PHOTOCHEMICAL GRID MODELING OF FOUR HIGH OZONE EPISODES IN THE NEW ENGLAND DOMAIN: CALGRID vs. UAM-IV

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1. Introduction

EARTH TECH has been retained by NESCAUM, on behalf of a consortium of New England states and industries, to conduct base case photochemical modeling simulations for four high ozone episodes with the CALGRID model. As the first task of this project, a technical memorandum (Technical Justification for CALGRID as an Alternative to the UAM-IV Model, 18 October 1996) presented a detailed evaluation for the 7-8 July 1988 episode that demonstrated that CALGRID performed better than the UAM-IV. EPA has requested (12 December 1996 and 24 March 1997 letters to DEP) that CALGRID be compared with UAM-IV for at least three primary episode days to confirm this improved performance. This report presents the modeling results and performance statistics for CALGRID and UAM-IV for the four high ozone days 17 August 1987 (14-17 August 1987 episode), 22 June 1988 (21-22 June 1988 episode), 8 July 1988 (7-8 July 1988 episode), and 11 July 1988 (10-11 July 1988 episode).

As specified by EPA, CALGRID version 1.81 was run with BEIS2 biogenics. Version 1.81 has the same updated CB-4 isoprene chemistry used in UAM-V. This version also has cell-specific sun angle and cloud cover. UAM-IV version 6.21 was run with BEIS inputs.

In section 2, several technical features of the CALGRID and UAM-IV models are described and contrasted. Section 3 presents the model inputs used to drive UAM-IV and CALGRID during the four episodes. Performance statistics and scoring used in the technical memorandum are reviewed in section 4. Section 5 presents the modeling results and performance statistics for both models for the four primary episode days.

2. Comparison of CALGRID and UAM-IV Technical Features

The CALGRID photochemical model is peer-reviewed (Yamartino et al., 1992), documented (Yamartino et al., 1989; Scire et al., 1989), and publicly available. It was developed by Sigma Research Corporation (now part of Earth Tech) scientists as an upgrade and modernization of UAM-IV. CALGRID represents a fully second-generation photochemical model for regulatory application. Modeling features to make the model backward compatible with UAM-IV were retained; however, CALGRID's more compact and streamlined preprocessor and input file style make it easier than UAM-IV to apply.

CALGRID contains state-of-the-science model improvements including:

- A vertical transport and diffusion scheme that incorporates the latest boundary layer formulations, permits several vertical level spacing approaches including dynamic, semi-logarithmic, and arbitrary level spacing, and accounts for all vertical flux components when employing either dynamic or fixed levels.

- A full resistance-based model for the computation of dry deposition rates as a function of geophysical parameters, meteorological conditions, and pollutant species.

- A chemical integration solver based on an adaptive time-step implementation of the quasi-steady state method of Hesstvedt et al. (1978) and Lamb (1983). This solver can efficiently and accurately handle the stiffest of modern schemes.

- Incorporation of more modern photochemical reaction schemes, such as the SAPRC mechanisms, that can more accurately address the roles of biogenic emissions and intermediate chemical products formed over multi-day episodes. In the current version of the model, the user can select between the SAPRC-90 and Carbon Bond IV chemical mechanisms.

- A horizontal advection scheme based on spectrally-constrained cubics (Yamartino, 1993) that conserves mass exactly, prohibits negative concentrations, and exhibits a level of numerical diffusion that is intermediate between class E and F (PGT class) dispersion.

CALGRID essentially uses the same dynamical equations as UAM-IV but, importantly, accounts for density variation with height to ensure exact mass conservation during all transport and diffusion operations. UAM-IV does not include density variation with height. Other improvements over UAM-IV include: (1) use of operator reversal to ensure second-order temporal accuracy, (2) use of three-dimensional space- and time-varying values of meteorological parameters such as photolysis coefficients, humidity, diffusivity, pressure, and temperature, and (3) on-the-fly computation of plume rise and entrainment for more precise initial vertical distribution of plume material.

There are good scientific reasons why CALGRID should perform more accurately than UAM-IV in the New England modeling domain. The Boston urban "plume" originates over land and, during the high ozone episodes, moves northeastward over the ocean, hugging the New Hampshire-Maine coastline. The land-sea difference in the thermal and turbulent structure of the planetary boundary layer results in large changes in temperature, wind direction and mixing profiles with distance from the shore. In this environment, UAM-IV is plagued by two limitations. The first is a lack of vertical resolution, which causes wind shears and temperature profile information to be lost to vertical averaging This leads to spurious instantaneous vertical transport via cell dilution as the UAM-IV layers expand. The second is that the numerical solution of the model equations is strained by the rapidly varying thickness of model layers along the coast. Errors in the estimate of fluxes across cell faces are larger, resulting in unrealistically large transport between land and marine environment along the sloping cell interfaces.

In its fixed layer mode, CALGRID is considerably less prone to several classes of numerical biases. The CALGRID model, in the New England domain application, was operated with all of the 14 layers provided by the CALMET meteorological model (Scire et al., 1995). This means there was no additional vertical averaging of the wind and temperature fields, as in UAM-IV. The CALGRID model has a 20 m thick first layer which is important for modeling thin polluted marine layers. The minimum UAM-IV first layer, on the other hand, is 50 meters, or more. The result is that CALGRID does considerably better than UAM-IV under conditions where ozone precursors from a coastal city such as Boston are transported out over water.

Another distinct advantage that CALGRID has over UAM-IV is the presence of a more realistic deposition algorithm that tracks the changes in plant uptake of ozone and other pollutants more closely. Diurnal and environmental changes in vegetation are not tracked with UAM-IV, except via changes in the aerodynamic resistance. This makes it possible for CALGRID to better track the dynamic range of the diurnal ozone variation. This is especially evident when coupled with a 20 m thick surface layer where predicted surface concentrations are quite responsive to changes in deposition velocity.

3. Description of Model Input Data

Both photochemical models use the same types of input data, although UAM-IV tends to aggregate/average the data more. The basic types of input data used by the models are:

- time-independent data on terrain and surface cover,
- time-independent data on chemistry parameters,
- time-dependent boundary and initial concentration data,
- time-dependent information on emissions, and
- time-dependent information on meteorological conditions.

