Improving Mass Conservation in Air Quality Models

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Outline

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  - Treatment of topography and **Mass Distribution**
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Introduction

Definition 1

- **(Mass) Consistency** is a quality of meteorological fields that satisfy the discrete continuity equation. The continuity equation is a statement of mass conservation for the air that contains the pollutants:

$$\frac{\partial \rho}{\partial t} + \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

where ρ is air density and u, v and w are the x-, y- and z-components of the wind vector.[*] For a grid with finite spacing and time steps the partial derivatives in the equation above can be expressed as differences; that form of the equation is referred to as the discrete continuity equation.

[*] For simplicity we wrote the continuity equation in Cartesian coordinates. The expression of the equation in coordinate systems used in air quality models is more complex.

Definition 2

- **Mass Conservation** in air quality models is defined as "no change in mass" (loss or gain) of a chemical element (e.g., sulfur, nitrogen, carbon) or inert species, except through boundary fluxes or source (e.g., emissions) and sink (e.g., deposition) processes that can be accounted for.
  - Since reactive species transform into other species their mass is not conserved. For example, SO_2 transforms into SO_4^{2-} (sulfate). The mass of sulfur (S) is conserved during this transformation. Hence we can speak of the mass conservation of a chemical element, in this case sulfur.
  - Changes in mass due to known and modeled processes are accountable therefore they do not violate mass conservation. For example, if a certain amount of sulfur is deposited the total mass of sulfur in the modeling domain is reduced by that amount.

Definitions 3

- **Mass distribution** is a term we will use to refer to the three-dimensional distribution of the pollutant mass in the modeling domain.
  - Mass distribution errors can be very important in the way they affect source-receptor relationships.

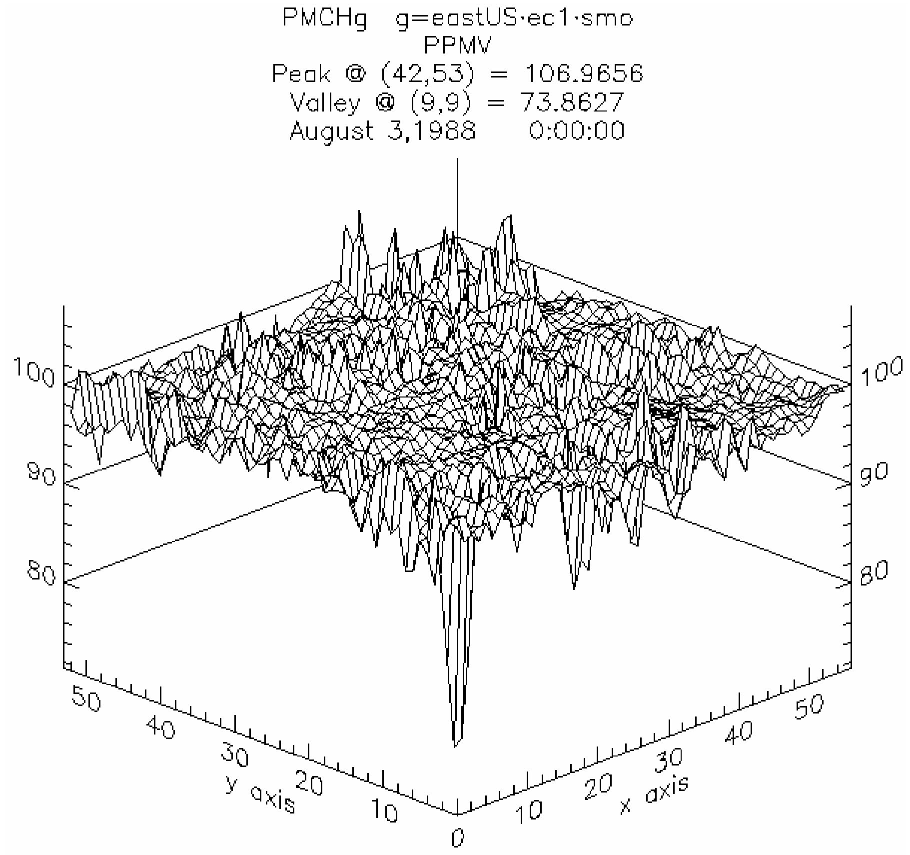
Background

Mass Conservation in SAQM

Odman, M. T. and A. G. Russell, 2000. Mass conservative coupling of non-hydrostatic meteorological models with air quality models, in Air Pollution Modeling and its Application XIII, (S.-E. Gryning and E. Batchvarova, Eds.), New York, Kluwer Academic/Plenum Publishers, pp. 651-660.

Inconsistency Problem

- AQMs cannot maintain a uniform tracer field when they use wind fields generated by non-hydrostatic MMs.
- This occurs because of the models having different
  - grid structures,
  - time steps,
  - finite-difference forms.
- Perturbations grow in time and may lead to instabilities.



Renormalization: A Flawed Approach

- Some existing AQMs try to correct the problem by
  - advecting air (or a calibration gas) along with pollutant species,
  - renormalizing species concentrations as:

$$c_i = \frac{\rho}{\rho^{adv}} c_i^{adv}$$

- This renormalization violates species mass conservation because of the non-linearity in advection schemes.
  - Non-linearities affect pollutant fields of different distribution differently. Many species, especially the emitted ones, have highly non-uniform spatial distributions. Renormalizing their concentrations based on the perturbation of a fairly uniform field can artificially increase or decrease mass.
- Lack of mass conservation is a serious error in AQMs.

Mass Conservative Method 1

- Wind or density fields, or both, must be adjusted for mass conservative coupling.
- The first method adjust the vertical velocity using the discrete continuity equation.
- Donor cell scheme is used for vertical advection

$$c_k^{n+1} = c_k^* - \frac{\Delta t}{\Delta z_k}\left(w_{k+1/2} c_k^* - w_{k-1/2} c_{k-1}^*\right)$$

- Vertical velocity can be solved directly

$$w_{k+1/2} = \frac{1}{\rho_k^*}\left(\frac{\Delta z_k}{\Delta t}\left(\rho_k^* - \rho_k^{n+1}\right) + w_{k-1/2}\rho_{k-1}^*\right)$$

Mass Conservative Method 2

- In Method 2, Bott's scheme is used for vertical advection
- This scheme is more accurate than the donor cell scheme, but it is non-linear.
- Vertical velocities must be solved iteratively.
- The secant iteration technique is used

$$w_{k+1/2}^{i+1} = w_{k+1/2}^{i} - \frac{w_{k+1/2}^{i} - w_{k+1/2}^{i-1}}{\rho_k^i - \rho_k^{i-1}} \left(\rho_k^i - \rho_k^{n+1} \right)$$

- Convergence may be slow depending on the tolerance

Mass Conservative Method 3

- The flux form of the equations are used:

$$\rho_{i,j,k}^{n+1} = \rho_{i,j,k}^{n} - \frac{\Delta t}{\Delta x}\left(F_{i+1/2}^{n} - F_{i-1/2}^{n}\right) - \frac{\Delta t}{\Delta y}\left(G_{j+1/2}^{n} - G_{j-1/2}^{n}\right) - \frac{\Delta t}{\Delta z}\left(H_{k+1/2}^{n} - H_{k-1/2}^{n}\right)$$

$$c_{i,j,k}^{n+1} = c_{i,j,k}^{n} - \frac{\Delta t}{\Delta x}\left(A_{i+1/2}^{n} - A_{i-1/2}^{n}\right) - \frac{\Delta t}{\Delta y}\left(B_{j+1/2}^{n} - B_{j-1/2}^{n}\right) - \frac{\Delta t}{\Delta z}\left(C_{k+1/2}^{n} - C_{k-1/2}^{n}\right)$$

- F,G,H are defined as donor cell fluxes; H is solved directly
- For consistency,

$$A = Fr_x;\, B = Gr_y;\, C = Hr_z$$

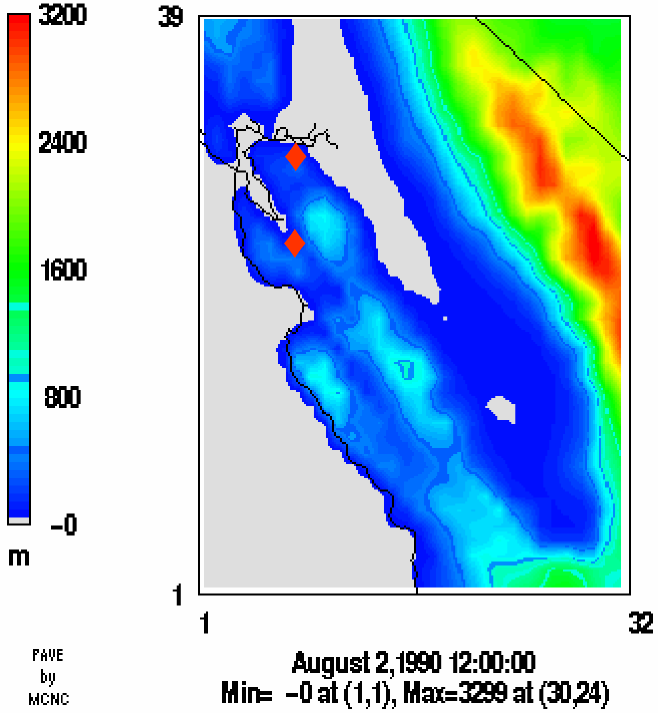
- Mixing ratios, $r=c/\rho$, are calculated using Bott's scheme

Simulations

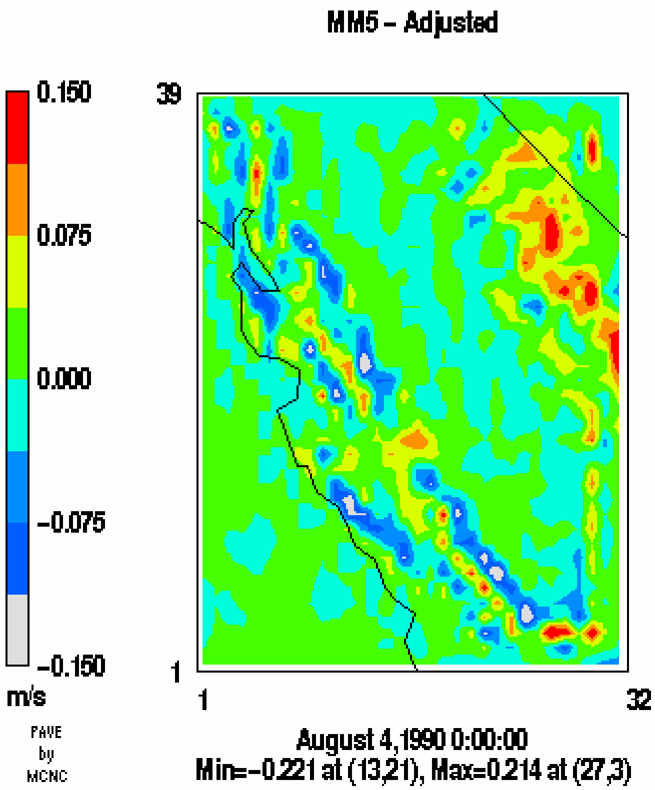
- SARMAP domain
  - 12-km grid, 32x39 grid cells
  - 15 layers, 60-m thick first layer
- An (imaginary) tracer experiment (PMCH) released from San Jose
  - Trajectory goes over complex coastal terrain
- A real tracer experiment (PMCP) released from Pittsburg
  - More flat terrain
- August 2-6, 1990 ozone episode

