

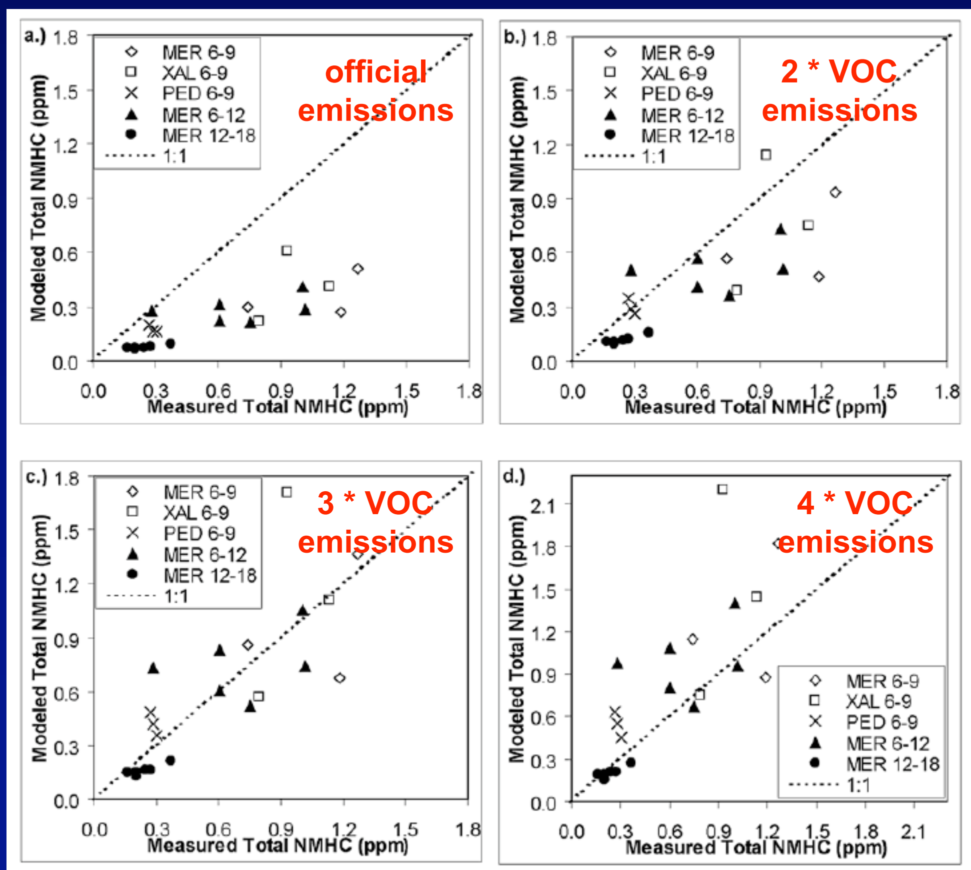


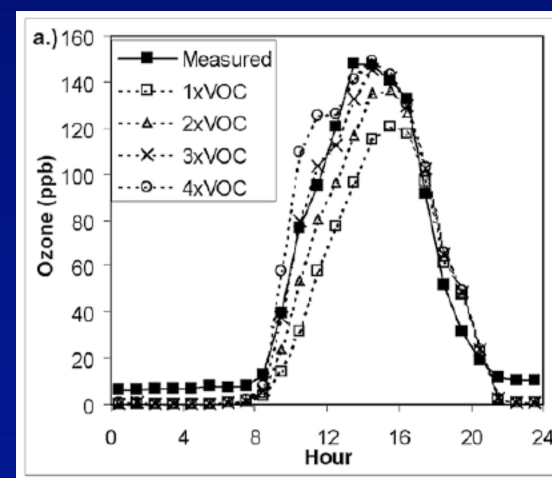


Emissions Estimates

West et al., *JGR*, 2004:

- RAMS (Δx = 2.25 km) coupled with the CIT photochemical model
- Six 2-day periods during IMADA 1997
- Vary official emission rates to best fit surface observations of trace gases