The information on terrain data for UAM-IV includes cell-average roughness lengths and a vegetation factor used to determine the deposition velocities of various pollutants. CALGRID uses all of the geographical data present in the CALMET output meteorological file, including terrain elevation, roughness length, albedo, leaf area index, and land cover type. Both models read in the rate coefficient information for Carbon Bond IV version 6.21 (CB4). The chemical parameters in the UAM-IV CHEMPARAM file were directly translated, number by number, to update the CALGRID CARBON4.MOD input file to match the latest EPA version. However, as noted earlier, CALGRID was modified to use the updated isoprene chemistry.

The sources of the time-dependent input data used by CALGRID and UAM-IV in the model evaluation and comparison are summarized in Table 3-1. More details are presented in the subsections that follow.

Table 3-1. Sources of the data used to exercise UAM-IV and CALGRID in the New England photochemical modeling domain.

Data Type	UAM-IV Input File	Data Origin	CALGRID Input File	Data Origin
Geophysical	TERRAIN	U.S. Geological Survey (USGS) gridded land use/land cover (LULC) data	CALMET.DAT	CALMET GEO.DAT input file prepared from USGS LULC and Digital Elevation Mapping (DEM) data
Emissions	EMISSIONS (surface)	Emissions Processing System (EPS2.0) output using state inventory data - UAM-BEIS, UAM-BEIS2 biogenic emissions processor	AREM.DAT (surface)	Same as UAM-IV
	PTSOURCE (elevated)	EPS2.0 output using state inventory data	PTEMARB.DAT (elevated)	Same as UAM-IV
Meteorology	DIFFBREAK	Extraction from hourly CALMET.DAT file using CAL2UAM extraction program	CALMET.DAT	Run CALMET5.0 with Aerometric Information Retrieval System (AIRS), National Weather Service (NWS), and buoy meteorological data
	WINDS	Extraction from hourly CALMET.DAT using CAL2UAM UAMWND processor	"	"
	TEMPERATURE	Extraction from hourly CALMET.DAT file using CAL2UAM	"	"
	METSCALARS	Estimation using CALMET.DAT station information, EPA SUNFUNC routine and other UAM-IV pre-processors in CAL2UAM	"	"
	REGIONTOP	Estimated using DIFFBREAK, minimum layer thickness, and constant height top option in CAL2UAM	CALGRID.INP	Set to match UAM-IV

Table 3-1. (Continued) Sources of the data used to exercise UAM-IV and CALGRID in the New England photochemical modeling domain.

Data Type	UAM-IV Input File	Data Origin	CALGRID Input File	Data Origin
Initial Concentrations	AIRQUALITY	Extracted from ROM "BASE88RR" run	ICON.DAT	Reformat of UAM-IV file
Boundary Concentrations	TOPCONC	Extracted from ROM "BASE88RR" run	TCON.DAT	Reformat of UAM-IV file
	BOUNDARY	Extracted from ROM "BASE88RR" run. NY SIP UAM-IV concentrations overlaid on "BASE88RR" extractions for July 1988 episodes.	BCON.DAT	Reformat of UAM-IV file

3.1 Emissions Data

The base year emissions data consist of daily files of gridded hourly surface and elevated point source emissions for each CB4 specie emitted. These daily UAM-IV model-ready emissions files were supplied by the Massachusetts DEP. In addition to the aggregated input files, individual files for mobile source emissions, low-level point source emissions, area source emissions, and biogenic emissions were supplied. The biogenic emission files used for the model performance evaluation were produced with version 2 of the EPA Biogenic Emissions Inventory System model (BEIS2) for CALGRID, but, as agreed upon with EPA, the original BEIS model for UAM-IV.

CALGRID requires reformatting of the UAM-IV emissions data, but no other conversion is needed when CB4 is being used. Rather than exercising a separate plume rise model as UAM-IV does, CALGRID estimates plume rise internally. The estimates of plume rise produced by CALGRID should be more accurate since the actual temperature profile of the atmosphere is used rather than the simple two-segment fit based on the domain-wide vertical temperature gradients above and below the mixing height ("TGRADABOVE" and "TGRADBELOW") employed by the UAM-IV plume rise processor.

3.2 Meteorological Data

CALMET version 5.0 was used to create gridded wind, temperature, mixing height, and other fields from hourly observed data provided by the Massachusetts DEP. These output data were directly mapped into CALGRID without averaging because the horizontal grid dimensions and vertical layer structures were defined identically in the CALMET and CALGRID models for this study. On the other hand, UAM-IV requires substantial processing of the CALMET output data file (or alternatively the raw observational data) in order to create the WINDS, DIFFBREAK, TEMPERATUR, METSCALARS, TERRAIN, and REGIONTOP files. The CALMET post-processing was done using the recommendations in Volume 2 of the UAM-IV user's manual (Morris et al., 1990). EARTH TECH developed a processor called CAL2UAM that uses the UAMWND and various other UAM preprocessor routines (e.g., SUNFUNC) to produce UAM-IV input files from the CALMET output file. The winds and other variables are averaged and aggregated over the domain to provide winds for the coarser UAM vertical layers and domain-wide hourly METSCALARS. UAMWND does a linear vertical interpolation and a momentum conservation weighting of winds in the column. No divergence minimization was applied to reduce the magnitude of the vertical winds. The temperature field and the mixing height were used to estimate the domain-wide temperature lapse rates. The station and sounding relative humidity information was directly averaged to create a domain-volume-average estimate of the water vapor concentration.

UAM-IV is a clear sky model with chemical photolysis rates estimated using a Los Angeles haze layer and a 320 Dobson Units (DU) columnar ozone depth. CALGRID was exercised using NWS-interpolated cloud cover with a 320 DU columnar ozone thickness. The CALMET model outputs the PGT stability class, roughness length, Monin-Obukhov length, and a convective scaling velocity for each surface grid cell. This information is used in CAL2UAM, along with information from the UAM-IV preprocessor user's manual, in order to estimate an appropriate exposure class. Both models assumed the same fixed model top of 3300 m.

3.3 Boundary and Initial Conditions

Lateral and top boundary conditions that were extracted using the EPA ROM-UAM interface software. For the two July 1988 episodes, UAM-IV simulations were available for the New York domain. Since the New York modeling domain overlaps Connecticut, UAM-IV runs conducted by the New York DEC were used to estimate boundary conditions on the southern border of the New England domain, with ROM boundary conditions for the nonoverlapping borders. Direct mapping from UTM zone 18 to UTM zone 19 was conducted. The mixing heights in both cases were obtained using CALMET on a 5 km grid. When intercompared, the mixing height differences were small. As a result, direct layer-to-layer mapping of the concentrations was used, rather than doing mass adjustments.