Tracer Experiment

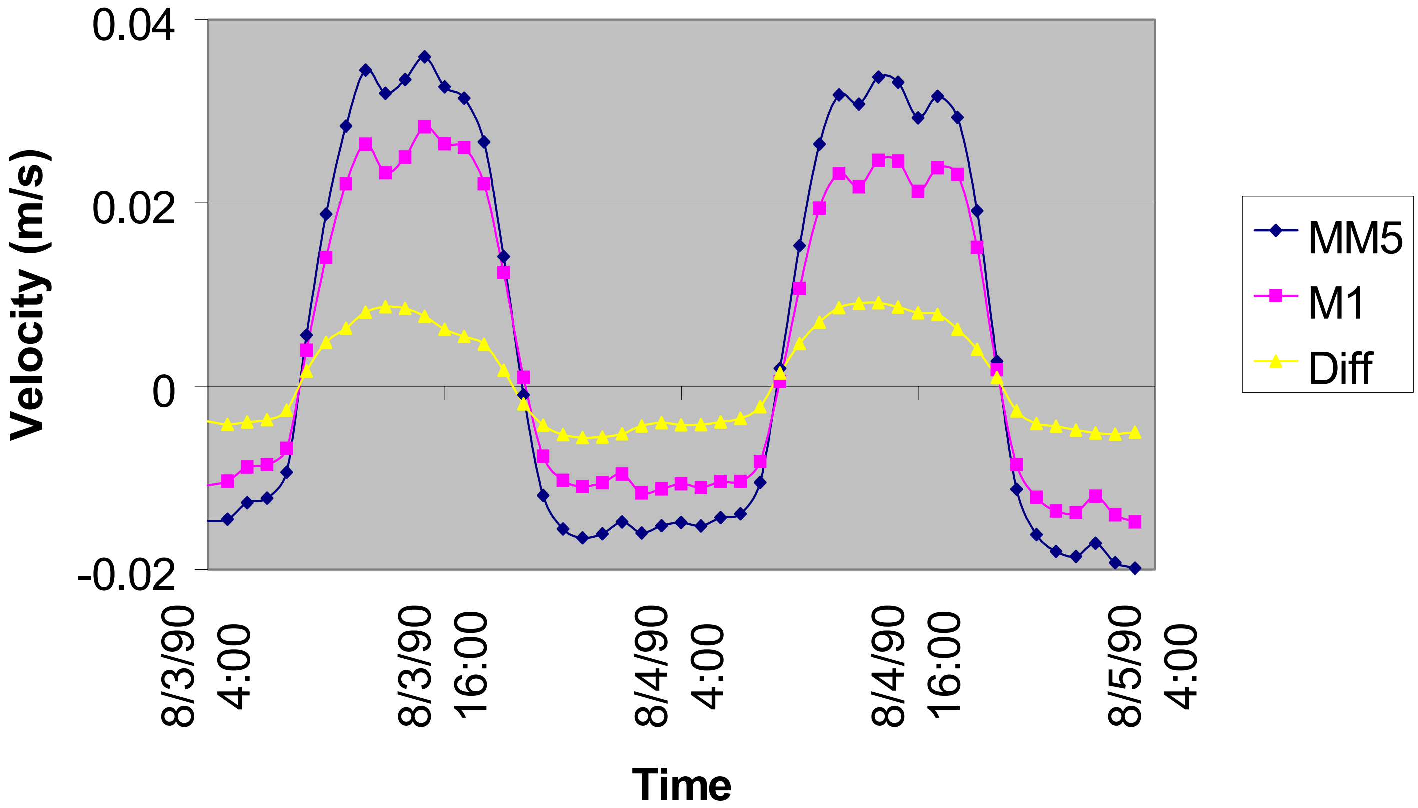
Terrain Height



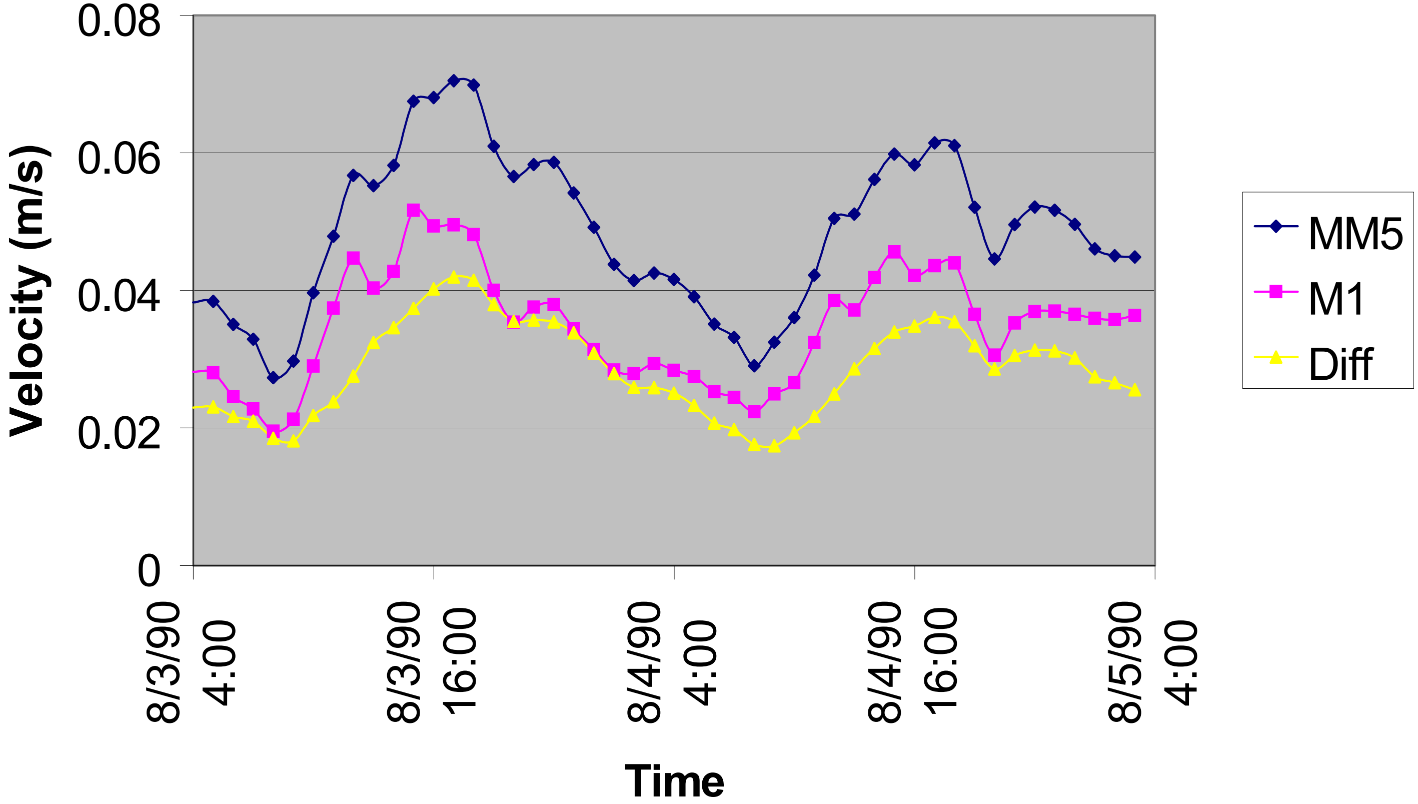
Layer 1 W-Difference



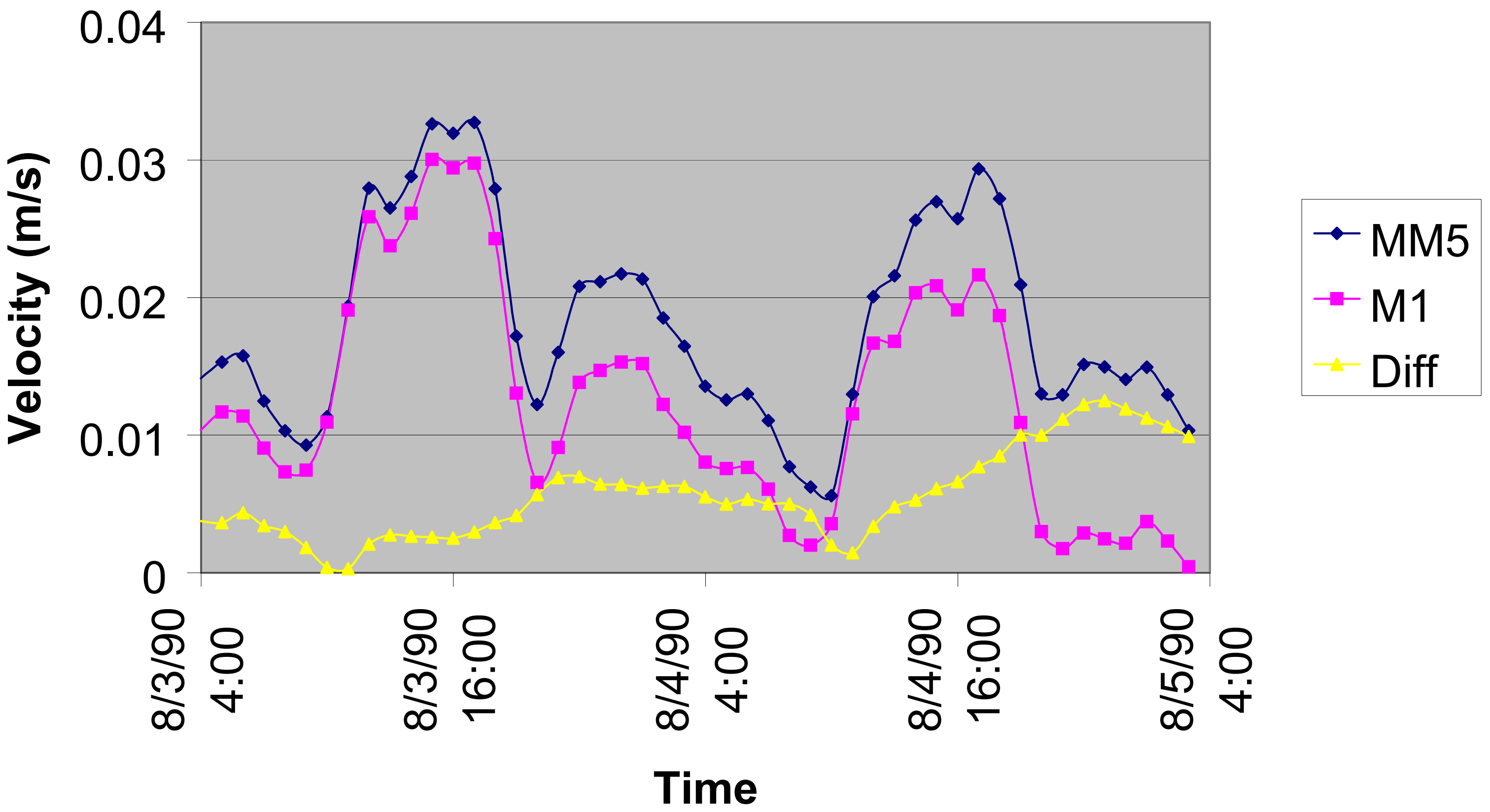
Layer 1 *w* (Mean)



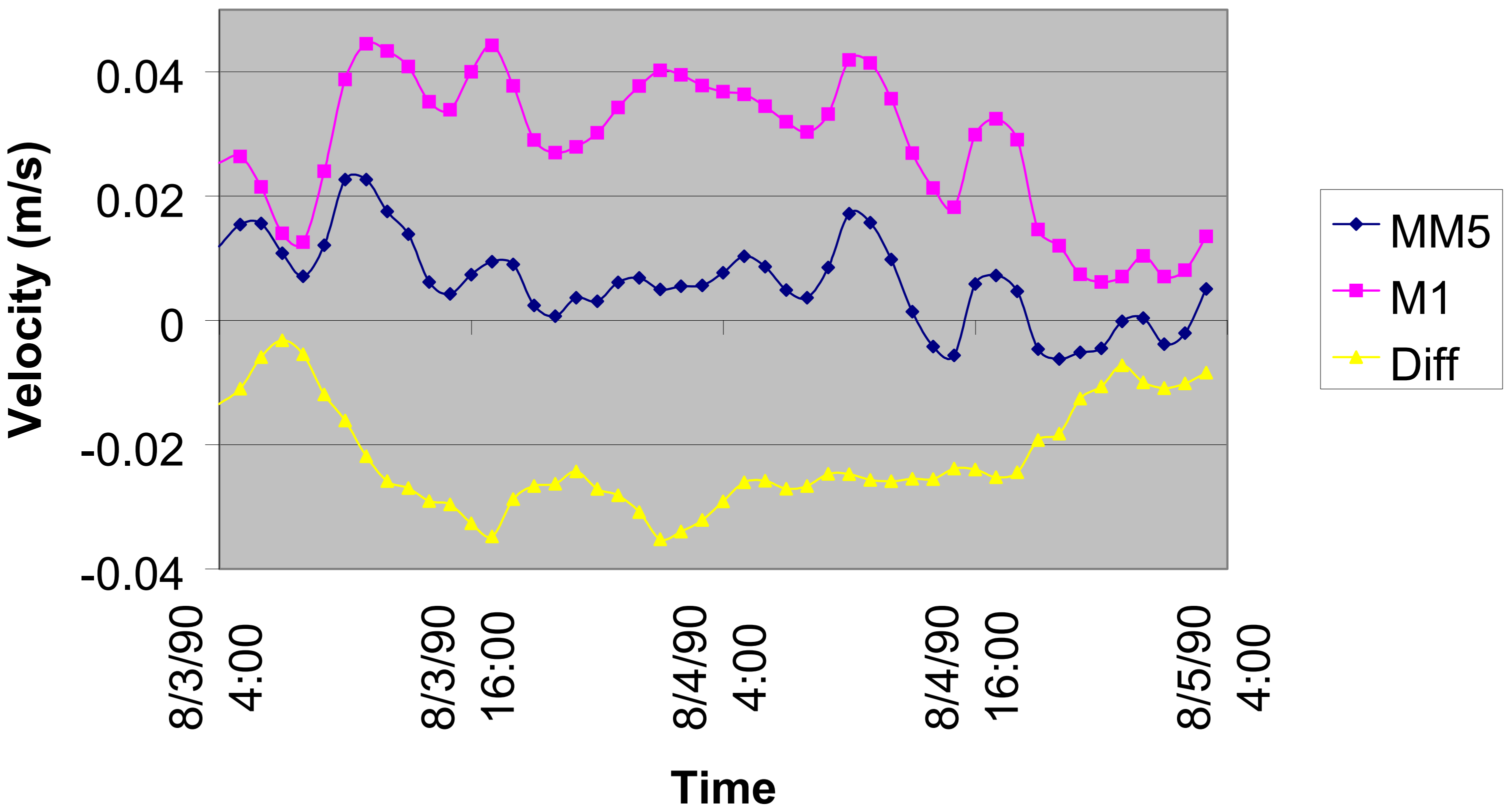
Layer 1 *w* (Standard Deviation)



Layer 5 *w* (Mean)



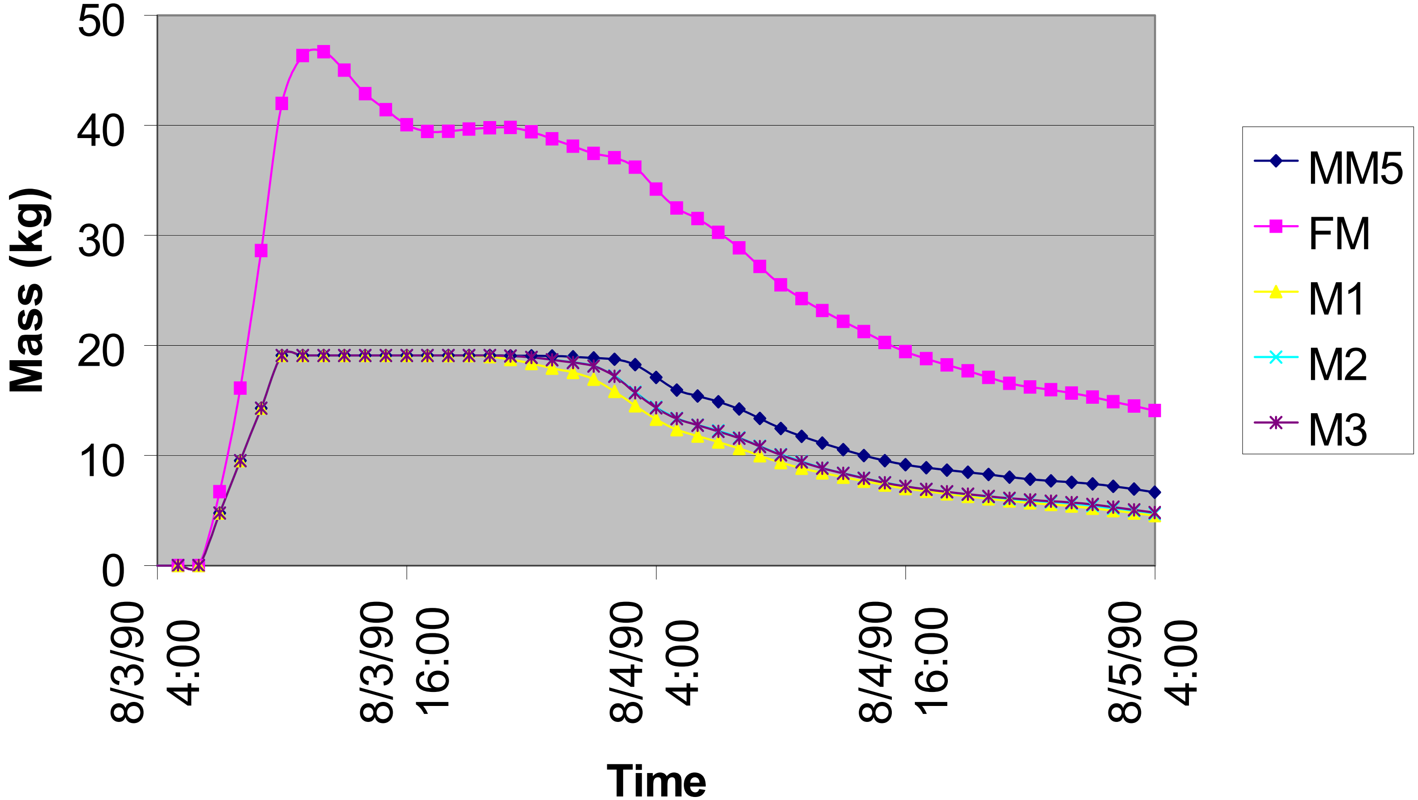
Layer 11 *w* (Mean)



