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Transport and Dispersion Model Predictions of Elevated Source Tracer Experiments in the Copenhagen Area: Comparisons of Hazard Prediction and Assessment Capability (HPAC) and National Atmospheric Release Advisory Center (NARAC) Emergency Response Model Predictions

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PREFACE

The U.S. Government has invested heavily in sophisticated computer models to predict the transport and dispersion (T&D) and the ensuing human effects of Chemical, Biological, Radiological, and Nuclear (CBRN) agents and materials. As new modeling capabilities are added, there is a continuing need to verify and validate T&D models through rigorous comparisons to field trial data. Since 2000, IDA has taken part in verification and validation activities connected with the Hazard Prediction and Assessment Capability (HPAC) model developed by the Defense Threat Reduction Agency (DTRA). In past studies we have compared the predictions of HPAC to several field trial data sets, covering a broad range of release conditions, terrain, and weather conditions. Additional insight into model performance and capabilities can be gleaned by comparing the model predictions of two or more models to field trial data and to one another, which is the approach taken in the present study. The second model used in this study is the National Atmospheric Release Advisory Center (NARAC) model, developed by the Lawrence Livermore National Laboratory (LLNL). Two previous collaborative IDA/LLNL studies compared HPAC and NARAC. The first was an exhaustive comparison of HPAC and NARAC predictions to the well-known *Prairie Grass* field trial data. The second study compared HPAC and NARAC predictions for 17 hypothetical releases (a model-to-model comparison). In that study there was general good agreement between HPAC and NARAC. There were some significant differences between HPAC and NARAC for elevated releases, suggesting distinct modeling choices between the two models for elevated releases. Prompted by these results and by a review of vertical transport modeling in the NARAC model by Dr. J. Weil, IDA and LLNL undertook the present study to compare HPAC and NARAC to the Copenhagen releases – a set of ten elevated releases conducted in the late seventies. This document presents the details of this comparison.

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CONTENTS

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EXECUTIVE SUMMARY

EXECUTIVE SUMMARY

A. BACKROUND

This study is part of a continuing effort to support the verification and validation activities associated with DTRA's HPAC model. The specific area of interest in this study is that of elevated releases. In a previous study that compared HPAC to LLNL's NARAC model for a set of hypothetical releases, sizeable differences were observed between HPAC and NARAC for some elevated releases. In those releases HPAC significantly overpredicted the NARAC ground dosages; the HPAC plume exhibited a faster settling rate and larger vertical diffusivity. Prompted by these results, IDA teamed with LLNL to undertake the present study, which compares HPAC and NARAC predictions to a set of ten elevated release experiments – *The Copenhagen Field Trials* – carried out in Copenhagen, Denmark in the late 1970s.

B. STUDY FRAMEWORK

The design of the study was to run each of the models using as much information (e.g., meteorology, terrain, release parameters) as they could ingest, in order to get the best possible "scientific" predictions. This required a great deal of coordination between IDA and LLNL during the initial phases of this work. We emphasize that this was *not* an operational comparison between the two models. IDA performed all of the HPAC runs, while LLNL performed all of the NARAC runs. LLNL provided IDA with spreadsheets containing the Copenhagen sampler data (ground truth concentration data), as well as the meteorological data for each release (mainly wind speeds and directions), which they extracted from the original Copenhagen published literature. LLNL also sent all of their predictions to IDA and IDA performed the comparison analyses.

C. OVERVIEW OF COPENHAGEN RELEASES

The Copenhagen releases comprise a set of ten continuous release Sulfur Hexafluoride (SF_6) tracer experiments conducted in Gladsaxe, Copenhagen in 1978 and 1979. The tracers were released from a TV tower 115 m above ground level (AGL). All releases were roughly 1.5 hours in duration with flow rates ranging from 2.4 - 4.7 gs^{-1}. The downwind region of the release (East of the release) was mainly residential, with an estimated surface roughness of 0.6 m. Releases were conducted under neutral boundary layer conditions (3 releases) and unstable boundary layer conditions (7 releases). Sampling arcs were placed at rough distances of 2 km, 4 km, and 6 km from the release point. Approximately 20 samplers per arc were employed for each release and not all arcs were used for all of the releases. Average concentrations at each sampler were measured over 3 successive 20 minute sampling intervals.

D. HPAC TERRAIN/SURFACE MODES AND WEATHER INPUTS

Four HPAC terrain and surface type combinations were investigated, summarized in the table below.

TABLE 1: HPAC Terrain and Surface Type Run Modes

Mode	Terrain	Surface Type
1	Enabled	Constant surface roughness = 0.6 m
2	Enabled	Landcover data
3	Flat	Constant surface roughness = 0.6 m
4	Flat	Landcover data

Three meteorological input options (referred to as modes herein) were examined for the HPAC runs – a "Full Met" mode and two "Operational" excursions.

The full met mode employed all of available meteorological inputs that could be used by HPAC, namely wind speed, wind direction, and temperature, all at 10-minute intervals, as well as Monin-Obukhov length[1] and inversion height. The operational excursions employed only wind speed and direction (Excursion 1) or wind speed, wind direction, and temperature (Excursion 2). The full met mode was used with all four terrain/surface modes, while the operational excursions were used with terrain/surface Mode 1 only.

E. SUMMARY OF RESULTS

Graphical and statistical comparisons of HPAC and NARAC predictions to the observed one hour average concentrations were performed. The statistical metrics employed were: Fractional Bias (FB), Normalized Absolute Difference (NAD), Normalized Mean Square Error (NMSE), Bounded Normalized Mean Square Error (BNMSE), and FACx, the fraction of prediction to observation concentration ratios within a factor of x^2. We employed Fac2, Fac5, and Fac10. All comparison metrics were computed on a release-by-release basis using concentrations that were paired in space and time and for all data/prediction pairs within the release. Average statistics were also computed by averaging each of the metrics over the releases.

On the whole, HPAC performed best when including terrain and constant surface roughness (Mode 1).

The summary statements that follow apply to HPAC Mode 1 with full met. Similar results were found with the other modes and met options. As measured by the fractional bias, HPAC underpredicted all 9 releases considered for analysis (the first release was not used), while NARAC underpredicted 7 of the 9 releases. HPAC underpredicted NARAC for all of the releases. Table 1 below shows comparative results for HPAC and NARAC for all prediction/observations pairs used in the analysis. HPAC underpredictions relative to the data and to NARAC are clear from the table.

Differences between HPAC and NARAC for all metrics except Fac2, Fac5, and Fac 10 were found to be statistically significant at the 2% level (and at the 1% level using multivariate ANOVA for the combined metrics FB, NAD, BNMSE, Fac2, Fac5, and Fac10).

TABLE 2: Selected Statistical Comparisons of HPAC and NARAC Predictions of the Elevated Copenhagen Releases

	NARAC	HPAC	OBSERVATIONS
Mean (ng/m^3)	690	347	846
Median (ng/m^3)	394	210	399
Fac2	0.419	0.332	
Fac5	0.740	0.732	
Fac10	0.834	0.883	
Fraction underpredicted	0.570	0.774	
Fraction overpredicted	0.430	0.226	
Fraction NARAC > HPAC	0.728		
Fraction HPAC > NARAC	0.272		

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1 The height at which buoyant and inertial convective accelerations are equal.

2 Excluding prediction/observation pairs having zero predictions or zero observations.

Analyses of time sequences of HPAC concentration contours show that the HPAC plume reaches the ground and extends well above the release height in a short time scale, suggesting a large vertical diffusivity (perhaps larger than that of NARAC). With this in mind, we speculate that the "missing" mass in the HPAC simulations either remains lofted or reaches the ground *before the sampling arcs* for these elevated releases. Based on this study, we recommend that the HPAC/SCIPUFF developer reexamine the algorithm and parameterization associated with the representation of vertical diffusivity for elevated releases. The goal of such a reexamination would be to simply identify and trace the original case for verification and validation of these elevated release features.

The major findings of this study are as follows. The main finding is that both HPAC and NARAC underpredict the 1-hour average ground concentrations of the elevated Copenhagen releases, with the HPAC underpredictions being much more pronounced than those of NARAC. With respect to the statistics FB, NAD, NMSE, and BNMSE, the differences between HPAC and NARAC are statistically significant at the 2 percent level. Multivariate ANOVA hypothesis applied to FB, NAD, BNMSE, Fac2, Fac5, and Fac10 shows that HPAC and NARAC differ at the 1% level of significance. Resampled HPAC and NARAC summed concentration MOEs are also well separated. The 4 HPAC terrain /landcover modes and the 3 met options do not "fix" the severe HPAC underpredictions. Finally, the HPAC vertical slice concentration contours suggest that the modeled HPAC vertical diffusivity is larger than what was present during the releases.

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OUTLINE

- **MOTIVATION FOR THIS STUDY: A REVIEW OF PAST HPAC/NARAC COMPARISONS**

- **REVIEW OF THE *COPENHAGEN TRACER EXPERIMENTS***

- **COMPARISON PROTOCOLS, HPAC RUN MODES AND WEATHER MODES**

- **STANDARD STATISTICS AND MEASURES OF EFFECTIVENESS (MOES)**

- **INDIVIDUAL RELEASES**

- **ANALYSIS OF RESULTS**

- **SUMMARY**

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BRIEFING REPORT

INTRODUCTION

This work was funded by the Defense Threat Reduction Agency (DTRA) as part of validation efforts for their Hazard Prediction Assessment Capability (HPAC) model. IDA was tasked by DTRA to provide independent technical analyses of the HPAC system in support of the DTRA validation efforts. The work carried out in this study is the third in a series of works that involve HPAC and the National Atmospheric Release Advisory Center (NARAC) model, developed by the Lawrence Livermore National Laboratory (LLNL). NARAC currently serves as the Department of Homeland Security (DHS) hazardous material atmospheric transport and dispersion model within the Interagency Modeling and Atmospheric Assessment Center (IMAAC). The purpose of the study was to advance the HPAC and NARAC model physics using field data from the Copenhagen tracer releases conducted in the late seventies. This study was not intended to be an operational intercomparison or evaluation between the HPAC and NARAC systems, as much of the information used is typically not available during an operation response. The companion evaluation of the NARAC modeling system by Weil is also available [Ref. 3].

INTRODUCTION

- **Preface**
  - **Institute for Defense Analyses (IDA) is a non-profit research and development center, serving the Office of the Secretary of Defense, Defense Agencies, Unified Combatant Commands, and the Joint Staff.**
  - **For this task, we provide <u>independent</u> technical analyses to support model validation efforts.**

- **Atmospheric Transport and Dispersion Models are Required by U.S. Government**
  - **DOD: chemical and biological attacks on the battlefield or at military facilities**
  - **DHS: terrorist attacks on homeland**

- **Models Examined in this Study**
  - *Hazard Prediction and Assessment Capability (HPAC): DTRA*
  - *National Atmospheric Release Advisory Center (NARAC) Model : DHS/LLNL-DOE*

BRIEF MODEL DESCRIPTIONS

The HPAC and NARAC methodologies are summarized in the slide. The modeling approaches for the two models are quite distinct - HPAC uses a puff formulation, while NARAC uses a particle propagation formulation. Additionally, meteorological data are assimilated by unique sub-models for the 2 models.

Version numbers of the models and sub-models used in this comparison are also listed. Both models have been used extensively in their respective arenas. Additional descriptions of these models can be found in IDA papers P-3554, P-3555, references [1] and [2], respectively on the next slide.

BRIEF MODEL DESCRIPTIONS

- **HPAC - Version 4.04, Service Pack 3 (4.04.012)**
  - *Second-Order Closure Integrated Puff Model (SCIPUFF)*
    - Lagrangian model that uses Gaussian puff method; turbulent dispersion parameterization is based on second-order closure theory, allowing for estimation of concentration mean *and* variance
    - Version 2.2
  - *Stationary Wind Fit and Turbulence (SWIFT)*
    - Mass-consistent wind field model
  - Applied to military planning and various national defense problems
- **NARAC**
  - *Lagrangian Operational Dispersion Integrator (LODI)*
    - Lagrangian Monte Carlo model: Solves 3D advection-diffusion equation by integrating a stochastic differential equation
    - Version 1.0 2003 Dec23 (Random number seed 79836158.0000000)
  - *Atmospheric Data and Parameterization Tool (ADAPT)*
    - Data assimilation tool that constructs meteorological fields using a variety of interpolation techniques and atmospheric parameterizations
    - Version DEV2.12
  - Serves as the primary atmospheric transport and dispersion modeling system for the Department of Homeland Security (DHS) Interagency Modeling & Atmospheric Assessment Center (IMAAC) and Department of Energy (DOE) Atmospheric Release Advisory Center (ARAC)

PREVIOUS HPAC-NARAC COMPARISIONS

Two previous studies that compare HPAC and NARAC are listed in the slide. The *Prairie Grass* field trials were examined in an extensive comparison in Warner S., Platt, N., Heagy, J. F., Bradley, S., Bieberbach, G., Sugiyama, G., Nasstrom, J. S., Foster, K. T, and Larson, D., 2001: *User-Oriented Measures of Effectiveness for the Evaluation of Transport and Dispersion Models*, IDA Paper P-3554, 797 pp, January 2001 (reference [1]). Both HPAC and NARAC compared favorably to these short-range field trials, performing best for unstable releases. NARAC was found to be somewhat more conservative than HPAC for low threshold dose comparisons (NARAC displayed fewer false negatives and more false positives).

HPAC and NARAC were also compared in a model-to-model study: Warner, S., Heagy, J. F., Platt, N., Larson, D., Sugiyama, G., Nasstrom, J. S., Foster, K. T., Bradley, S., and Bieberbach, G., 2001: *Evaluation of Transport and Dispersion Models: A Controlled Comparison of Hazard Prediction and Assessment Capability (HPAC) and National Atmospheric Release Advisory Center (NARAC) Predictions*, IDA Paper P-3555, 251 pp, May 2001 (reference [2]). Seventeen releases were analyzed with good overall agreement found between HPAC and NARAC. Slight model differences were observed as functions of particle size and atmospheric stability. Some significant differences (shown in the next two slides) were observed as a function of release height.

PREVIOUS HPAC – NARAC COMPARISONS

- *Prairie Grass* Field Experiment

  - *Similar model performance* - both models performed best for releases that occurred during unstable conditions

  - NARAC somewhat more "conservative" (overpredictive) than HPAC with respect to predicting hazard regions (i.e., samplers at which a low threshold is exceeded)
    - Fewer false negatives
    - Higher false positives

  - [1] Warner S., Platt, N., Heagy, J. F., Bradley, S., Bieberbach, G., Sugiyama, G., Nasstrom, J. S., Foster, K. T, and Larson, D., 2001: *User-Oriented Measures of Effectiveness for the Evaluation of Transport and Dispersion Models*, IDA Paper P-3554, 797 pp, January 2001.

- "Model-to-Model" Comparisons for 17 Simple Releases

  - Overall, very close agreement, *but only after carefully ensuring the comparability of input parameters and model settings*

  - Differences detected as a function of
    - particle size (slight differences)
    - atmospheric stability (slight differences)
    - release height (some significant differences)

  - [2] Warner, S., Heagy, J. F., Platt, N., Larson, D., Sugiyama, G., Nasstrom, J. S.,Foster, K. T., Bradley, S., and Bieberbach, G., 2001: *Evaluation of Transport and Dispersion Models: A Controlled Comparison of Hazard Prediction and Assessment Capability (HPAC) and National Atmospheric Release Advisory Center (NARAC) Predictions*, IDA Paper P-3555, 251 pp, May 2001.

PREVIOUS MODEL-TO-MODEL STUDY-EXAMPLE DIFFERENCES IN SURFACE DOSAGE FOR HPAC & NARAC PREDICTIONS OF ELEVATED RELEASES

The slide shows surface dosage contours for HPAC (Blue --) and NARAC (Red -) for two elevated releases (MvM 3 and MvM 15) considered in the model-to-model study [2]. MvM 3 was a gas release (SF_6) carried out under stable conditions with a boundary layer height of 100 m and release height of 80 m, while MvM 15 was a particle release carried out under neutral conditions with a boundary layer height of 500 m and release height of 750 m. In each case the HPAC surface dosage contours cover much larger areas than corresponding NARAC dosage contours (NARAC predicts lower surface concentrations than HPAC for these releases).
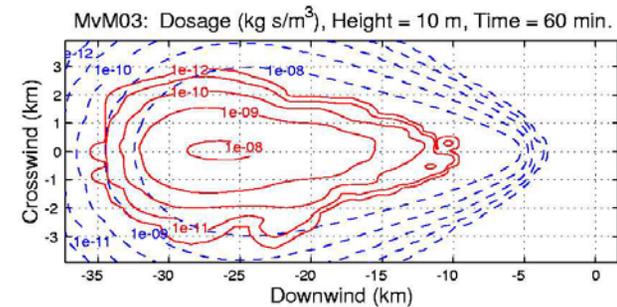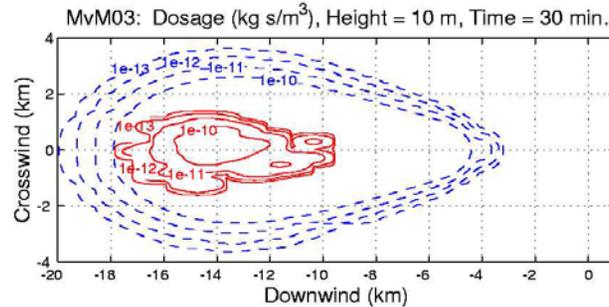
PREVIOUS MODEL-TO-MODEL STUDY
Example Differences in Surface Dosage for
HPAC & NARAC Predictions of Elevated Releases

HPAC (Blue --) and NARAC (Red -) surface dosage contours for two elevated release scenarios: MvM 3 at 30 and 60 Minutes and MvM 15 at 120 and 180 minutes. Each release shows significant NARAC underpredictions with respect to HPAC (from reference [2]).
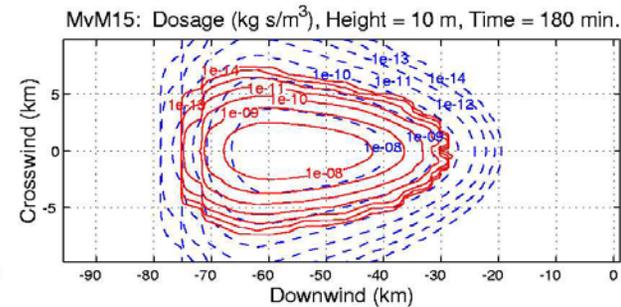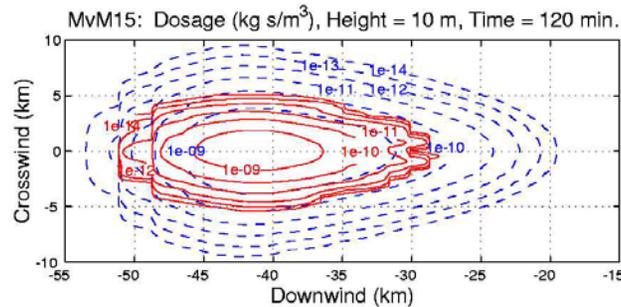
MvM 3

1 kg instantaneous "gas" release
Stable boundary layer
Release height = 80 m
Boundary layer height =100 m

MvM 15

1 kg instantaneous "particle" release
Neutral boundary layer
Release height = 750 m
Boundary layer height = 500 m

PREVIOUS MODEL-TO-MODEL STUDY NARAC AND HPAC INSTANTANEOUS CONCENTRATIONS: VERTICAL SLICE FOR ELEVATED RELEASE MVM 3

The figure in the slide shows a comparison of HPAC and NARAC concentration contours over time for the elevated release MvM 3 [2]. The HPAC contours show enhanced settling and enhanced vertical dispersion with respect to the NARAC contours, indicating distinct modeling choices for the two models.

