Improving Mass Conservation in CAMx and CMAQ

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CCOS Technical Committee Meeting
September 14, 2006

Background

- CAMx and CMAQ take meteorological inputs from a mesoscale model (MM5).
- Since the grids, the time-steps, and the finite-difference forms are not the same, we face an "inconsistency" problem.
- If no action is taken air quality models may crash.
- CAMx adjusts the vertical wind.
- CMAQ adjusts the density and the concentration fields. This approach leads to mass conservation errors.
  - Version 4.5 provides an option to adjust the vertical wind.

Definitions to Remember

- **Mass Conservation** is defined as "no change in mass" except through boundary fluxes or source and sink processes that can be accounted for.
- **Mass distribution** refers to the three-dimensional allocation of the pollutant mass in the modeling domain.

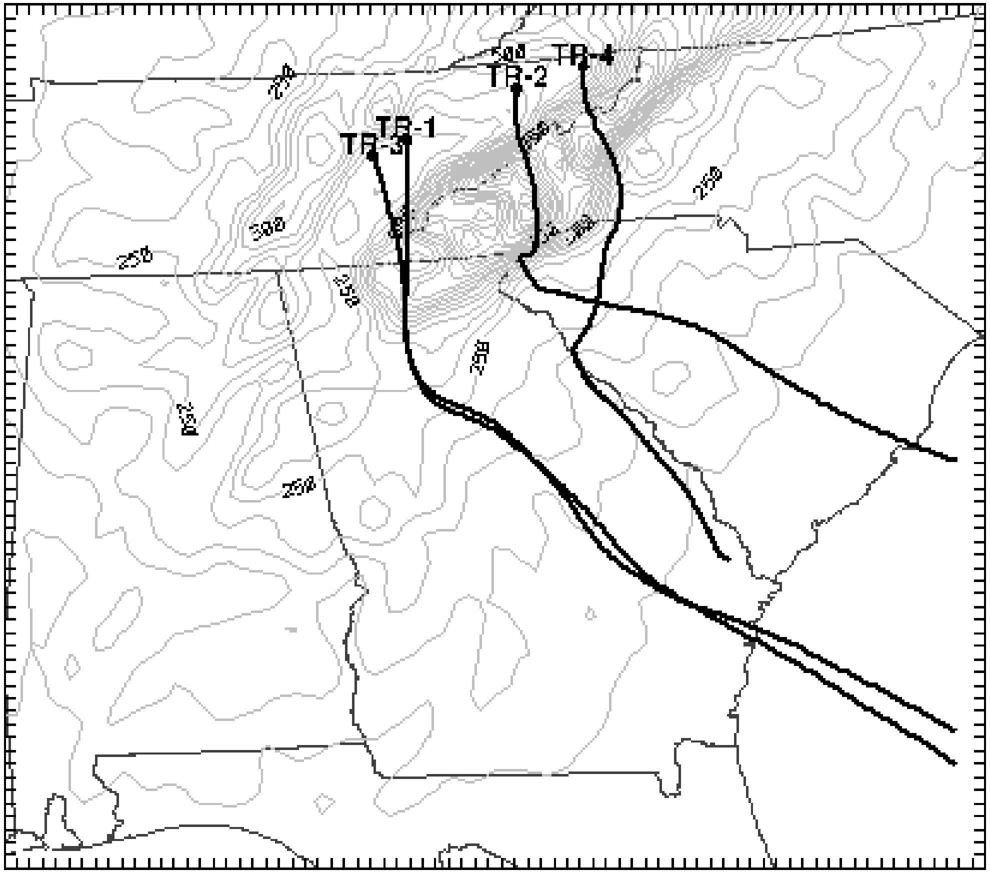
Mass Conservation in CMAQ

Hu, Y., M. T. Odman, and A. G. Russell, "Mass conservation in the Community Multiscale Air Quality model," *Atmospheric Environment*, vol. **40**, no. 7, pp. 1199–1204, March 2006.