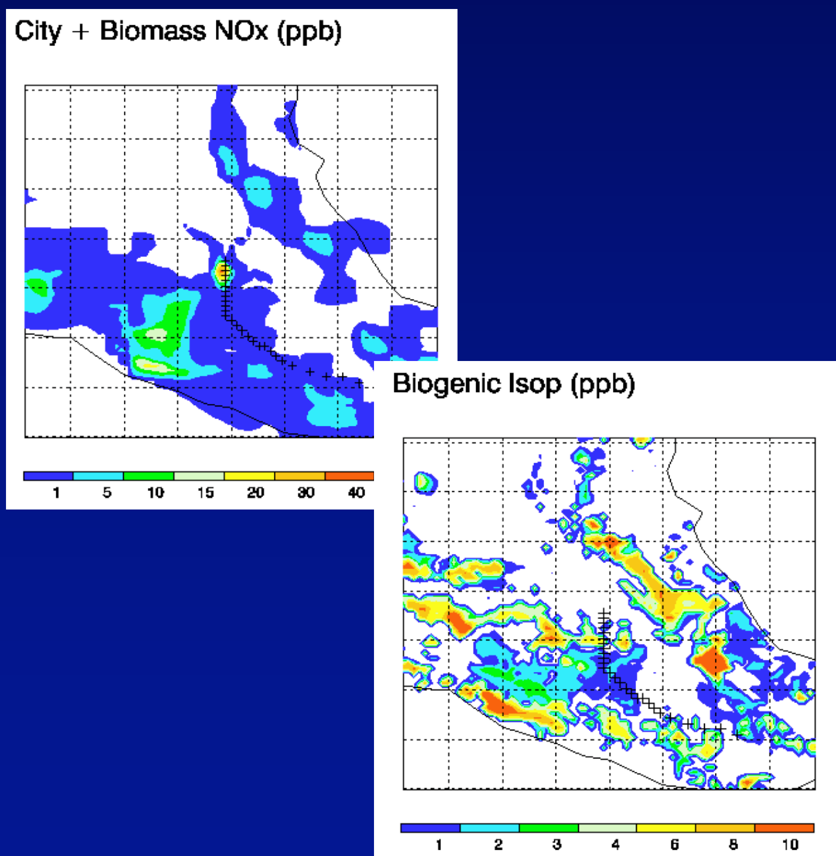


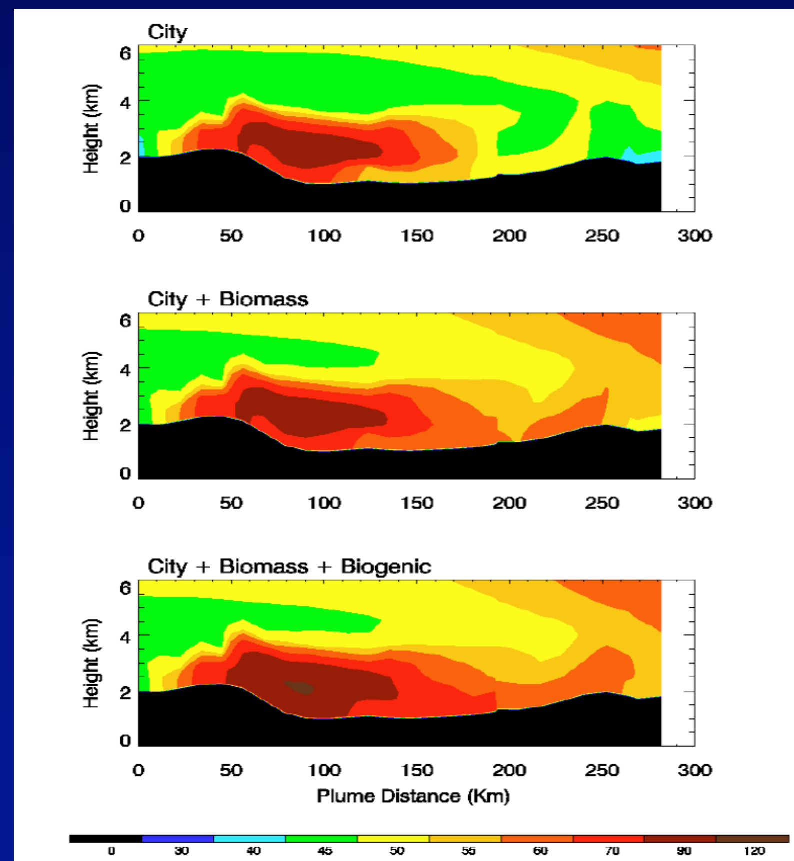


Biogenic Emissions

Tie, *5th MM5/WRF Workshop*, 2004:

- WRF-chem (Δx = 6 km)
- Ozone production enhanced downwind of Mexico City as a result of biogenic emissions





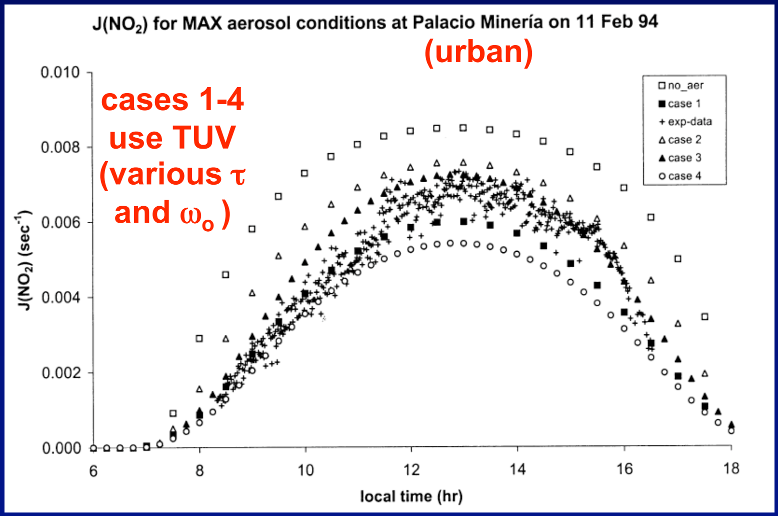
Photolysis Rates

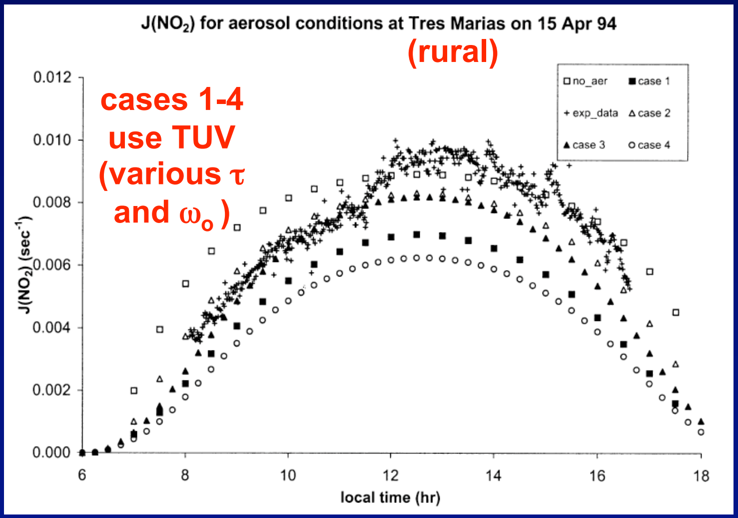
Ruiz-Suarez et al., *Atmos. Environ.*, 1993:

- Theoretical calculations of photolysis rates, no aerosols

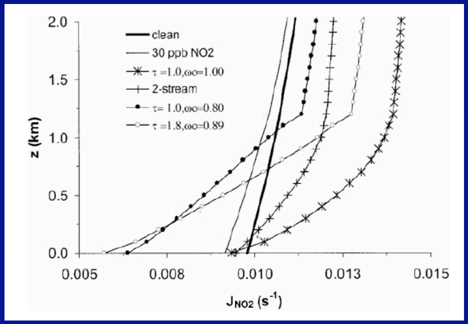
Castro et al., *Atmos. Environ.*, 1997, 2001:

- Aerosols affect ultraviolet radiation and thus affect photochemistry

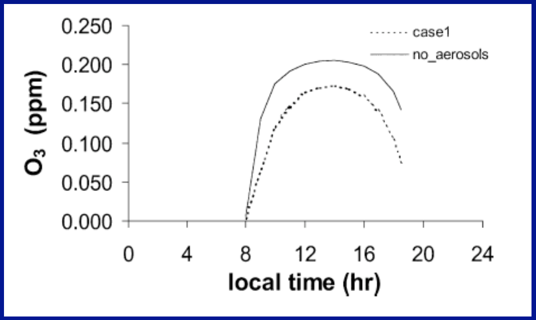




Variation of JNO_2 with Height



Effect of Aerosols on Ozone



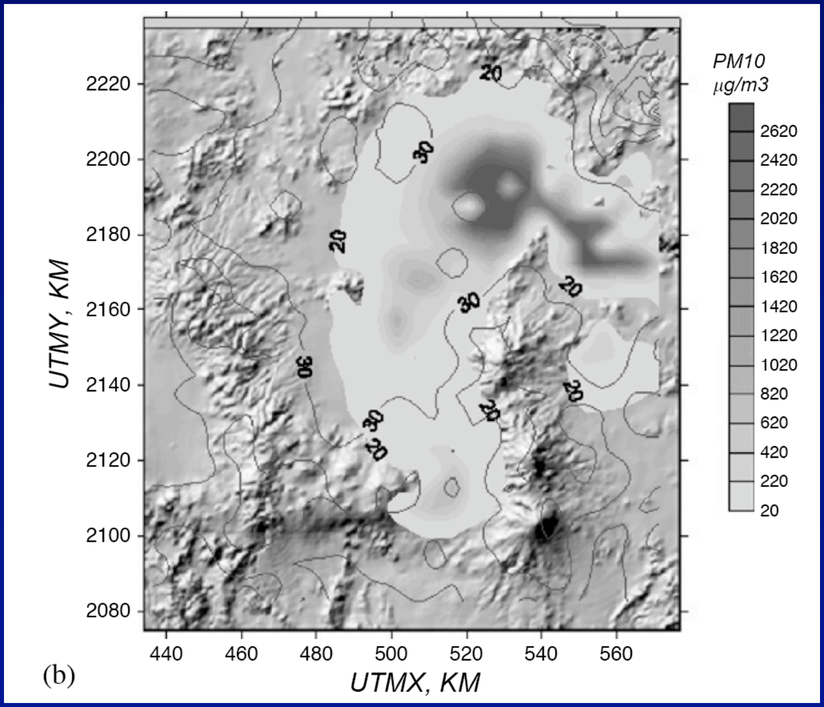
Particulates

Dust modeling

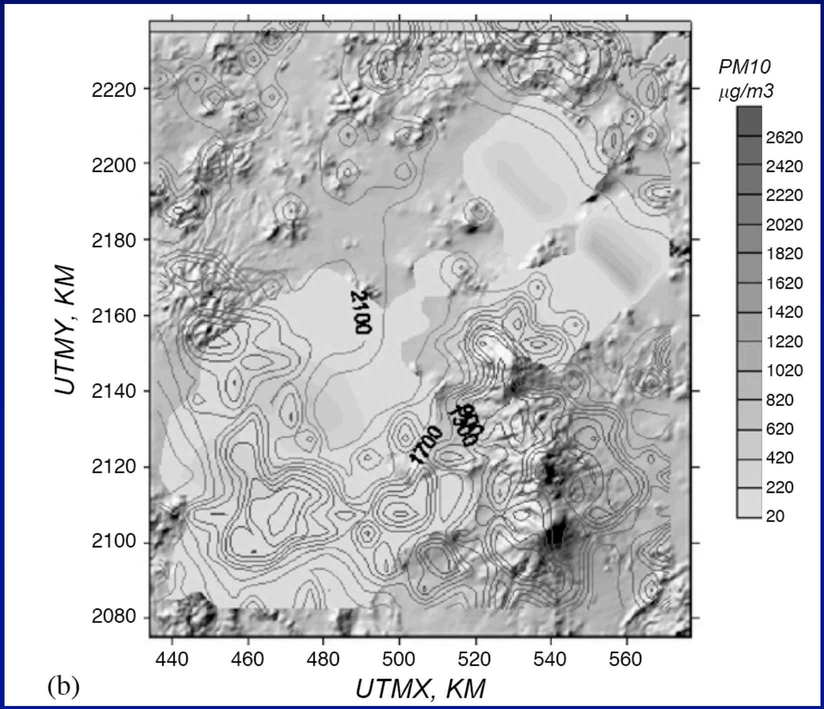
Villasenor et al., *Atmos. Environ.*, 2003:

- CALMET/CALPUFF (Δx = 5 km)
- Simulate PM10, no chemical transformation
- Examine how soil dust emission from agricultural fallow land affect downwind areas during the dry season

Simulated PM10 at 06 LST 5 March



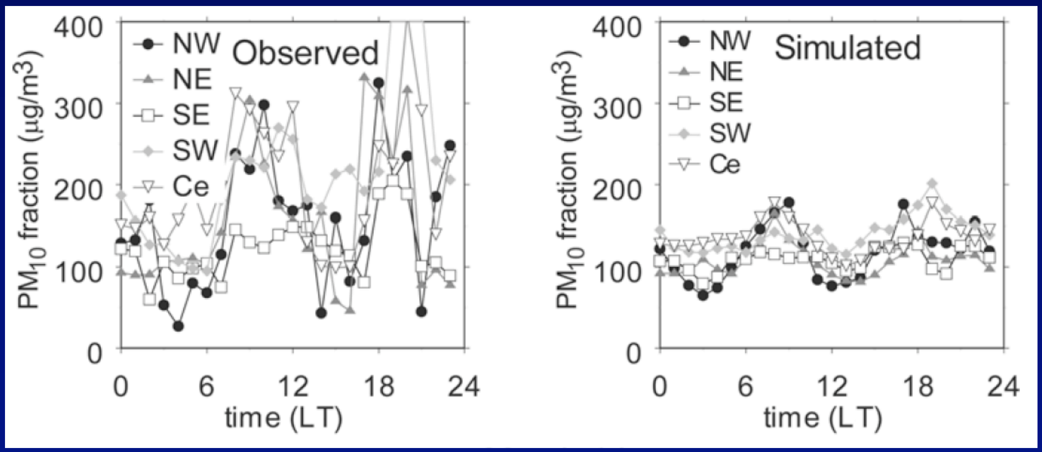
Simulated PM10 at 18 LST 5 March



Visibility

Munoz-Alpizar et al., *JGR*, 2002:

- NARCM, (Δx = 50, 10, 2 km)
- 3 case study periods during IMADA 1997, long spin-up period
- Better resolution of the size distribution leads to better predicted visibility



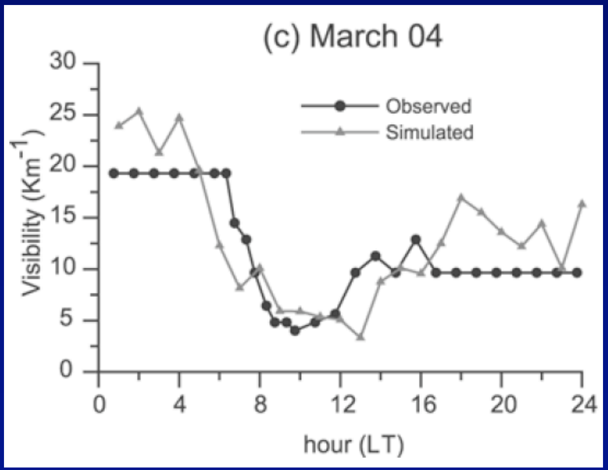


Table 2. Twenty-Four-Hourly Average Particulate Matter 2.5 ($PM_{2.5}$) Concentrations Measured and Simulated at Different Sites of the RAMA Stations[a]

Site	2 March Obs. $PM_{2.5}$	2 March Sim. $PM_{2.5}$	4 March Obs. $PM_{2.5}$	4 March Sim. $PM_{2.5}$	14 March Obs. $PM_{2.5}$	14 March Sim. $PM_{2.5}$
TLA	27	40	35	43	54	44
MER	32	36	49	52	35	28
PED	23	34	32	54	26	46
XAL	41	29	66	38	53	28
NET	54	53	83	59	44	53
CES	38	28	55	39	32	41

Equilibrium Models

San Martini et al., *Atmos. Environ.*, 2005:

Moya et al., *Atmos. Environ.*, 2001:

- SEQUILIB, SCAPE2, ISOROPIA, GFEMN equilibrium models compared
- Input HNO_3, NH_3, H_2SO_4, HCL, temperature, and RH from IMADA 1997
- partitioning of nitrate and ammonium between gas and particulate phases
- Dynamic approach, instead of equilibrium, is more suitable in reproducing aerosol behavior during the afternoon

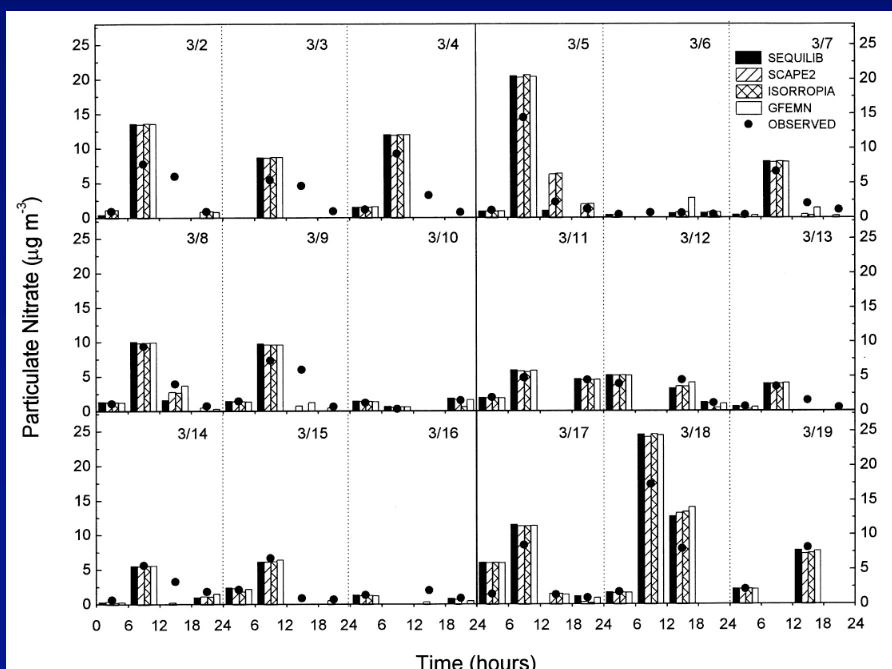


Table 8
SCAPE2 and MADM performance for $PM_{2.5}$ species at the MER site on 2 and 14 March 1997 for the afternoon sampling periods (12:00–18:00 h)

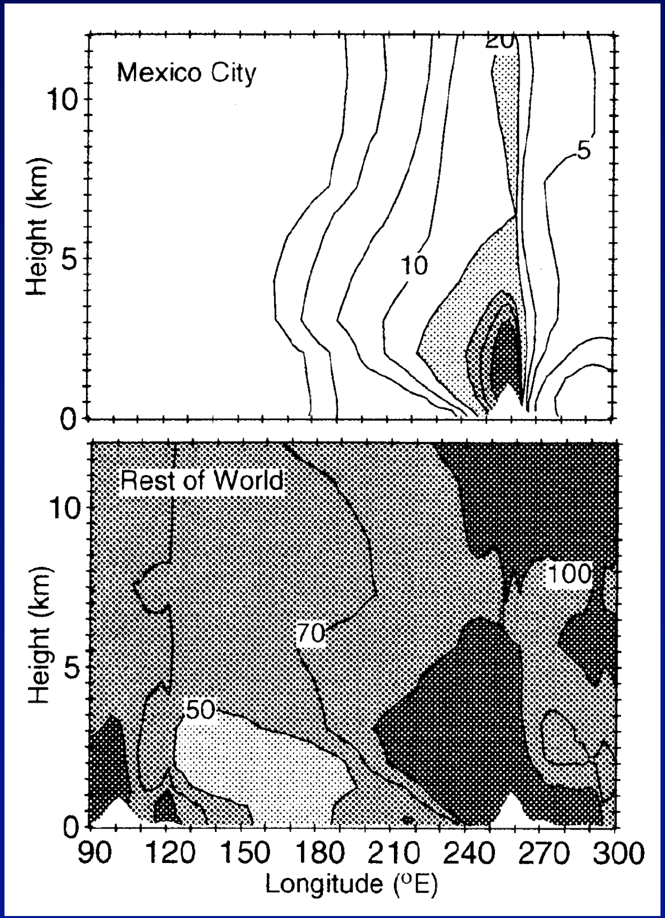
Species	Date	Mean predicted SCAPE2 ($\mu g\,m^{-3}$)	Mean predicted MADM ($\mu g\,m^{-3}$)	Mean observed ($\mu g\,m^{-3}$)
Predicted nitrate	02/03/1997	0.00	2.80	5.95
	14/03/1997	0.23	2.29	3.25
Predicted ammonium	02/03/1997	0.31	1.32	1.89
	14/03/1997	1.15	1.94	1.80