PREVIOUS MODEL-TO-MODEL STUDY
NARAC and HPAC Instantaneous Concentrations:
## Vertical Slice for Elevated Release MvM 3

NARAC and HPAC 10^{-9} kg/m³ (1000 ng/m³) instantaneous concentration contours at t = 10, 20, 30, 40, 50, and 60 minutes. The material is moving from right to left. The HPAC contours show much greater vertical diffusion and descend at a greater rate (from reference [2]).

NARAC

HPAC

MvM 3 Release Description

1 kg instantaneous "gas" release
Stable boundary layer
Release height = 80 m
Boundary layer height =100 m

MvM03: Concentration (kg/m³),Vertical Slice at y = 0 km
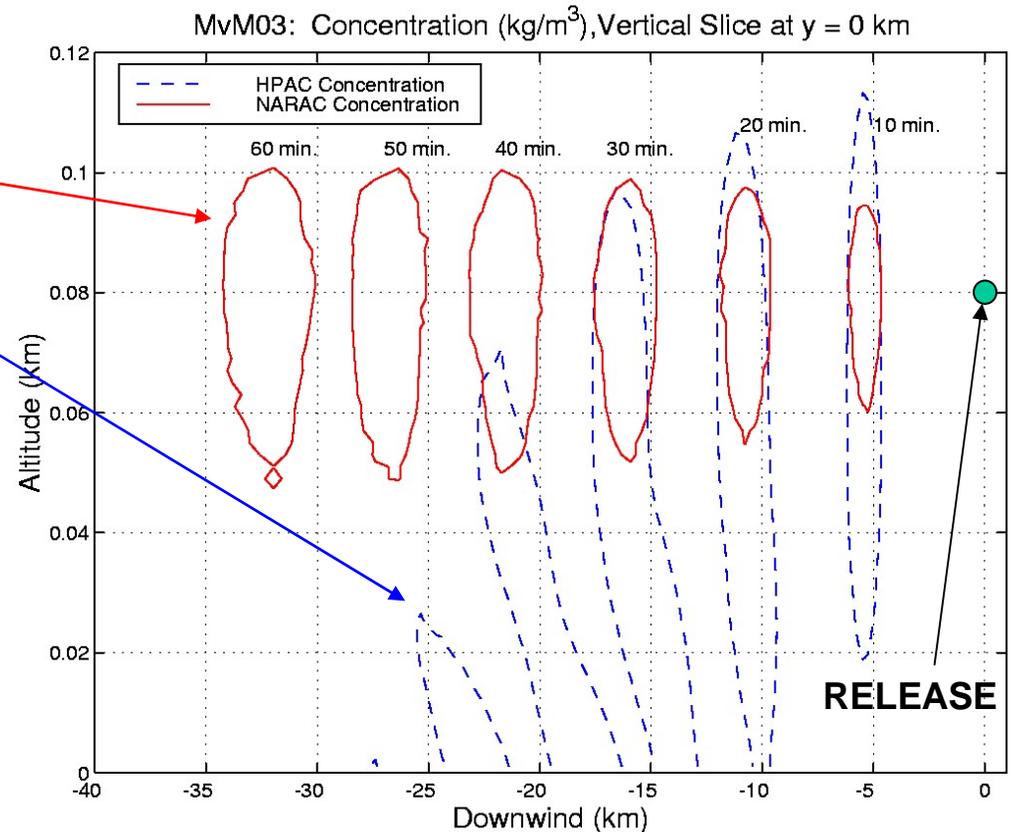
RECENT ANALYSES SUGGEST NEED FOR ELEVATED RELEASE EXAMINATIONS

Recent studies with HPAC and NARAC suggest there is a need for enhanced modeling capabilities for elevated releases for both models. Comparisons of HPAC to the Over-Land Wind Dispersion (OLAD) field experiment data showed under-predictions for some of the elevated releases. A recent review of NARAC (Weil, J. C., *Review of Approaches and Data Sets for Evaluation of the NARAC Modeling System*, Cooperative Institute in Environmental Sciences Report no. UCRL-TR-2011989, September 2003), identified the need for more complete testing of NARAC vertical dispersion formulations. This report specifically recommends comparisons of NARAC to the Copenhagen Tracer Experiments. The recommended evaluation of the NARAC modeling system with the Copenhagen field data was performed. In summary, the NARAC predictions were in good overall agreement (60 percent of the NARAC predictions were within a factor of 2 of the observations after accounting for the meteorological uncertainty) See [3] for more details including a discussion of the NARAC vertical dispersion parameterization. We note that the Copenhagen releases were conducted under unstable or neutral conditions with release heights well below the boundary layer height. Therefore, the present study is unlikely to explain the previously noted model-to-model differences. However, we expect the results of this study will further characterize this issue.

RECENT ANALYSES SUGGEST NEED FOR ELEVATED RELEASE EXAMINATIONS

- **Over-Land Along-Wind Dispersion (OLAD) Field Experiment**
  - HPAC under-predictions of some elevated releases

- **Recent Review for NARAC Evaluation Approaches**
  - **[3] Weil, J. C., *Review of Approaches and Data Sets for Evaluation of the NARAC Modeling System*, Cooperative Institute for Research in Environmental Sciences Report no. UCRL-TR-201989, September 2003.**
  - Identifies several attributes of field experiments that would support future NARAC evaluation
  - Calls for more complete testing of vertical dispersion formulations
  - Specifically recommends Copenhagen Tracer Experiments of 1978/1979

- **Weil, J. C., *Evaluation of the NARAC Modeling System: Final Report to the Lawrence Livermore National Laboratory*, Cooperative Institute for Research in Environmental Sciences Report no. UCRL-TR-217329, September 2004.**
  - Evaluated NARAC with both Copenhagen field data and a Large Eddy Simulation particle model
  - Demonstrated overall good agreement between NARAC predictions and Copenhagen field data (60% of the NARAC predictions were within a factor of 2 of the observations after accounting for wind direction uncertainty)
  - Evaluated NARAC vertical dispersion parameterization: overall parameterization was reasonable, although for elevated releases under unstable atmospheric conditions NARAC modestly underpredicts surface concentrations near the source

OVERVIEW OF COPENHAGEN RELEASES

The releases considered in this study were conducted in the Gladsaxe region of Copenhagen and cover a period from 14 September 1978 though 19 July 1979 [refs. 4, 5, 6]. Ten separate continuous releases of the tracer gas Sulfur Hexafluoride (SF_6) were carried out. Release durations were all approximately 1.5 hours and SF_6 flow emission rates ranged from 2.4 gs^{-1} to 4.7 gs^{-1}. All sources were situated on a TV tower 115 meters above ground level (AGL). The downwind region of the release site (mainly East of the releases) was residential, with an estimated surface roughness of 0.6 m [4]. Three releases were conducted under neutral boundary layer conditions, while 7 were conducted under unstable boundary layer conditions. Weather measurements were taken at several heights along the TV tower; measurements included temperature, wind speed, and wind direction at 10-minute intervals. Hourly averaged vertical and cross-wind wind speed fluctuations were also measured near the point of the releases. Three "arcs" of SF_6 samplers were employed in the experiments at distances of roughly 2 km, 4 km, and 6 km from the release location. Each sampling unit contained 3 plastic bags that were inflated sequentially in 20-minute sampling periods, for a net sampling period of one hour per sampler. Details of the sampling methodology can be found in [4] and [5]. Approximately 20 samplers per arc were employed in the releases and not all arcs were used for all of the releases.

OVERVIEW OF COPENHAGEN RELEASES

- The Copenhagen releases comprised 10 continuous release SF_6 tracer experiments conducted in Gladsaxe Copenhagen, spanning 14 Sep. 1978 to 19 July 1979. Release durations were roughly 1.5 hour, with flow emission rates ranging from 2.4 - 4.7 gs^{-1}.

- All tracers were released from a TV tower at 115 m AGL. The downwind region of the release (East of the release) was mainly residential, with an estimated surface roughness of 0.6 m.

- Releases were conducted under neutral boundary layer conditions (3 releases) and unstable boundary layer conditions (7 releases).

- Temperature, wind speed and direction measurements were taken at various heights along the tower at 10 minute intervals. Hourly averaged vertical and lateral wind fluctuations were also measured near the release point.

- Sampling arcs were placed at rough distances of 2 km, 4 km, and 6 km from the release point. Approximately 20 samplers per arc were employed for each release. Not all arcs were used for all of the releases.

- Average concentrations at each sampler were measured over 3 successive 20 minute sampling intervals.

COPENHAGEN REFERENCES

The three main Copenhagen release references are listed on the slide.

COPENHAGEN REFERENCES

[4] Gryning, Sven-Erik, *Elevated Source SF$_6$-Tracer Dispersion Experiments in the Copenhagen Area*, Ph.D. Thesis, Technical University of Denmark, Risø National Laboratory, Risø-R-446, 1981.

[5] Gryning, Sven-Erik, Lyck, E., *Atmospheric Dispersion for Elevated Sources in an Urban Area: Comparison Between Tracer Experiments and Model Calculations*, Journal of Climate and Applied Meteorology <u>23</u>, 651-660, April 1984.

[6] Gryning, Sven-Erik, Lyck, E., *The Copenhagen Tracer Experiments: Reporting of Measurements*, Risø National Laboratory, Risø-R-1054, August 2002.

RELEASE SPECIFICS

The release location is shown in this 4 km x 4 km overhead photograph, which also shows the residential area east (downwind) of the release point. Since the image date is 2005, details of the downwind region are not expected to match those present in 1978 and 1979. Quantitative details of the 10 releases are shown in the table. Local Copenhagen time is two hours later than UTC, so with the exception of the first (9/14/78) release, the releases were carried out in early to mid afternoon.

RELEASE SPECIFICS

Release location

UTM : (342580 m Easting, 6179610 m Northing),
Zone 33 = (55.7366° N, 12.4927° E)
Release height: 115 m AGL

Residential area: surface roughness = 0.6 m [4]
(Note: a surface roughness of 0.5 m is associated
with mixed forest, towns and cities)

Note: 2005 overhead photo
Dimensions: 4 km x 4 km
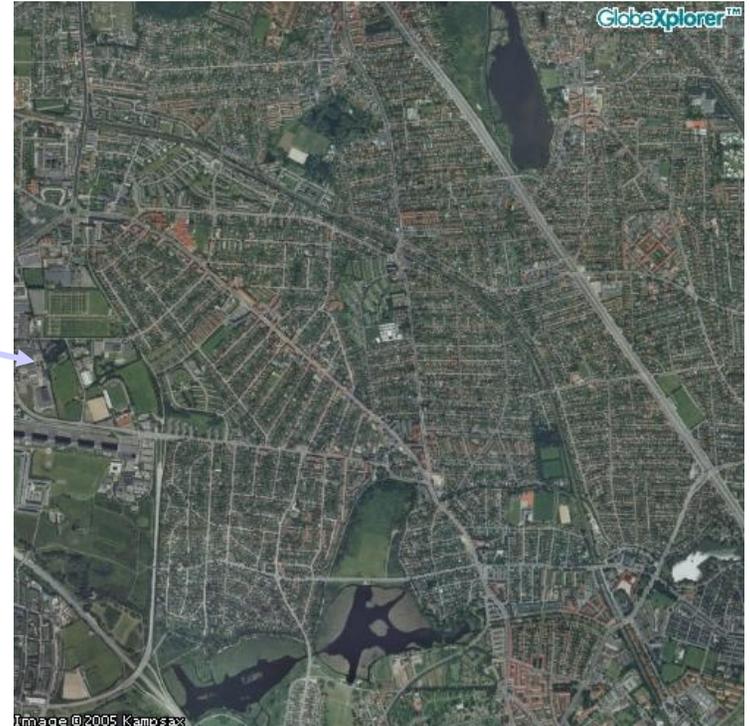
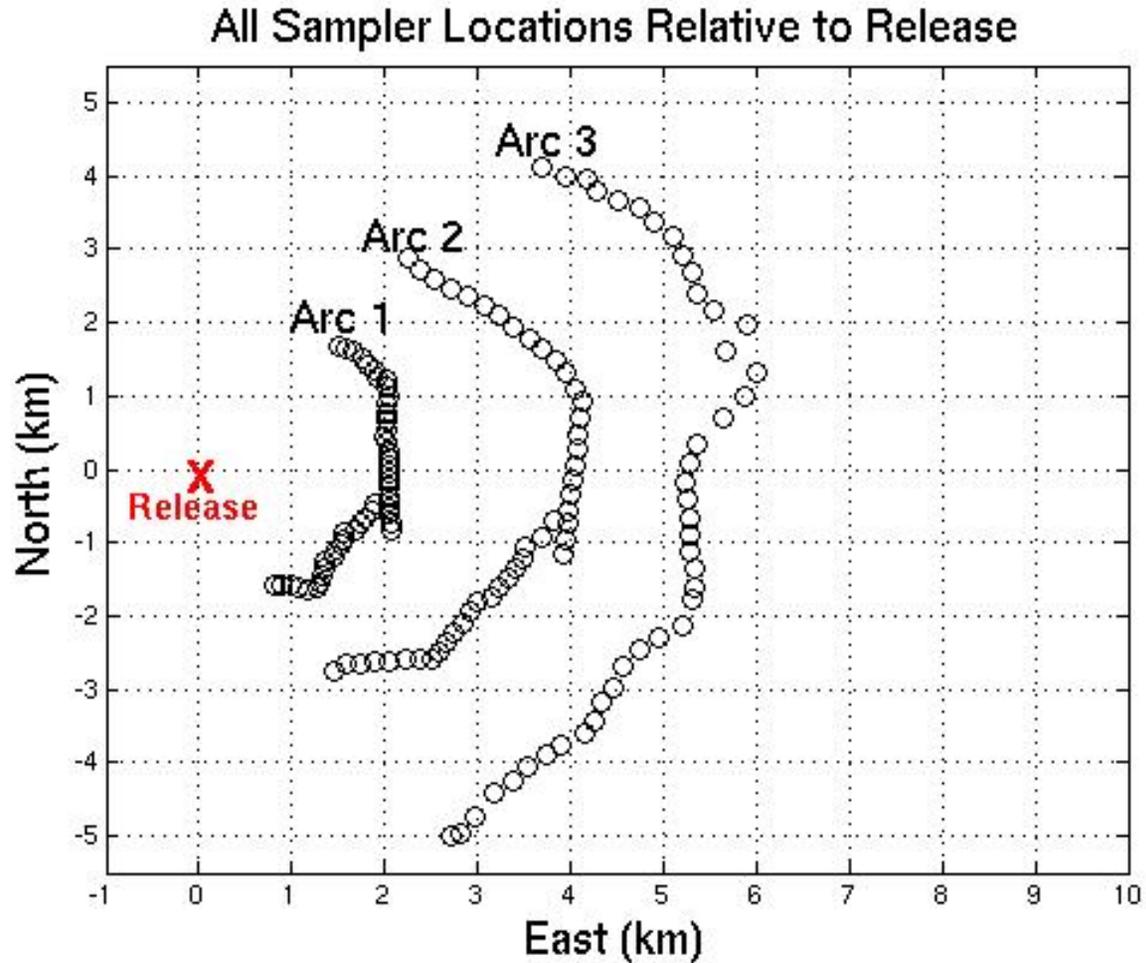| Number	Date	Release start (UTC)	Release stop (UTC)	Release duration (hr:min)	Sampling start (UTC)	Sampling stop (UTC)	Sampling duration (hr:min)	Tracer release rate (g/s)
1	9/14/78	14:00	15:25	1:25	14:23	15:23	1:00	4.70
2	9/20/78	11:45	13:17	1:32	12:17	13:17	1:00	3.20
3	9/26/78	10:21	11:40	1:19	10:40	11:40	1:00	3.20
4	10/19/78	10:47	12:18	1:31	11:13	12:13	1:00	3.20
5	11/3/78	12:02	13:21	1:19	12:20	13:20	1:00	2.30
6	11/9/78	11:46	13:27	1:41	12:26	13:26	1:00	3.20
7	4/30/79	11:41	13:02	1:21	12:02	12:42	0:40	3.10
8	6/27/79	11:25	12:45	1:20	11:45	12:45	1:00	2.40
9	7/6/79	11:30	12:55	1:25	11:50	12:50	1:00	3.00
10	7/19/79	10:50	12:20	1:30	11:15	12:18	1:03	3.30

SAMPLER LAYOUT - ALL SAMPLERS

The figure shows the Copenhagen sampler locations with Easting (x) and Northing (y) coordinates relative to the release point (0, 0). The three sampler arcs are roughly 2 km, 4 km, and 6 km from the release location. Approximately 20 samplers per arc were used for each release and not all arcs were active for all of the releases. The UTM coordinates of the samplers are given in a backup slide. Activated samplers for each release are also pictured in a backup slide.