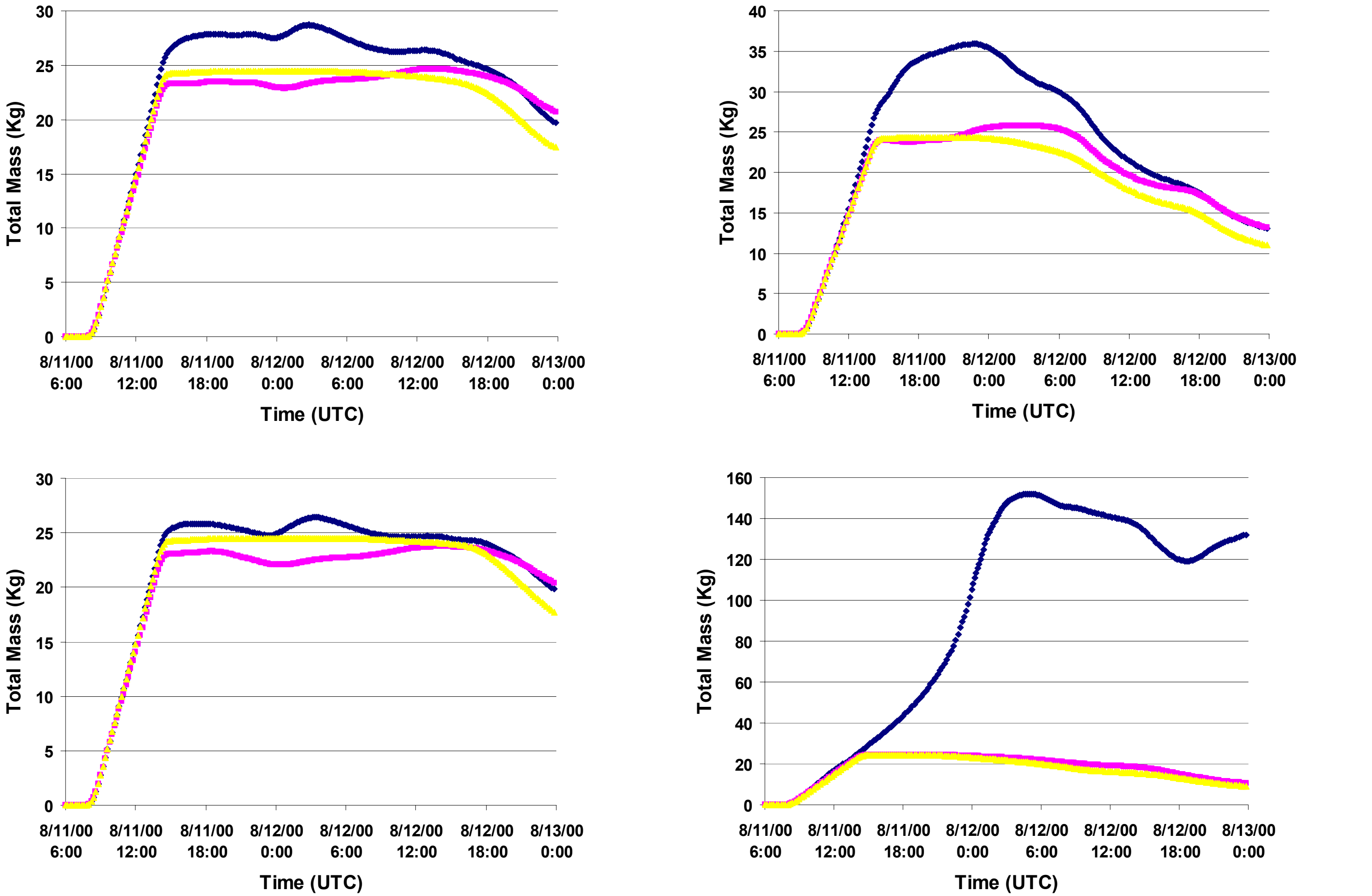
Overview of the Paper

- We made CMAQ mass-conservative by incorporating the vertical velocity adjustment of Odman and Russell (2000).
  - This method (Method 1) requires first-order vertical advection.
  - Another method (Method 2) provided by Odman and Russell allows higher-order advection schemes such as Bott and PPM.
- An imaginary tracer experiment was simulated over southeastern United States.
  - The grid resolution was 12-km.
  - Inert tracers were released from 4 different locations in the Tennessee Valley.

Imaginary Tracer Test



Mass Conservation Error in CMAQ



Trajectory Analysis

Trajectory	Age (hr)	Trajectory Position						Distance Apart (m)
		Unadjusted winds			**Adjusted winds**			
		Col	Row	Lay	Col	Row	Lay	
Tracer-1	12	33	35	6	33	35	6	202
	24	46	23	9	46	23	9	4,739
Tracer-2	12	39	46	8	39	46	8	474
	24	48	42	9	47	43	9	13,724
Tracer-3	12	33	35	7	33	35	7	1,871
	24	49	22	9	48	22	9	7,786
Tracer-4	12	46	48	4	46	48	4	2,604
	24	45	36	9	44	36	9	3,350

Phase-1 Report

Phase-1 Tasks

1. Document sources of mass conservation problems in CAMx and CMAQ air quality models
2. Characterize errors associated with existing CCOS modeling results arising from mass conservation problems
3. Identify improved means for dealing with mass conservation issues in CAMx and CMAQ
4. Document findings of Phase 1, develop a work plan for Phase 2, and meet with the Technical Committee

Task 1-1: Documentation

- We provided a technical memorandum on March 31, 2006.
  - There are no obvious mass conservation problems in CAMx.
  - However, given the complex terrain of the CCOS domain, there may be mass distribution issues.
  - The new vertical advection option in CMAQ Version 4.5 seems to have taken care of the mass conservation problem.
  - However, a new inconsistency is discovered between the meteorological preprocessor and the model itself.

Task 1-2: Characterization

- Benchmarking
- Tracer tests
- Tests with chemistry and deposition
- Trajectory analysis
- Terrain analysis
- Parallelization of the CAMx code
  - This was not in our scope of work

Benchmarking

- We simulated the July 29-August 2, 2000 episode in the CCOS domain (4-km) using the inputs provided by ARB.
- Ozone results differed from the outputs provided by ARB
  - On average, 1.5 ppb over the domain
  - Point-wise as much as 83 ppb
- Differences are most likely due to using CAMx Version 4.21 instead of 4.03
- "*Overall ozone model performance statistics did not change appreciably*." **Bruce Jackson**
- CAMx Version 4.21 will be used for the rest of the project.