Global Climate Modeling

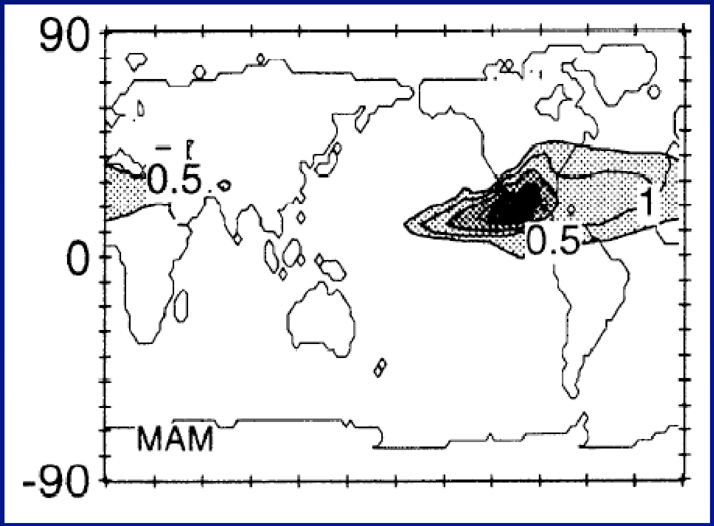
Barth and Church, *JGR*, 1999:

- CCM3, (Δx = 2.8 degrees)
- Sulfate from Mexico City, Southeast China, and rest of the world
- Mexico City emits ~1% of global anthropogenic sulfur emissions, contributes to ~1% of global sulfate burden

Annually Averaged Sulfate
(15 - 25 N)



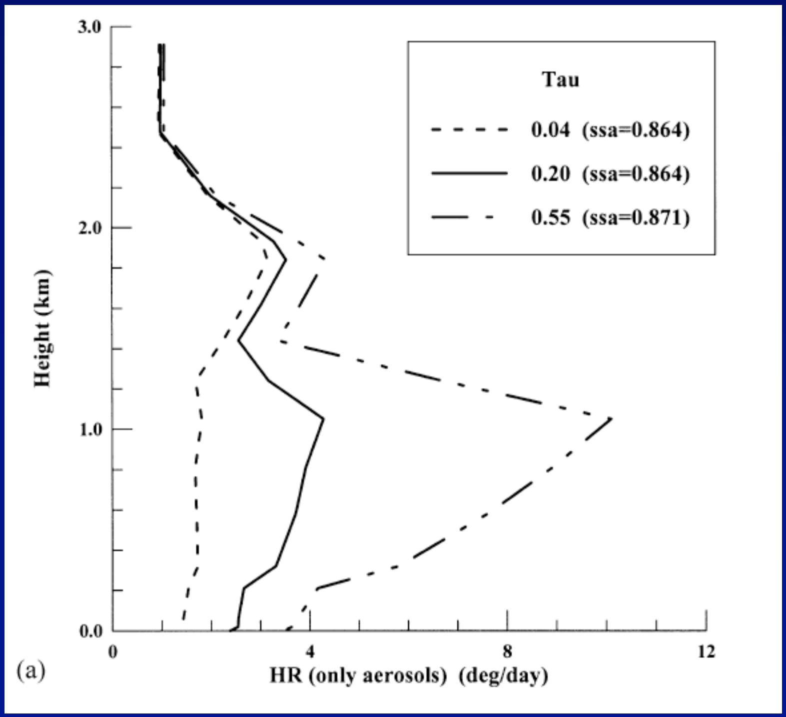
Sulfate Column Burden from
Mexico City (March - May)

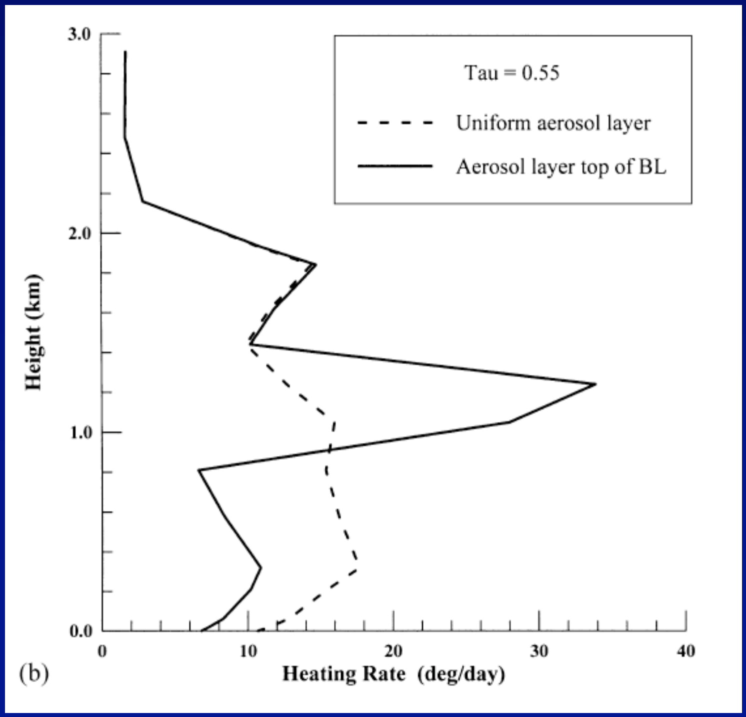


Climate Impacts of Aerosols

Raga et al., *Atmos. Environ.*, 2001:

- Radiative transfer model
- Reduction of ~18% in solar radiative flux for τ = 0.55
- Photolysis rates reduced by 18-21% at the surface and increased by 15-17% above the boundary layer





Pre-Field Campaign Modeling

MIRAGE Activities

- Predict downwind chemical evolution
- Determine transport pathways during months of Feb., Mar., and Apr.
- Modeling meeting held at UNAM in Mexico City on 15 March 2005