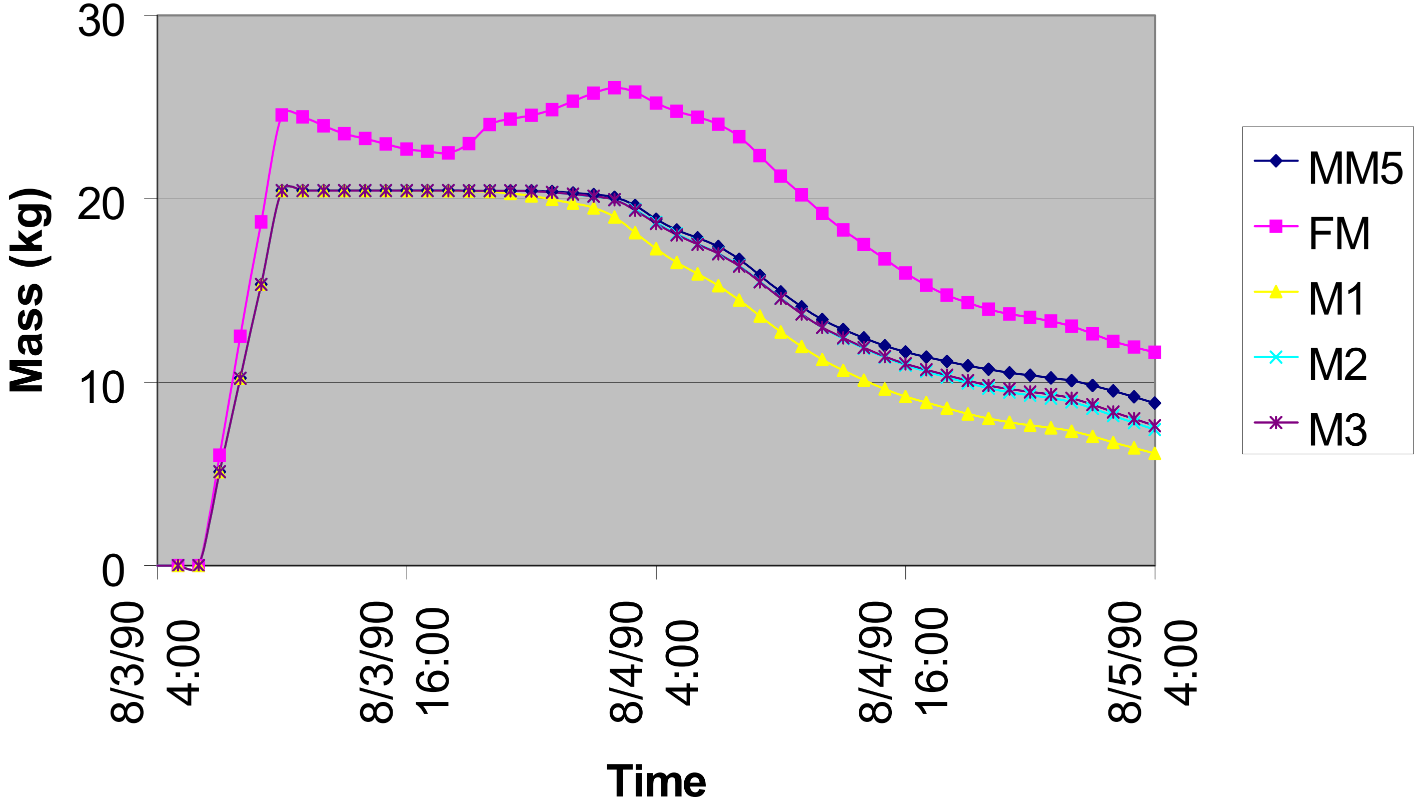
Adjustments to Vertical Velocity

- Correlate with the slope of terrain
- On an average, 25-35%
- Smallest in the morning and largest in the afternoon
- In the first layer (60 m) maximum adjustment is ~ 0.2 m/s when *w* is ~ 0.4 m/s.
- In the PBL the adjustments decrease with altitude.
- In the free troposphere the adjustments start increasing.
- The adjusted vertical velocity is nonzero at the top.

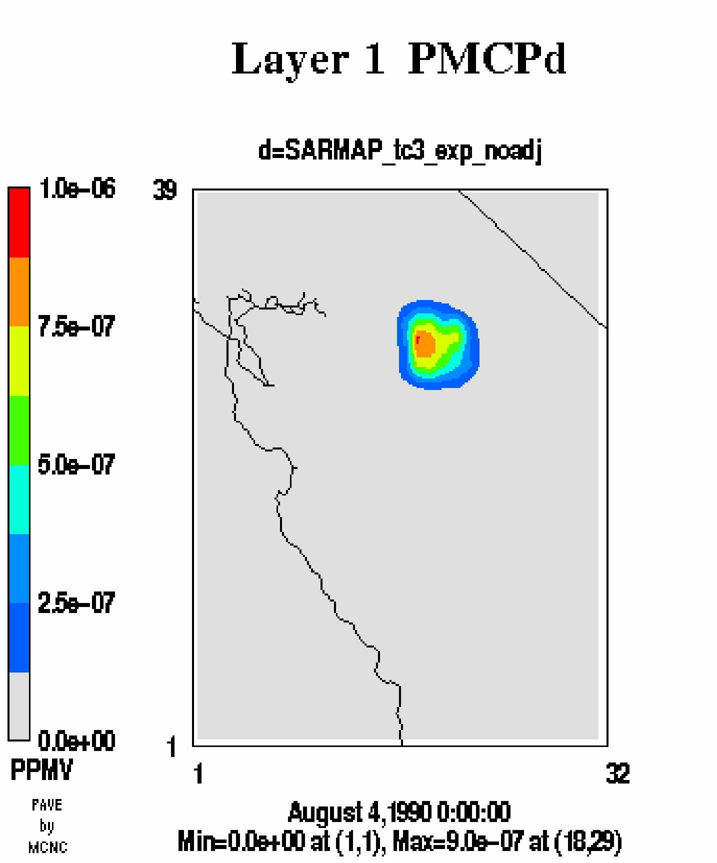
Total PMCH Mass
(Released from San Jose)

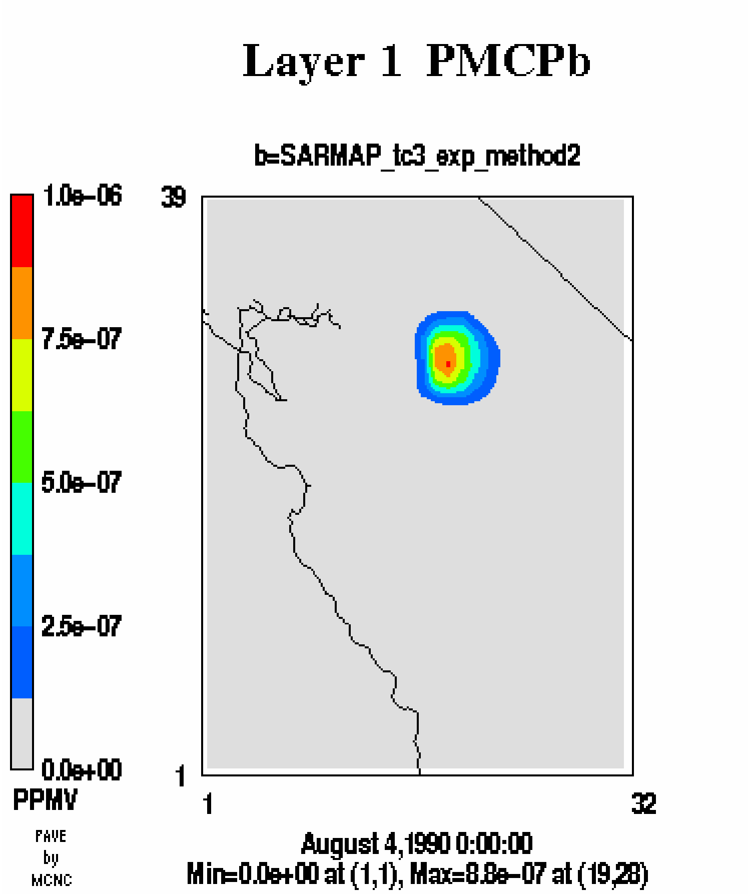


Total PMCP Mass (Released from Pittsburg)



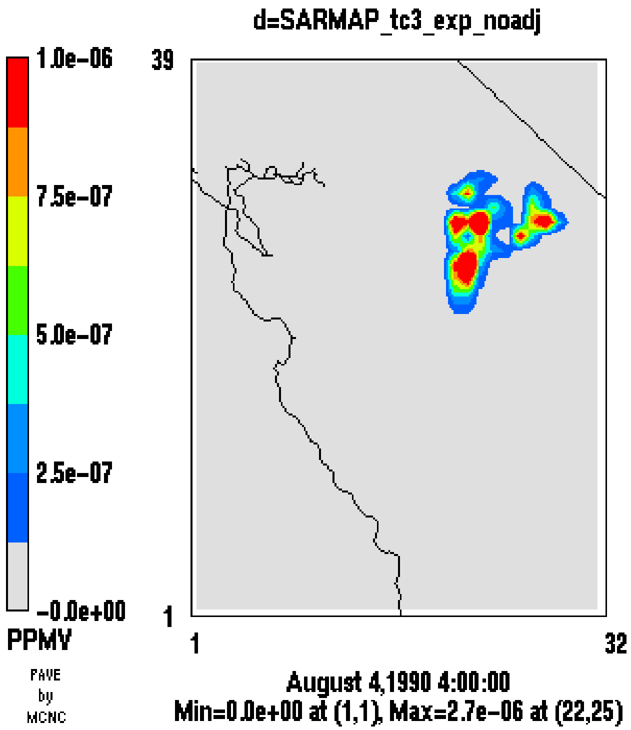
PMCP (11 hr after release)



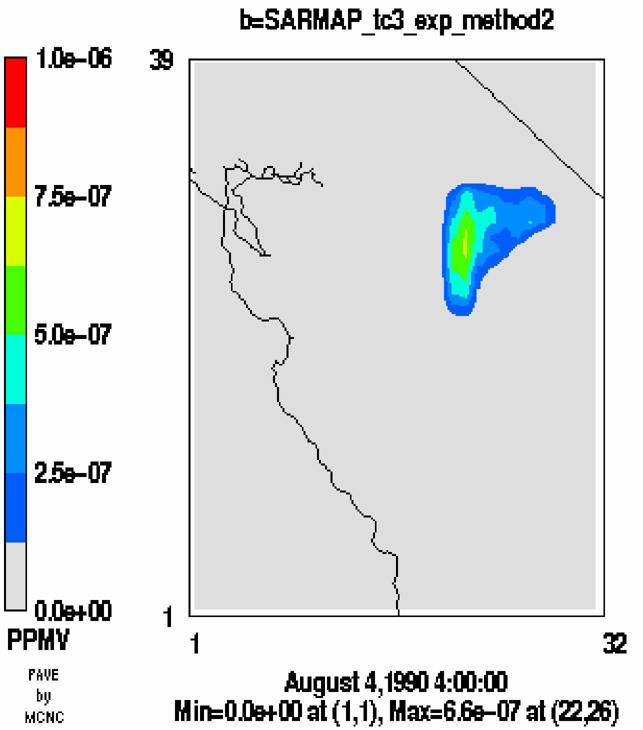


PMCP (15 hr after release)