All Sampler Locations Relative to Release

METEOROLOGICAL OVERVIEW OF RELEASES

The table at the top of the slide, adapted from Table 1 in [5], shows the overall meteorological conditions for the 10 releases. The Monin-Obukhov length (L), inversion height (zi), friction velocity (not listed in the table), and Pasquill stability class for the releases are derived parameters. Details for their origin are described in [5]. The derived Pasquill stability class appears to be inconsistent with the zi/L ratio for some of the releases. For example, release 10, with a zi/L ratio of –5.5, has an assigned stability class of D (neutral), even though release 6, with a zi/L ratio of –1.4, is declared class C (slightly unstable). The box at the bottom of the slide summarizes the meteorological measurements and their altitudes above ground level (AGL) taken along the TV tower. Wind speed, wind direction, and temperature data were taken at 10-minute intervals at the indicated altitudes. Vertical and cross-wind wind speed fluctuation measurements were one hour averages. All meteorological data for the HPAC and NARAC runs were extracted from data tables in reference [6].

METEOROLOGICAL OVERVIEW OF RELEASES

Number	Date	Mean Wind Speed (m/s) 115 m	Mean Wind Speed (m/s) 10 m	Hourly Averaged Wind Fluctuations σ_v (m/s)	Hourly Averaged Wind Fluctuations σ_w (m/s)	L: Monin-Obukhov Length (m)	z_i: Inversion Height (m)	z_i/L	Pasquill Stability Class
1	9/14/78	8.9	-	1.14	0.68	-	-	-	D: Neutral
2	9/20/78	3.4	2.1	0.98	0.83	-46	1980	-43.0	C: Slightly Unstable
3	9/26/78	10.6	4.9	1.39	1.07	-384	1920	-5.0	C: Slightly Unstable
4	10/19/78	5.0	2.4	0.85	0.68	-108	1120	-10.4	C: Slightly Unstable
5	11/3/78	4.6	2.5	0.47	0.47	-173	390	-2.3	C: Slightly Unstable
6	11/9/78	6.7	3.1	0.77	0.71	-577	820	-1.4	C: Slightly Unstable
7	4/30/79	13.2	7.2	2.26	1.33	-569	1300	-2.3	D: Neutral
8	6/27/79	7.6	4.1	1.61	0.87	-136	1850	-13.6	B-C: Moderately Unstable
9	7/6/79	9.4	4.2	1.35	0.72	-72	810	-11.3	B-C: Moderately Unstable
10	7/19/79	10.5	5.1	1.71	0.98	-382	2090	-5.5	D: Neutral

Table adapted from reference [5]; Friction velocity for each release also estimated

Release height for all releases: 115 m AGL

Meteorological measurements taken along TV tower

- **Temperature**
  - **Heights: 2m, 40m, 80m, 120m, 160m, 200m AGL**
  - **10 minute intervals**
- **Wind speed**
  - **Heights: 10m, 60m, 120m, 200m AGL**
  - **10 minute intervals**
- **Wind direction**
  - **Heights: 10m, 120m, 200m AGL**
  - **10 minute intervals**
- **Crosswind (s_v) and vertical (s_w) wind fluctuations**
  - **Height: 115m AGL (release height)**
  - **One hour averages**

NARAC MODEL RUN PROTOCOLS

The NARAC runs for this study were performed by Lawrence Livermore National Laboratory (LLNL) researchers. All releases were modeled, except for release 1 (9/14/78), which was omitted because of a lack of consistent input meteorology data relative to the other releases (complicating a best-physics analysis). One hour average SF_6 concentrations were computed over the collection times given in the table in slide 11; concentrations were computed at the sampler locations and on an approximate 20 km x 20 km horizontal grid with 100 m grid resolution. The 10-minute wind speed and direction data were averaged over one hour (to be consistent with the sigma v and sigma w averaging times) and these one hour averages were used for the NARAC input winds. Other NARAC meteorological inputs were: friction velocity, Monin-Obukhov length, surface roughness (0.6 m), inversion height, and lateral wind fluctuations (σ_v). Parameters that were not used included vertical wind fluctuations (σ_w), Pasquill stability class (this information is duplicative after specifying the Monin-Obukhov length), and temperature. For simplicity, terrain was not used as an input for the NARAC calculations reported here (there was negligible difference between runs with and without terrain). The averaging time for the NARAC calculations was set to one hour.

NARAC MODEL RUN PROTOCOLS

- **Model runs performed by LLNL**
  - **All releases modeled except for 09/14/78 release**
  - **1 hour average SF$_6$ concentrations computed at sampler locations and on ~ 20 km x 20 km horizontal grid with 100 m grid resolution**

- **Meteorological inputs**
  - **Wind speed and direction (1 hour averages)**
  - **Friction velocity**
  - **Monin-Obukhov (MO) length**
  - **Surface roughness (0.6 m)**
  - **Inversion height**
  - **Sigma v (lateral wind fluctuations)**

- ***Not used*****:**
  - **Sigma w (vertical wind fluctuations)**
  - **Pasquill stability class (this information is duplicative after specifying the Monin-Obukhov length)**
  - **Temperature**

- **Terrain not used**

- **One hour averaging times**

HPAC MODEL RUN PROTOCOLS

The HPAC runs for this study were performed by IDA research staff. All releases were modeled except for release 1 (9/14/78). This release could not be modeled because of an invalid weather profile (.prf file) [error # 99 in the .log file from the SCIPUFF Weather Input Model (SWIM)]. We speculate that the cause of this error is the absence of any co-located wind speed and wind direction data along the tower; this did not occur for any of the other releases. Twenty-minute average SF_6 concentrations as well as one-hour concentrations were computed at the sampler locations and on the NARAC grid discussed in the previous slide. HPAC runs employed the raw 10-minute wind speed, wind direction, and temperature data. Other HPAC meteorological inputs were: Monin-Obukhov length, surface roughness (0.6 m), inversion height, and Pasquill stability class. Parameters that were not used included friction velocity (HPAC does not accept this as input), vertical wind fluctuations (σ_w), and lateral wind fluctuations (σ_v). While HPAC does accept σ_w and σ_v as inputs, it does so only for preparation of hazard areas, not concentration outputs. Terrain was used as an input for the HPAC calculations, however terrain was toggled off for some excursion runs. The averaging time for all HPAC calculations was set to 20 minutes; this matches the collection time (3 sampler bags per sampler, 20-minutes each) [4, 5].

HPAC MODEL RUN PROTOCOLS

- **Model runs performed by IDA**
  - **All releases modeled except for 09/14/78 release**
    - **SCIPUFF Weather Input Model (SWIM) reports invalid weather profile (.prf file); error # 99 in .log file**
    - **Error possibly due to absence of any co-located wind speed and wind direction data**
  - **20 minute average concentrations and 1 hour average concentrations computed**
- **Meteorological inputs**
  - **Wind speed and direction (10 minute updates)**
  - **Temperature (10 minute updates)**
  - **MO length**
  - **Pasquill stability class (overridden by MO length, when MO is also used)**
  - **Surface roughness**
  - **Inversion height**
- ***Not used*:**
  - **Friction velocity (HPAC cannot accept)**
  - **Sigma v and Sigma w (fluctuation inputs used only for creation of HPAC hazard areas)**
- **Terrain used (excursion runs performed without terrain)**
- **20 minute averaging times (matches collection times)**

FOUR HPAC TERRAIN/ SURFACE MODES EXAMINED

Four HPAC terrain and surface mode combinations were investigated. Modes 1 and 2 employed terrain, while modes 3 and 4 did not. Modes 1 and 3 used a constant surface roughness of 0.6 m, while modes 2 and 4 used the HPAC internal landcover database. One finding uncovered in these investigations was that when HPAC sampler coordinates for Mode 3 (no terrain, surface roughness = 0.6 m) were entered in UTM coordinates, the output concentrations (in the .smp file) were zero at all sampler locations and all times. The other three modes did not display this behavior. Converting the Mode 3 sampler coordinates to latitude and longitude alleviated the zero output problem, although without having access to the HPAC source code, it is not possible to know the exact representation of the internal UTM to lat/lon conversion that HPAC employs. Sampler conversions were carried out with GEOTRANS 2.2.6, a National Geospatial Intelligence Agency (NGA) conversion utility available at **http://earth-info.nima.mil/GandG/geotrans**. It would be useful to allow UTM coordinates to be used for all sampler files, irrespective of terrain or landcover usage, and we suggest that the HPAC developer consider adding this functionality.[2]

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[2] According to the HPAC developer this functionality exists, however there is no mention of it in the HPAC/SCIPUFF documentation.

FOUR HPAC TERRAIN/ SURFACE MODES EXAMINED

- *Mode 1: Terrain on, Surface roughness = 0.6 m*
- *Mode 2: Terrain on, Landcover enabled*
- *Mode 3: Terrain off, Surface roughness = 0.6 m*
- *Mode 4: Terrain off, Landcover enabled*
- **HPAC output sampler specifications**
  - **UTM sampler coordinates used for both terrain "on" cases and terrain "off", landcover "enabled" case**
  - **UTM coordinates *do not work* with terrain "off", surface roughness = 0.6 m case; *concentration outputs in .smp file are all zeros***
    - **Lat/lon coordinates required to get nonzero output**
    - **Lat/lon conversions made with GEOTRANS 2.2.6 (NGA utility, available at http://earth-info.nima.mil/GandG/geotrans/)**
    - **Unknown whether internal HPAC conversions match those of GEOTRANS 2.2.6**
    - **Recommend HPAC add UTM functionality with terrain off**
      - *Have recently learned that this capability does exist in HPAC, although there is no mention of it in the HPAC/SCPIFF technical documentation*

THREE HPAC METEOROLOGICAL INPUT OPTIONS EXAMINED

Three meteorological input options were examined for the HPAC runs – a "Full Met" mode and two "Operational" excursions. The full met mode employed all of available meteorological inputs that could be used by HPAC, namely wind speed, wind direction, and temperature, all at 10-minute intervals, as well as Monin-Obukhov length, and inversion height. Pasquill stability information was also entered into the HPAC profiles (.prf files), however, according to the SCIPUFF Technical Documentation [7], this is ignored when the Monin-Obukhov length is also entered. The operational excursions employed only wind speed and direction (Excursion 1) or wind speed, wind direction, and temperature (Excursion 2). The full met mode was used with all four terrain/surface modes, while the operational excursions were used with terrain/surface Mode 1 only.

THREE HPAC METEOROLOGICAL INPUT OPTIONS EXAMINED

- **"Full" meteorology**
  - **Wind speed and direction at 10 minute intervals**
  - **Temperature at 10 minute intervals**
  - **Inversion height**
  - **Monin-Obukhov length**
  - **PGT stability category (overridden by MO length)**
  - *Employed with all 4 HPAC terrain/surface modes*
- **Excursion 1: "Operational" meteorology**
  - **Wind speed and direction at 10 minute intervals**
  - *Employed with terrain on, SR=0.6 m (Mode 1) only*
- **Excursion 2: "Operational with temperature" meteorology**
  - **Wind speed and direction at 10 minute intervals**
  - **Temperature at 10 minute intervals**
  - *Employed with terrain on, SR=0.6 m (Mode 1) only*

STATISTICAL COMPARISON METRICS EMPLOYED

The slide shows five comparison metrics employed in our analyses, where C_P stands for predicted concentration and C_O stands for observed concentration. These metrics are: Fractional Bias (FB), Normalized Absolute Difference (NAD), Normalized Mean Square Error (NMSE), Bounded Normalized Mean Square Error (BNMSE), and FACx, the fraction of prediction to observation concentration ratios within a factor of x, excluding prediction/observation pairs with zero predictions or zero observations. We employ Fac2, Fac5, and Fac10 in this study. In this study all comparison metrics are computed on a release-by-release basis using concentrations that are paired in space and time and for all data/prediction pairs within the release. Additionally, average metrics are computed by averaging each of the metrics over the nine releases.

STATISTICAL COMPARISON METRICS EMPLOYED

Fractional Bias (FB):

$$FB = \frac{(\overline{C_P} - \overline{C_O})}{0.5(\overline{C_P} + \overline{C_O})}$$

Normalized Absolute Difference (NAD):

$$NAD = \frac{\sum_{i=1}^{n} |C_P^{(i)} - C_O^{(i)}|}{\sum_{i=1}^{n} |C_P^{(i)} + C_O^{(i)}|} = \frac{\overline{|C_P - C_O|}}{\overline{C_P} + \overline{C_O}}$$

Normalized Mean Square Error (NMSE):

$$NMSE = \frac{\overline{(C_P - C_O)^2}}{\overline{C_P}\,\overline{C_O}}$$

Bounded Normalized Mean Square Error (BNMSE):

$$BNMSE = \frac{\sum_{i=1}^{n}(C_P^{(i)} - C_O^{(i)})^2}{\sum_{i=1}^{n}(C_P^{(i)} + C_O^{(i)})^2} = \frac{\overline{(C_P - C_O)^2}}{\overline{(C_P + C_O)^2}}$$

FACx = fraction of cases for which $1/x \leq C_P/C_O \leq x$ **, excluding prediction/ observation pairs for which** $C_P=0$ **or** $C_O=0$**. Specifically, we employ Fac2, Fac5, and Fac10.**

All metrics are computed for each release over all concentrations, paired in space and time

35

AREA-BASED MEASURE OF EFFECTIVENESS (MOE): FALSE NEGATIVES AND FALSE POSITIVES

The figure in the slide shows three areas used in formulating the Area-based Measure of Effectiveness (MOE), the overlap area, AOV, the false negative area, AFN, and the false positive area, AFP.

Area-Based Measure of Effectiveness (MOE):
False Negatives and False Positives
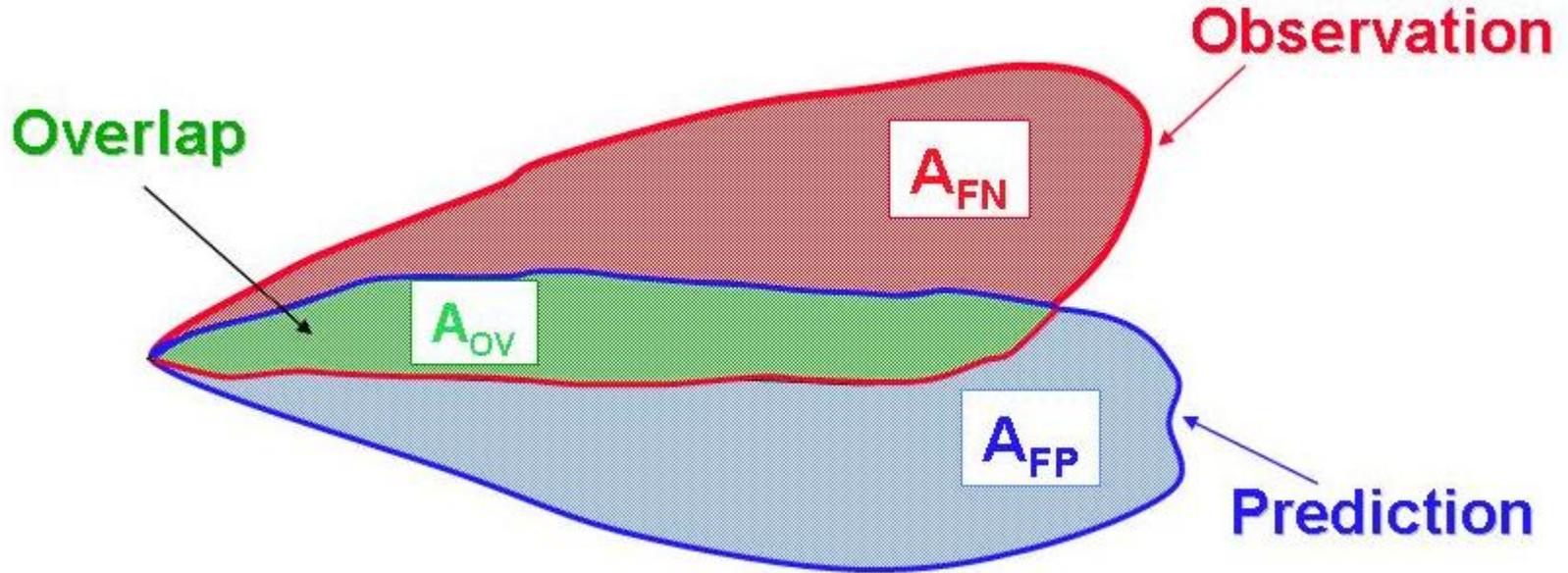
A_{FN} = Area of *False Negative*
A_{OV}= Area of Overlap
A_{FP} = Area of *False Positive*

A_{OB} = Area of Observation = A_{OV}+A_{FN}
A_{PR} = Area of Prediction = A_{OV}+A_{FP}

AREA-BASED MEASURE OF EFFECTIVENESS (MOE): FALSE NEGATIVE AND FALSE POSITIVE FRACTIONS

The slide shows the definition of the false negative fraction f_{FN} and false positive fraction f_{FP}. The two-dimensional MOE has x and y coordinates given respectively by MOEx $=1- f_{FN}$ and MOEy$=1- f_{FP}$.