Tracer Tests: Site Selection

- 10 imaginary release sites were selected based on the likelihood of potential mass conservation errors.

1. CHEVRON PRODUCTS CO.	6. IMC CHEMICALS, INC.
2. MIRANT DELTA, LLC	7. CAL. PORTLAND CEMENT CO.
3. KAISER CEMENT CORP.	8. GUARDIAN INDUSTRIES CORP.
4. LIBBEY OWENS FORD	9. AERA ENERGY, LLC
5. EXXON CORPORATION	10. DUKE ENERGY MOSS LANDING

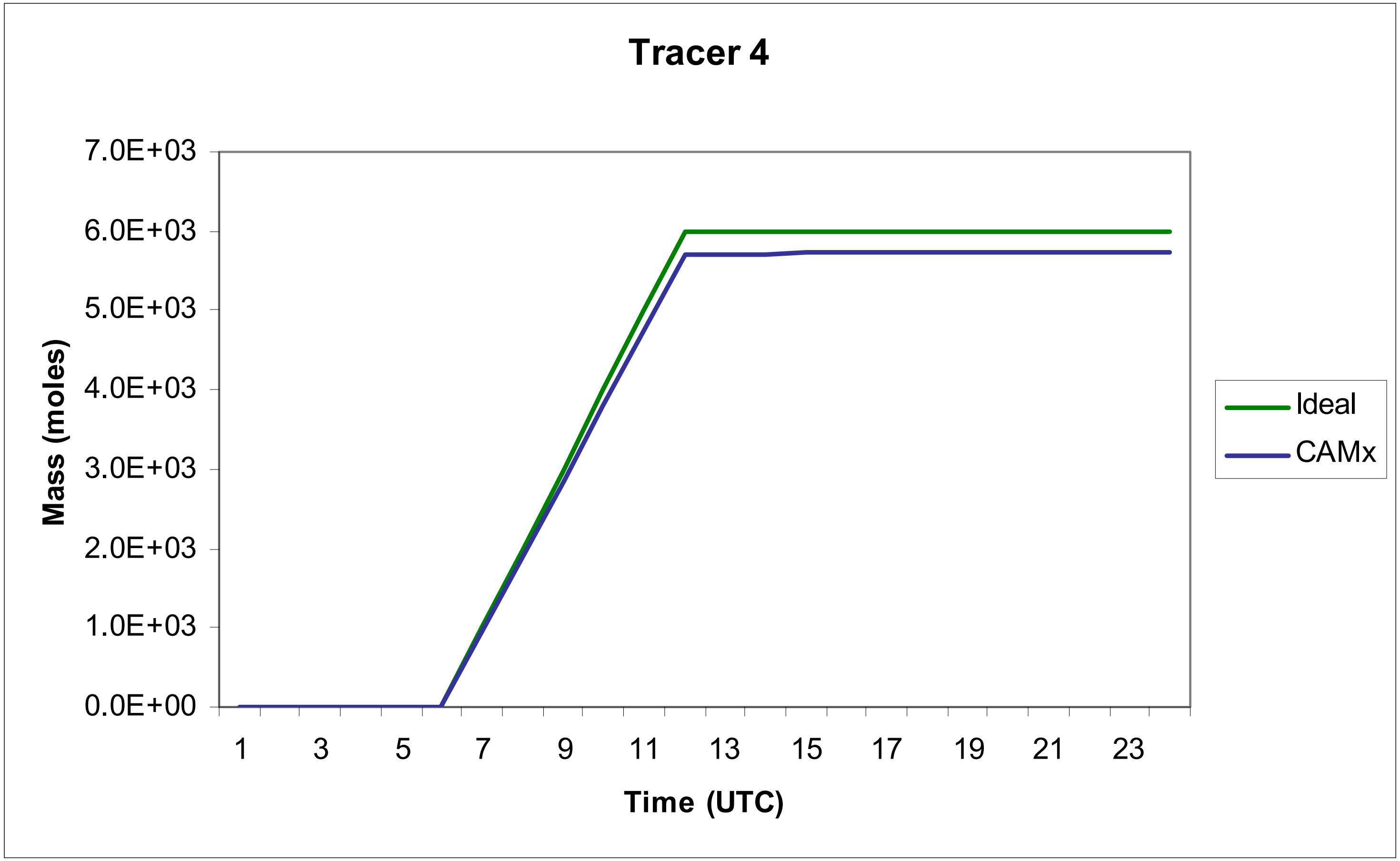
- The factors affecting our selection were:
  - Major NO_x source
  - Plume likely to travel over complex terrain, experience wind divergence and remain in the domain for some time


TRA05
TRA01
TRA02
TRA04
TRA03
TRA10
TRA08
TRA06
TRA09
TRA07

Nighttime Releases

- All releases start at 6 UTC
- Every day a different inert tracer is released from each site at effective stack height
  - Total of 50 tracers (10 stacks times 5 days)
- At the rate of 1000 moles/hour for six hours.
  - at 12 UTC, the total amount of tracer is 6000 moles
- Reactive tracer (RTRAC) feature of CAMx is used to track the tracers
- We modified the CAMx code to output the mass and mass-flux information for the tracers.
  - This is only done for reactive species in Version 4.21