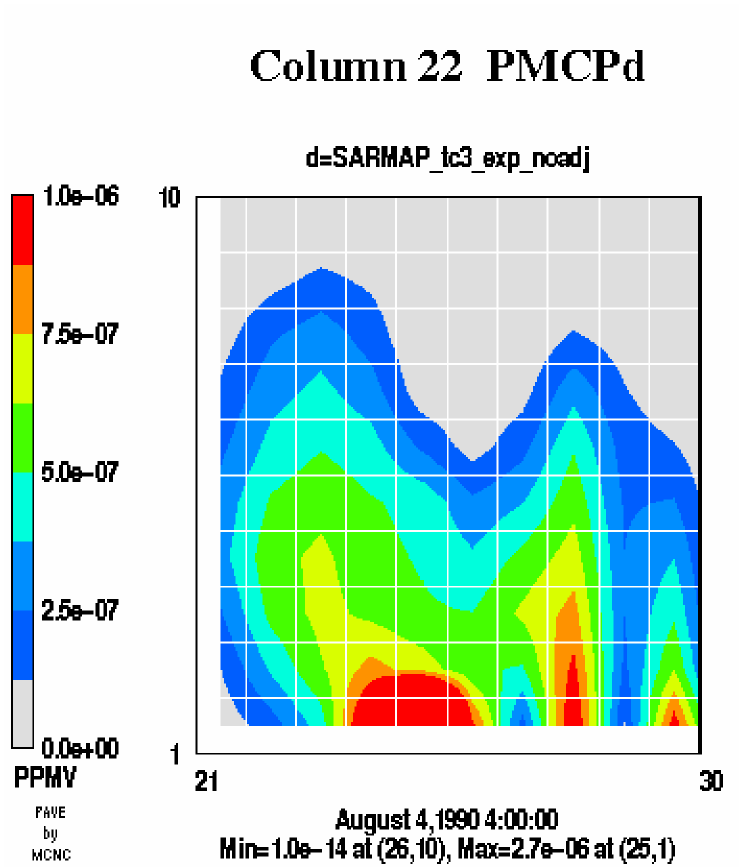
Layer 1 PMCPd

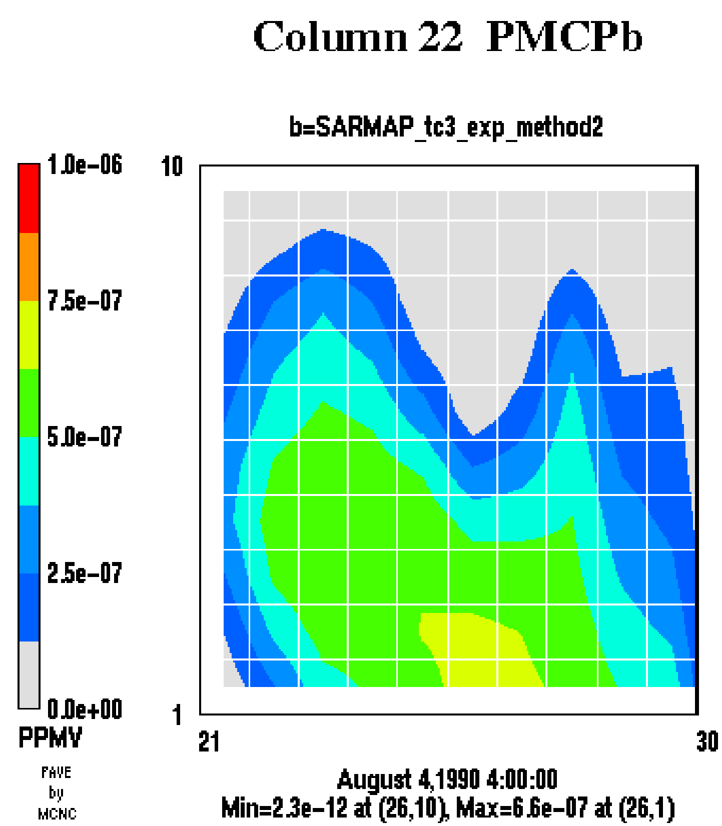


Layer 1 PMCPb



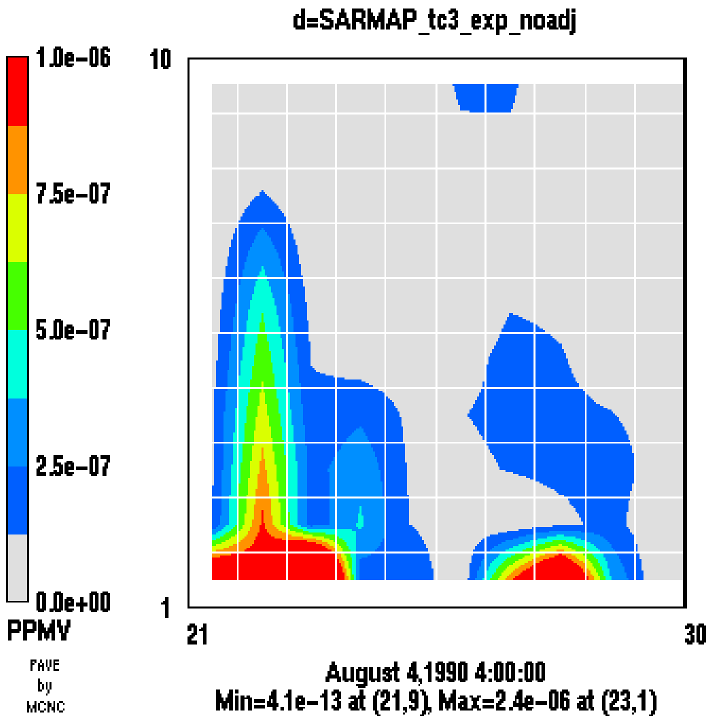
PMCP Vertical Slice (N-S)



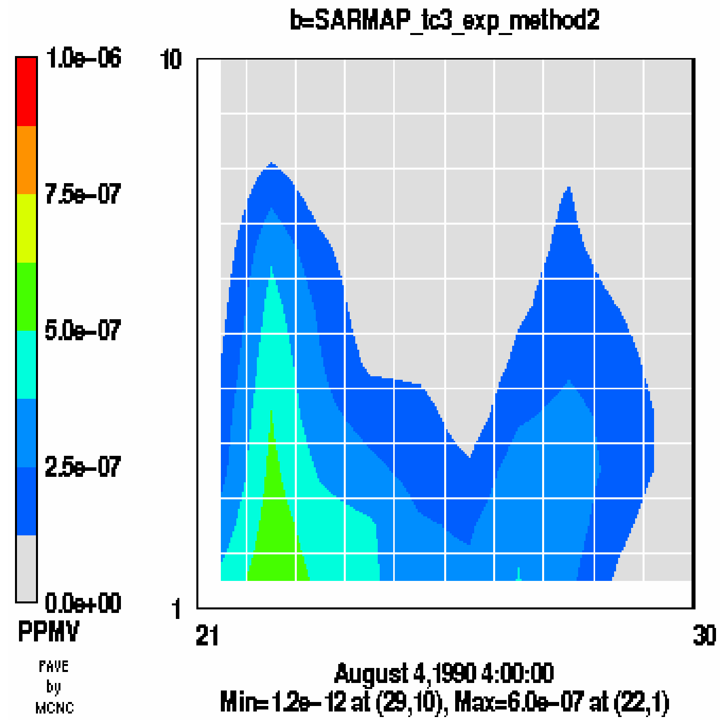


PMCP Vertical Slice (E-W)

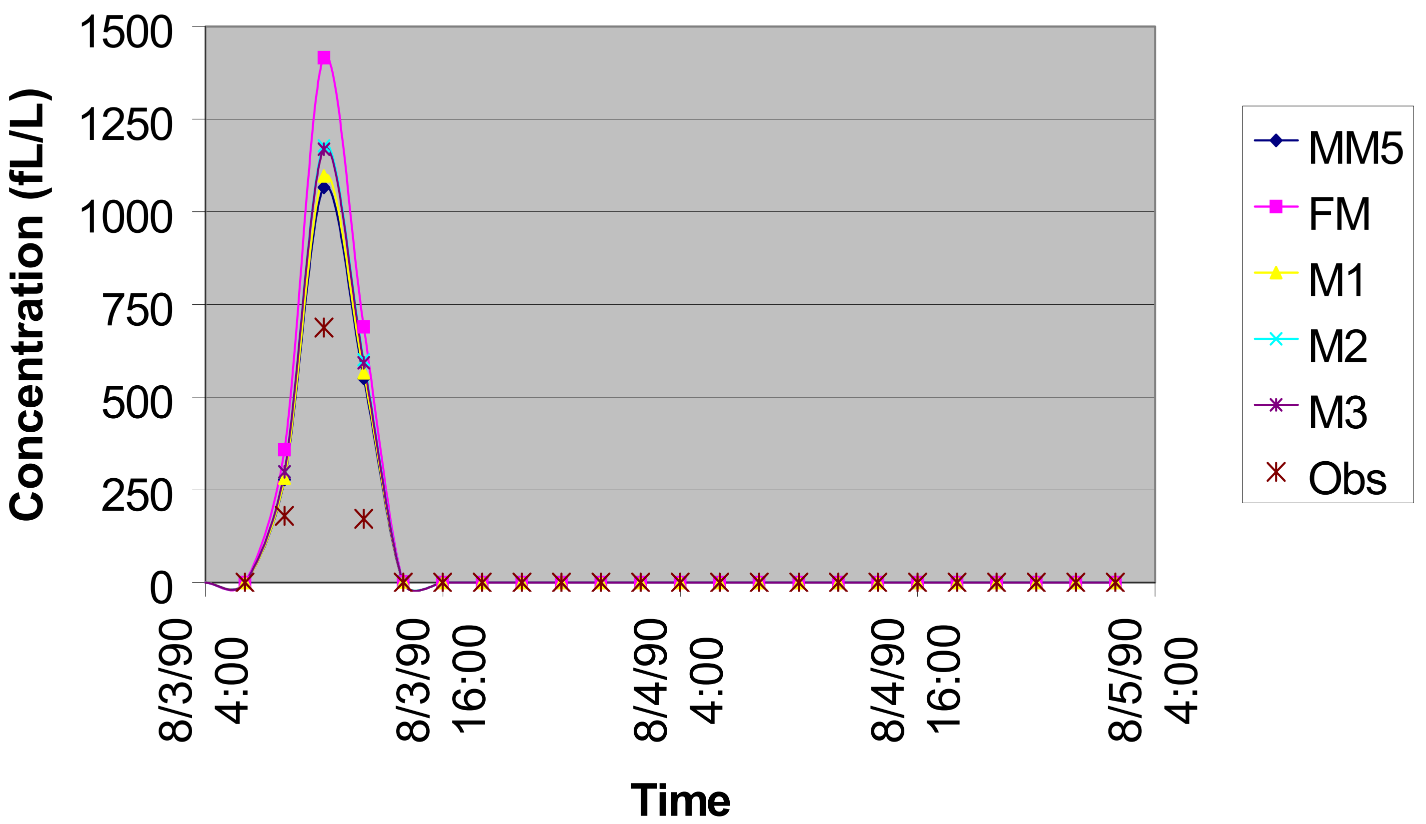
Row 28 PMCPd



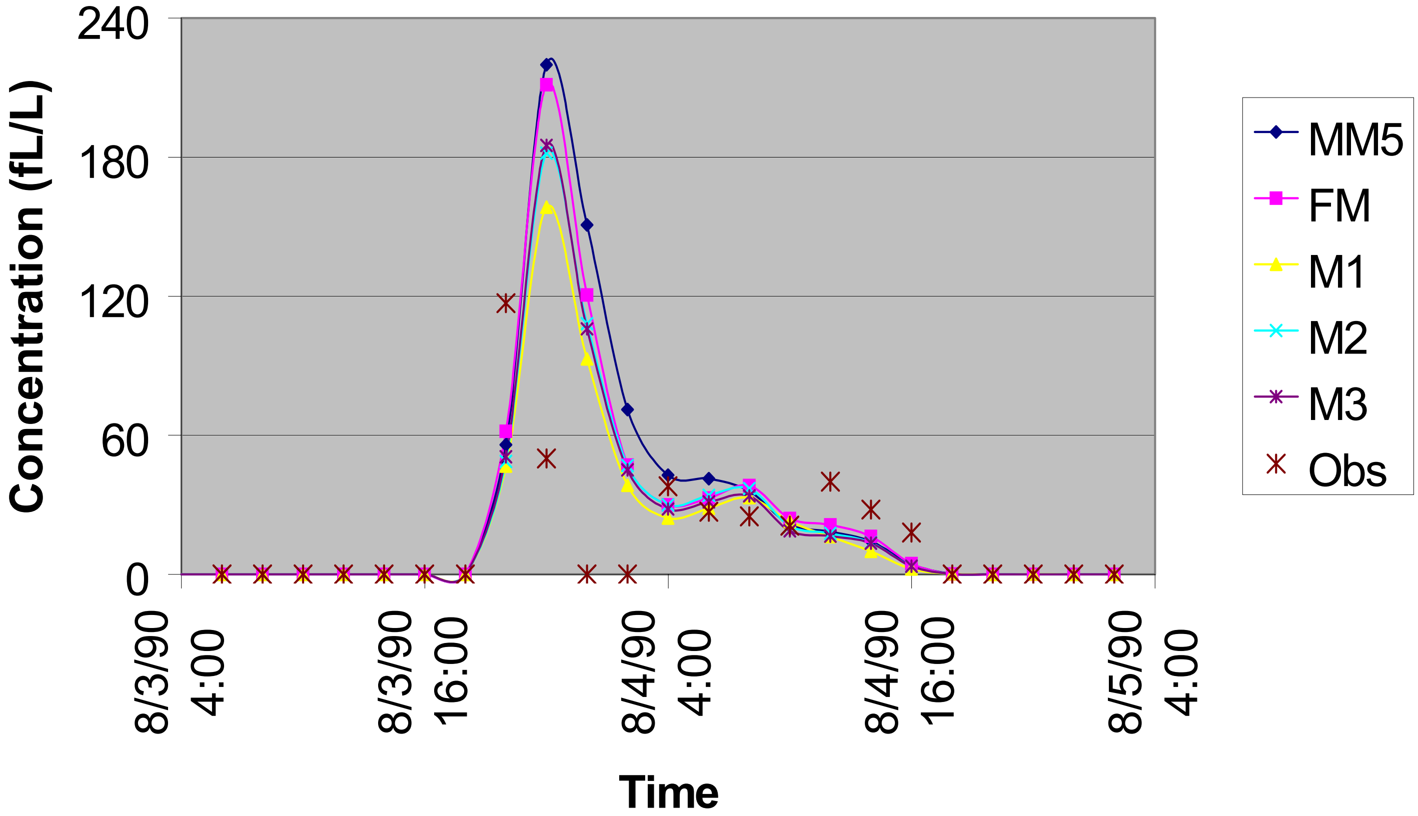
Row 28 PMCPb



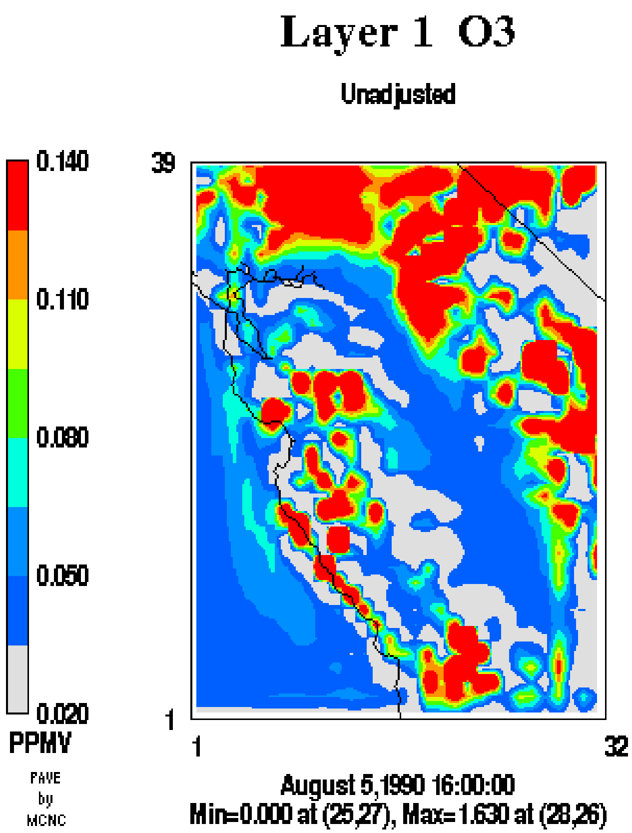
PMCP at Brentwood (30 km)