4. Description of the Model Evaluation and Comparison Methodology

The model evaluation methodology was based on four EPA-recommended (EPA, 1991) statistics. The New England domain was divided into five subdomains by the Massachusetts DEP to capture different influences and transport processes. A scoring scheme was devised by the DEP to compare the performance of UAM-IV and CALGRID. This scheme uses estimates of the statistical measures in the domain and each subdomain to develop a single composite measure.

The statistics were generated for the four high ozone days 17 August 1987, 22 June 1988, 8 July 1988, and 11 July 1988.

4.1 Statistical Performance Measures

The four statistics are defined in equations 4-1 through 4-4 and have the following percentage evaluation targets:

- A_U - unpaired highest prediction accuracy 20%,
- D - normalized bias for C_o> 60 ppb 15%
- E_d - gross error for C_o > 60 ppb 30%
- A - average station peak prediction accuracy 30%

where C_o is the observed concentration. Note that since the convention for residual concentrations of observed minus predicted is used, a positive value is an underprediction.

Unpaired Highest-Prediction Accuracy

$$A_u = \frac{C_o(.,.) - C_p(.,.)}{C_o(.,.)} \times 100\% \qquad (4\text{-}1)$$

where

A_U	=	unpaired highest-prediction accuracy (quantifies the difference between the magnitude of the highest 1-hour observed value and the highest 1-hour predicted value, regardless of location
$C_o(.,.)$	=	maximum 1-hour observed concentration over all hours and monitoring stations
$C_P(.,.)$	=	maximum 1-hour predicted concentration over all hours and surface grid squares

Normalized Bias

$$D = \frac{1}{N_T} \sum_{i=1}^{N} \sum_{j=1}^{H_i} \frac{C_O(i,j) - C_P(i,j)}{C_O(i,j)} \times 100\% \qquad (4\text{-}2)$$

where

D	=	normalized bias obtained from all hourly prediction-observation pairs with hourly observed values > 60 ppb
N	=	number of monitoring stations
H_i	=	number of hourly prediction-observation pairs for monitoring station i
N_T	=	total number of station-hours
$C_O(i, j)$	=	observed value at monitoring station i for hour j
$C_P(i, j)$	=	predicted value at monitoring station i for hour j

Gross Error of All Pairs >60 ppb

$$E_d = \frac{1}{N_T} \sum_{i=1}^{N} \sum_{j=1}^{H_i} \frac{|C_O(i,j) - C_P(i,j)|}{C_O(i,j)} \times 100\% \qquad (4\text{-}3)$$

where

E_d	=	normalized gross error for all hourly prediction-observation pairs for hourly observed values >60 ppb
N_T	=	total number of station hours (defined previously)
N	=	number of monitoring stations
H_i	=	number of hourly prediction-observation pairs for monitoring station i
$C_O(i, j)$	=	observed value >60 ppb at monitoring station i for hour j
$C_P(i, j)$	=	predicted value at monitoring station i for hour j

Average Station Peak Prediction Accuracy

$$A = \frac{1}{N} \sum_{i=1}^{N} \left| \frac{C_O(i,t_i) - C_P(i,t_i)}{C_O(i,t_i)} \right| \times 100\% \qquad (4\text{-}4)$$

where

A	=	mean paired peak prediction accuracy averaged over all monitoring stations
N	=	number of monitoring stations
$C_O(i, t_i)$	=	peak observed value at monitoring station i for hour t_i
$C_P(i, t_i)$	=	predicted value at monitoring station i for hour t_i

The pairing in time at sites provides a valuable indication of the match in timing between the observed and predicted maximum concentrations. The predictions at the monitors for the pairing in space is done using bilinear interpolation (EPA, 1991) between the four grid cell centers that surround the monitor.

4.2 Model Subdomains

To examine local performance, the Massachusetts DEP divided the modeling domain into five subdomains. These five subdomains are shown in Figure 4-1. They are:

1. Maine, coastal New Hampshire, northern coastal Massachusetts,
2. Northeast Massachusetts, Merrimack Valley
3. southeast Massachusetts and Rhode Island
4. Central Massachusetts,
5. Connecticut and Vermont.

The Connecticut and Vermont subdomain, at the request of the DEP, was excluded from the performance evaluation because most of the monitors in this region are in the New York SIP modeling domain. There are nine monitors in subdomain 1, seven in subdomain 2, six in subdomain 3, and seven in subdomain 4.