Tracer from Libbey Owens Ford on July 31



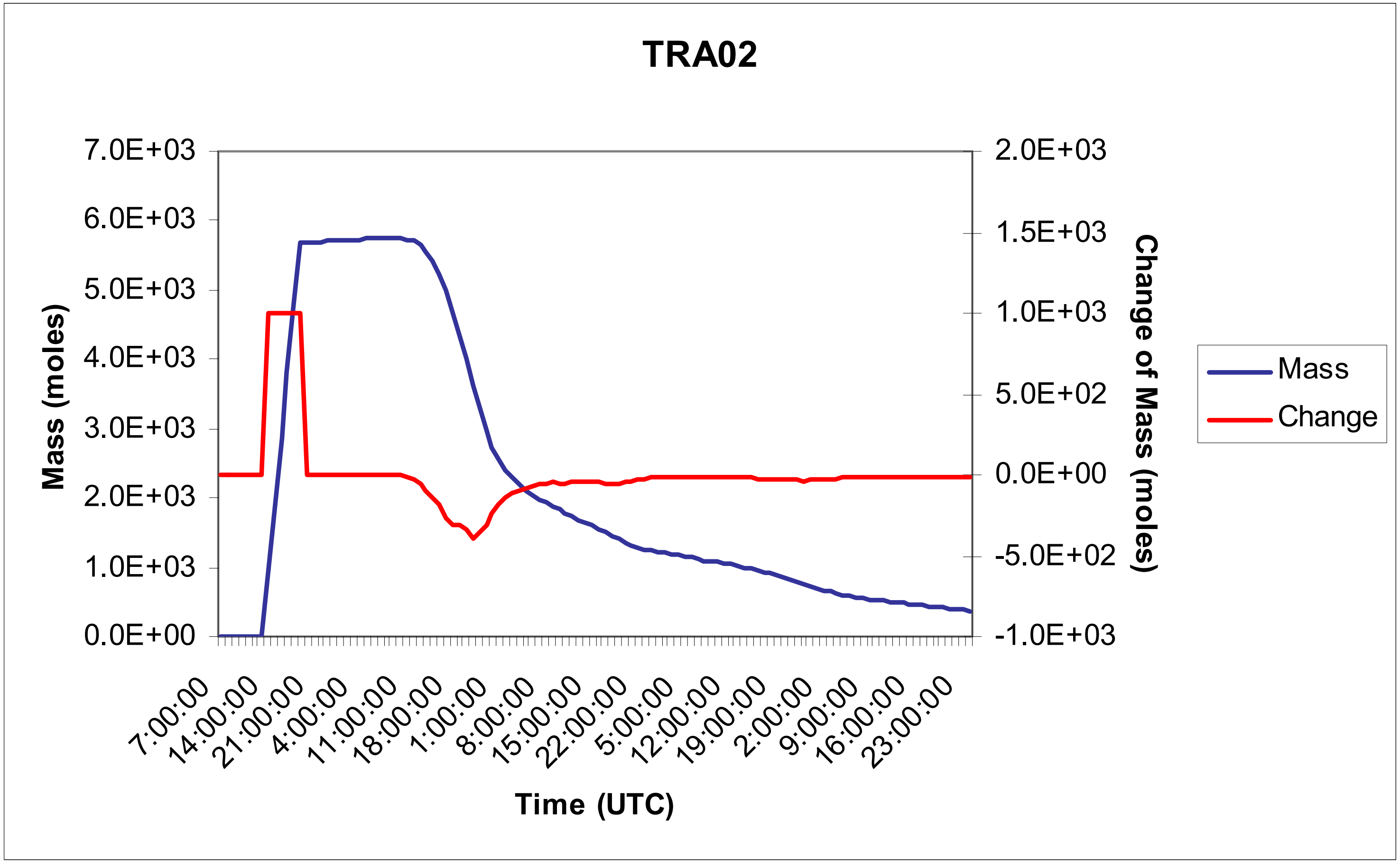
Mass Accounting Error in CAMx

- Due to an error in the computation of grid cell volumes 5% of the tracer mass appeared to be lost.
- Note that this error did not affect tracer concentrations; it only affected the mass accounting.
- We corrected this error by dividing the grid cell volume by the square of the map scale in SUBROUTINE MASSUM.

Daytime Releases

- Same setup as nighttime releases, except the releases start at 13 UTC instead of 6 UTC
- The mass increase reached about 1% for the tracer released from Mirant Delta, LCC plant on July 29, 2000 (next slide)
  - This has to be a mass conservation error.
- Unaccounted mass changes ranged between 3.5% gain and 5.5% loss.
  - Note that we normalized the error by the final mass while CAMx uses the largest mass change.
- Ground-level (area) releases were also simulated from the same sites but the errors were smaller.