Area-Based Measure of Effectiveness (MOE):
False Negative and False Positive Fractions

False Negative Fraction $= \dfrac{\text{Area predicted to be } not \text{ hazardous, but } is \text{ hazardous}}{\text{Total area of observed (true) hazard}}$

For a uniform population density, of those people exposed, this is the fraction who were not warned

$$f_{FN} = \frac{A_{FN}}{A_{OB}}$$ ⟹ $$MOE_x \equiv 1 - f_{FN} = 1 - \frac{A_{FN}}{A_{OB}} = \frac{A_{OB} - A_{FN}}{A_{OB}} = \frac{A_{OV}}{A_{OB}}$$

False Positive Fraction $= \dfrac{\text{Area predicted to } be \text{ hazardous, but } is \, not \text{ hazardous}}{\text{Total area of predicted hazard}}$

For a uniform population density, of the people predicted to be exposed, this is fraction who were inadvertently warned

$$f_{FP} = \frac{A_{FP}}{A_{PR}}$$ ⟹ $$MOE_y \equiv 1 - f_{FP} = 1 - \frac{A_{FP}}{A_{PR}} = \frac{A_{PR} - A_{FP}}{A_{PR}} = \frac{A_{OV}}{A_{PR}}$$

$$MOE = (MOE_X, MOE_Y) = (1-F_{FN}, 1-F_{FP}) = (A_{OV}/A_{OB}, A_{OV}/A_{PR})$$

The figure in the slide shows the two-dimensional MOE space, which is the unit square. Every model prediction/observation comparison corresponds to a point in this MOE space. A "perfect" MOE of (1, 1) represents complete agreement between predictions and observations, while a MOE of (0, 0) represents no overlap between model predictions and observations. From the definition of MOEx and MOEy it is straight-forward to show that the diagonal line MOEy=MOEx corresponds to the case where the prediction area is the same as the truth area, APR=AOB. Below the diagonal, the false positive fraction is larger than the false negative fraction and the model is said to *overpredict* the observations; for MOEx=1, the model predictions completely surround the observations (no false negative). Above the diagonal, the false positive fraction is smaller than the false negative fraction and the model is said to *underpredict* the observations; for MOEy=1, the observations completely surrounds the model predictions (no false positive).

$$\text{MOE} \equiv \left(\text{MOE}_x, \text{MOE}_y\right) = \left(1 - f_{FN}, 1 - f_{FP}\right) = \left(\frac{A_{OV}}{A_{OB}}, \frac{A_{OV}}{A_{PR}}\right)$$

Observation surrounds prediction

(0,1)

(1,1)

Prediction and observation overlap perfectly

Predicted area = Observed area

$\dfrac{A_{OV}}{A_{PR}}$

Decreasing False Positive

Prediction surrounds observation

No overlap between observation and prediction

(0,0)

Decreasing False Negative

(1,0)

$\dfrac{A_{OV}}{A_{OB}}$
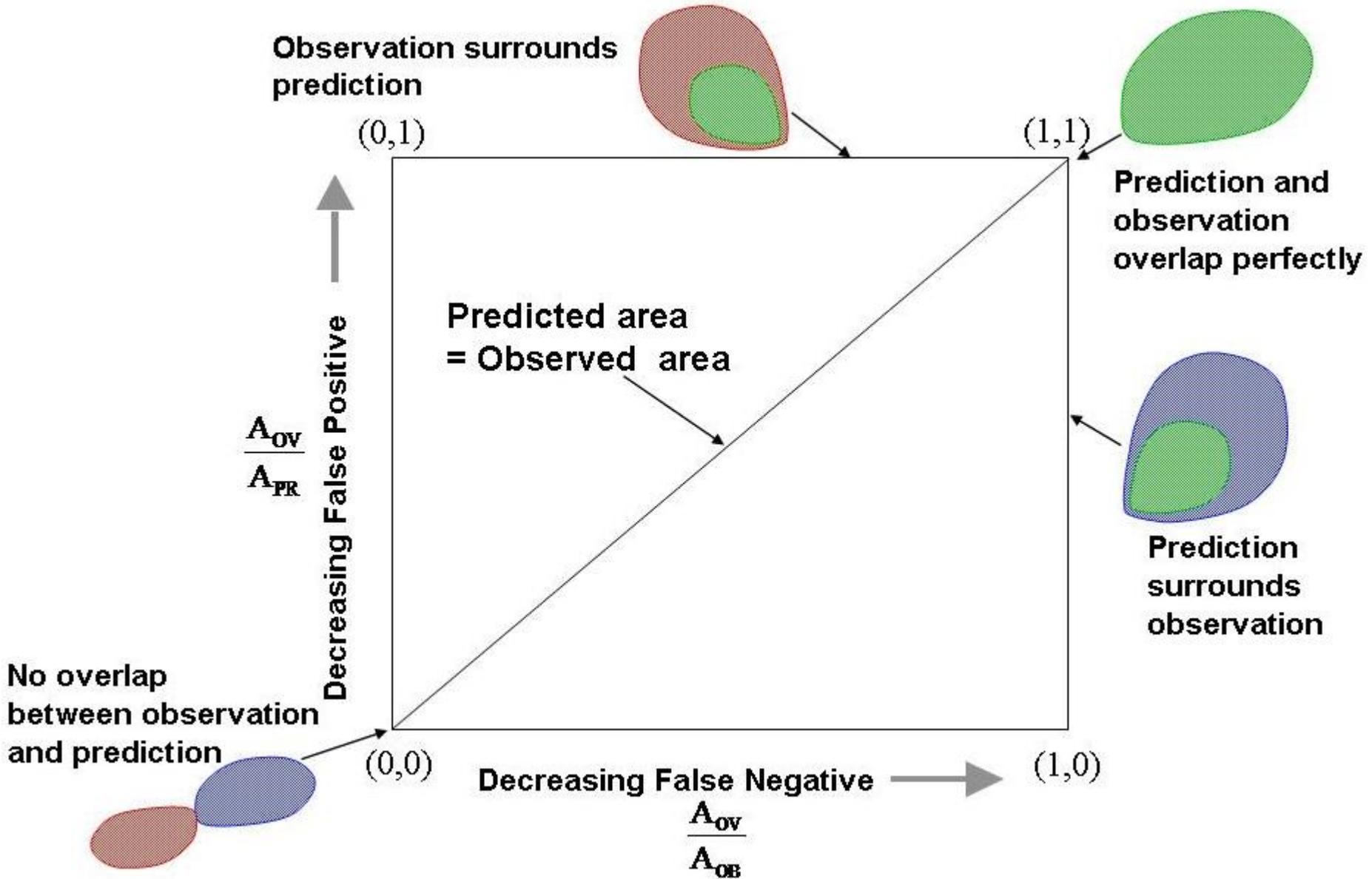
SUMMED CONCENTRATION AND THRESHOLD MOES

The slide gives the definition of two kinds of MOES. The summed concentration MOE scores the model based on the marginal differences between the predicted and observed concentrations. The threshold MOE scores the model based on the *number of samplers* that are predicted and observed to be above a given concentration threshold T. As for the previous statistics, all MOEs are computed on a release-by-release basis using concentrations that are paired in space and time and for all data/prediction pairs within the release. A more detailed description of the two-dimensional MOE can be found in reference [8] and references therein.

Overlap (A_{OV}), False Negative (A_{FN}) and False Positive (A_{FP}) "areas" for predictions and observations at N Samplers: i=1,2, …, N

$$A_{OV} = \sum_{i=1}^{N} A_{OV}(i)$$

$$A_{FN} = \sum_{i=1}^{N} A_{FN}(i)$$

$$A_{FP} = \sum_{i=1}^{N} A_{FP}(i)$$

where…

For Summed Concentration MOEs

$$A_{OV}(i) = \min\{C_p^{(i)}, C_o^{(i)}\}$$

$$A_{FN}(i) = \begin{cases} C_o^{(i)} - C_p^{(i)} & \text{if } C_o^{(i)} > C_p^{(i)} \\ 0 & \text{otherwise} \end{cases}$$

$$A_{FP}(i) = \begin{cases} C_p^{(i)} - C_o^{(i)} & \text{if } C_p^{(i)} > C_o^{(i)} \\ 0 & \text{otherwise} \end{cases}$$

For Threshold MOEs with threshold T

$$A_{OV}(i) = \begin{cases} 1 & \text{if } C_o^{(i)} \geq T \text{ and } C_p^{(i)} \geq T \\ 0 & \text{otherwise} \end{cases}$$

$$A_{FN}(i) = \begin{cases} 1 & \text{if } C_o^{(i)} \geq T \text{ and } C_p^{(i)} < T \\ 0 & \text{otherwise} \end{cases}$$

$$A_{FP}(i) = \begin{cases} 1 & \text{if } C_o^{(i)} < T \text{ and } C_p^{(i)} \geq T \\ 0 & \text{otherwise} \end{cases}$$

All MOEs are computed for each release over all concentrations, paired in space and time

INDIVIDUAL RELEASES: GRAPHICAL COMPARISONS

The nine slides that follow are identical in format and show graphical comparisons of HPAC and NARAC predicted 1-hour average concentrations and observations. The HPAC results that are shown are for Mode 1 (terrain on, constant surface roughness = 0.6 m), which turned out to yield the best HPAC-based predictions (as is shown later in this document). The meteorology option was "full met" in all cases.

Individual Releases:
Graphical Comparisons

The top row shows the predicted HPAC (left) and NARAC (middle) 1-hour average concentrations and observations (in ng/m^3) at the sampler locations. The HPAC predictions are for Mode 1 (terrain on, constant surface roughness=0.6 m) with full met. Only 2 sampler arcs (2 km and 4 km) were employed in this release. The release point is the red star at the origin. The bar colors mean the following. The height of a green bar represents the concentration value where the predicted and observed concentrations agree (overlap) at a sampler location. A red bar represents the additional concentration observed, but not predicted by the model (a false negative). A yellow bar represents the additional concentration predicted, but not observed by the model (a false positive).

The HPAC predictions are seen to underpredict the observations noticeably more than NARAC (HPAC has more false negatives). The NARAC plume appears to be shifted to the right of the observations when viewed from the release location. This would account for the excess NARAC overpredictions (yellow bars) relative to HPAC (NARAC has more false positives). The figure on the top right shows a log-log plot of the predicted versus observed concentrations for HPAC (blue circles) and NARAC (red squares). The dashed diagonal lines are factor of two lines above and below the main diagonal. The HPAC underpredictions and the NARAC overpredictions are clearly seen. The plot in the bottom left shows the summed concentration MOEs. The 1-hour average concentration MOEs are represented by the letter H – blue for HPAC and red for NARAC. The plot shows, quantitatively, the qualitative result observed from the sampler plots, namely that HPAC exhibits a higher false negative fraction than NARAC, while NARAC exhibits a higher false positive fraction than HPAC for this release. Also shown are the HPAC MOEs for the 3 20-minute average concentration measurement periods (blue 1, 2, and 3). The plot in the bottom right shows the threshold MOEs based on a threshold of 20 ng/m^3. This value is roughly twice the method level of detection (MLOD) of 12 ng/m^3 for the sampler measurement devices employed in the Copenhagen trials [5]. It is clear from this plot that NARAC and HPAC are each able to predict this low threshold concentration reasonably well.

The table in the bottom center shows 6 statistics for HPAC and NARAC for this release. The HPAC underprediction is evident from the large negative fractional bias, FB = -0.77. The NARAC value of FB = 0.005 is a reflection of compensating over and under predictions observed in the sampler plot. Other statistics indicate better NARAC performance for this release, for example the smaller NARAC NAD and BNMSE values.

HPAC, Terrain, SR=0.6 m, Full Met   **NARAC**   **Predictions vs Observations**

9/20/78: Hour Average, HPAC, Terrain, SR=0.6 m

9/20/78: Hour Average, NARAC

1 Hour Average Predictions vs Observations: 9/20/78
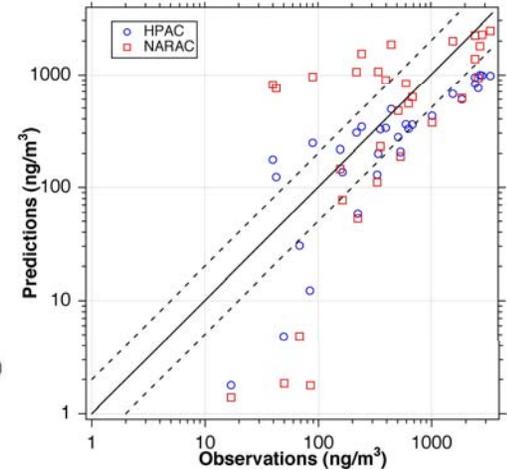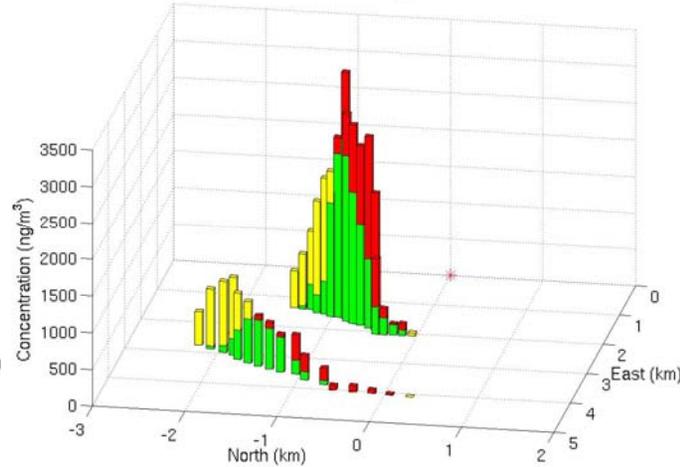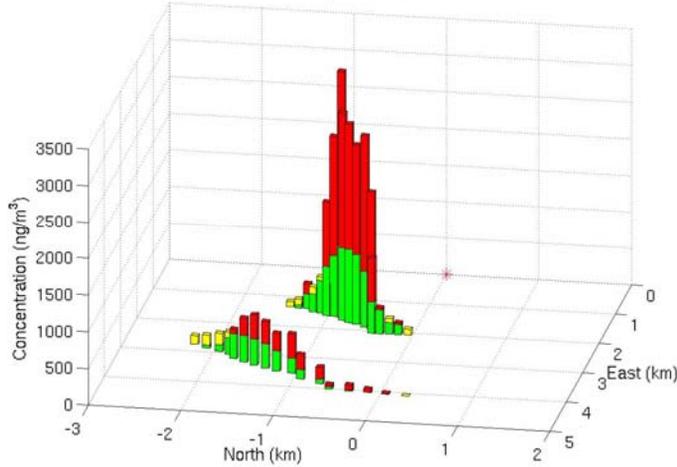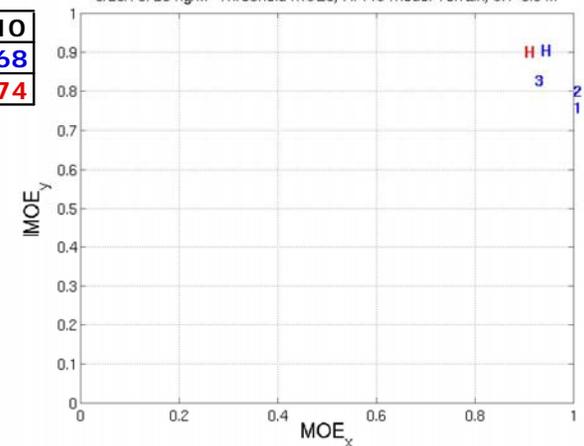
Summed Concentration MOEs   **Standard Statistics**   **20 ng/m³ Threshold MOEs**

9/20/78: Summed Conc. MOEs; HPAC Mode: Terrain, SR=0.6 m
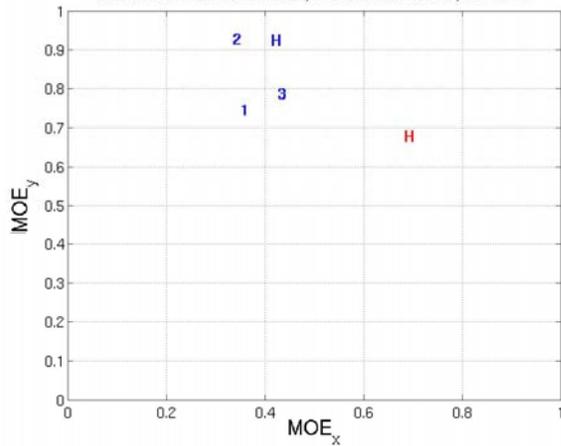
	FB	NAD	BNMSE	FAC2	FAC5	FAC10
HPAC	-0.766	0.430	0.234	0.387	0.903	0.968
NARAC	0.005	0.320	0.089	0.387	0.742	0.774

9/20/78: 20 ng/m³ Threshold MOEs; HPAC Mode: Terrain, SR=0.6 m

9/26/78 1-HOUR AVERAGES

HPAC underpredictions relative to NARAC are again clear from the sampler concentration figures. The NARAC plume again appears to be shifted to the right with respect to the observations. The qualitative performance of NARAC and HPAC for this release is the same as was found in the 9/20/78 release.