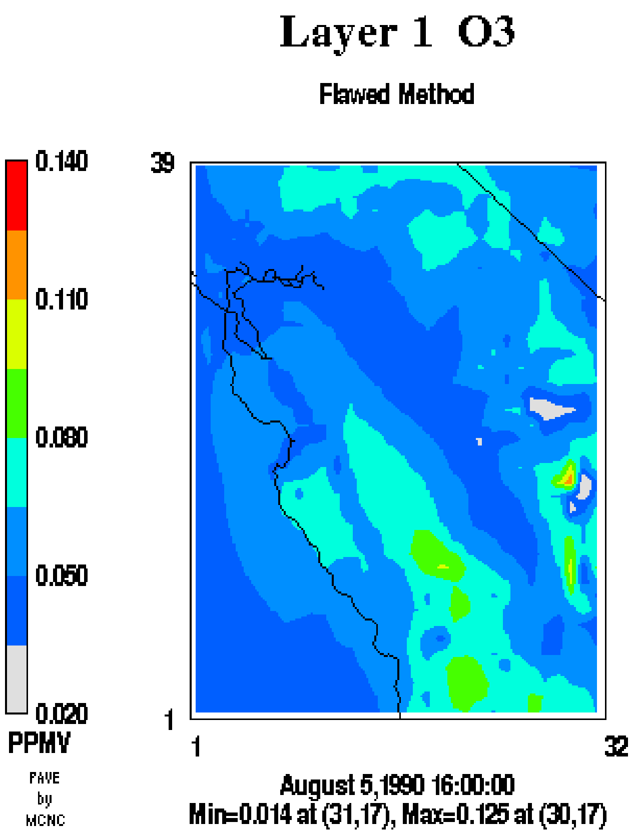


PMCP at Friant (220 km)