4.3 Model Performance Scoring

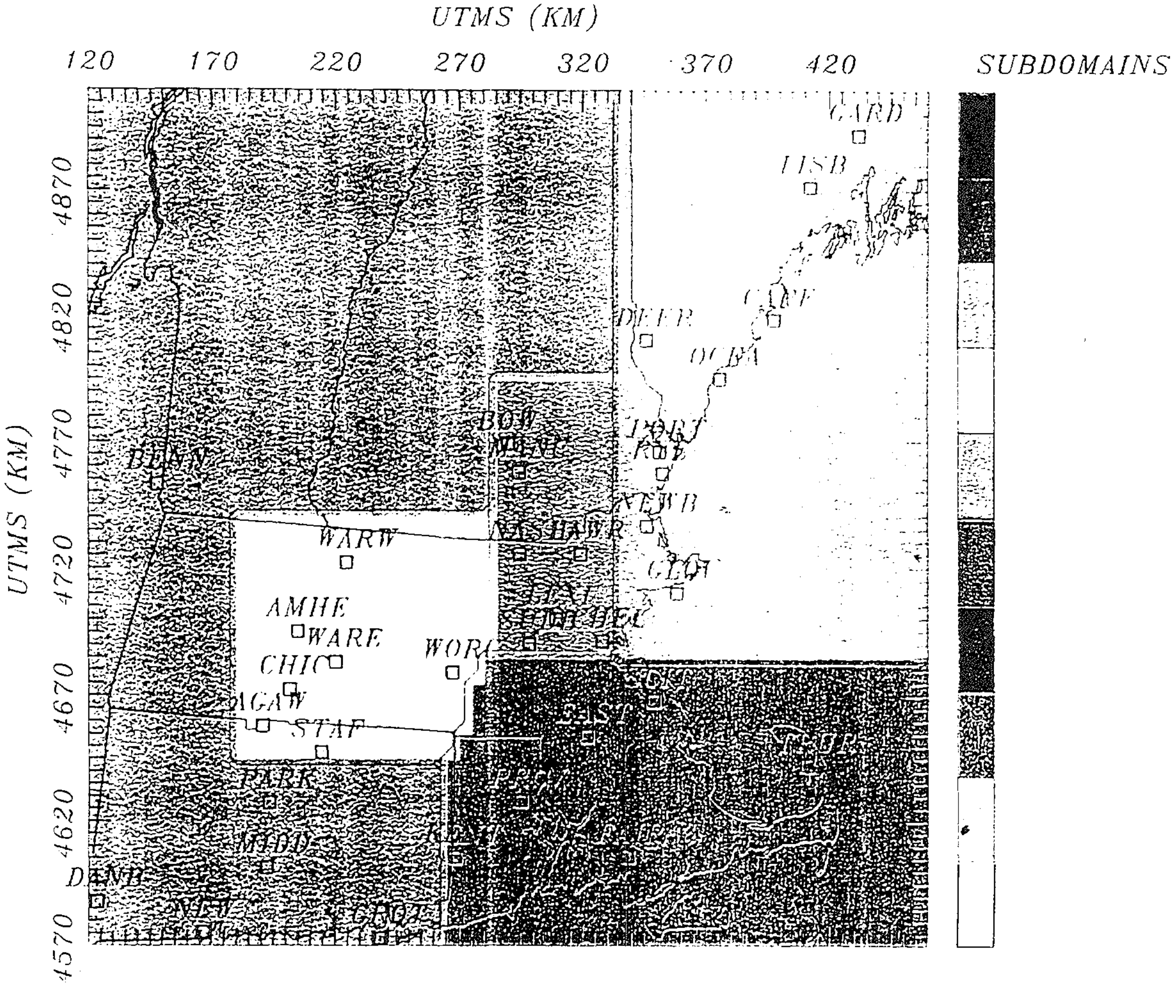
The scoring scheme developed by the Massachusetts DEP is based on the four statistical measures and their targets. A maximum of one point is awarded for each measure for the whole domain and for each of the four subdomains, or a maximum of twenty points. No points are awarded if the value of the performance measure is outside of the target. The maximum of one point is awarded if the performance is perfect (0% for the statistical measure). No points are awarded for performance outside of the target value. For performance between perfect and the target value, a linear interpolation is used. For example, if the bias is plus or minus 10% for a given subdomain, then 0.3333 points are awarded (1 - 10%/15%).

5.0 Performance of CALGRID and UAM-IV

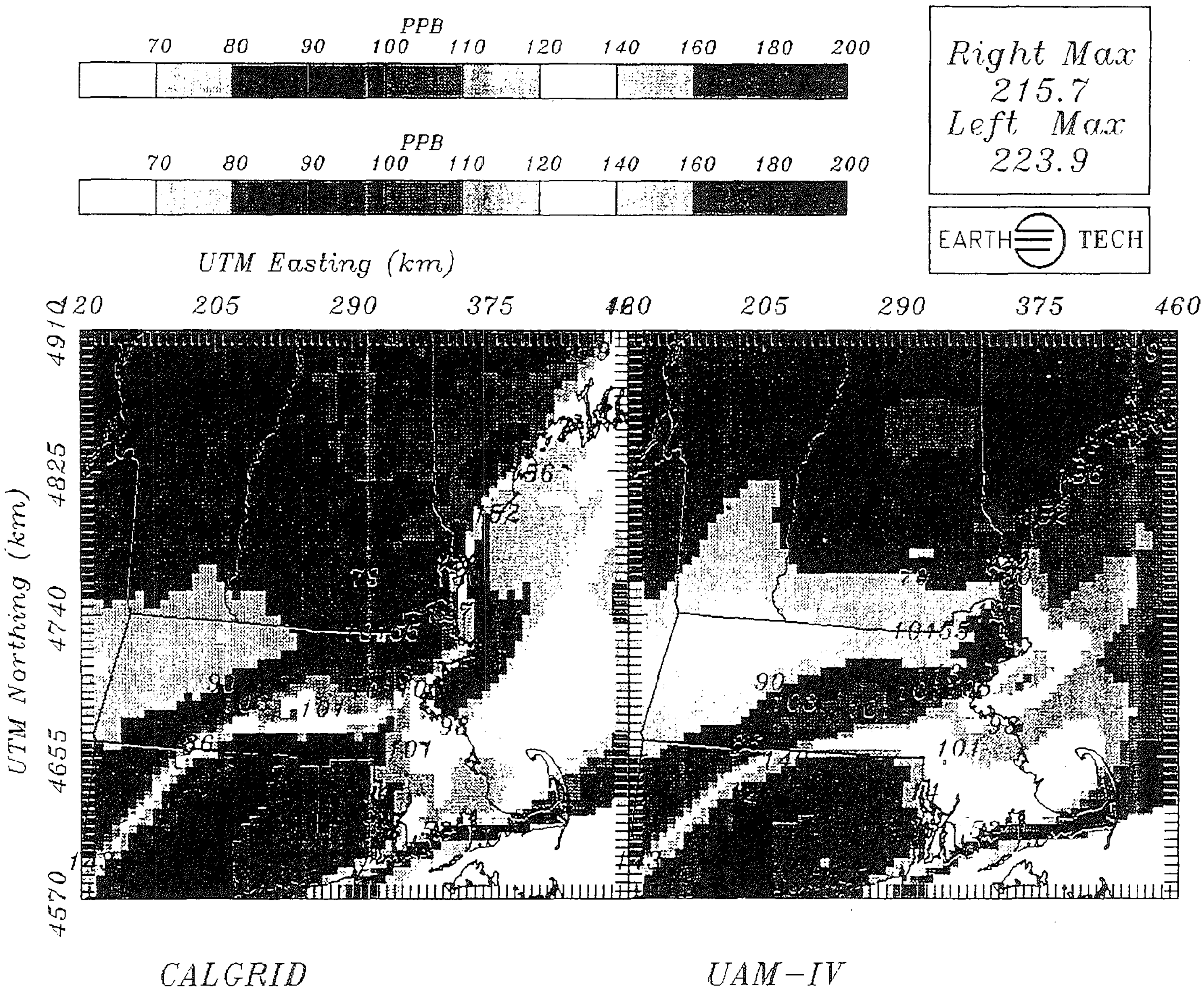
5.1 17 August 1987

The maximum hourly ozone concentrations for 17 August 1987 for both the CALGRID and UAM-IV model are shown in Figure 5-1. CALGRID produces higher ozone concentrations along the ozone transport corridor. This results in better agreement with the 156 ppb and 152 ppb observations in Maine, as well as the 180 ppb observation on the New Hampshire coast. Both models match the low observed values in north central Massachusetts and interior New Hampshire and Maine. UAM-IV better matches the moderate ozone concentrations in southeast Massachusetts. The values near the southern boundary of the domain, however, are primarily generated by the inflow boundary conditions, which are predicted by ROM.