Tracer from Mirant Delta, LLC (July 29-August 2)



Tests with Chemistry and Deposition

- We defined a sub-domain consisting of 3×3×20 grid cells around the Mirant Delta, LLC plant.
- Using the Integrated Process Rate (IPR) feature of CAMx we tracked the hourly average concentrations in the sub-domain as well as the rates of the following processes:
  - point and area source emissions
  - lateral advection and diffusion (through the N-E-S-W sides)
  - vertical advection and diffusion through the top
  - dry and wet deposition
  - chemistry


IPR-BOX

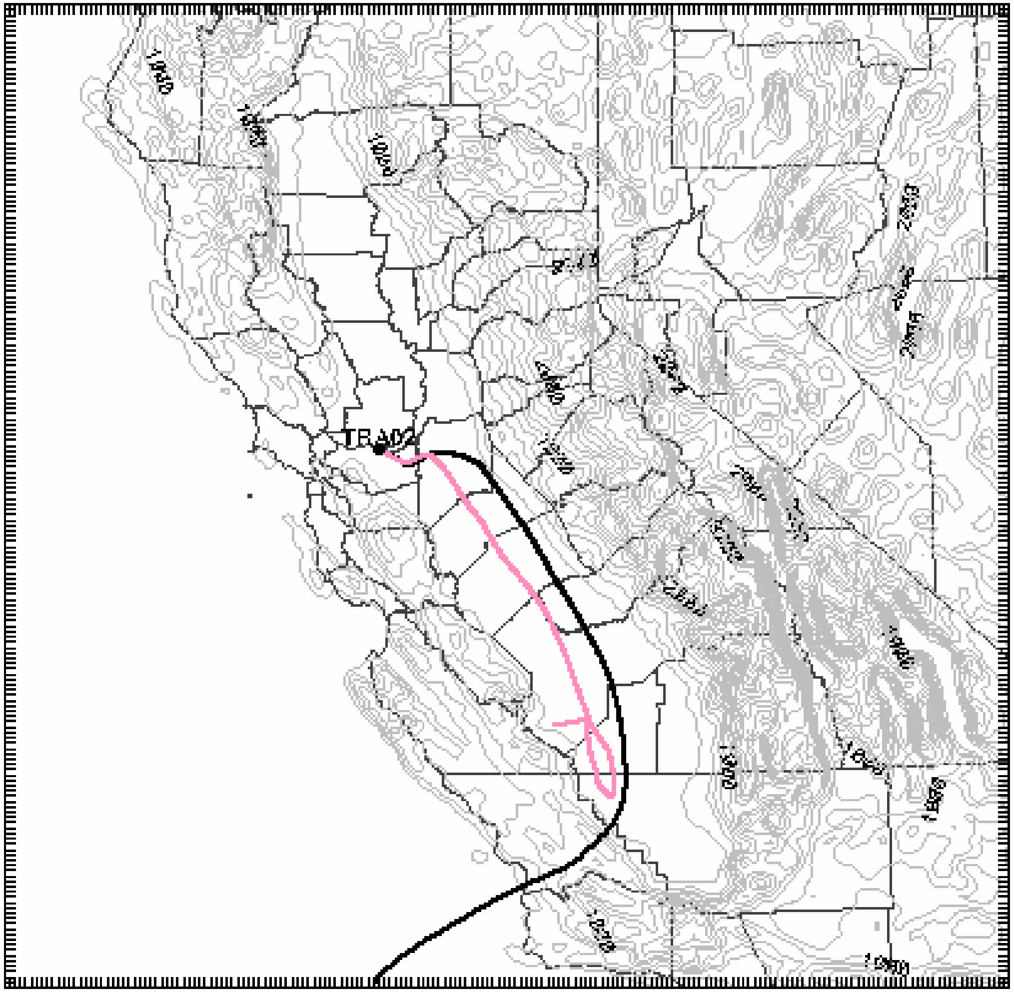
Unaccounted Mass of Nitrogen Species

Species	Absolute Error (moles)	Relative Error (%)
HNO3	-155.1	-0.70%
HNO4	-0.00102	-2.50%
HONO	-5.292	-1.18%
MPAN	-1.9842	-0.74%
NO	46.74	1.23%
NO2	-111.82	-0.29%
NPHE	0.6887	37.23%
PAN	-76.064	-0.85%
PAN2	33.968	0.95%
PBZN	0.045066	0.62%
RNO3	-9.732	-0.88%
XN	4.1921	0.54%