9/26/78 1-HOUR AVERAGES
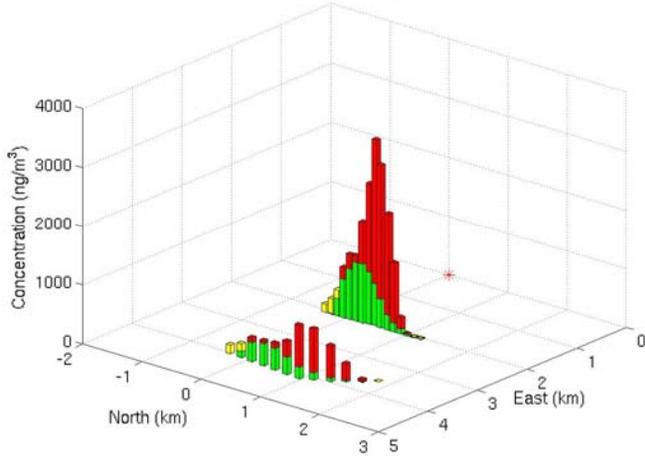
HPAC, Terrain, SR=0.6 m, Full Met

NARAC
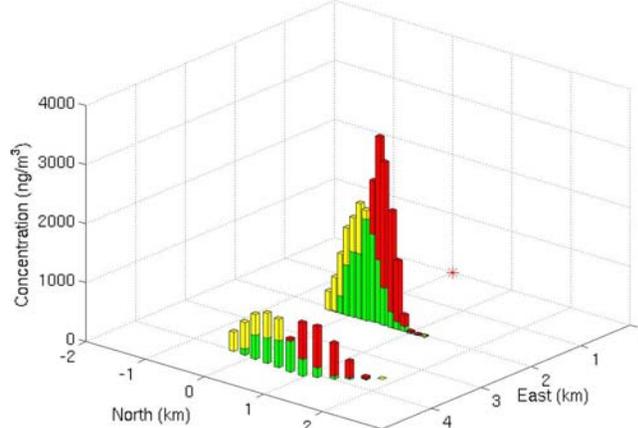
Predictions vs Observations
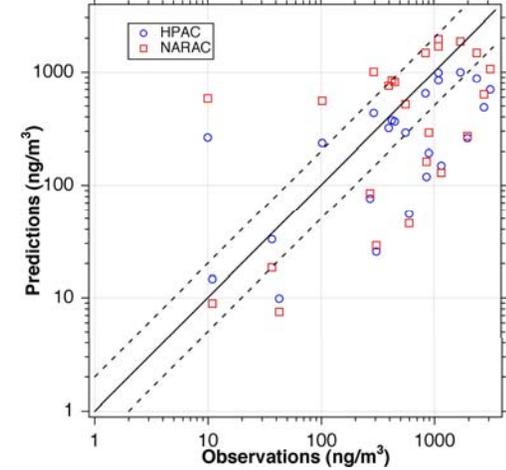
Summed Concentration MOEs
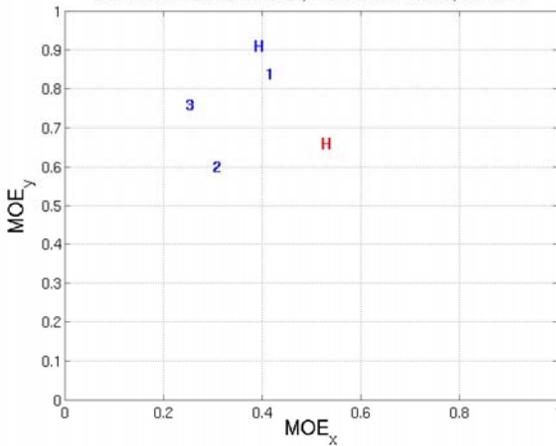
Standard Statistics

	FB	NAD	BNMSE	FAC2	FAC5	FAC10
HPAC	-0.814	0.461	0.296	0.458	0.708	0.875
NARAC	-0.236	0.418	0.184	0.417	0.667	0.875

20 ng/m³ Threshold MOEs

49
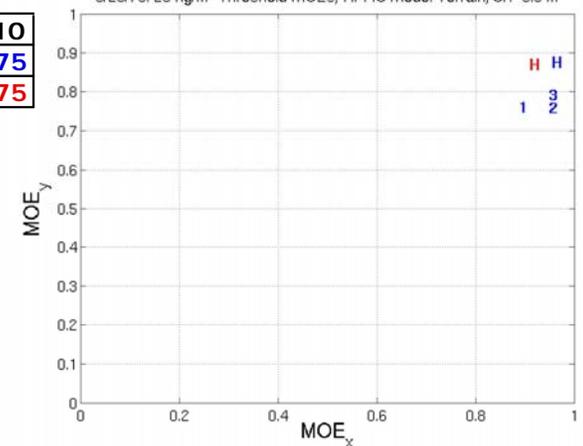
10/19/78 1-HOUR AVERAGES

Significant HPAC underpredictions are seen at all three arcs. Large NARAC overpredictions are consistent with a right-going NARAC plume shift, as in the two previous releases.

10/19/78 1-HOUR AVERAGES

HPAC, Terrain, SR=0.6 m, Full Met


10/19/78: Hour Average, HPAC, Terrain, SR=0.6 m
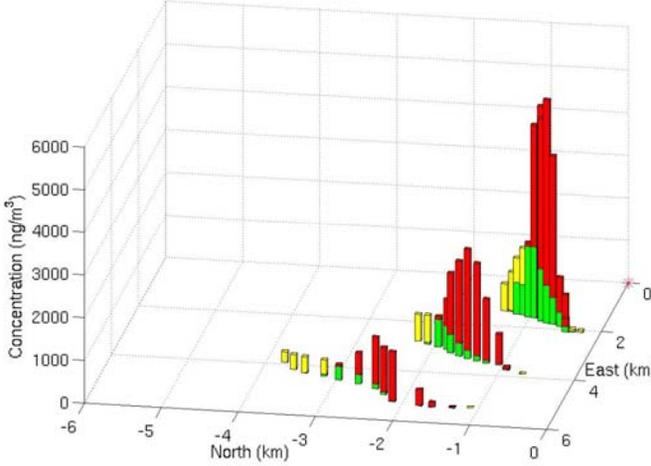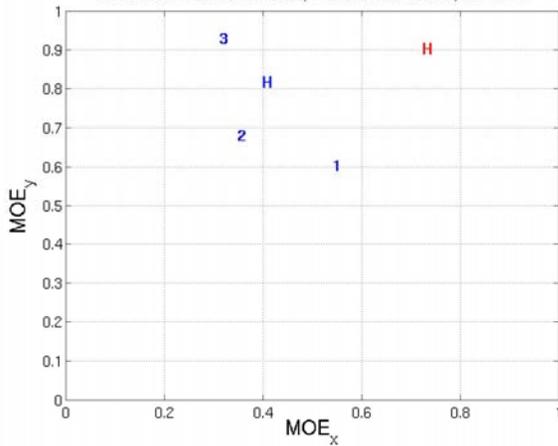
NARAC

10/19/78: Hour Average, NARAC
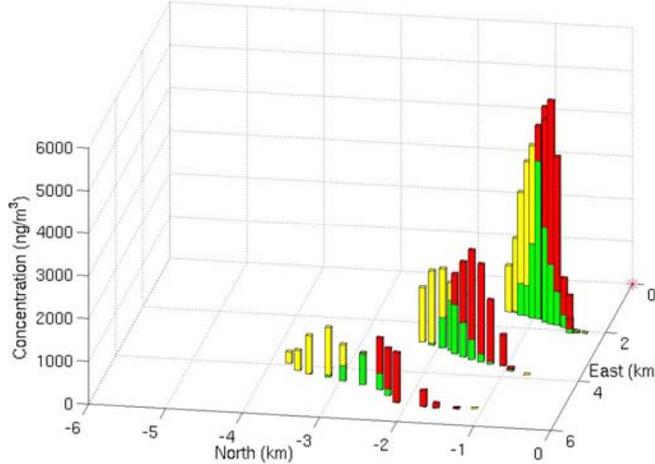
Predictions vs Observations

1 Hour Average Predictions vs Observations: 10/19/78
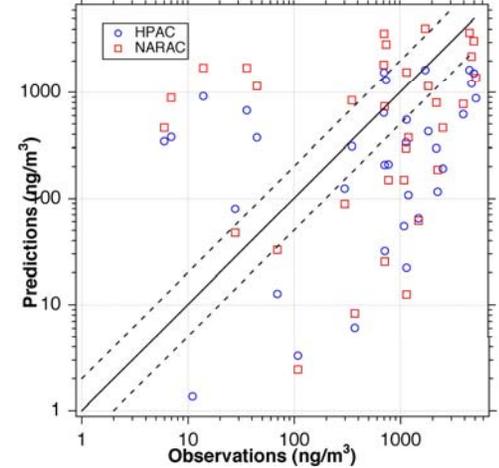
Summed Concentration MOEs

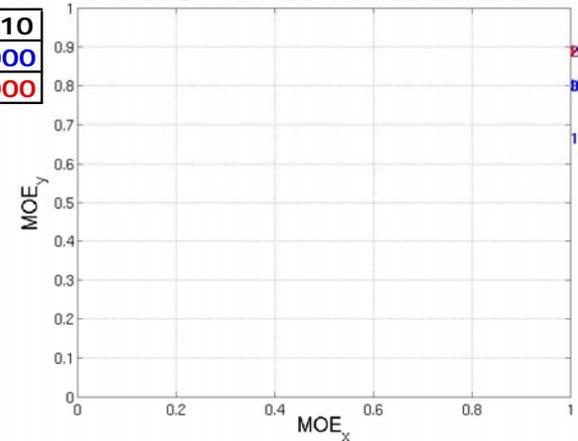10/19/78: Summed Conc. MOEs; HPAC Mode: Terrain, SR=0.6 m
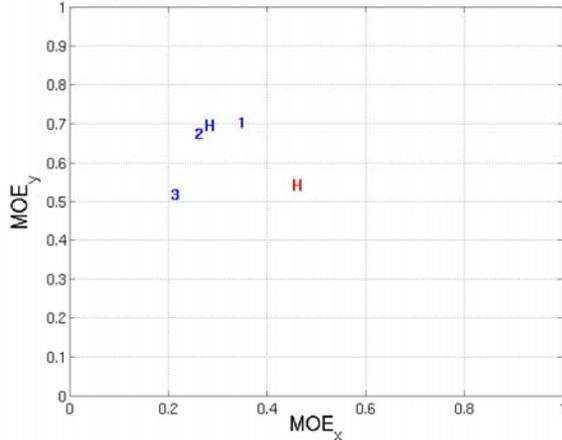
Standard Statistics

	FB	NAD	BNMSE	FAC2	FAC5	FAC10
HPAC	-0.873	0.607	0.373	0.118	0.441	0.618
NARAC	-0.184	0.508	0.213	0.182	0.515	0.667

20 ng/m³ Threshold MOEs

10/19/78: 20 ng/m³ Threshold MOEs; HPAC Mode: Terrain, SR=0.6 m
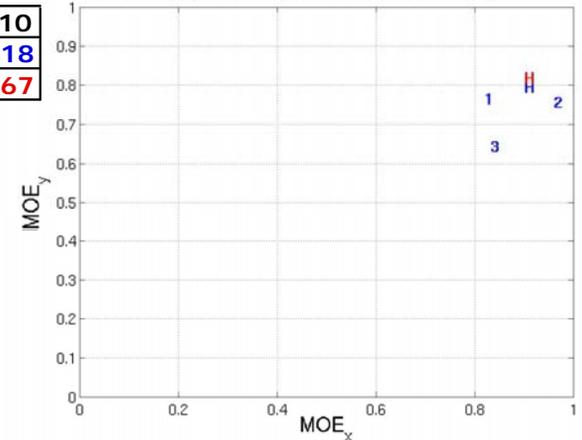
11/3/78 1-HOUR AVERAGES

HPAC underpredictions are higher than those of NARAC. The HPAC false positive fraction is also higher than that of NARAC, due possibly to a right-going HPAC plume shift. Since there were only 10 samplers activated for this release, the results may not represent overall model performance for this release.

11/3/78 1-HOUR AVERAGES
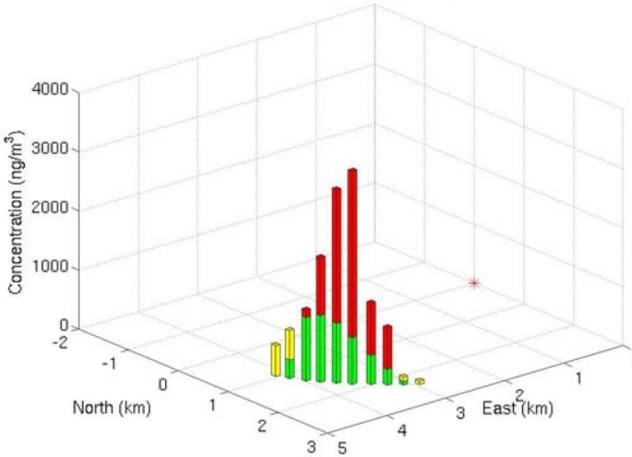
HPAC, Terrain, SR=0.6 m, Full Met

NARAC
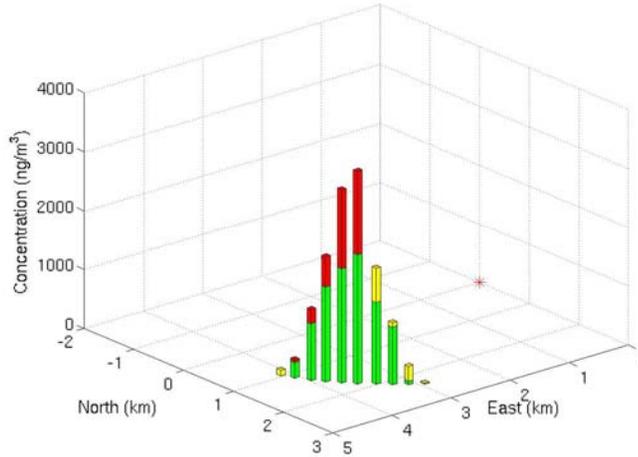
Predictions vs Observations
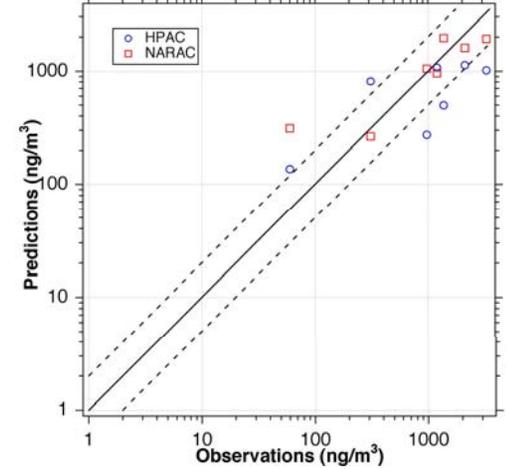
Summed Concentration MOEs

Standard Statistics

	FB	NAD	BNMSE	FAC2	FAC5	FAC10
HPAC	-0.687	0.464	0.260	0.250	1.000	1.000
NARAC	-0.220	0.197	0.049	0.875	0.875	1.000

20 ng/m³ Threshold MOEs

53

11/9/78 1-HOUR AVERAGES

Significant HPAC false negatives are observed in all three arcs. NARAC false positives are consistent with a right-going NARAC plume shift with respect to the observations.
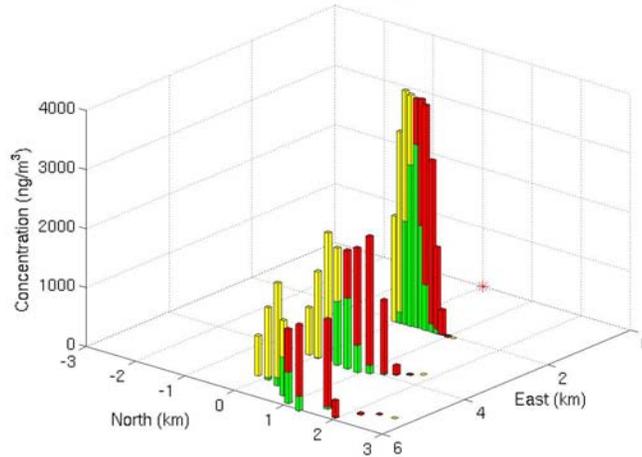
11/9/78 1-HOUR AVERAGES

HPAC, Terrain, SR=0.6 m, Full Met

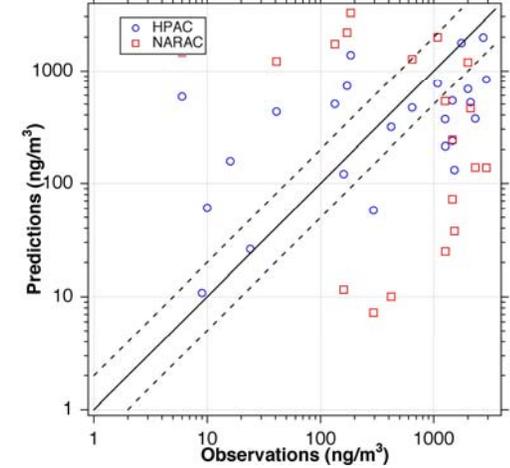11/9/78: Hour Average, HPAC, Terrain, SR=0.6 m
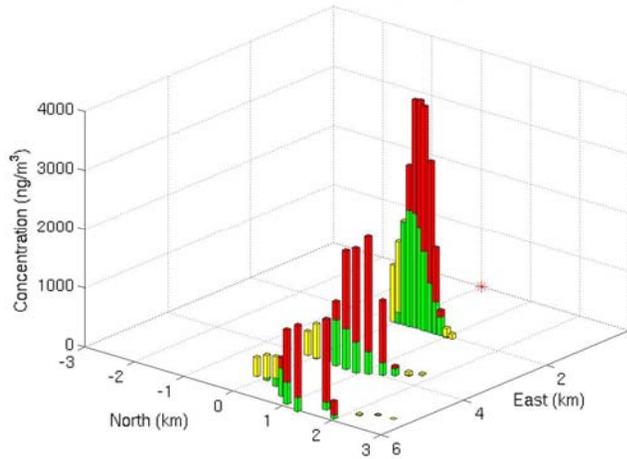
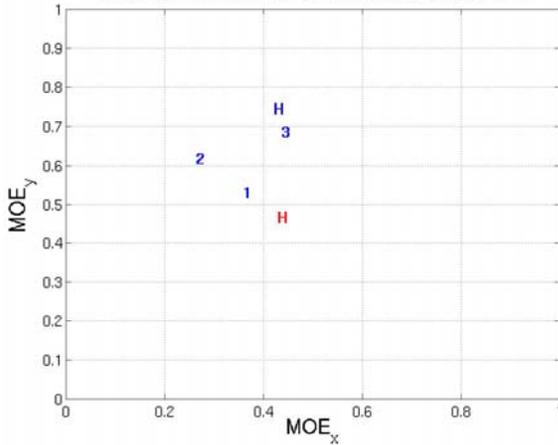**NARAC**

11/9/78: Hour Average, NARAC

Predictions vs Observations

1 Hour Average Predictions vs Observations: 11/9/78

Summed Concentration MOEs

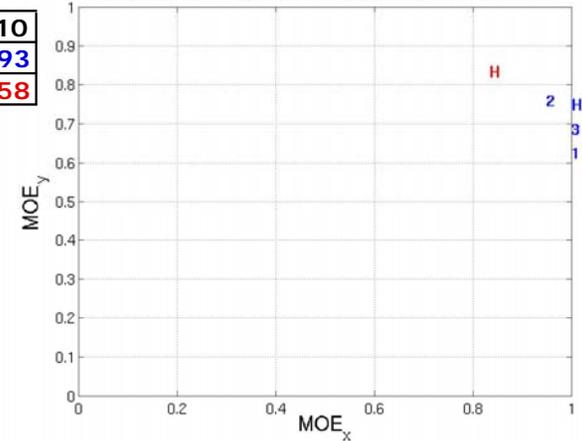11/9/78: Summed Conc. MOEs; HPAC Mode: Terrain, SR=0.6 m