UCAR | NCAR | Milagro | ACD | MIRAGE is a project of the Atmospheric Chemistry Division

Modeling

Madronich (NCAR), Tie (NCAR), Fast (PNNL), de Foy (MIT)

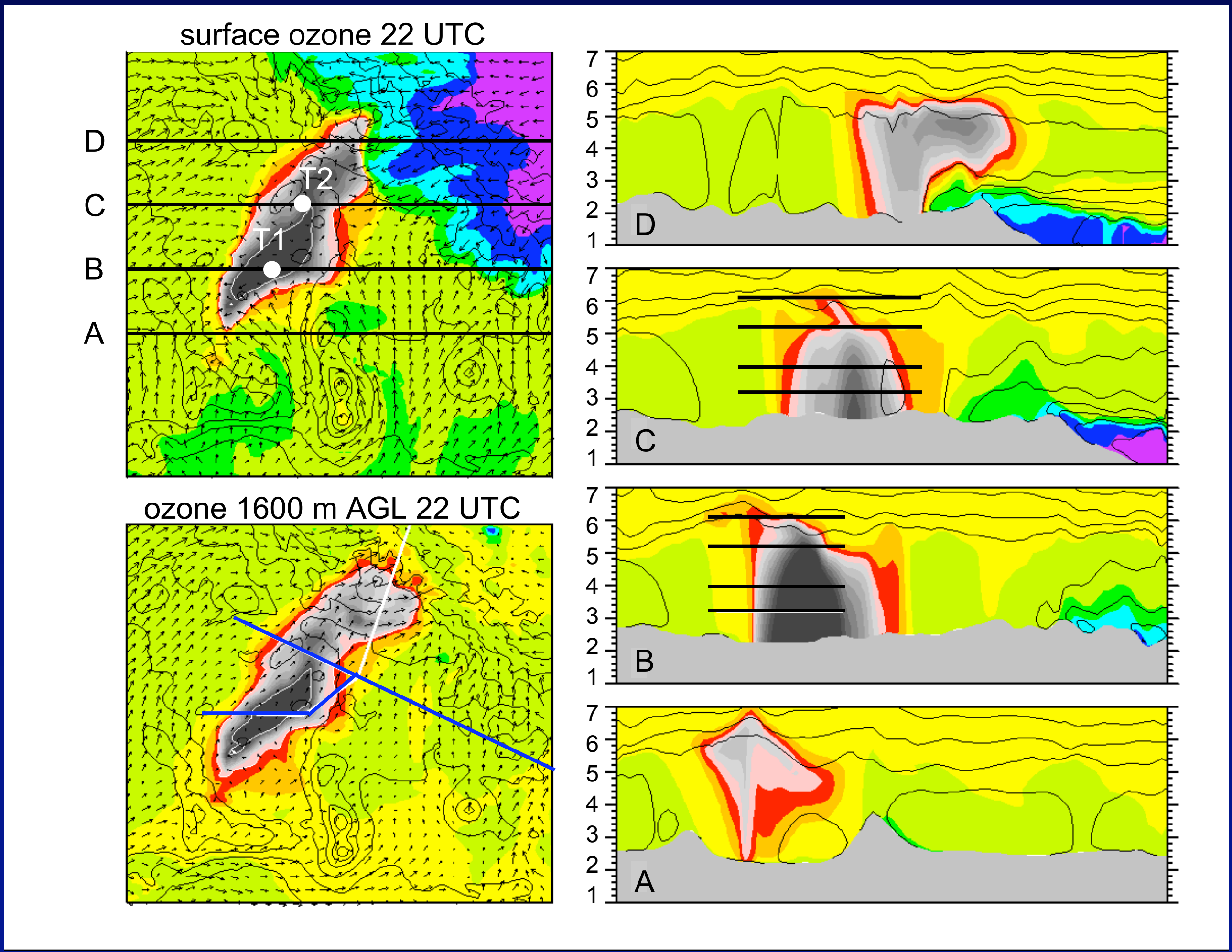
The following models were used as part of the MIRAGE-Mexico planning process:

- Box → chemical evolution as simulated by NCAR master mechanism over 5 days
- WRF → 13 out of 29 days (15 Feb - 14 Mar 2004) had outflow of CO column towards NE
- RAMS → dispersion for 14 days simulated between 24 Feb - 18 Mar 1997
- MM5 → forward and back trajectories (Apr -May 2003), NE and SW pathways
- Trajectories → radar wind profiler or HYSPLIT (Feb - Mar 2002, 2003), large fraction towards NE

MIRAGE is a project of the Atmospheric Chemistry Division at the National Center for Atmospheric Research