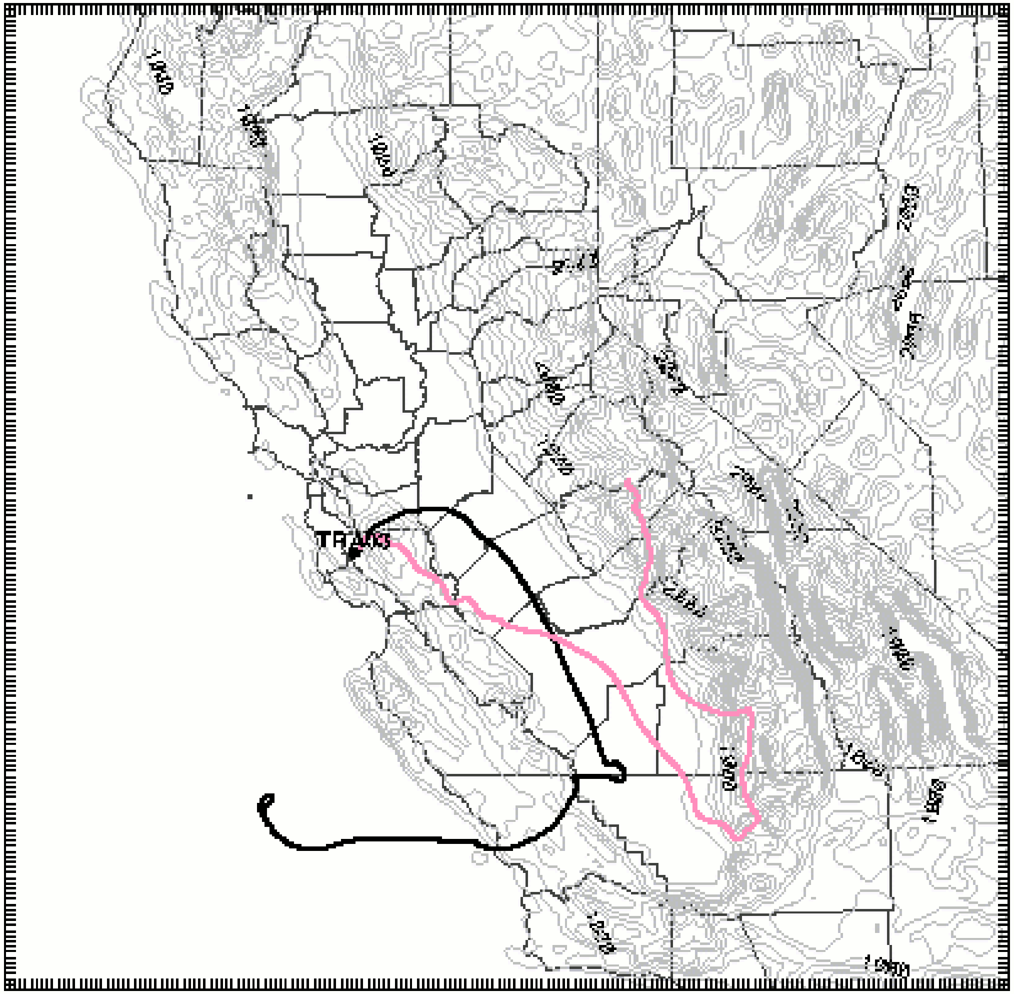
Trajectory Analysis

- We calculated forward trajectories using 2 sets of winds:
  1. MM5 hourly outputs of U, V, and W interpolated temporally to the advection time-steps used in CAMx
  2. Same U and V as the first set, but W as re-diagnosed by CAMx
- Each trajectory starts at 13 UTC on July 30 from the effective stack height.
- In the following slides, the trajectory in **black** is obtained by using the MM5 winds and the one in **red** is calculated by using the vertical wind as adjusted by CAMx.

Trajectories for Mirant Delta, LLC



Trajectories for Kaiser Cement Corp.