Standard Statistics

	FB	NAD	BNMSE	FAC2	FAC5	FAC10
HPAC	-0.557	0.462	0.194	0.321	0.643	0.893
NARAC	-0.083	0.554	0.250	0.208	0.417	0.458

20 ng/m³ Threshold MOEs

11/9/78: 20 ng/m³ Threshold MOEs; HPAC Mode: Terrain, SR=0.6 m

4/30/79 1-HOUR AVERAGES

Both HPAC and NARAC appear to have significant left-going plume shifts with respect to sampler observations. Every HPAC prediction is below its paired observation, as evidenced in the log-log concentrati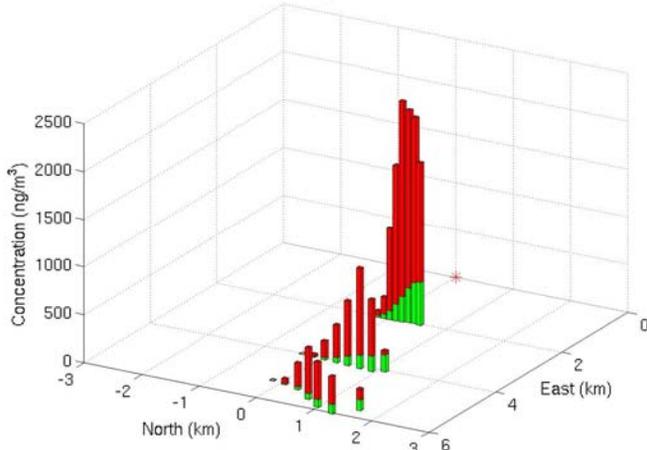on plot (top right) and the summed concentration MOE plot (lower left), which shows a zero false positive fraction. NARAC shows significant false negatives, as well.
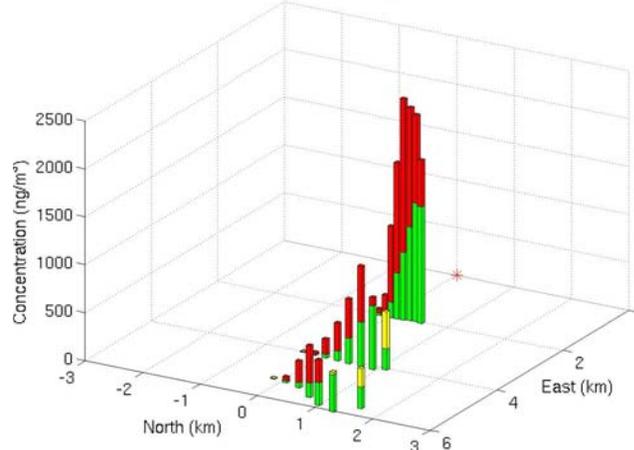
4/30/79 1-HOUR AVERAGES

HPAC, Terrain, SR=0.6 m, Full Met

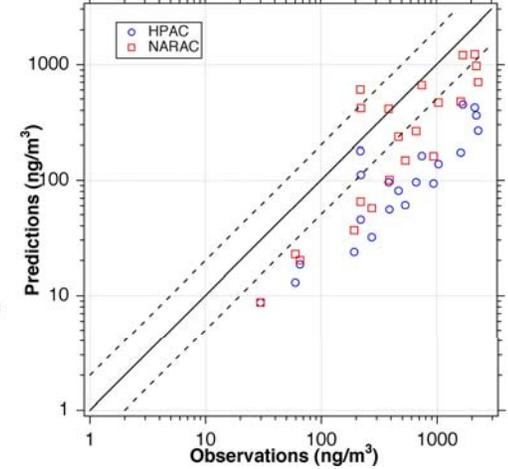4/30/79: Hour Average, HPAC, Terrain, SR=0.6 m
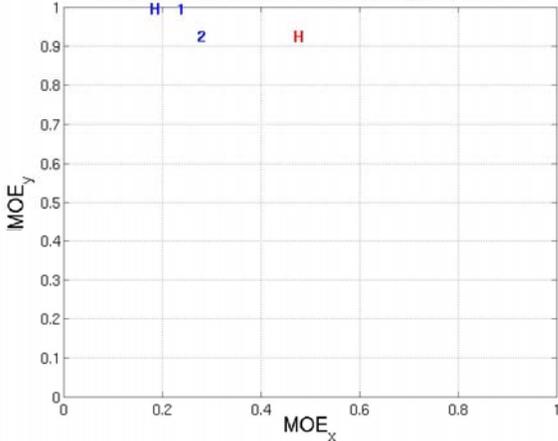
NARAC

4/30/79: Hour Average, NARAC

Predictions vs Observations

1 Hour Average Predictions vs Observations: 4/30/79

Summed Concentration MOEs

4/30/79: Summed Conc. MOEs; HPAC Mode: Terrain, SR=0.6 m

Standard Statistics

	FB	NAD	BNMSE	FAC2	FAC5	FAC10
HPAC	-1.402	0.703	0.518	0.048	0.429	0.952
NARAC	-0.660	0.381	0.154	0.286	0.905	1.000

20 ng/m³ Threshold MOEs

4/30/79: 20 ng/m³ Threshold MOEs; HPAC Mode: Terrain, SR=0.6 m

57

6/27/79 1-HOUR AVERAGES

Again, left-going plume shifts appear to be present in the HPAC and NARAC predictions. Significant underpredictions (false negatives) accompany both models, with HPAC having the larger false negative fraction. NARAC has the larger false positive fraction.

6/27/79 1-HOUR AVERAGES

HPAC, Terrain, SR=0.6 m, Full Met

6/27/79: Hour Average, HPAC, Terrain, SR=0.6 m

NARAC

6/27/79: Hour Average, NARAC

Predictions vs Observations

1 Hour Average Predictions vs Observations: 6/27/79
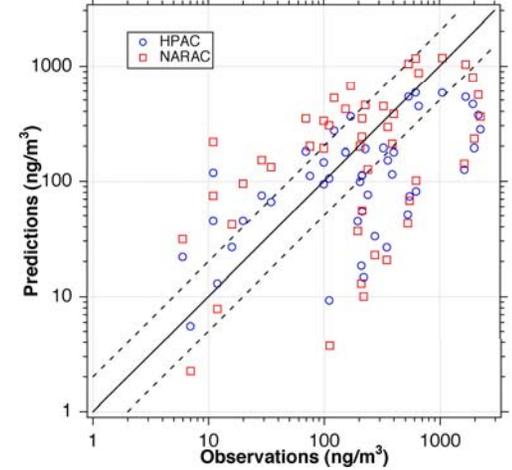
Summed Concentration MOEs

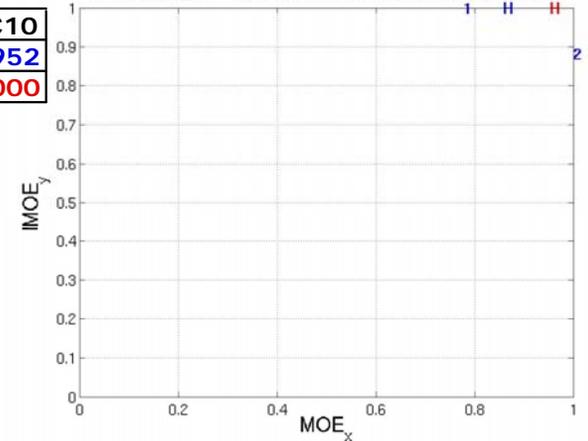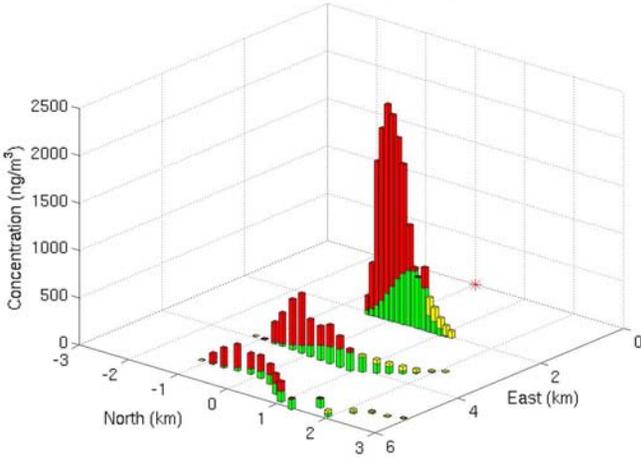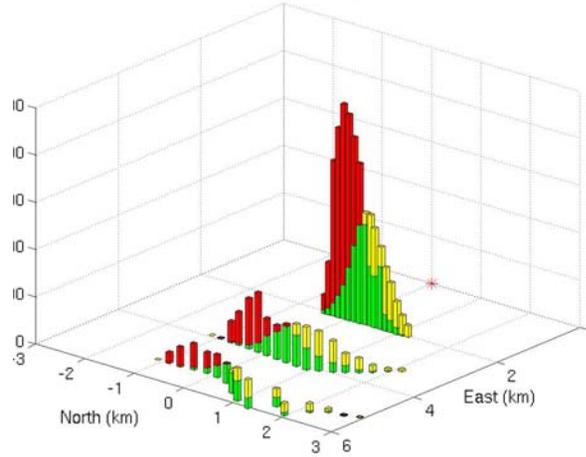6/27/79: Summed Conc. MOEs; HPAC Mode: Terrain, SR=0.6 m
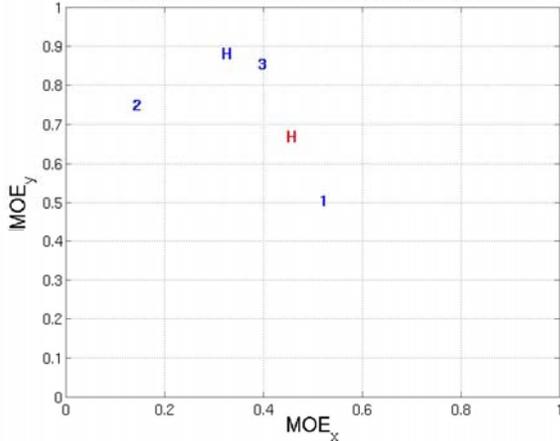
Standard Statistics

	FB	NAD	BNMSE	FAC2	FAC5	FAC10
HPAC	-0.945	0.536	0.424	0.370	0.717	0.826
NARAC	-0.400	0.464	0.276	0.348	0.652	0.826

20 ng/m³ Threshold MOEs

6/27/79: 20 ng/m³ Threshold MOEs; HPAC Mode: Terrain, SR=0.6 m

59
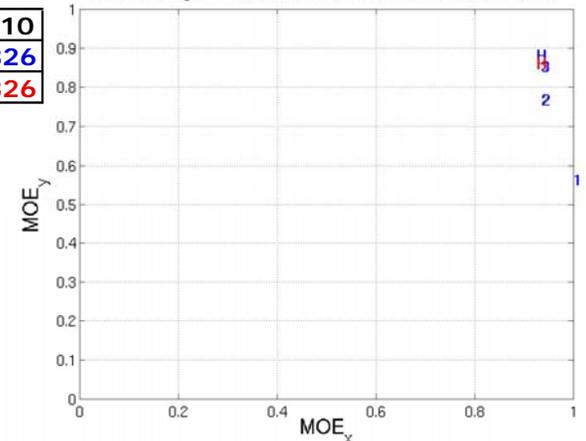
7/6/79 1-HOUR AVERAGES

For this release, HPAC false negatives are concentrated in the 2 km arc. By comparison, NARAC exhibits very few false negatives; those present are also primarily in the 2 km arc. NARAC has the larger false positive fraction, with the bulk of the false positives falling in the 4 km and 6 km arcs. Interestingly, the Fac2 performance of the two models is nearly the same – 0.600 for HPAC and 0.641 for NARAC, yet the graphs and summed concentration MOEs show substantially different model performance.

7/6/79 1-HOUR AVERAGES

HPAC, Terrain, SR=0.6 m, Full Met   *NARAC*   *Predictions vs Observations*

7/6/79: Hour Average, HPAC, Terrain, SR=0.6 m

7/6/79: Hour Average, NARAC
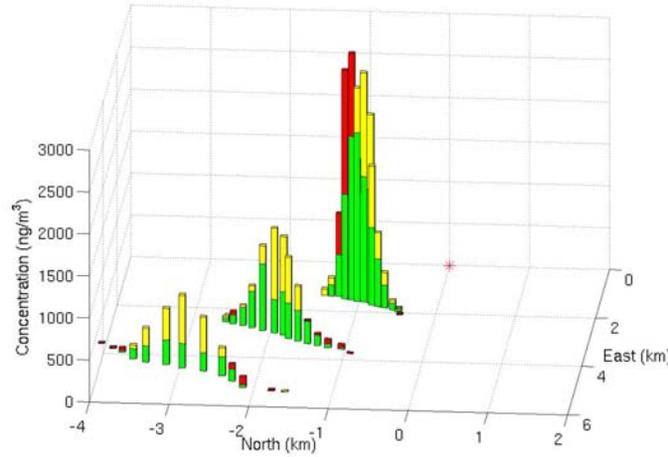
1 Hour Average Predictions vs Observations: 7/6/79
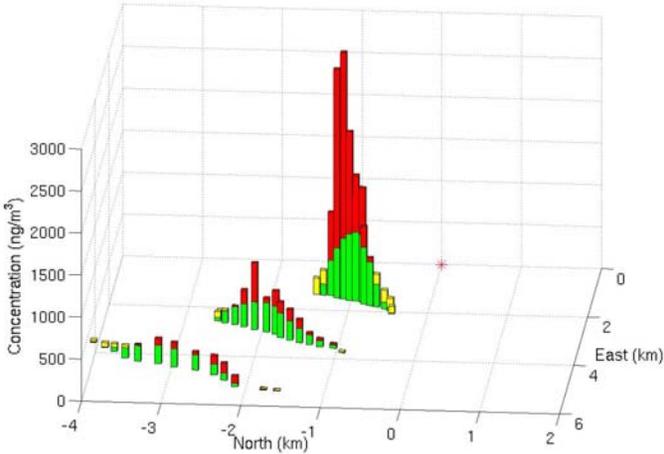
Summed Concentration MOEs   *Standard Statistics*   *20 ng/m³ Threshold MOEs*
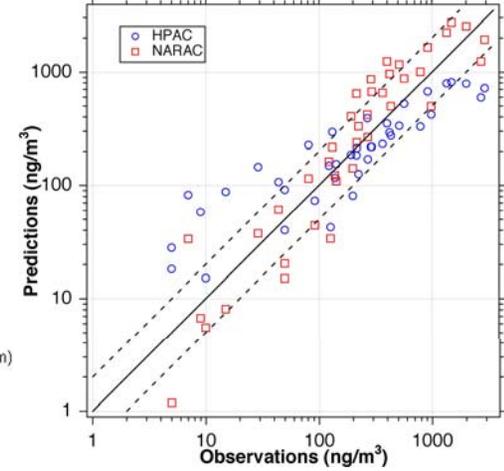
7/6/79: Summed Conc. MOEs; HPAC Mode: Terrain, SR=0.6 m
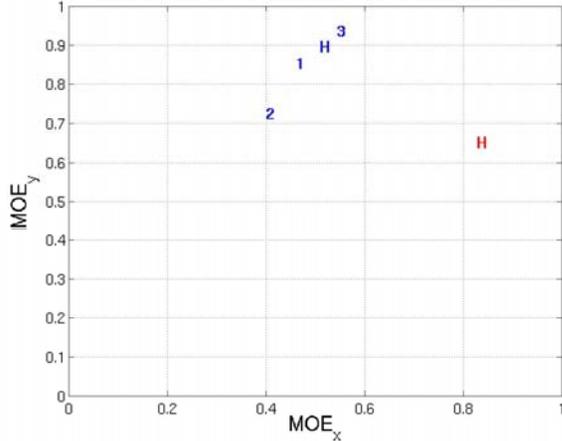
	FB	NAD	BNMSE	FAC2	FAC5	FAC10
HPAC	-0.551	0.351	0.230	0.600	0.875	0.975
NARAC	0.239	0.271	0.075	0.641	1.000	1.000

7/6/79: 20 ng/m³ Threshold MOEs; HPAC Mode: Terrain, SR=0.6 m
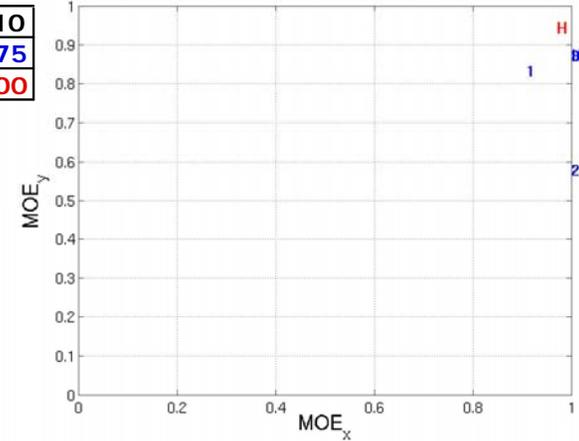
7/19/79 1-HOUR AVERAGES

The HPAC plume appears to have a left-going shift, as in the 4/30/79 and 6/27/79 releases. Large HPAC false negatives are observed on all arcs. NARAC false negatives are prominent in the 2 km arc. NARAC has the higher false positive fraction and the smaller false negative fraction.