MAX-Mex Activities

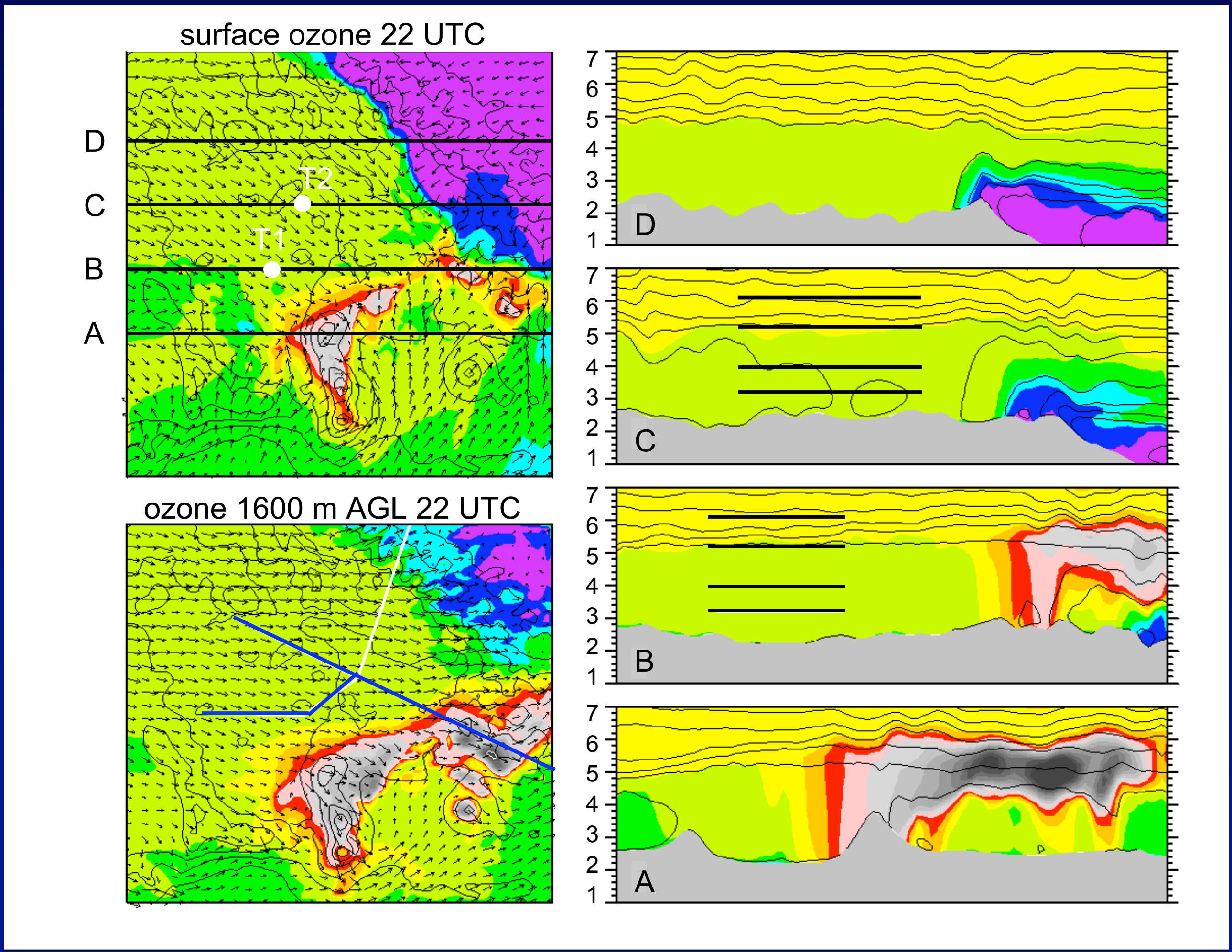
- WRF-chem simulations of IMADA 1997 periods to evaluate proposed T1 & T2 surface measurements and G-1 flight plans



<u>1 March 1997</u>

good day for
T1-T2 scenario

MAX-Mex Activities (2)

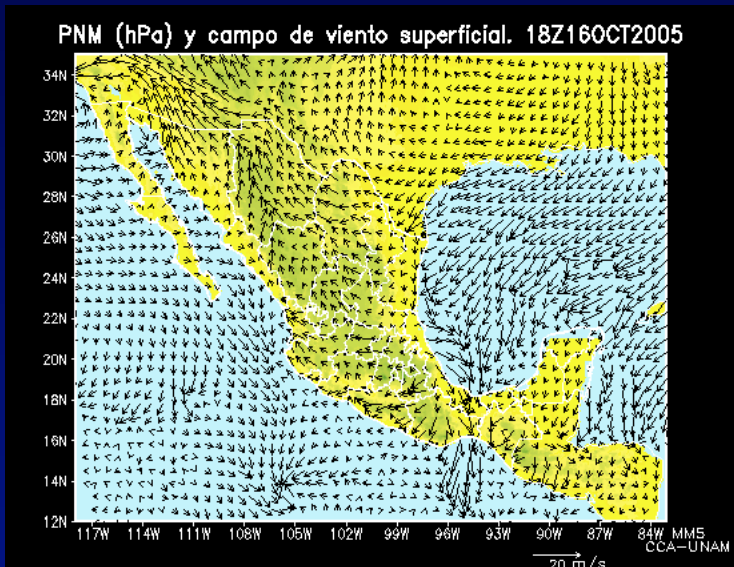


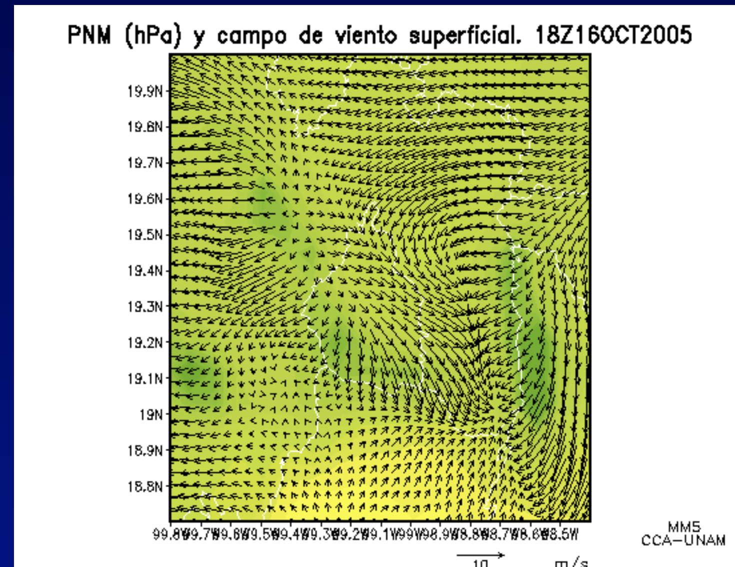
13 March 1997

not a good day for T1-T2 scenario

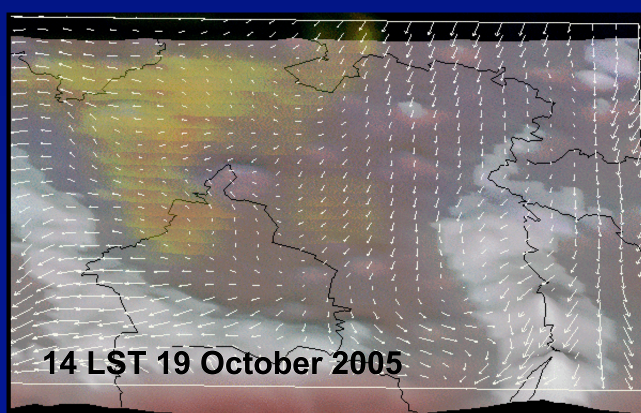
Operational Modeling

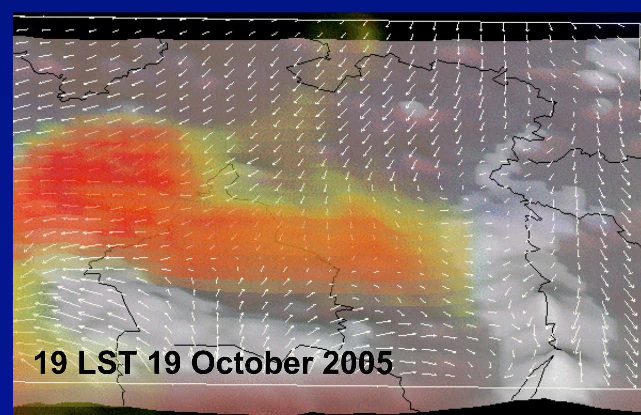
- Meteorological Forecasts - MM5 currently operational for Mexico