MODEL EVALUATION SUBDOMAINS IN NEW ENGLAND



Maximum Daily Ozone for August 17, 1987.



Comparison of CALGRID and UAM-IV models
New England Domain - August 17, 1987

PERFORMANCE EVALUATION STATISTICS

CALGRID with BEIS2	MAINE	NH/MA	RI/MA	Central MA	All	EPA Target
Unpaired Peak Accuracy	-10.4	**-35.6**	**-75.0**	**-50.2**	**-24.4**	20%
Ave. Paired Peak Accuracy	-0.8	8.1	**-43.5**	1.7	-9.1	30%
Normalized Bias	2.2	**26.4**	**-34.4**	-12.5	-3.5	15%
Gross Error	19.4	**32.4**	**35.2**	19.5	25.7	30%
UAM-IV with BEIS						
Unpaired Peak Accuracy	9.4	-7.5	**-56.1**	**-26.4**	-19.8	20%
Ave. Paired Peak Accuracy	29.3	23.8	**-31.2**	20.2	9.4	30%
Normalized Bias	**31.3**	**42.2**	**-22.7**	11.1	**17.0**	15%
Gross Error	**34.1**	**44.1**	24.2	23.7	**32.2**	30%

Notes:
1. Units are percent
2. Negative values - predicted exceeds observed
3. Positive values - observed exceeds predicted
4. Values in **bold face** exceed target

PERFORMANCE EVALUATION SCORES

CALGRID with BEIS2	MAINE	NH/MA	RI/MA	Central MA	All	Total
Unpaired Peak Accuracy	0.5	0.0	0.0	0.0	0.0	0.5
Ave. Paired Peak Accuracy	1.0	0.7	0.0	0.9	0.7	3.3
Normalized Bias	0.9	0.0	0.0	0.2	0.8	1.8
Gross Error	0.4	0.0	0.0	0.4	0.1	0.8
Total	2.7	0.7	0.0	1.5	1.6	**6.5**
UAM-IV with BEIS						**Total**
Unpaired Peak Accuracy	0.5	0.6	0.0	0.0	0.0	1.2
Ave. Paired Peak Accuracy	0.0	0.2	0.0	0.3	0.7	1.2
Normalized Bias	0.0	0.0	0.0	0.3	0.0	0.3
Gross Error	0.0	0.0	0.2	0.2	0.0	0.4
Total	0.6	0.8	0.2	0.8	0.7	**3.1**

The statistical comparison of the two models is shown in Table 5-1. The overprediction of both models in southeast and central Massachusetts, likely due to the ROM boundary conditions is apparent. In the northern half of the domain (subdomains Maine and New Hampshire/Massachusetts), CALGRID better matches the observations. Of note are the paired statistics, represented by the average paired peak accuracy, the bias, and the gross error. Although UAM-IV does well on unpaired peak accuracy, where any prediction north of Boston is compared with the highest in Maine, New Hampshire and northern Massachusetts, UAM-IV underpredicts by 20%-30% at the monitor sites in this region.

The scoring scheme shows that CALGRID has 6.5 points and UAM-IV has 3.1 points. A perfect model would have 20 points.

5.2 22 June 1988

The maximum hourly ozone concentrations for 22 June 1988 for both the CALGRID and UAM-IV model are shown in Figure 5-2. CALGRID produces higher ozone concentrations in the ocean from Massachusetts to Maine and UAM-IV produces slightly higher concentrations in the north central Connecticut and south central Massachusetts region.

This episode day has the very high observed concentrations in the southern half of the domain, but the ROM boundary conditions underestimate the boundary ozone concentrations. This hampers the performance of both models. More realistic boundary conditions should improve model performance and lead to a more meaningful comparison.

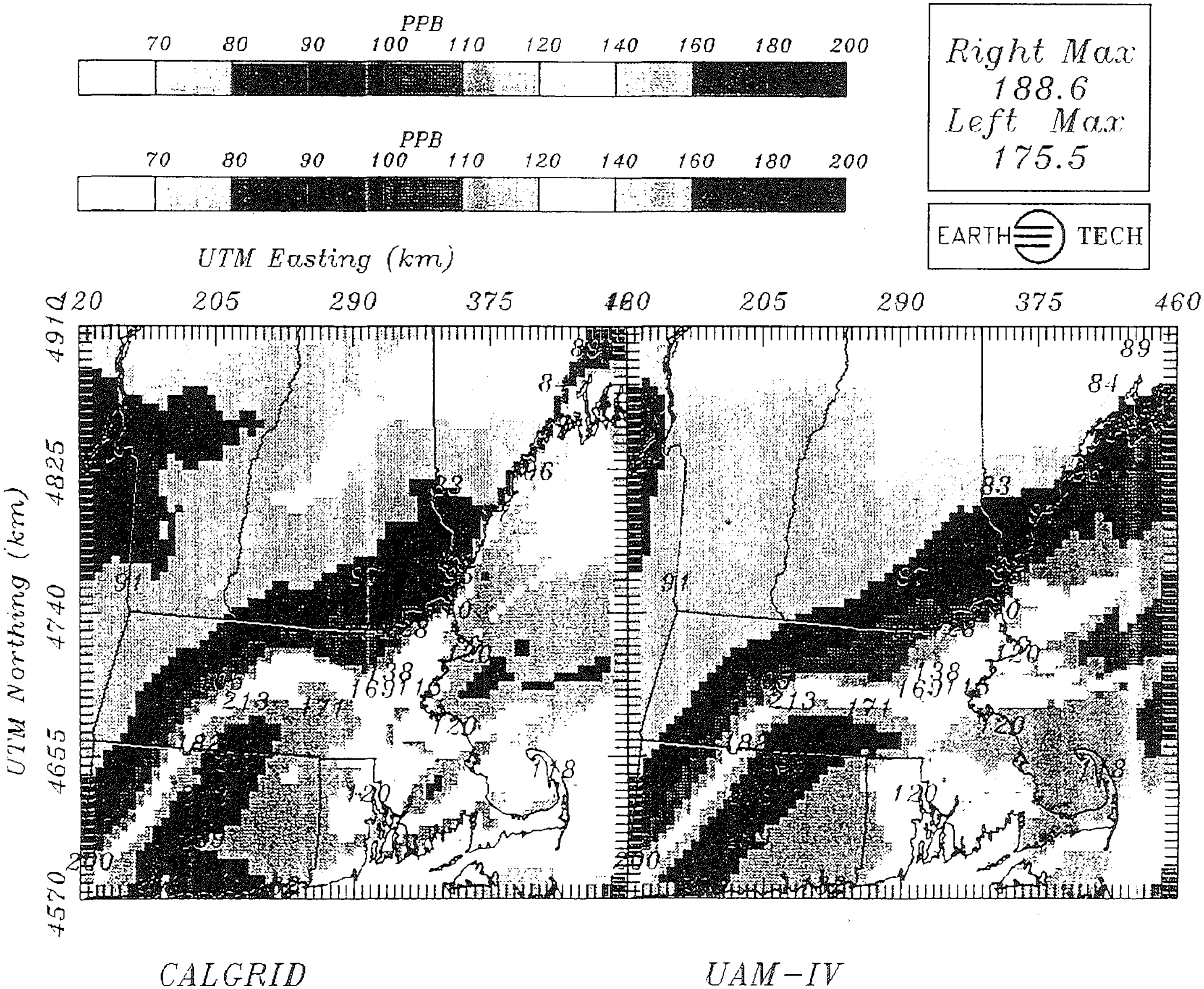
The statistical comparison of the two models is shown in Table 5-2. Both models underpredict at the monitor sites, as seen with the paired statistics. With the unpaired peak accuracy, both models overpredict in the two regions with ocean coverage (Maine and RI/MA), where there are no monitors to verify the predictions, and underestimate in the two land-based regions (NH/MA and Central MA).