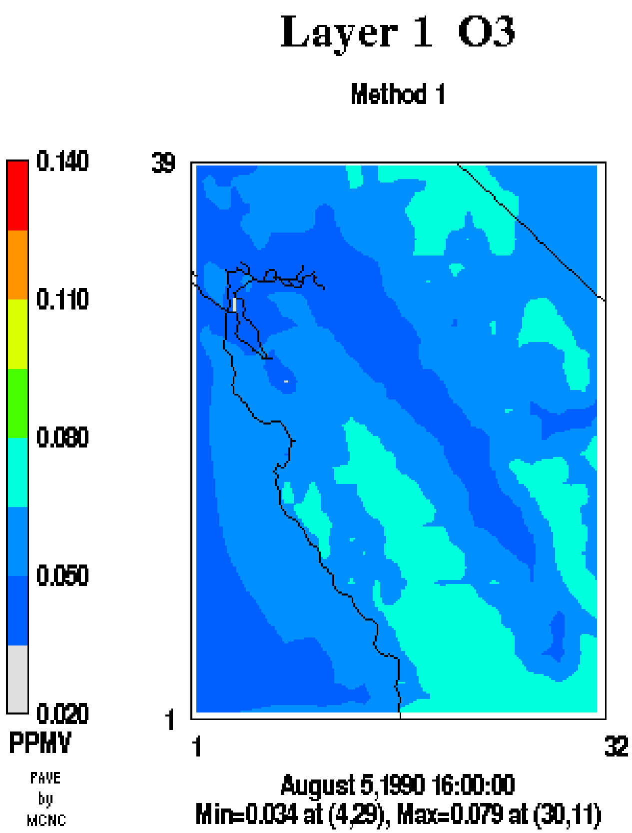


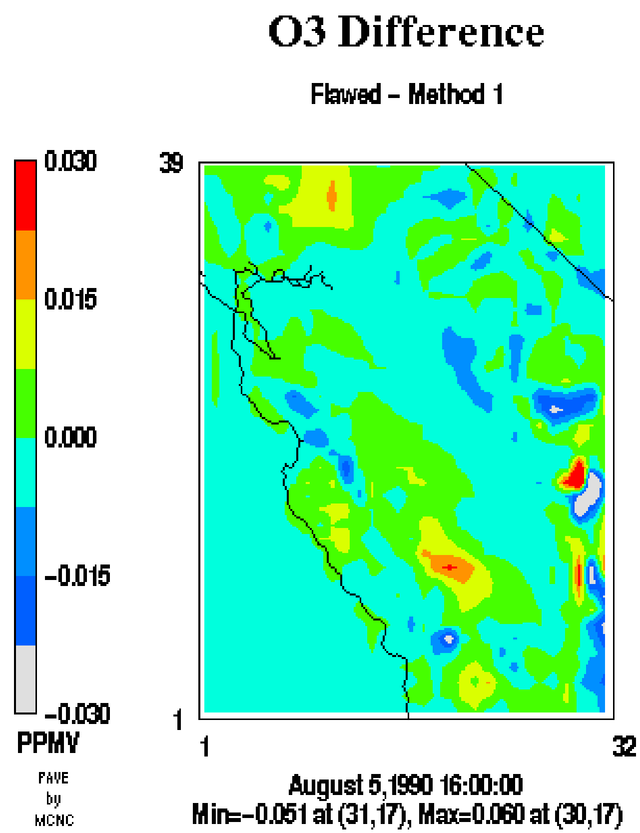
Morning Ozone



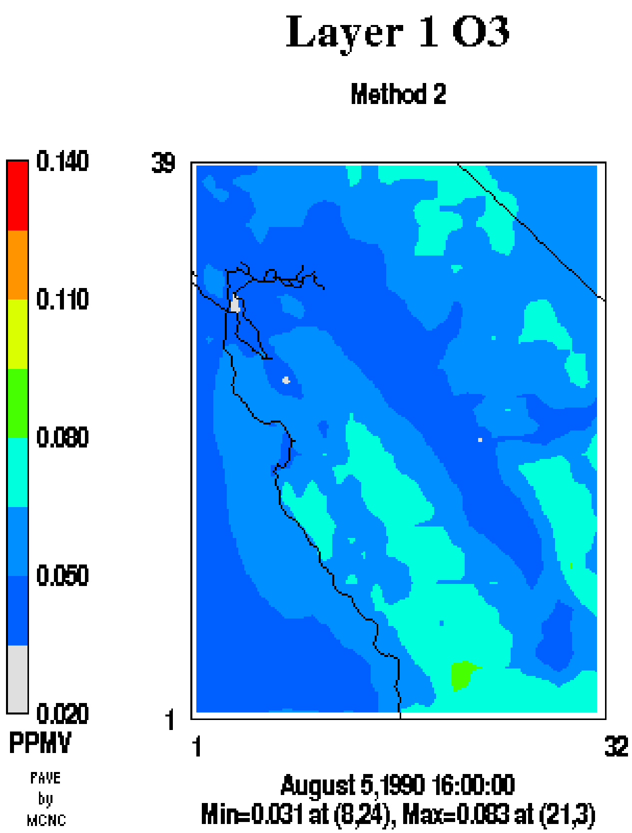


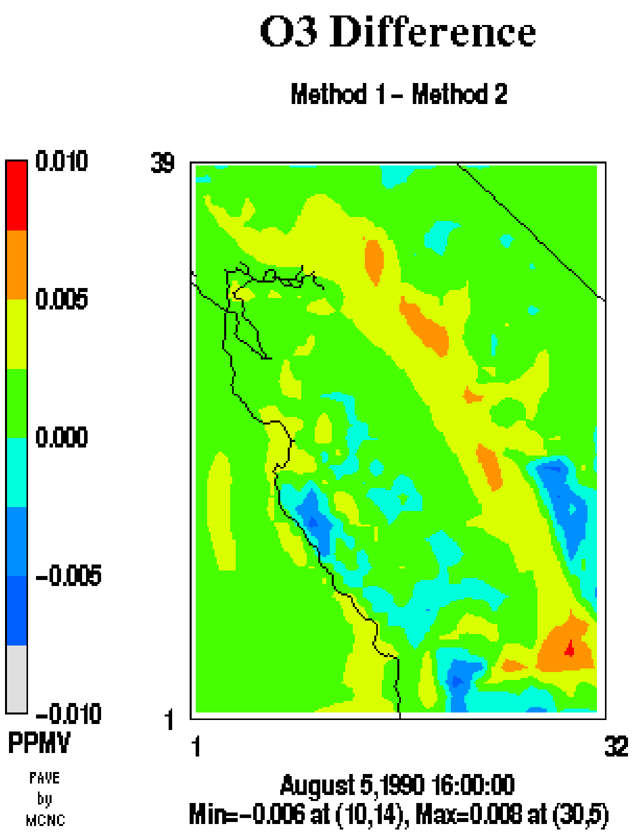
Morning Ozone



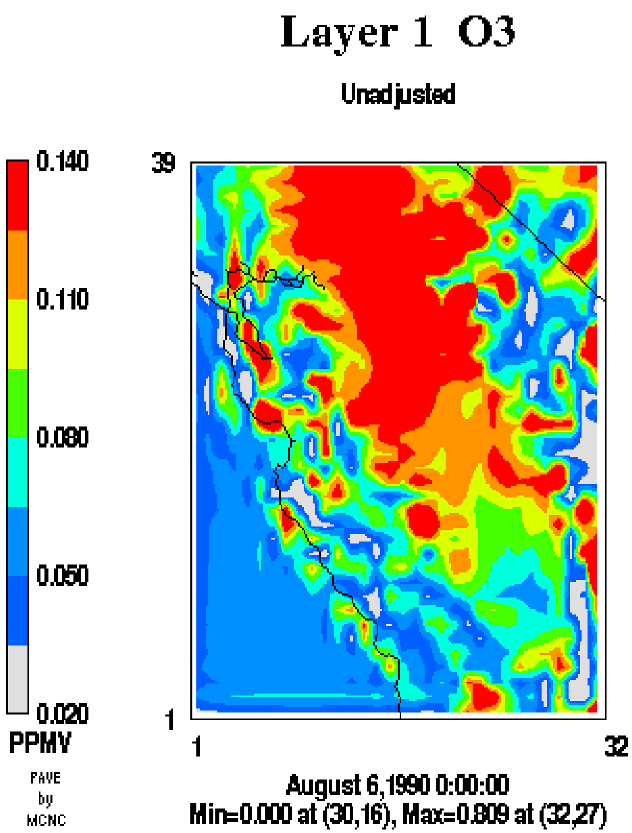


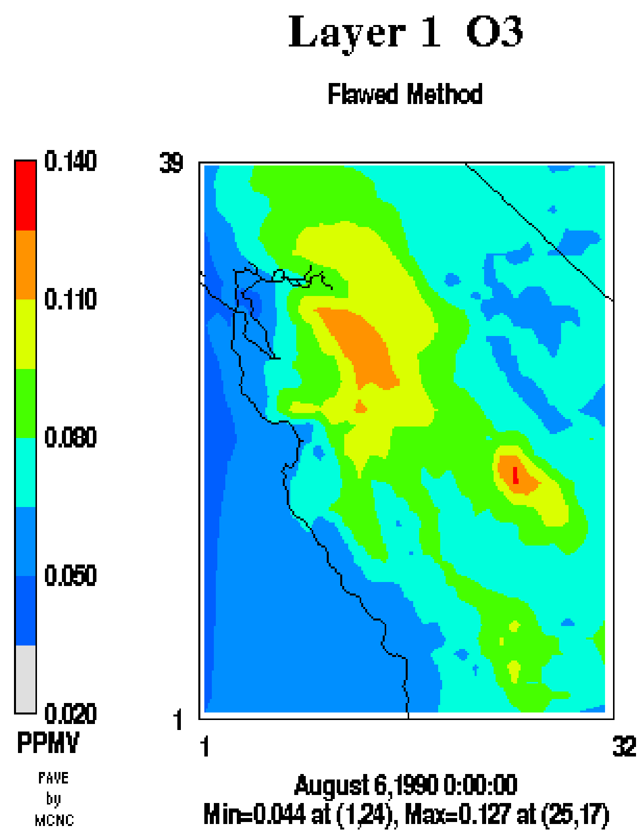
Morning Ozone



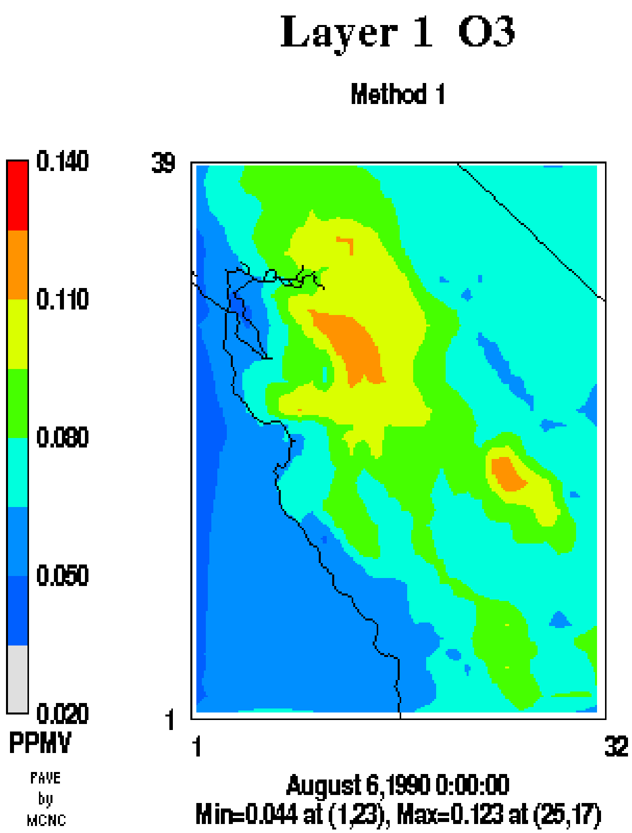


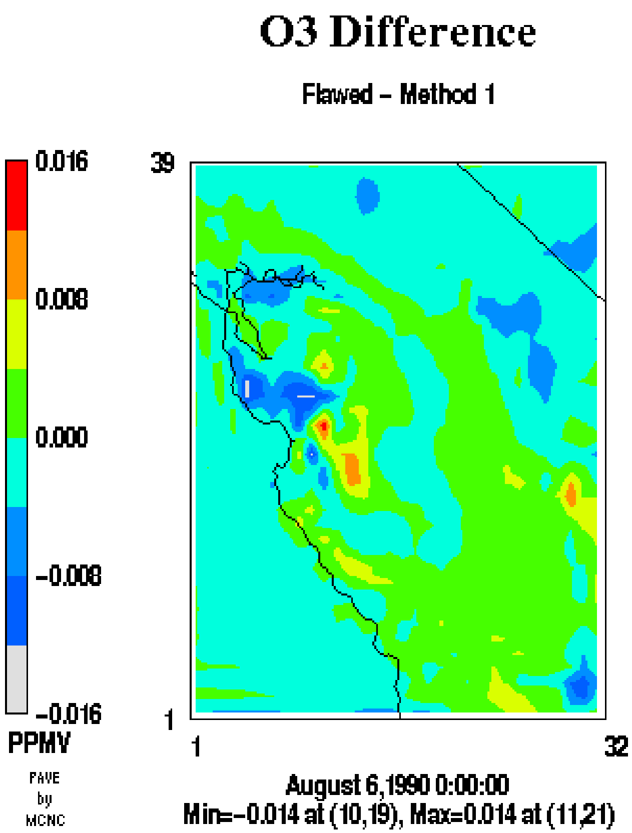
Afternoon Ozone



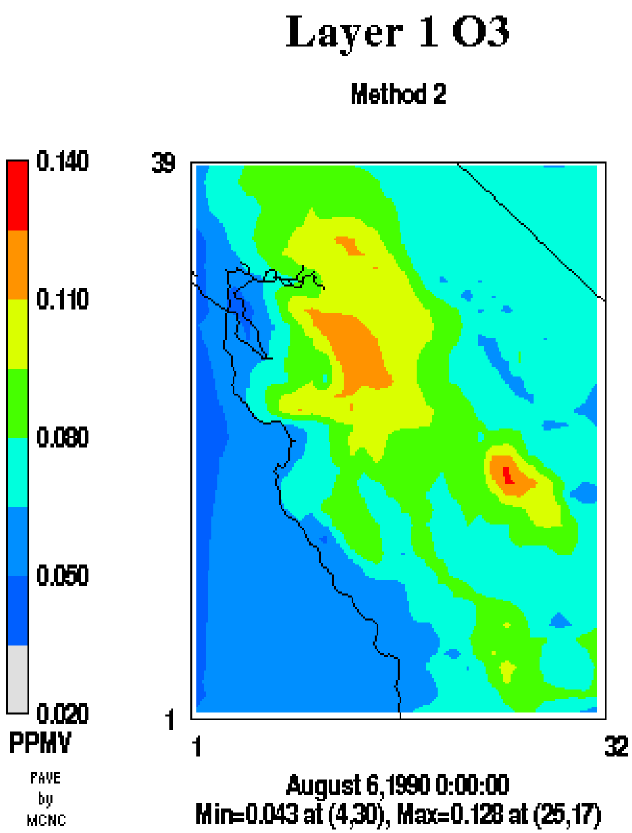


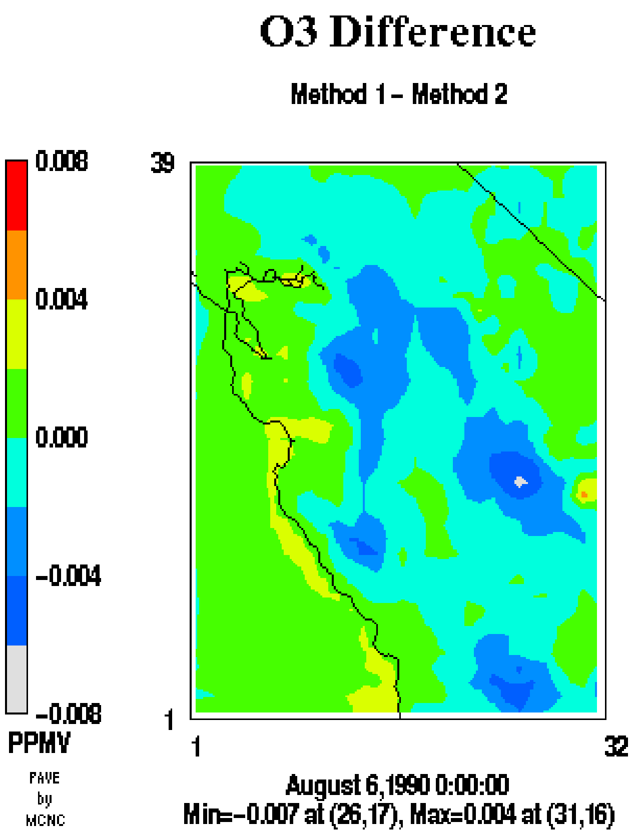
Afternoon Ozone



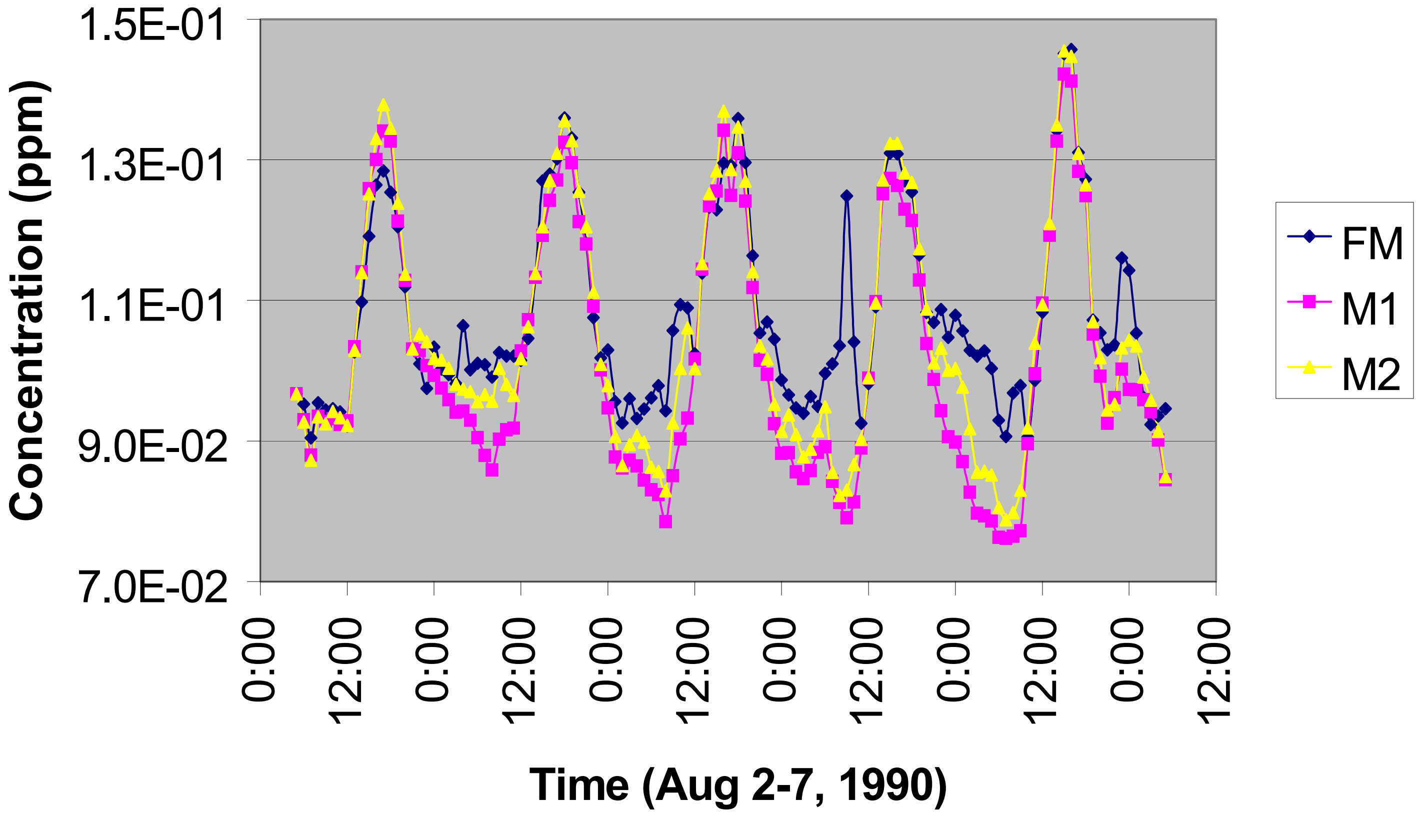


Afternoon Ozone

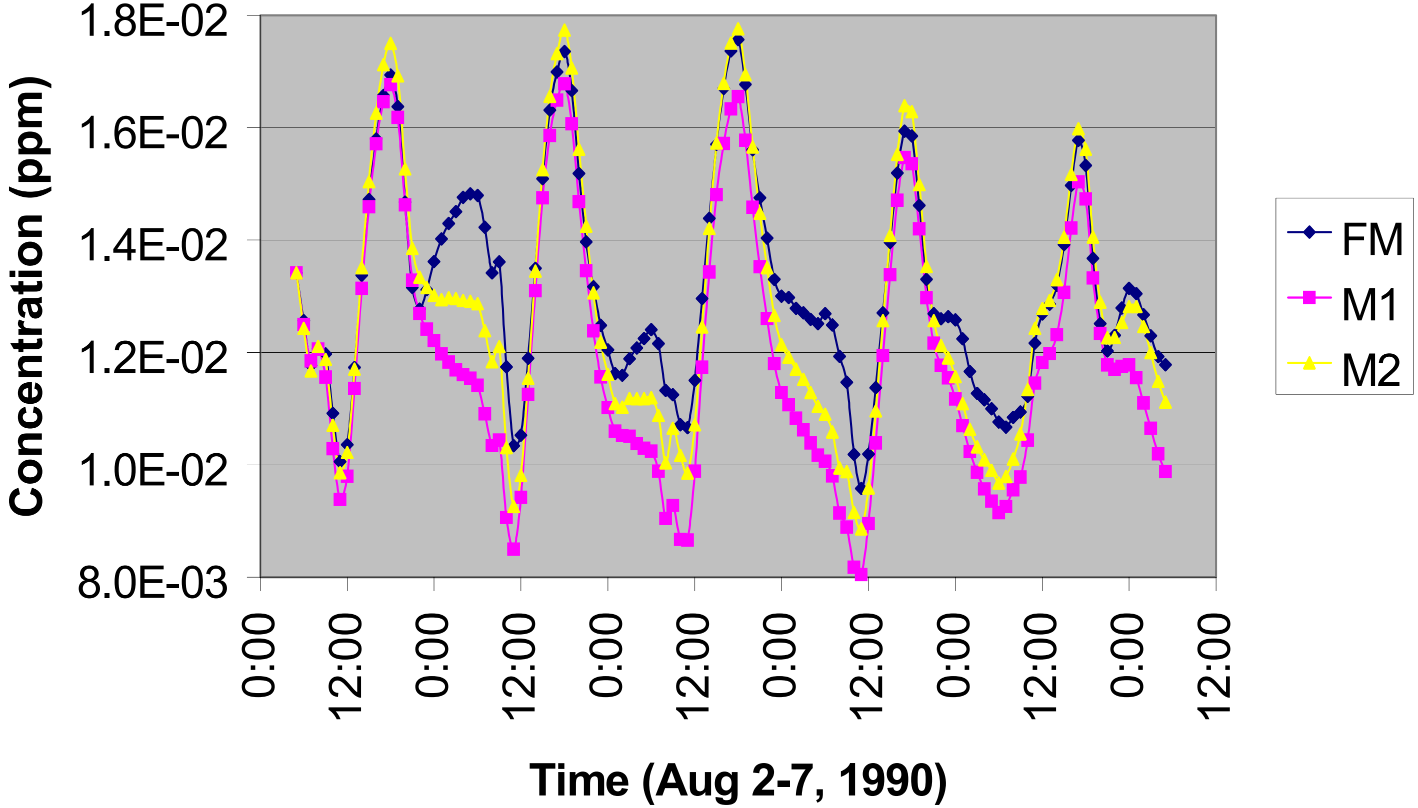




Ozone (Maximum)



Ozone (Standard Deviation)



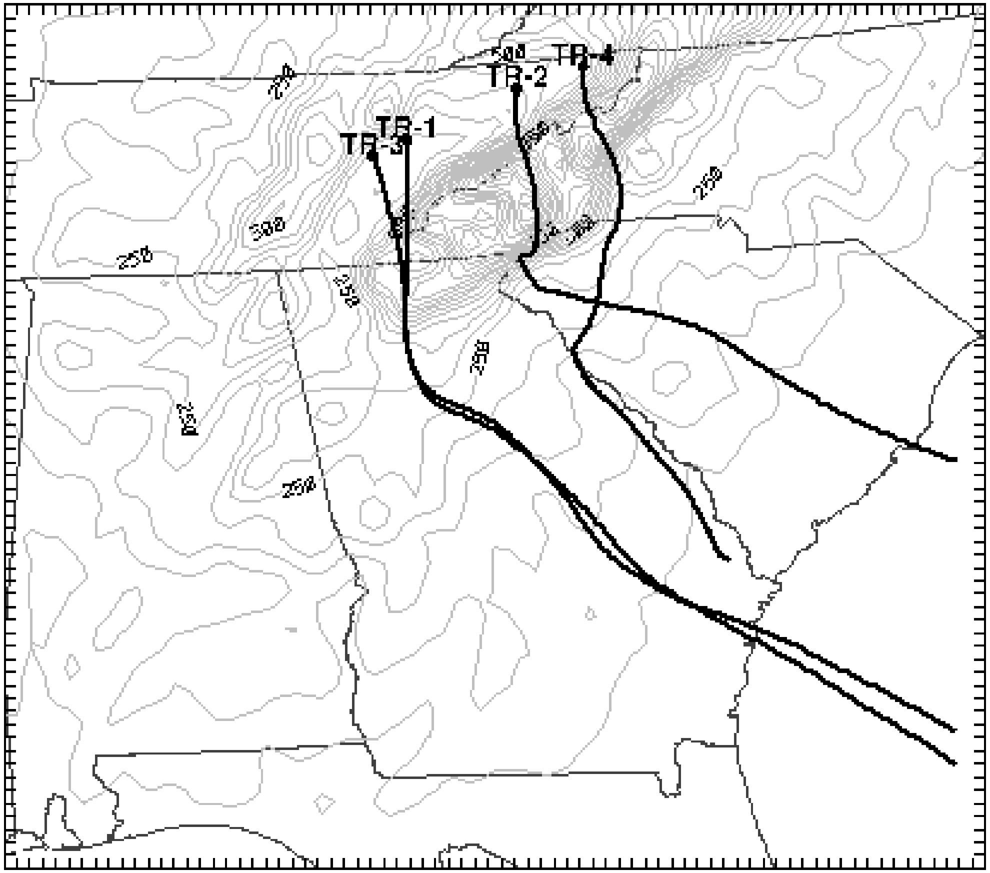
Mass Conservation in CMAQ

Hu, Y., M. T. Odman, and A. G. Russell, 2005. "Mass conservation in the Community Multiscale Air Quality model," *Atmospheric Environment*, in press.