- Air Quality Forecasts - in development





Summary

Overall Model Performance

Meteorology:

- Models qualitatively reproduce primary thermally-driven flows, but forecasts contain errors in timing and magnitude of these flows
- Complex flows in valley contribute to large wind direction/speed errors at specific locations at times
- Models are unable to produce strong vertical shears in the CBL
- Forecasting during conditions with weak synoptic forcing will be more problematic than strong synoptic forcing conditions
- While maximum afternoon CBL height well simulated, models do not represent well the rapid CBL growth in the late morning

Chemistry:

- Despite uncertainties in emissions and meteorology, diurnal ozone variations are often similar observations (peak values usually under-predicted)
- Limited information on how well models simulate ozone precursors

Particulates:

- Simulated PM2.5 and PM10 mass is usually too low
- Despite available data, little information on how well 3-D models simulate aerosol composition, size distribution, and aerosol optical properties

Future Modeling

Research Needs:

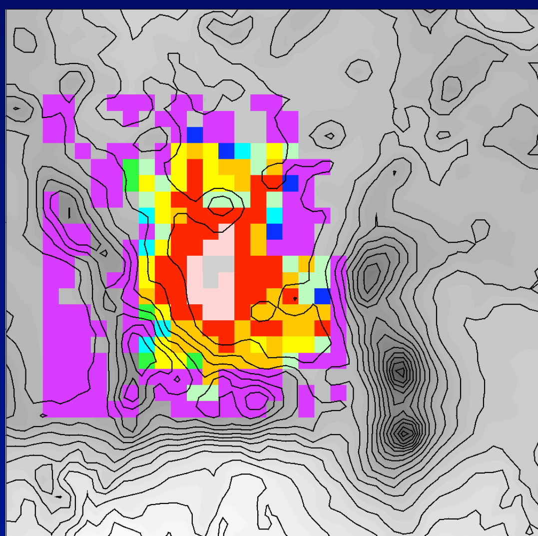
- Concurrent meteorology, chemistry, and particulate measurements to fully evaluate models so that they can be used to test scientific hypotheses
- Urban canopy parameterizations for mechanical mixing and surface heating over the city
- Better lower boundary conditions - soil moisture, satellite derived quantities
- Improved PBL parameterizations
- Data assimilation, both meteorology and chemistry
- Investigate the model performance in simulating clouds over central Mexico and the role of clouds on processing and mixing trace gases and particulates
- Improved emission estimates: higher spatial resolution, more hydrocarbon and primary particulate species, and information on biomass burning

Emission Rates

Sources of Gridded Emission Rates:

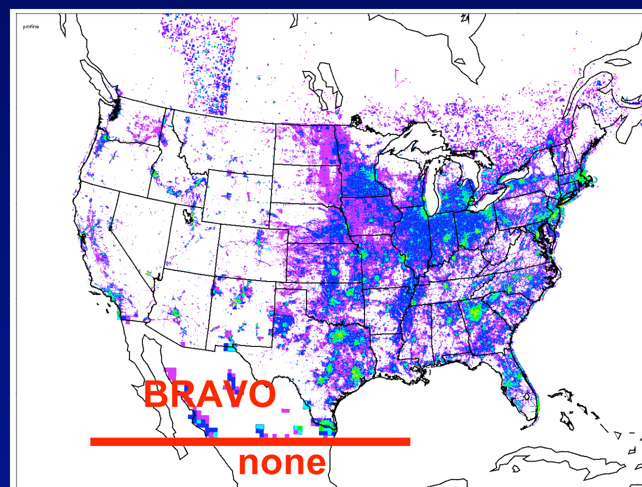
- Need better emissions inventories so that models can be used to address scientific questions with fewer uncertainties

Mexico City inventory



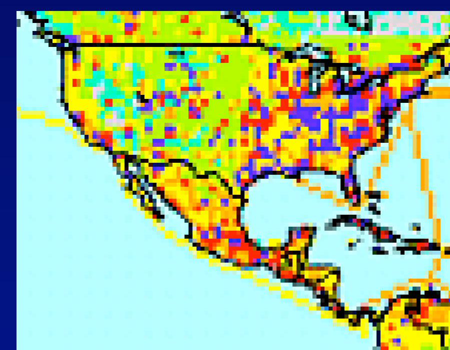
Δx = 4.5 km

NEI99 inventory



Δx = 4 km

EDGAR inventory



Δx = 1 degree

Implications for MILAGRO 2006

Inside the Valley:

- Much is known about transport and mixing within the valley, but it is not always forecasted well because of the complexity of the flows
- Are the uncertainties in the local conditions in the valley important for regional and long-range transport?

Outside the Valley:

- Preliminary modeling studies have been performed to simulate downwind transport from Mexico City, but
- Performance of models in simulating regional and long-range transport cannot be verified because of a lack of direct evidence

Implications for MILAGRO 2006 (2)

Operational:

- Expect differences between model predictions and embrace uncertainty
- Models will be useful in predicting downwind plume location, but beware of forecasts with high degrees of confidence
- Need to rely on near real-time field measurements

Research:

- Scientific objectives of previous modeling studies different than the objectives of MAX-Mex and MIRAGE-Mex
- It will take several years before 2006 observations can be fully exploited by modeling studies

Implications for MILAGRO 2006 (3)

Testing Conceptual Models

Then:

- Model predictions employed to develop a conceptual model of diurnal evolution of pollutants in the valley
- Same-day recirculation of pollutants possible
- Little multi-day accumulation of pollutants

Now:

- 2006 campaigns will provide data to test these hypotheses