7/19/79 1-HOUR AVERAGES

HPAC, Terrain, SR=0.6 m, Full Met   **NARAC**   **Predictions vs Observations**

7/19/79: Hour Average, HPAC, Terrain, SR=0.6 m
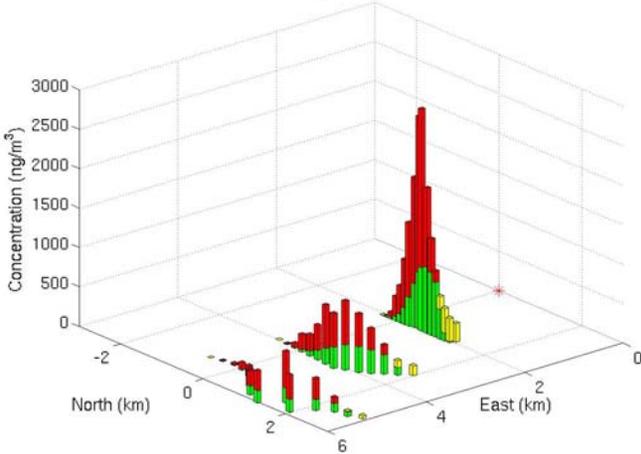
7/19/79: Hour Average, NARAC
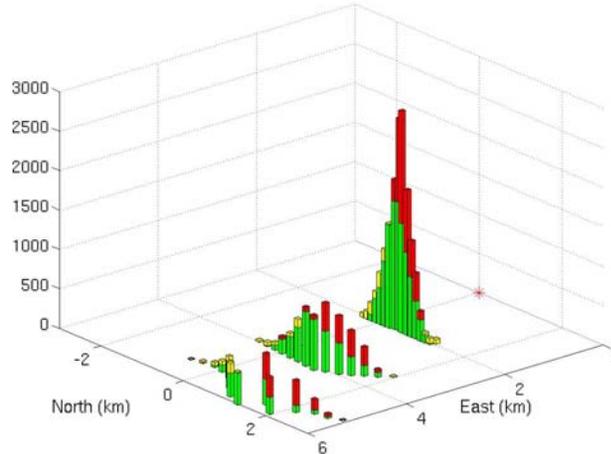
1 Hour Average Predictions vs Observations: 7/19/79

Summed Concentration MOEs   **Standard Statistics**   **20 ng/m³ Threshold MOEs**
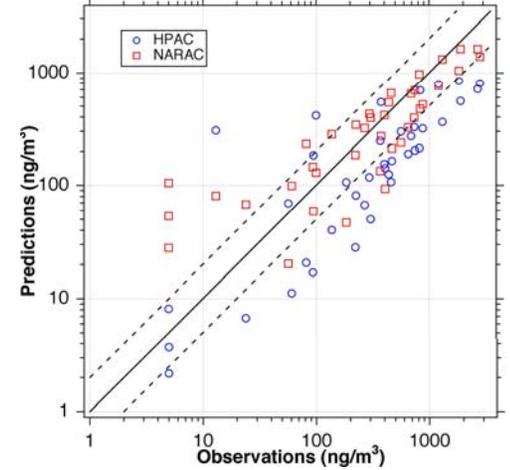
7/6/79: Summed Conc. MOEs; HPAC Mode: Terrain, SR=0.6 m
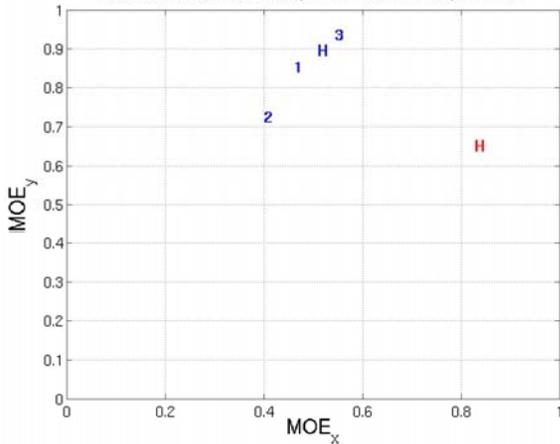
	FB	NAD	BNMSE	FAC2	FAC5	FAC10
HPAC	-0.781	0.469	0.248	0.256	0.872	0.974
NARAC	-0.261	0.216	0.058	0.615	0.897	0.949

7/19/79: 20 ng/m³ Threshold MOEs; HPAC Mode: Terrain, SR=0.6 m

63
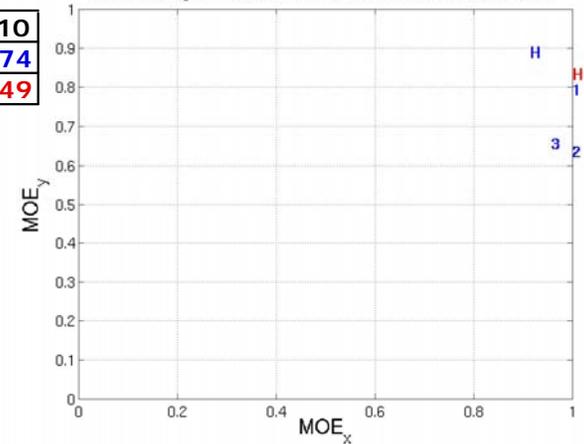
OVERALL NARAC AND HPAC PERFORMANCE: STATISTICAL COMPARISONS

The following several slides focus on the overall performance of HPAC and NARAC.

Graphical and statistical comparisons of the two models are shown.

Overall NARAC and HPAC Performance: Statistical Comparisons

HPAC & NARAC NORMALIZED ABSOLUTE DIFFERENCE:
1 HOUR AVERAGE CONCENTRATIONS; FOUR HPAC MODES, FULL MET

The graph shows the normalized absolute difference (NAD) performance of NARAC and all four HPAC modes using full met for all releases. With the exception of the 11/9/79 release, NARAC NAD values (red filled squares) are smaller than HPAC NAD values for all 4 HPAC modes. The smallest HPAC NAD value for every release is the one performed with constant surface roughness; of those, the majority are HPAC Mode 1: terrain on, surface roughness = 0.6 m (blue filled diamonds).

HPAC & NARAC Normalized Absolute Difference: 1 Hour Average Concentrations; Four HPAC Modes, Full Met
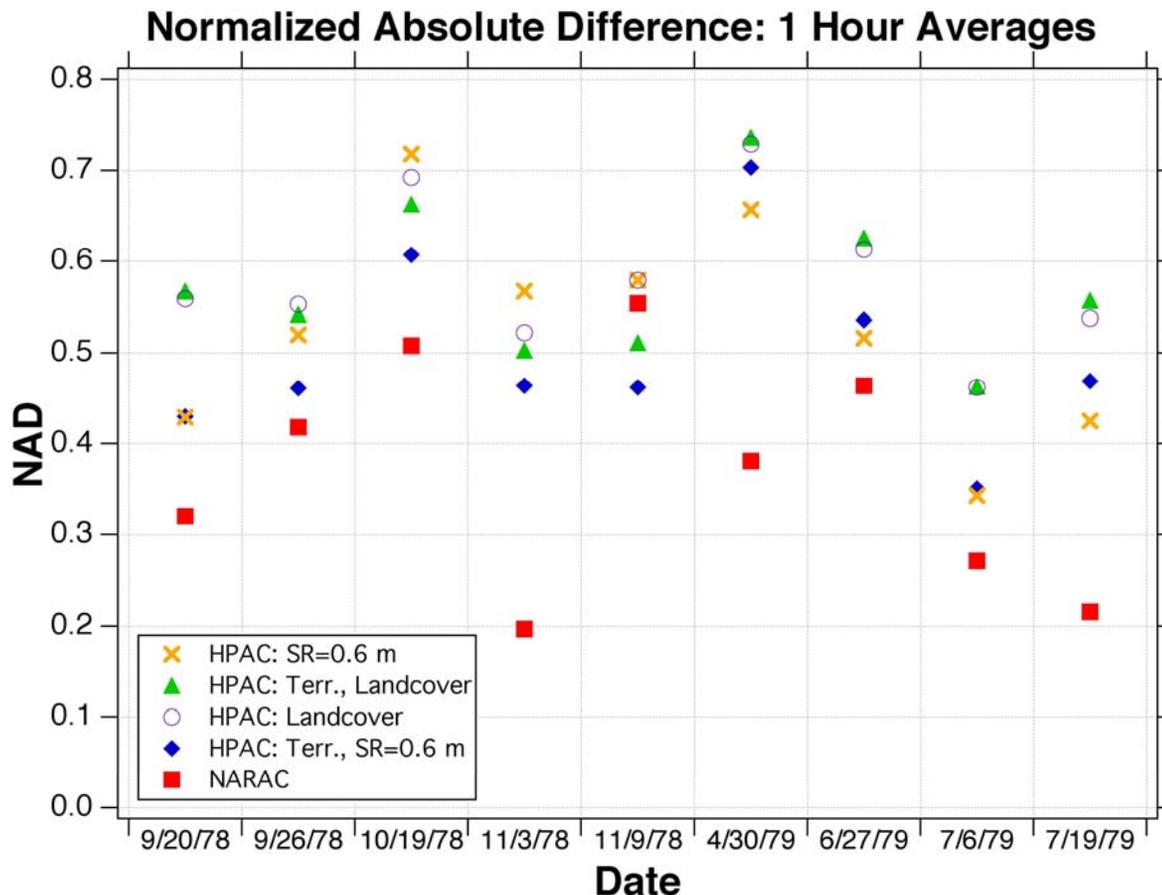
- **With the exception of the 11/9/79 release, NARAC NAD values are smaller than HPAC NAD values for all 4 HPAC modes**
- **The smallest HPAC NAD value for every release is the one performed with constant surface roughness; of those, the majority are HPAC Mode 1: Terrain on, SR=0.6m**

HPAC & NARAC FRACTIONAL BIAS: 1 HOUR AVERAGE CONCENTRATIONS; FOUR HPAC MODES, FULL MET

The graph shows the fractional bias (FB) performance of NARAC and all four HPAC modes using full met for all releases. Every HPAC mode underpredicts every release (FB<0), while NARAC underpredicts 7 of the 9 releases (the two exceptions are the 9/20/78 and 7/6/79 releases). For every release, all HPAC modes underpredict NARAC (i.e., all HPAC modes have more negative FBs). The least negative HPAC FB value for every release is one performed with constant surface roughness; of those, the majority are HPAC Mode 1 (terrain on, surface roughness = 0.6 m) (blue filled diamonds). This result is consistent with the NAD result in the previous slide.

HPAC & NARAC Fractional Bias: 1 Hour Average Concentrations; Four HPAC Modes, Full Met
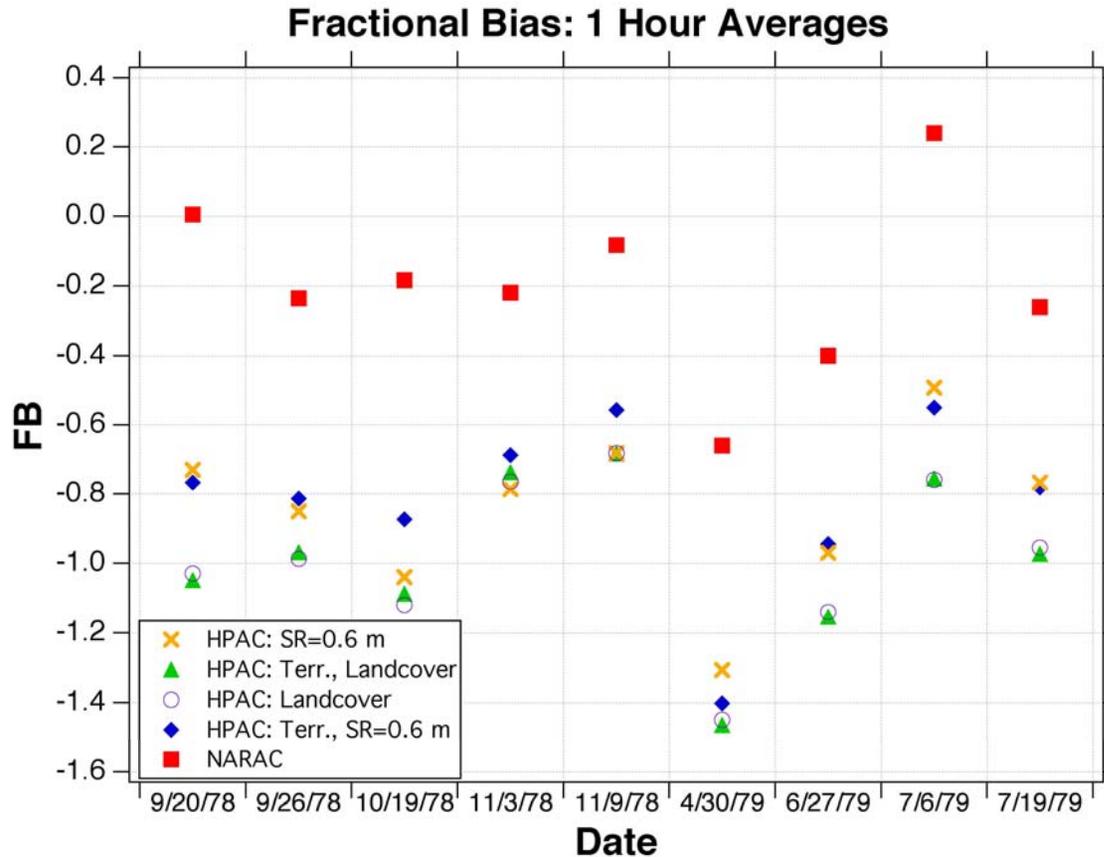
- **HPAC underpredicts (FB < 0) every release for all 4 modes**
- **NARAC underpredicts 7 of the 9 releases (exceptions are 9/20/78 and 7/6/79)**
  FB values for all HPAC modes are more negative than NARAC for every release
- **The least negative HPAC FB value for every release is the one performed with constant surface roughness; of those, the majority are HPAC Mode 1: Terrain on, SR=0.6m**

HPAC AND NARAC AVERAGE STATISTICS: 1 HOUR AVERAGE CONCENTRATIONS; FOUR HPAC MODES, FULL MET

The table in the slide shows the average statistics of NARAC and the four HPAC modes with full met. With the exception of <Fac10>, NARAC average statistics (red) outperform HPAC average statistics for all HPAC modes. Again, with the exception of <Fac10>, HPAC Mode 1 (terrain on, surface roughness = 0.6 m) average statistics outperform the average statistics for all other HPAC modes.

HPAC and NARAC Average Statistics: 1 Hour Average Concentrations; Four HPAC Modes, Full Met

Average Statistics for 4 HPAC Modes (Full met) and NARAC

	\<FB\>	\<NAD\>	\<NMSE\>	\<BNMSE\>	\<FAC2\>	\<FAC5\>	\<FAC10\>
HPAC Mode 1: Terrain, SR=0.6	**-0.82**	**0.50**	**3.65**	**0.31**	**0.31**	**0.73**	0.90
HPAC Mode 2: Terrain, Landcover	-0.99	0.57	5.24	0.40	0.27	0.70	**0.91**
HPAC Mode 3: No terrain, SR=0.6	-0.85	0.53	3.85	0.34	0.30	0.68	0.86
HPAC Mode 4: No terrain, Landcover	-0.99	0.58	5.28	0.41	0.26	0.69	0.90
NARAC	**-0.20**	**0.37**	**1.31**	**0.15**	**0.44**	**0.74**	**0.84**

- ***With the exception of \<FAC10\>, NARAC average statistics outperform HPAC average statistics for all HPAC modes.***

- ***With the exception of \<FAC10\>, HPAC mode 1: Terrain on, SR=0.6 m average statistics outperform average statistics for all other HPAC modes.***

HPAC MODE 1, FULL MET AND NARAC:
ALL RELEASES - 1 HOUR AVERAGES

The plot in the top left shows a log-log plot of the HPAC (Mode 1, full met) and NARAC predictions versus observations in ng/m^3 for all releases. The plot on the right shows the normalized histograms of HPAC and NARAC predictions and observations. For low concentrations (~ 50 ng/m^3 and below) the three histograms are similar. Between ~50-500 ng/m^3 HPAC (blue) *overpredicts* both the NARAC predictions (red) and the observations (green).

At around 1000 ng/m^3 there is a peak in the NARAC histogram and a noticeable dip in the observation histogram. At ~ 2000 ng/m^3 and above, the NARAC and observation histograms track each other through ~ 4000 ng/m^3. The table shows summary statistics for HPAC and NARAC. The statistics show the significant underpredictive tendency of HPAC and the less pronounced underpredictive tendency of NARAC for these releases. The bottom two rows indicate the fraction of cases for which NARAC overpredicted HPAC (HPAC overpredicted NARAC).

HPAC Mode 1, Full Met and NARAC:
All Releases - 1 Hour Averages

	NARAC	HPAC	OBSERVATIONS
Mean (ng/m³)	690	347	846
Median (ng/m³)	394	210	399
Fac2	0.419	0.332	
Fac5	0.740	0.732	
Fac10	0.834	0.883	
Fraction underpredicted	0.570	0.774	
Fraction overpredicted	0.430	0.226	
Fraction NARAC > HPAC	0.728		
Fraction HPAC > NARAC	0.272		

10,000 RESAMPLED MOES; HPAC MODE 1, FULL MET AND NARAC: ALL RELEASES - 1 HOUR AVERAGES

The top figure shows 10,000 resampled HPAC and NARAC summed concentration MOEs for the 1-hour average concentrations for the 9 releases. The HPAC and NARAC clouds are clearly separated, with HPAC exhibiting more false negatives and fewer false positives than NARAC. The bottom figure shows 10,000 resampled HPAC and NARAC threshold MOEs based on a 20 ng/m^3 threshold. There is significant overlap between the HPAC and NARAC clouds, indicating similar low concentration (e.g., hazard area prediction) model performance. Since the detection limit is approximately 10 ng/m^3 , the instrument noise is high for this low concentration threshold. There are noticeable differences between the two models' relative performance when examining thresholds well above (> 10x) the instrument detection limit.