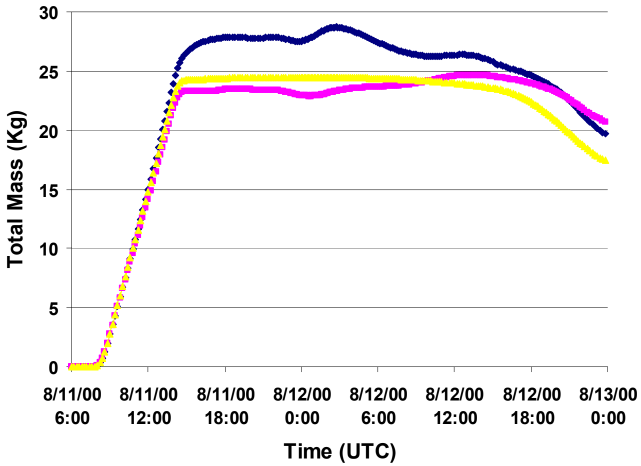
Overview of the Paper

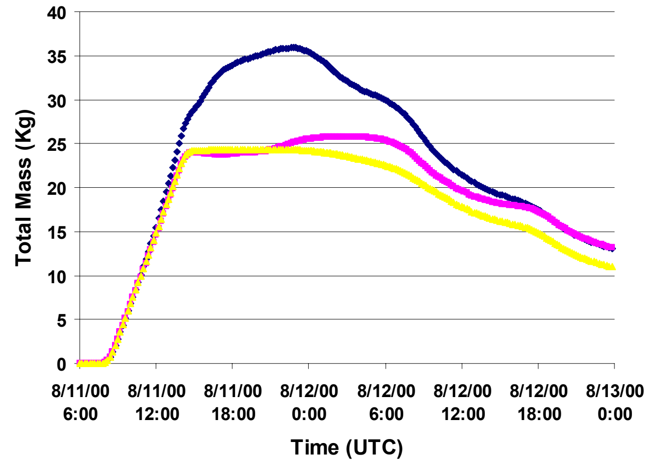
- CMAQ uses the renormalization method (flawed approach).
  – This may have changed in the latest release (Version 4.5)
- We made CMAQ mass-conservative by incorporating vertical velocity adjustment (Method 1).
- An imaginary tracer experiment was simulated over southeastern United States. In this experiment, inert tracers were released from four different locations in the Tennessee Valley.

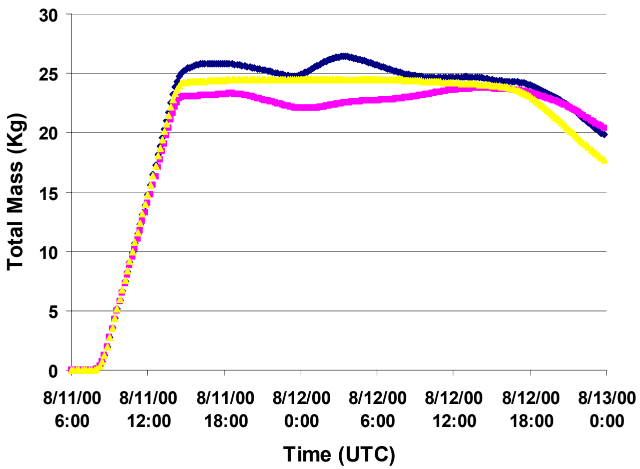
Imaginary Tracer Test

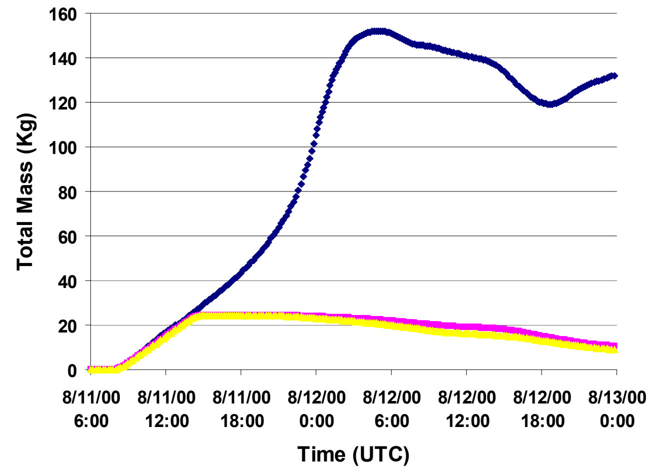


Mass Conservation Error in CMAQ









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

Conclusions of the 2 Papers

- Data from non-hydrostatic MMs may lead to instabilities in AQMs.
- Adjusting *w* is an effective way of achieving consistency without sacrificing mass conservation.
- Adjustments are largest, relative to *w,* when *w* is small.
- They do not significantly affect tracer transport.
- Tracer data are too uncertain to identify the best method.
- Ozone predictions by the three methods are similar.
- They differ significantly from the predictions by the renormalization (flawed) method over complex terrain.

Other Sources of Mass Conservation Error

- Chemical mechanisms
  - CB-4 mechanism and carbon balance…
- Aerosol and cloud modules
  - Recently, we discovered a mass conservation error in CAMQ's aerosol module by checking the sulfur balance and corrected it.[*]
- Establishing sulfur, nitrogen and carbon (in order of increasing difficulty) balance checks can help discover other potential errors.

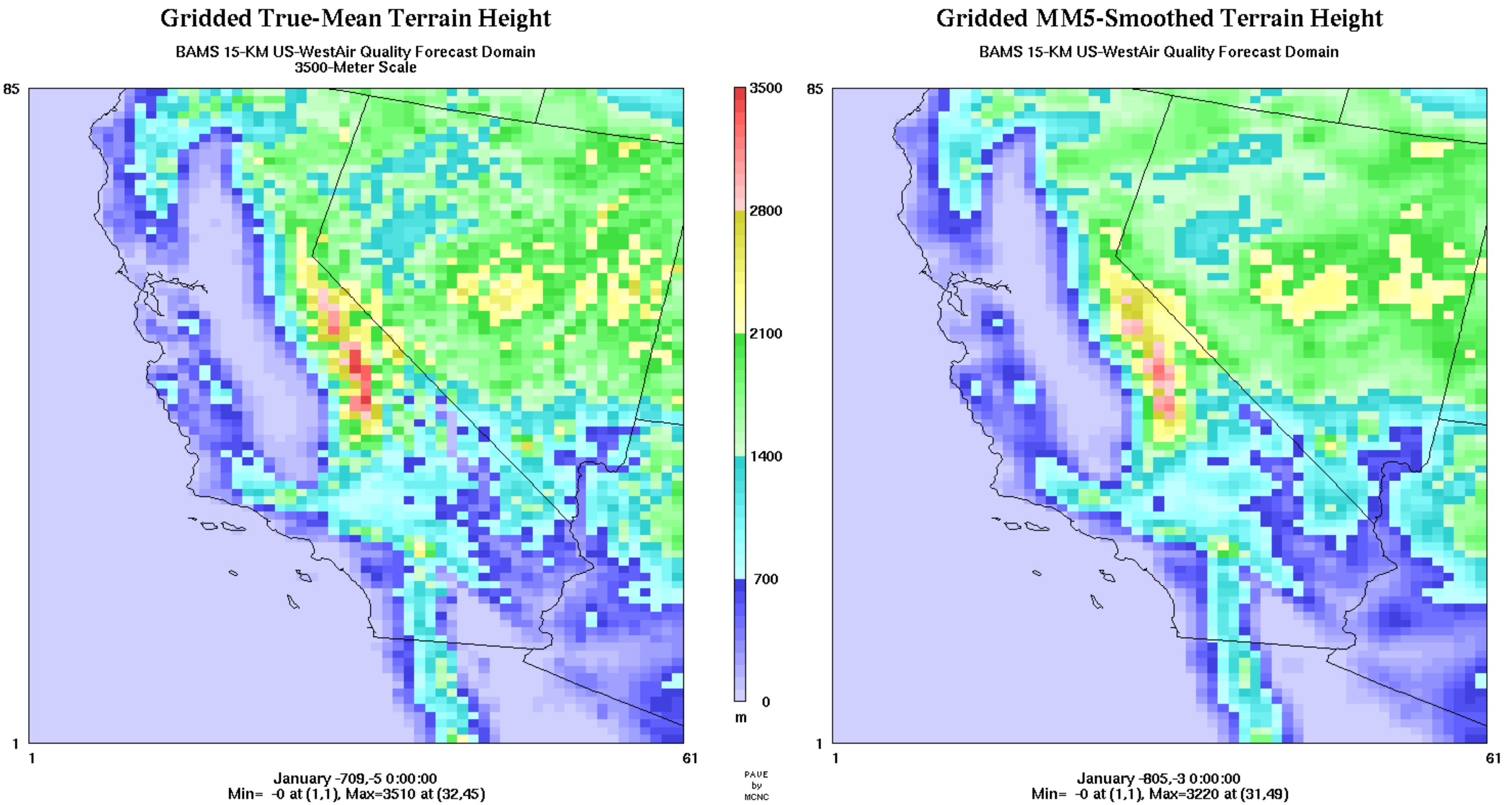
[*] More information about this error and its correction can be found at http://pah.cert.ucr.edu/vistas/results.shtml under "Evaluation of Mass Conservation Patch in CMAQ"

Mass Distribution

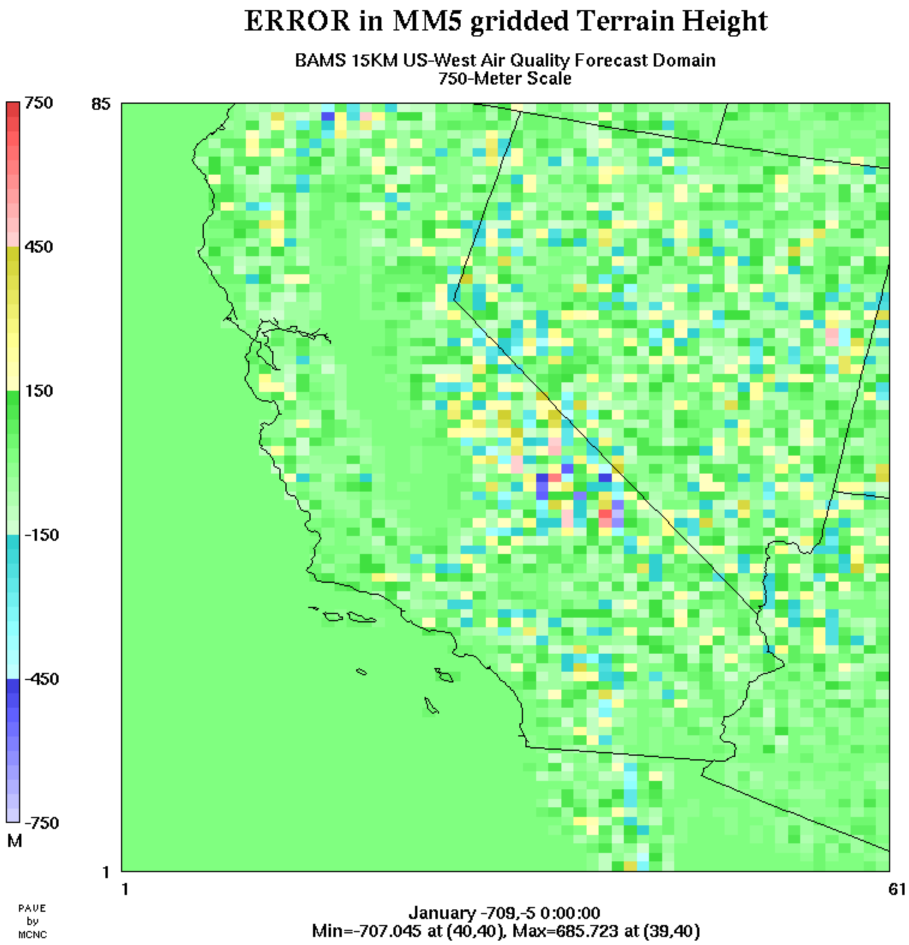
Treatment of Topography

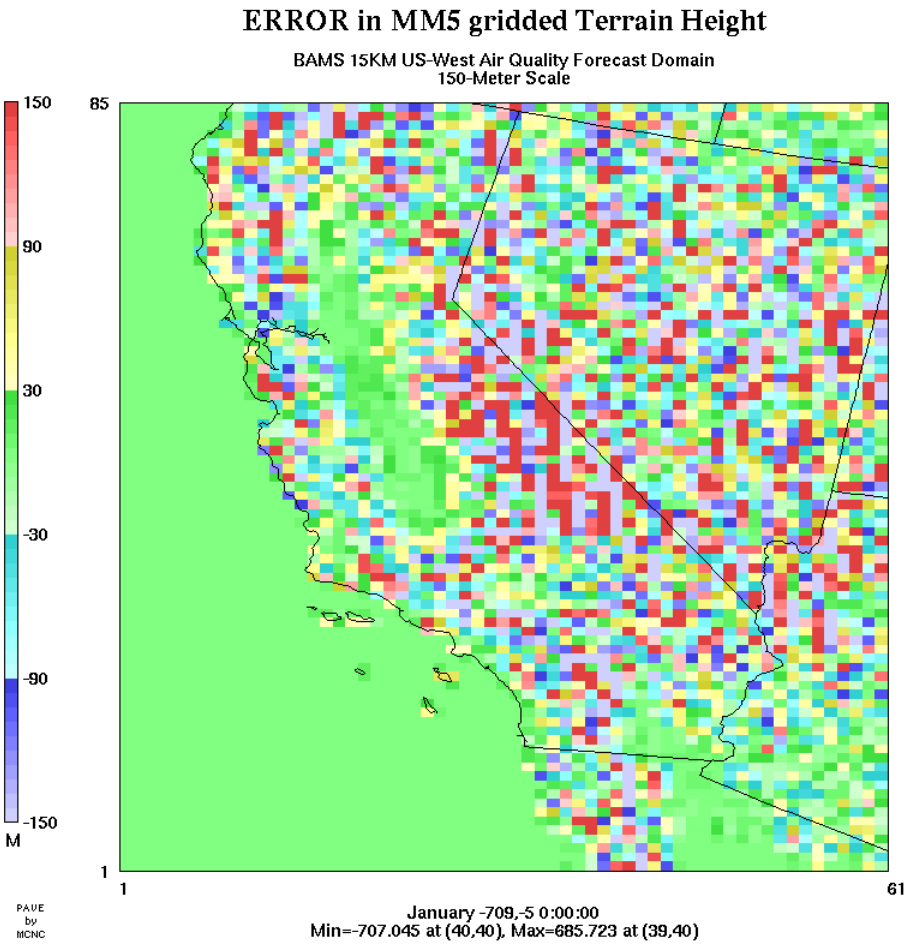
- Due to numerical stability issues in the dynamics, MM's view of the terrain elevation in each grid cell may be significantly different from the actual mean terrain elevation for that grid cell.
  - For example, MM5 applies at least $3\Delta x$ smoothing to the terrain.
- Moreover, there may be considerable terrain variation within each grid cell.
- This leads to two kinds of modeling errors:
  - grid scale terrain height errors,
  - sub-grid scale terrain variability and the consequent interaction between land surface and the modeled atmosphere.
- For example, emission sources and their plumes may be placed at very different altitudes in the model than the actual atmosphere.
- Similarly, deposition processes, particularly dry deposition, may be removing very different amounts of mass in the model than in the actual atmosphere.