The scoring scheme gives a slight edge to CALGRID, with 5.4 points to the 4.6 points for UAM-IV.

5.3 8 July 1988

Figure 5-3 shows the maximum hourly ozone concentrations for 8 July 1988 for both the CALGRID and UAM-IV model. CALGRID better matches the observed ozone concentrations along the New Hampshire and Maine coastal regions. The July 1988 episodes have the benefit of using UAM-IV boundary conditions, which improve the comparisons of both models in the southern half of the domain, although UAM-IV better captures the lower values in Rhode Island and Cape Cod.

Maximum Daily Ozone for June 22, 1988.



Comparison of CALGRID and UAM-IV models
New England Domain - June 22, 1988

PERFORMANCE EVALUATION STATISTICS

CALGRID with BEIS2	MAINE	NH/MA	RI/MA	Central MA	All	EPA Target
Unpaired Peak Accuracy	**-40.7**	17.0	-4.3	**26.5**	**26.6**	20%
Ave. Paired Peak Accuracy	4.2	25.0	20.7	24.9	18.4	30%
Normalized Bias	8.6	1.9	9.1	**16.3**	9.2	15%
Gross Error	26.9	20.3	**33.2**	27.9	29.1	30%

UAM-IV with BEIS						
Unpaired Peak Accuracy	-19.8	17.0	-12.6	**20.8**	**21.2**	20%
Ave. Paired Peak Accuracy	12.3	22.9	21.5	24.9	20.1	30%
Normalized Bias	**17.8**	7.4	**19.4**	3.3	9.6	15%
Gross Error	**30.5**	23.9	29.0	16.0	24.9	30%

Notes:
1. Units are percent
2. Negative values - predicted exceeds observed
3. Positive values - observed exceeds predicted
4. Values in **bold face** exceed target

PERFORMANCE EVALUATION SCORES

CALGRID with BEIS2	MAINE	NH/MA	RI/MA	Central MA	All	Total
Unpaired Peak Accuracy	0.0	0.1	0.8	0.0	0.0	0.9
Ave. Paired Peak Accuracy	0.9	0.2	0.3	0.2	0.4	1.9
Normalized Bias	0.4	0.9	0.4	0.0	0.4	2.1
Gross Error	0.1	0.3	0.0	0.1	0.0	0.5
Total	1.4	1.5	1.5	0.2	0.8	**5.4**

UAM-IV with BEIS						Total
Unpaired Peak Accuracy	0.0	0.1	0.4	0.0	0.0	0.5
Ave. Paired Peak Accuracy	0.6	0.2	0.3	0.2	0.3	1.6
Normalized Bias	0.0	0.5	0.0	0.8	0.4	1.6
Gross Error	0.0	0.2	0.0	0.5	0.2	0.9
Total	0.6	1.1	0.7	1.4	0.9	**4.6**