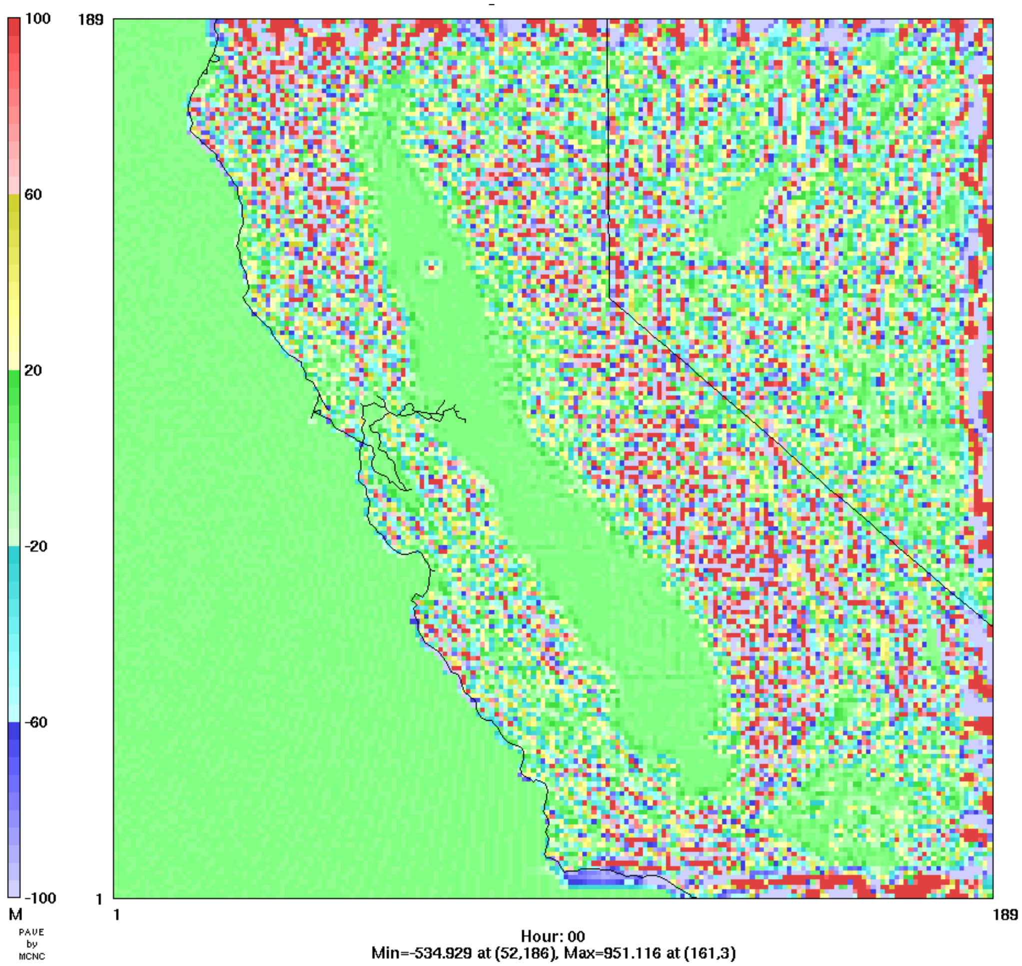


Terrain Analysis

- The "modeled terrain" in *MM5* **MMOUT** file was compared to the "true mean terrain" computed directly on the 4-km grid from USGS 30-second DEM data.
  - Elevation error due to MM5 smoothing ranges from -535 to 950 m
  - Standard deviation of the DEM terrain elevation values on each 4-km grid cell range from 0 to 550 m
  - Using the *Simple-Z* sub-grid scale terrain parameterization, DEM terrain penetrates up to Layer 22 (~1000 m) of MM5. The penetration is significant through layer 10 (~300 m).

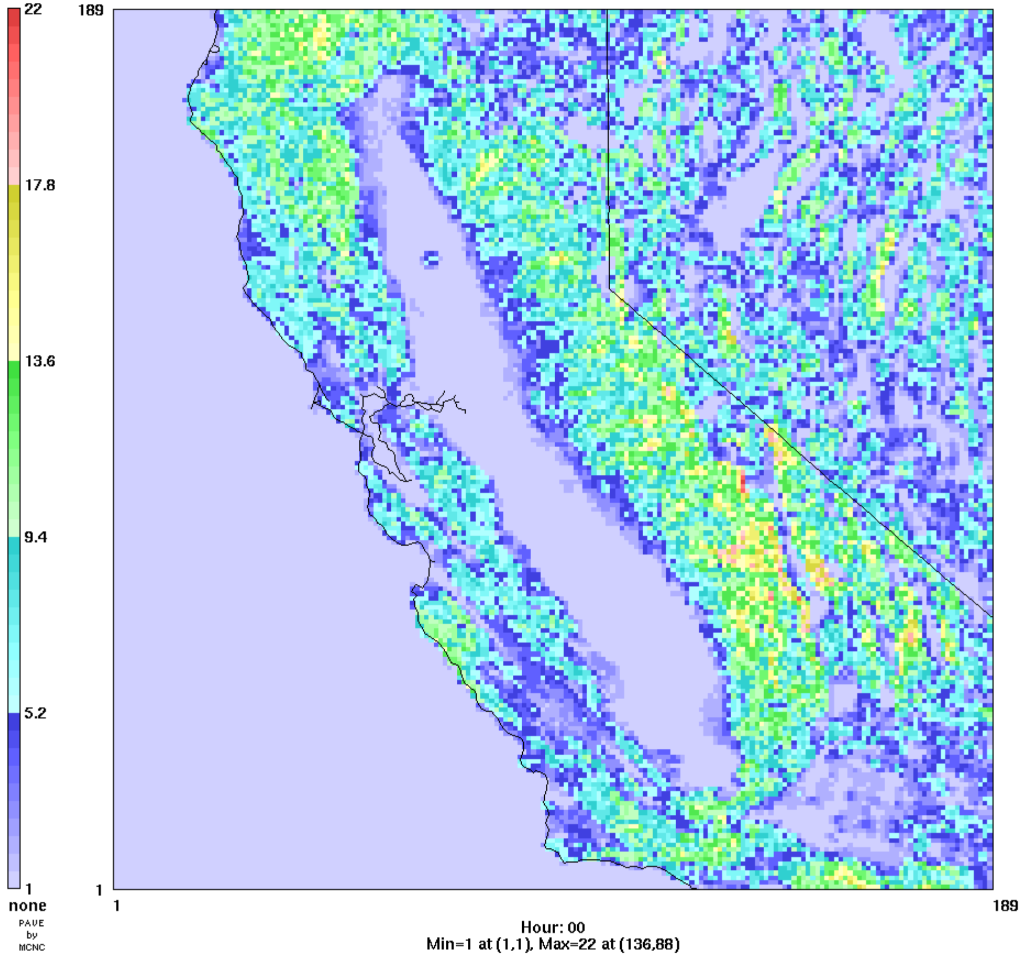
MM5 Terrain Height Error

(Scale here is from -100 to 100 m; Actual range is from -535 to 950 m)



Terrain Penetration in MM5 layers

(Layer 22 corresponds to about 1000 m)