Terrain Heights: USGS vs. MM5

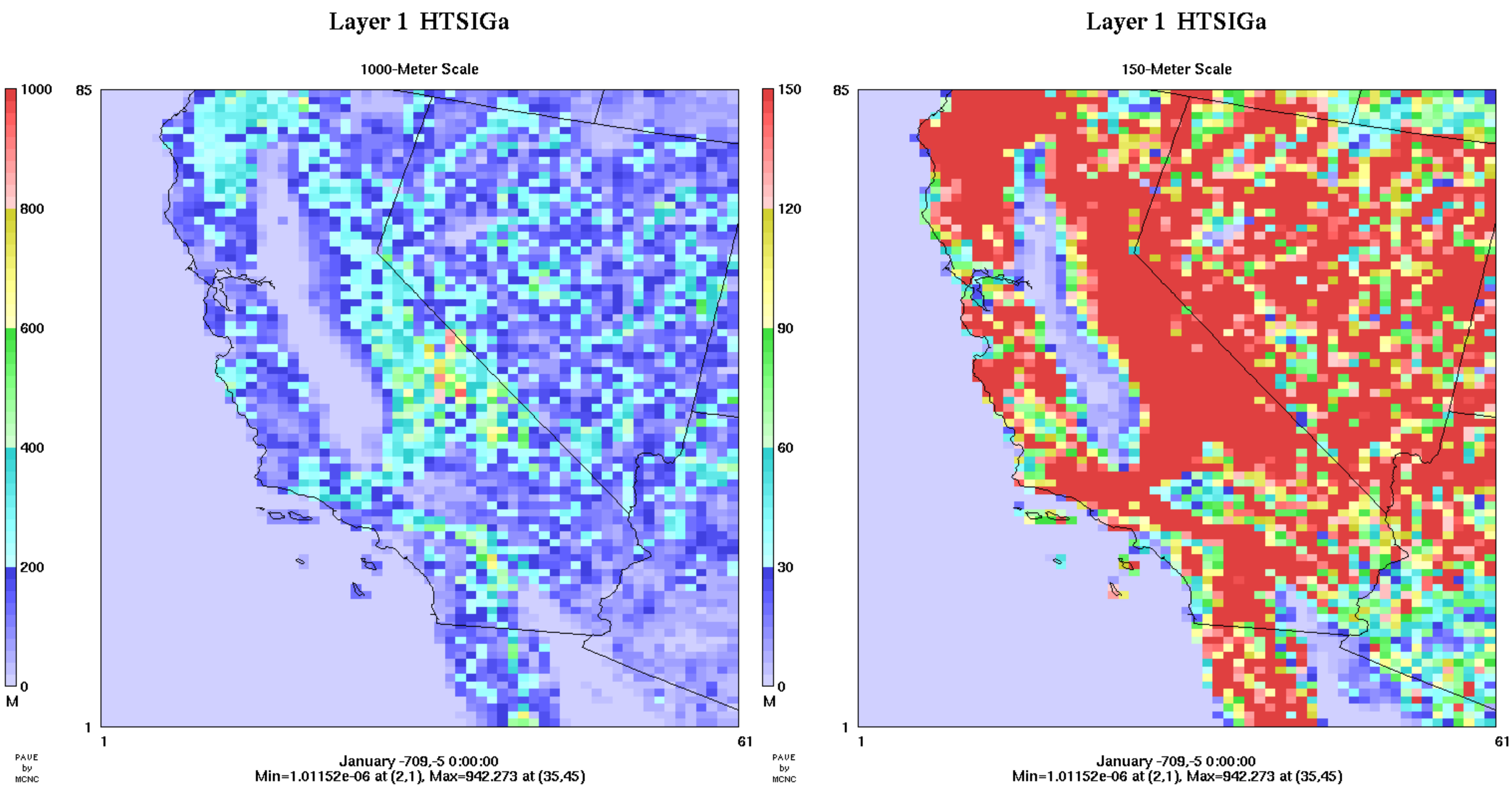


Error in Terrain Height





Standard Deviation of Terrain Height



Technical Approach

Phase 1

Task 1-1: Document sources of mass conservation problems in CAMx and CMAQ air quality models

- Review the air quality models (including preprocessors like MCIP) for sources of mass conservation and mass distribution problems
- Check if they are implemented in conservative form: the fluxes in and out of the modeling domain balance with the change in mass. This is the minimum requirement for mass conservation
- Review if deposition processes are formulated and implemented in conservative form, and whether this form is realistic for the complex topography of California

Task 1-1 (Continued)

- Review the chemical mechanisms of CAMx and CMAQ to see if there are any restrictions for building sulfur, nitrogen and carbon balance checks
- Search the most recent literature (2005) for new contributions
- Review the NOAA study mentioned in the RFP
- Examine the model formulations for being able to realistically simulate interactions with complex California terrain
  - How unrealistic is it to limit dry deposition to only a single model layer (surface layer) 20-40 meters thick?
  - Do models account for cloud impaction upon hill slopes?

Task 1-2: Characterize errors associated with existing CCOS modeling results arising from mass conservation problems

- Identify and acquire the computer codes and a complete set of model inputs and outputs for both CAMx and CMAQ as used in CCOS and 2004 SIP update air quality modeling efforts for central and northern California
- Replicate at least one existing CAMx and CMAQ base case simulation
- Conduct rigorous mass conservation tests using CAMx and CMAQ.
  - Release inert tracers from cells that contain major sources in the CCOS domain whose plumes travel over complex terrain or encounter large divergences in the wind fields
- Conduct similar tests with reactive species (SO_2, NO_X, VOC?) and check the chemical element (sulfur, nitrogen, carbon?) balance

Task 1-2 (Continued)

- Try to evaluate the effect upon pollutant mass of the unrealistic one-layer formulation of dry deposition both in CAMx and CMAQ
- Attempt to assess the effects of cloud impaction effects for California upon the mass balance between atmosphere and wet deposition
- Conduct error analyses of terrain elevation for CCOS domain and grid
- Estimate the potential impacts due to mass distribution errors in CAMx and CMAQ applications to CCOS

Task 1-3: Identify improved means for dealing with mass conservation issues in CAMx and CMAQ

- BAMS assessed the impacts of correcting mass-conservation errors on ozone concentrations over California using MAQSIP-RT (a close relative of CMAQ)
- Calculate the range of trajectory errors introduced by modifying the vertical wind in selected episodes of BAMS forecasts.
- Conduct simulations over the CCOS domain using CMAQ with Method 1, and assess ozone impacts and trajectory errors.
- Conduct a cost/benefit analysis for all the known methods as options for improving mass conservation in CAMx and CMAQ
- Recommend if one or more of these options should be implemented in Phase 2
- Recommend modifications to CAMx and CAMQ for other sources of mass conservation errors
- Address modifications in CAMx and CMAQ that may be needed to accommodate recommended modifications to prognostic meteorological models developed in the NOAA companion study

Task 1-3 (Continued)

- Mass distribution corrections: (BAMS)
  - Grid and sub-grid scale corrections to emissions
  - Better sub-grid scale terrain parameterization for dry deposition
- Considering recommended modifications to prognostic meteorological models developed in the NOAA companion study, conduct a cost/benefit analysis for the corrections mentioned above as options for improving mass distribution in CAMx and CMAQ.
  - Sub-grid scale correction from MM5 model terrain to USGS-derived high resolution terrain that BAMS uses in its determination of precipitation phase

Task 1-4: Document findings of Phase 1, develop a work plan for Phase 2, and meet with the Technical Committee

- Prepare a draft final report discussing the findings of Phase 1 activities (Tasks 1-1, 1-2, and 1-3)
- Prepare a draft work plan for proposed Phase 2 activities, including a discussion of schedule and required budget
- Participate in a one-day meeting with the CCOS Technical Committee in Sacramento, California, to discuss the findings of the study and comments on the draft final report for Phase 1 and, if appropriate, the draft work plan for Phase 2
- Prepare and submit a final report for Phase 1 and, if appropriate, a final work plan for Phase 2

Phase 2

Task 2-1: Develop, implement, and test improved mass conservation modules and procedures for CAMx and CMAQ

- Further develop the mass conservation corrections and mass distribution improvements discussed under Task 1-3, as necessary, to provide better adherence to the mass conservation principles
- Implement, test, and validate these corrections and improvements in CAMx and CMAQ
  - Whenever possible, implementation should be in the form of user-selectable options
- Conduct extensive code review and rigorous testing to verify code modifications and validate the implementation of each correction or improvement option

Task 2-2: Conduct CAMx and CMAQ simulations to assess changes to modeling results from use of the revised codes

- Conduct rigorous tests similar to those described under Task 1-2 to characterize any remaining mass conservation and trajectory errors
- Assess the improvement in mass distribution by simulating tracer experiments if tracer experiment data is available from CCOS
- Perform simulations using the revised CAMx and CMAQ codes developed under Task 2-1
- Compare the results from these simulations with those generated using the original codes as part of Task 1-2.
- Explain the reasons for the differences in results
- Perform a cost/benefit analysis (cost of computing versus improvement in results) for each implemented option to help future users determine which mass conservation option may be most appropriate for different types of model applications

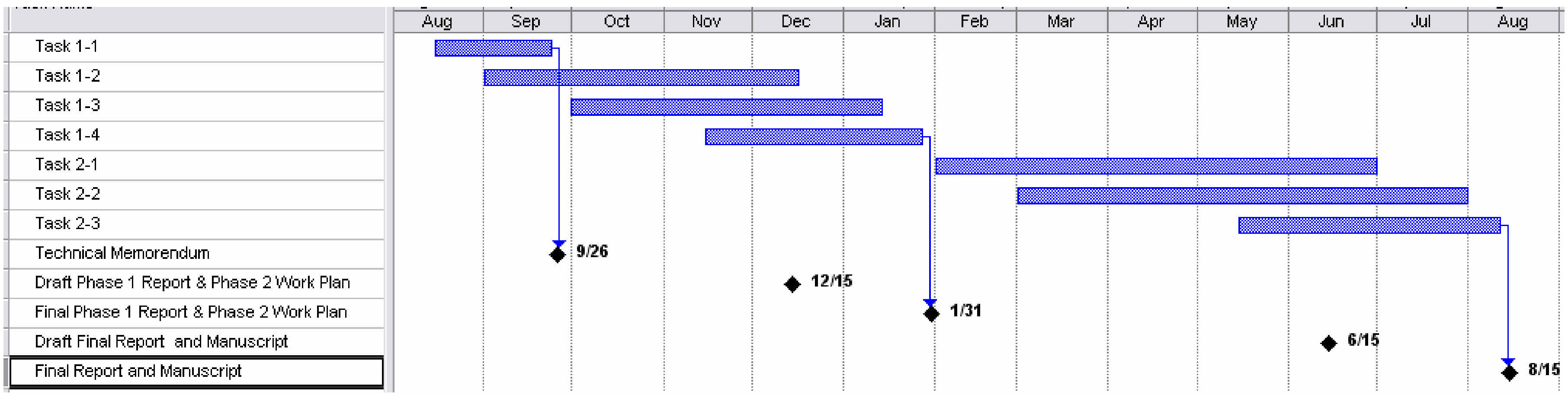
Task 2-3: Prepare study documentation and meet with the Technical Committee

- Document all code modifications made to CAMx and CMAQ, as well as the tests conducted for code validation
- Provide appropriate supplements to the user's guides.
- Submit these documents along with all modified code and input and output files used in testing
- Prepare and submit a draft final report discussing the findings of both Phase 1 and Phase 2 activities
- Participate in a one-day meeting with the CCOS Technical Committee in Sacramento, California, to discuss the findings of the study and comments on the draft final report
- Considering comments provided by the Technical Committee, prepare and submit a final report

Task 2-3 (Continued)

- Prepare and submit a draft manuscript suitable for publication in a peer reviewed journal
  - The manuscript will contain a discussion of the mass conservation problem along with an overview of existing methodology; a detailed description of novel methods developed in this project; a brief overview of the model setups, simulations, and the data used in evaluations; a detailed evaluation of the results; and conclusions.
- Considering comments provided by the Technical Committee, revise the manuscript and submit it to a peer-reviewed journal
- Continue revising until the paper is published

Schedule



Aug
Sep
Oct
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Dec
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Apr
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Jun
Jul
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Task 1-1
Task 1-2
Task 1-3
Task 1-4
Task 2-1
Task 2-2
Task 2-3
Technical Memorendum
Draft Phase 1 Report & Phase 2 Work Plan
Final Phase 1 Report & Phase 2 Work Plan
Draft Final Report and Manuscript
Final Report and Manuscript
9/26
12/15
1/31
6/15
8/15

Discussion

Questions

- CMAQ or just CAMx?
- Status of NOAA Study?
- $PM_{2.5}$ or just O_3?
- Particular emission sources of concern?
- Receptors of concern?
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- Your questions/comments