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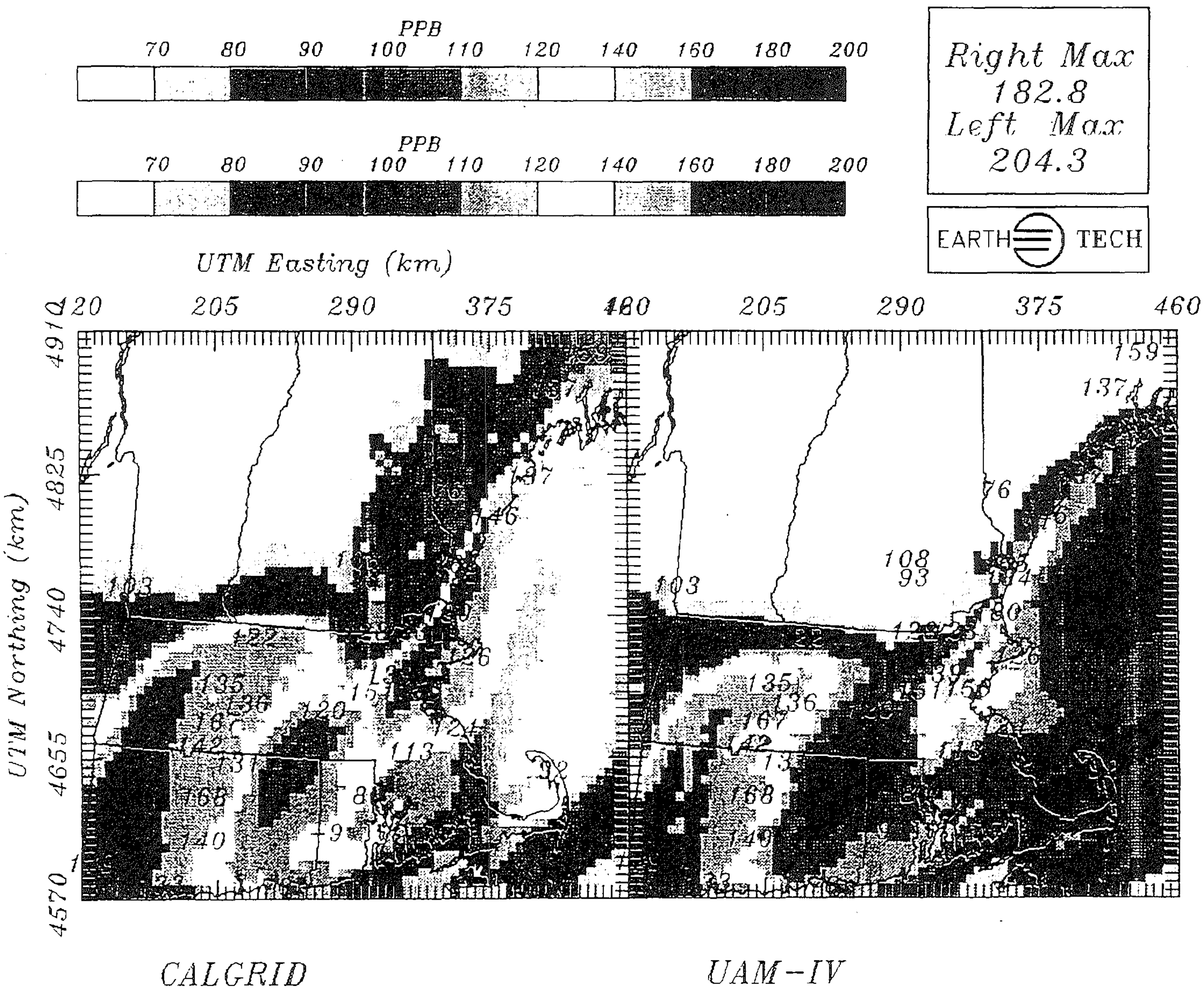
Predicted Surface Ozone for July 8, 1988.



Comparison of CALGRID and UAM-IV models
New England Domain - July 8, 1988

PERFORMANCE EVALUATION STATISTICS

CALGRID with BEIS2	MAINE	NH/MA	RI/MA	Central MA	All	EPA Target
Unpaired Peak Accuracy	-11.0	**-31.3**	**-34.3**	-0.8	-11.0	20%
Ave. Paired Peak Accuracy	18.8	28.8	7.5	20.0	14.8	30%
Normalized Bias	-2.0	**18.2**	**-22.9**	-0.1	-2.5	15%
Gross Error	24.1	27.9	29.7	20.0	25.4	30%
UAM-IV with BEIS						
Unpaired Peak Accuracy	11.2	-18.1	-11.8	4.0	0.7	20%
Ave. Paired Peak Accuracy	**35.8**	**39.3**	12.9	**32.6**	26.2	30%
Normalized Bias	**20.5**	**30.1**	**-16.1**	14.2	12.0	15%
Gross Error	27.6	**31.2**	22.7	23.6	26.7	30%

Notes:
1. Units are percent
2. Negative values - predicted exceeds observed
3. Positive values - observed exceeds predicted
4. Values in **bold face** exceed target

PERFORMANCE EVALUATION SCORES

CALGRID with BEIS2	MAINE	NH/MA	RI/MA	Central MA	All	Total
Unpaired Peak Accuracy	0.4	0.0	0.0	1.0	0.4	1.9
Ave. Paired Peak Accuracy	0.4	0.0	0.8	0.3	0.5	2.0
Normalized Bias	0.9	0.0	0.0	1.0	0.8	2.7
Gross Error	0.2	0.1	0.0	0.3	0.2	0.8
Total	1.9	0.1	0.8	2.6	1.9	**7.3**
UAM-IV with BEIS						**Total**
Unpaired Peak Accuracy	0.4	0.1	0.4	0.8	1.0	2.7
Paired Peak Accuracy	0.0	0.0	0.6	0.0	0.1	0.7
Normalized Bias	0.0	0.0	0.0	0.1	0.2	0.3
Gross Error	0.1	0.0	0.2	0.2	0.1	0.6
Total	0.5	0.1	1.2	1.1	1.4	**4.3**

The statistical comparison is shown in Table 5-3. CALGRID does better in the paired statistics (average paired peak accuracy, normalized bias, and gross error) and not as well in the unpaired peak accuracy. This is partly because CALGRID predicted higher concentrations over the ocean where there are no monitors to verify these predictions. It should be noted that high overwater ozone concentrations have been measured. For example, during the NARSTO-NE program, measurements on the Scotia Prince Ferry during a crossing from Nova Scotia on 1 August 1995 found the highest ozone value of 166 ppb ozone about 100 km to the east of Portland over the ocean.

The scoring scheme gave 7.3 points to the CALGRID model and 4.3 points to the UAM-IV model.

5.4 11 July 1988

The final episode day to be compared is 11 July 1988. The plot comparing the highest hourly ozone concentrations is shown Figure 5-4. Once again, only CALGRID produces the observed ozone along the Maine coast. CALGRID also more closely matches the higher observed concentrations in eastern and southeast Massachusetts.

The general underprediction of UAM-IV is seen in the statistical performance of Table 5-4. CALGRID also displays a general underprediction in the paired statistics, but to a much smaller degree. CALGRID overpredicts the unpaired peak accuracy statistic for three of the four subdomains.