Parallelization of the CAMx code

- The simulations we conducted with CAMx took longer than we planned for.
- When we executed the code in parallel, we did not get the expected speedup in turnaround.
- About two thirds (2/3) of the time, one processor was doing all the work while others were sitting idle.
- Upon review of the code we discovered that more than 20% of it consists of serial computations.
  - For example, the diffusion code was not parallelized.
- Dr. Carlie Coats parallelized the "low hanging fruit" reducing the serial code to about 1.5%, and improving the turnaround on an 8-processor machine by a factor of 2.7

Task 1-3: Recommendations

- CAMx is not “strictly” mass conservative. Up to 1% increases were observed in the masses of inert tracers released from the stacks of some major NOx emitters in the CCOS domain. CAMx re-diagnoses the vertical wind component in order to satisfy the continuity equation. A similar technique by Odman and Russell (2000) led to strict mass conservation in two other models (MAQSIP & CMAQ) and could be tried in CAMx.
- After correcting a mass accounting error, the unaccounted mass still ranges from -5.5% to +3.5% in inert tracer tests. In tests with chemistry and deposition, the unaccounted mass remained of the same order except for a few species whose masses became too small. Mass accounting errors are not necessarily mass conservation errors. Nevertheless, mass accounting in CAMx could be tightened.

Task 1-3: Recommendations (Continued)

- In our daily air quality forecasting for Atlanta, CMAQ Version 4.5 crashed on 4 occasions which are probably due to the new vertical advection module. During our initial review of the code we did not see any measures for a special case considered in Odman and Russell (2000). A special treatment of this case could avoid the crashes.
- The method used for adjusting the vertical wind both in CAMx and CMAQ necessitate the use first-order accurate advection, which leads to excessive numerical diffusion. Odman and Russell (2000) suggested an iterative wind adjustment technique that allows the use of higher-order schemes for vertical advection. This technique could be incorporated into CAMx as well as CMAQ.

Task 1-3: Recommendations (Continued)

- The deviation of the trajectories from those obtained by using MM5 winds is due to vertical wind shear. A compromise between the trajectory and mass conservation errors could be sought. For example, whenever the vertical wind shear is large, the density could be adjusted instead of the vertical wind.
- To the extent that a higher input time frequency is used for meteorological data, the magnitude of the inconsistency problem (i.e., imbalance of the continuity equation) would be reduced. Smaller adjustments to the wind (or density) fields would be needed therefore trajectory errors would also be reduced. In addition, a 15-minute input frequency could capture some gravity waves that are probably entirely missed by the current 1-hour input frequency.

Task 1-3: Recommendations (Continued)

- MM5 significantly flattens the terrain of the CCOS domain so the mean terrain height is in error. In addition, there is considerable terrain variability within each grid cell. For these reasons, CCOS modeling results are probably subject to significant mass distribution problems. Special treatments could be added to CAMx and CMAQ to account for the interactions of complex terrain with emissions and deposition processes.
  - Several terrain corrections could be implemented with the SMOKE emission model considering how CAMx calculates the plume rise. These include temperature corrections for biogenic emissions, vertical allocation of area source emissions and stack height corrections for major point sources.
  - The dry deposition module could be modified from 2-D to 3-D (i.e., layered deposition) to account for terrain effects.

Task 1-4: Documentation

- Phase-1 draft final report
- Phase-2 draft work plan
- Both summarized in this presentation
- They will be finalized based on your comments…

Phase-2 Plan

Phase-2 Tasks

1. Develop, implement, and test improved mass conservation modules and procedures for CAMx and CMAQ
2. Conduct CAMx and CMAQ simulations to assess changes to modeling results from use of the revised codes
3. Prepare study documentation and meet with the Technical Committee

Task 2-1: Implementation

- Incorporate vertical wind adjustment “Method 1” of Odman and Russell (2000) to achieve strict mass conservation
- Review the mass accounting in CAMx in search of possible errors
- Incorporate “Method 1” into CMAQ Version 4.5 to see if it takes care of the crashes
- Incorporate vertical wind adjustment “Method 2” of Odman and Russell (2000) to allow for higher-order vertical advection schemes

Task 2-1: Implementation (Continued)

- Develop a new vertical wind adjustment method that will consider vertical wind shear to reduce the deviation of the trajectories from those obtained by using MM5 winds
- Produce higher frequency (15-min) meteorological inputs by rerunning MM5
- Implement terrain corrections in the SMOKE emission model considering how CAMx employs the 2-D emissions data and generate new emissions inputs that would improve the allocation of plumes to vertical model layers
- Modify the dry deposition module of CAMx from 2-D to 3-D in order to account for terrain effects
- Continue the parallelization of the CAMx code

Task 2-2: Simulation

- Simulate the July 29-August 2, 2000 episode using the modified CAMx and CMAQ codes.
  - After each alternative methodology or improvement option
- Compare the results from these simulations with those generated using the original codes.
  - Evaluate the impacts of the modifications
- Perform a cost-benefit analysis for each option
  - Report cost of computing versus improvement in results

Task 2-3: Documentation

- Document all code modifications made to CAMx & CMAQ and the tests conducted for code verification
- Supplement the user's guides
- Submit all modified code and input/output files used in testing
- Prepare draft final report discussing the findings of Phases 1 & 2
- Prepare a draft manuscript suitable for publication in a peer reviewed journal.
- Present to the CCOS Technical Committee
- Finalize report and manuscript based on comments provided by the Committee