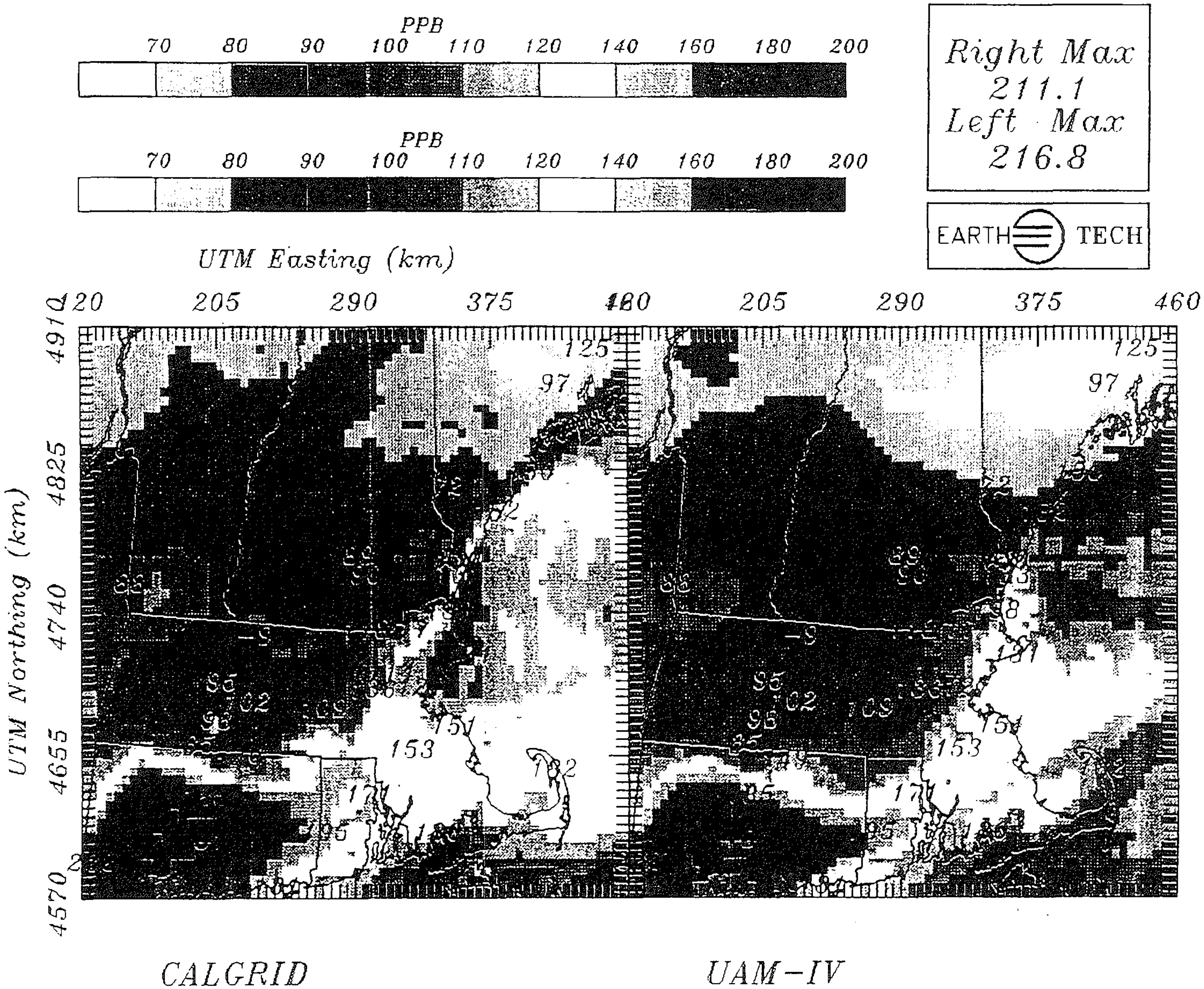
The scoring scheme gives 8.9 points to CALGRID and 5.0 points to UAM-IV.

5.5 Conclusions

The CALGRID model scored higher than UAM-IV for each of the four primary episode days. Statistically, over the whole domain, CALGRID was less than the EPA target values for peak accuracy, bias and gross error for July 8 and July 11, and only exceeded the unpaired peak accuracy for August 17 and June 22. The more stringent average paired peak accuracy was met on both these days. Unpaired peak accuracy is not particularly meaningful because there are usually no monitors to verify the highest predicted concentrations. The relative CALGRID scores would have been even higher if unpaired peak accuracy was not considered. UAM-IV was also less than the EPA target values for July 8 and July 11, but also exceeded the unpaired peak accuracy for June 22 and exceeded both the bias and gross error targets for August 17. If better boundary conditions for June 22 and August 17 were used, instead of the ROM predictions, performance should be improved for these two days.

The comparisons for these four high ozone days show a consistently better performance with CALGRID than with UAM-IV for the New England domain.

Maximum Daily Ozone for July 11, 1988.



Comparison of CALGRID and UAM-IV models
New England Domain - July 11, 1988

PERFORMANCE EVALUATION STATISTICS

CALGRID with BEIS2	MAINE	NH/MA	RI/MA	Central MA	All	EPA Target
Unpaired Peak Accuracy	**-20.1**	-15.7	**20.6**	-3.0	2.3	20%
Ave. Paired Peak Accuracy	18.0	9.7	29.8	20.7	17.1	30%
Normalized Bias	7.1	10.9	1.4	6.7	2.1	15%
Gross Error	21.4	15.3	21.2	12.4	20.0	30%
UAM-IV with BEIS						
Unpaired Peak Accuracy	9.9	13.6	17.0	16.5	4.9	20%
Ave. Paired Peak Accuracy	**33.3**	14.4	**31.4**	23.5	23.6	30%
Normalized Bias	**20.8**	14.7	10.5	12.6	11.0	15%
Gross Error	26.5	20.2	20.7	17.6	23.0	30%

Notes:

1. Units are percent
2. Negative values - predicted exceeds observed
3. Positive values - observed exceeds predicted
4. Values in **bold face** exceed target

PERFORMANCE EVALUATION SCORES

CALGRID with BEIS2	MAINE	NH/MA	RI/MA	Central MA	All	Total
Unpaired Peak Accuracy	0.0	0.2	0.0	0.8	0.9	1.9
Ave. Paired Peak Accuracy	0.4	0.7	0.0	0.3	0.4	1.8
Normalized Bias	0.5	0.3	0.9	0.6	0.9	3.1
Gross Error	0.3	0.5	0.3	0.6	0.3	2.0
Total	1.2	1.7	1.2	2.3	2.5	**8.9**
UAM-IV with BEIS						**Total**
Unpaired Peak Accuracy	0.5	0.3	0.2	0.2	0.8	1.9
Ave. Paired Peak Accuracy	0.0	0.5	0.0	0.2	0.2	1.0
Normalized Bias	0.0	0.0	0.3	0.2	0.3	0.7
Gross Error	0.1	0.3	0.3	0.4	0.2	1.4
Total	0.6	1.2	0.8	1.0	1.5	**5.0**

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