Resampled Summed Concentration MOEs:
All Releases, 1 Hour Averages

*The Summed Concentration MOE tests a model's ability to predict the **amount of material at the samplers***

- *HPAC exhibits sizeable false negatives and few false positives*
- *NARAC exhibits fewer false negatives and somewhat more false positives*
- *The performance of HPAC and NARAC is clearly separated*

*The Threshold MOE tests a model's ability to predict the **number of samplers that exceed the threshold**, in this case a low value of 20 ng/m³ (~ 2 times minimum detectable concentration)*

- *False negatives and false positives for HPAC and NARAC are greatly reduced with respect to Summed Concentration MOE*
- *HPAC and NARAC show very similar performance*

Resampled 20 ng/m³ Threshold MOEs:
All Releases, 1 Hour Averages
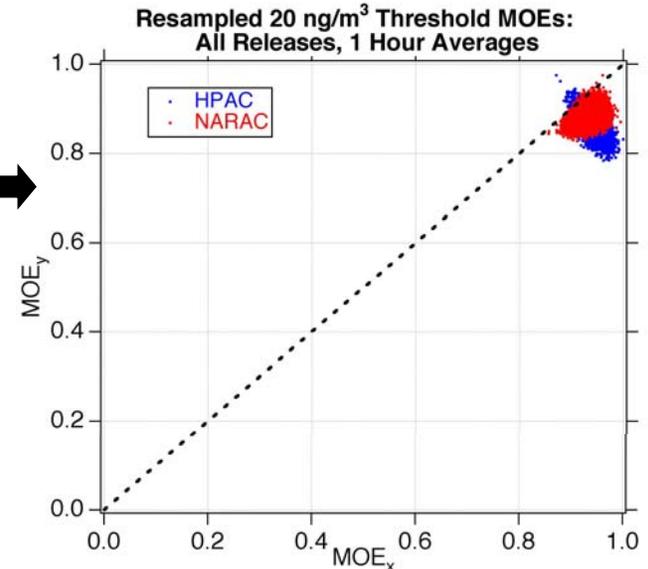
HPAC AND NARAC SUMMED CONCENTRATION MOE DIFFERENCES (NARAC-HPAC): 1 HOUR AVERAGE CONCENTRATIONS

The figure on the left shows the summed concentration MOE differences between NARAC and HPAC (NARAC MOE minus HPAC MOE). Two of the nine differences lie in the (+,+) quadrant, showing fewer false negatives and fewer false positives for NARAC. The remaining differences lie in the (+,-) quadrant, showing fewer false negatives and more false positives for NARAC. Sampler plots for the two (+, +) differences are also shown.
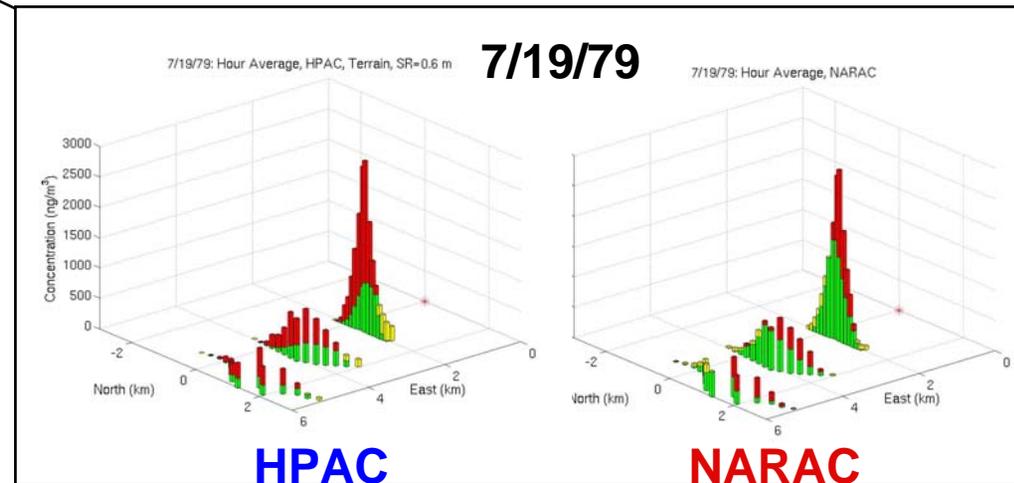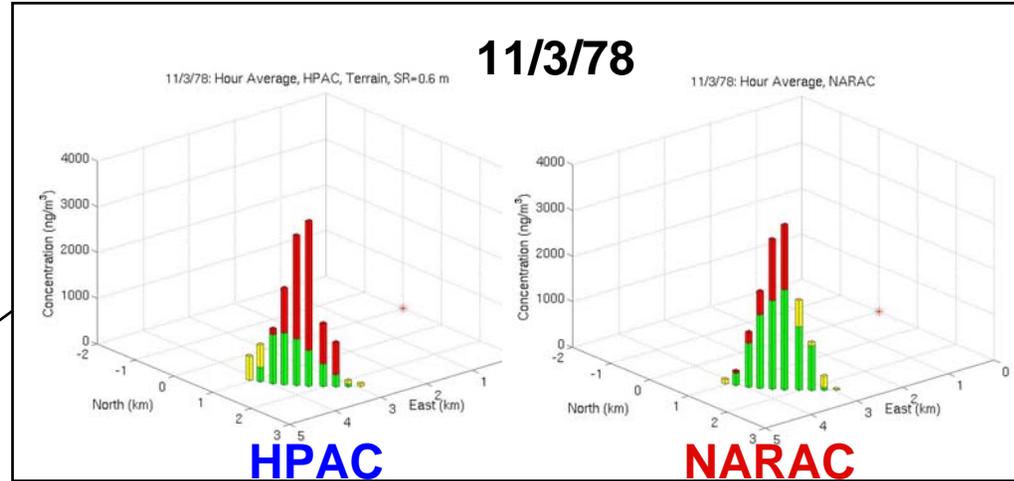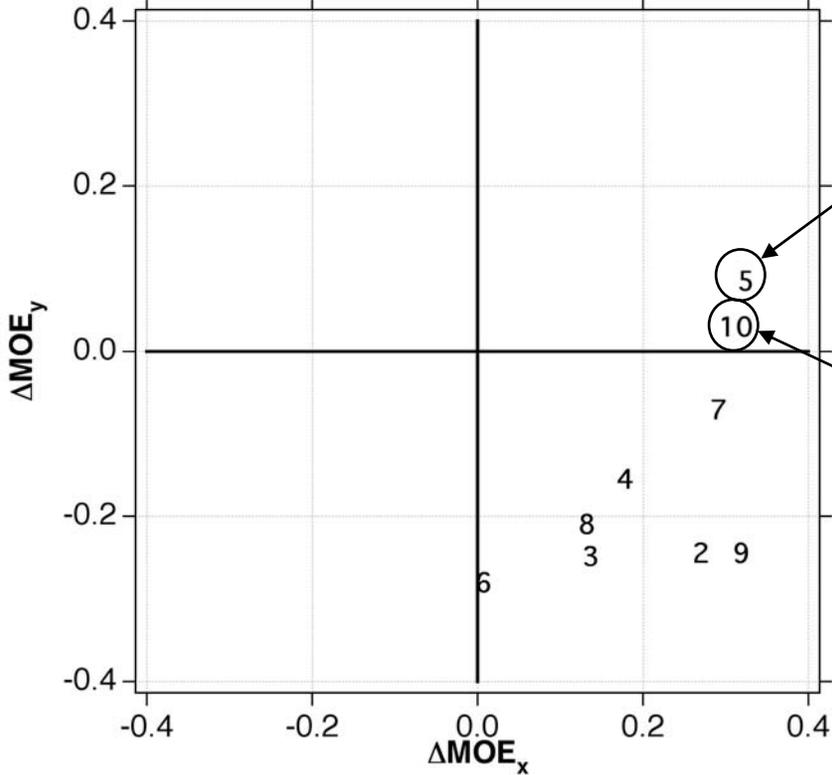
MODE 1 HPAC VS NARAC STATISTICAL DIFFERENCES:
1 HOUR AVERAGE CONCENTRATIONS

The slide shows the results of applying statistical hypothesis testing to the HPAC (Mode 1, full met) and NARAC statistics for the nine releases. The null hypothesis is that NARAC and HPAC do not differ. The *nonparametric* statistical test that is applied is a randomization test (the permutation test) on the paired differences between HPAC and NARAC statistics. A description of this technique with an application to urban T&D field trials can be found in reference [9] and references therein. Under the null hypothesis, the observed differences for each release are equally likely to be positive or negative. The test generates all

2^9=512 permutations of the 9 paired differences, computes their mean values, orders the absolute mean differences, and computes the probability (the p-value) of matching or exceeding that value. The p-value for the observed absolute mean difference is then obtained. Under this test the FB, NAD, NMSE, and BNMSE differences are all statistically significant at the 2% level (p-value < 0.02; see green values in the table). That is, for these statistics we reject the null hypothesis that HPAC and NARAC are the same at the 98 percent level. Similar results were found for the 3 other HPAC modes with full met.

Mode 1 HPAC vs NARAC Statistical Differences: 1 Hour Average Concentrations

- **Differences in HPAC and NARAC statistics were examined for statistical significance**
  - *Null hypothesis: HPAC and NARAC do not differ*
  - *Applied randomization test on paired differences (aka permutation test) and compute mean values over all permutations (standard nonparametric statistical test)*
  - *For these small data sets (9 paired differences), there are $2^9 = 512$ possible means => p-values can be computed exactly*
- **Findings**
  - *For HPAC Mode 1 (Full met), FB, NAD, NMSE, and BNMSE differences are all statistically significant at 2% level (p-value < 0.02), e.g., green values in table below*
  - *Similar findings for 3 other HPAC modes (Full met)*

| | 1 Hour Avg. Conc. Standard Statistics: Terrain, Surface Roughness = 0.6 m | | | | | | | | | | | | | |
| | FB | | NAD | | NMSE | | BNMSE | | FAC2 | | FAC5 | | FAC10 | |
	HPAC	NARAC	HPAC	NARAC	HPAC	NARAC	HPAC	NARAC	HPAC	NARAC	HPAC	NARAC	HPAC	NARAC
9/20/78	-0.766	0.005	0.430	0.320	2.536	0.753	0.234	0.089	0.387	0.387	0.903	0.742	0.968	0.774
9/26/78	-0.814	-0.236	0.461	0.418	2.847	1.400	0.296	0.184	0.458	0.417	0.708	0.667	0.875	0.875
10/19/78	-0.873	-0.184	0.607	0.508	4.140	1.838	0.373	0.213	0.118	0.182	0.441	0.515	0.618	0.667
11/3/78	-0.687	-0.220	0.464	0.197	1.941	0.344	0.260	0.049	0.250	0.875	1.000	0.875	1.000	1.000
11/9/78	-0.557	-0.083	0.462	0.554	1.779	2.029	0.194	0.250	0.321	0.208	0.643	0.417	0.893	0.458
4/30/79	-1.402	-0.660	0.703	0.381	8.654	1.439	0.518	0.154	0.048	0.286	0.429	0.905	0.952	1.000
6/27/79	-0.945	-0.400	0.536	0.464	5.542	2.639	0.424	0.276	0.370	0.348	0.717	0.652	0.826	0.826
7/6/79	-0.551	0.239	0.351	0.271	2.527	0.809	0.230	0.075	0.600	0.641	0.875	1.000	0.975	1.000
7/19/79	-0.781	-0.261	0.469	0.216	2.848	0.573	0.248	0.058	0.256	0.615	0.872	0.897	0.974	0.949
Mean Value	-0.820	-0.200	0.498	0.370	3.646	1.314	0.309	0.150	0.312	0.440	0.732	0.741	0.898	0.839
p-value	0.0039		0.0195		0.0078		0.0078		0.1719		0.9297		0.4688	

MULTIVARIATE ANALYSIS OF VARIANCE (MANOVA) APPLIED TO METRICS: 1 HOUR AVERAGE CONCENTRATIONS

Another method to analyze the statistical metrics is to apply multivariate analysis of variance (MANOVA) [10] to several metrics simultaneously. The method involves construction of two matrices H and E (reviewed in the slide) and computing the largest eigenvalue of the matrix $P=HE^{-1}$.

[10] Morrison, Donald F., *Multivariate Statistical Methods*, 3rd Ed., McGraw-Hill, 1990.

An F statistic is applied to a function of the largest eigenvalue to estimate significance (note that unlike the previous test, this test is a *parametric* statistical test). The test was applied to the metrics FB, NAD, BNMSE, FAC2, FAC5, and FAC10. The H and E matrices are shown along with the largest eigenvalue, F statistic, and significance. Under this test the HPAC and NARAC differences are significant at a level of less than 1%.

Multivariate Analysis of Variance (MANOVA) Applied to Metrics: 1 Hour Average Concentrations

- **Multivariate Analysis of Variance (MANOVA): Method to estimate the significance of several metrics *taken together***
  - Two matrices formed (c.f., Morrison, Donald F., *Multivariate Statistical Methods*, 3rd Ed., McGraw-Hill, 1990, p. 210)
    - H: "Hypothesis sum of squares matrix"
    - E: "Error sum of squares matrix"
  - Form the matrix product $P=HE^{-1}$
  - Compute largest eigenvalue of P
  - Significance is computed from F statistic applied to a function of the largest eigenvalue (note: this is a *parametric* statistical test)

- **Results**
  - Multivariate ANOVA applied to: FB, NAD, BNMSE, FAC2, FAC5, and FAC10
  - SPSS used to perform analysis*

H Matrix	FB	NAD	BNMSE	FAC2	FAC5	FAC10	E Matrix	FB	NAD	BNMSE	FAC2	FAC5	FAC10
FB	1.727	-0.357	-0.443	0.357	0.025	-0.165	FB	1.027	-0.231	-0.257	0.348	0.264	-0.041
NAD	-0.357	0.074	0.092	-0.074	-0.005	0.034	NAD	-0.231	0.216	0.162	-0.332	-0.31	-0.192
BNMSE	-0.443	0.092	0.113	-0.091	-0.007	0.042	BNMSE	-0.257	0.162	0.151	-0.21	-0.226	-0.118
FAC2	0.357	-0.074	-0.091	0.074	0.005	-0.034	FAC2	0.348	-0.332	-0.21	0.644	0.417	0.283
FAC5	0.025	-0.005	-0.007	0.005	0	-0.002	FAC5	0.264	-0.31	-0.226	0.417	0.632	0.396
FAC10	-0.165	0.034	0.042	-0.034	-0.002	0.016	FAC10	-0.041	-0.192	-0.118	0.283	0.396	0.384

  - Largest eigenvalue of $P=HE^{-1}$: $\lambda=3.223$
  - F statistic: F=5.909
  - **Significance: p=0.003 => Reject null hypothesis that HPAC and NARAC results are the same at a significance level of less than 1%**

*Reviewer Dr. Dennis DeRiggi provided this analysis

HPAC "OPERATIONAL" METEOROLOGY PERFORMANCE

The graph in the slide shows the FB performance of HPAC Mode 1 with the three meteorology options, Full met (blue filled diamonds), Operational (black stars), and Operational with Temperature (green circles), along with the NARAC FB values (red filled squares). With the exception of the 11/3/79 release, Operational and Operational with Temperature HPAC predictions performed better than or as well as Full met predictions; NAD, NMSE, and BNMSE show the identical trend. We note that the 11/3/79 release has a boundary layer height of 390 m, which is the lowest reported boundary layer height of all of the Copenhagen releases. The graph shows that adding temperature to the operational-only met did not improve the predictions. At this point it is not clear why the Operational meteorology outperforms the Full meteorology for these releases.

HPAC "Operational" Meteorology Performance

FB for 3 HPAC Met. Options: 1 Hour Averages
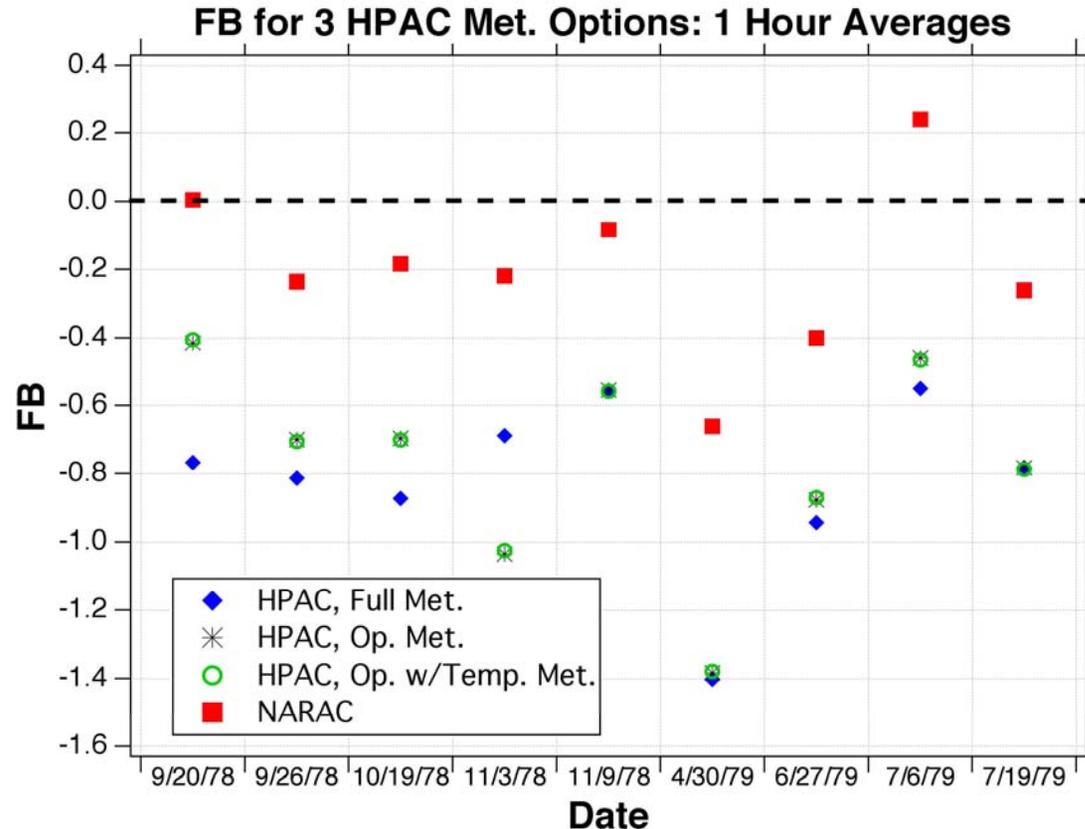
- *With the exception of the 11/3/78 release, "Operational" and "Operational with Temperature" HPAC predictions performed better than or as well as "Full Met" predictions (other measures show identical trend). Note that 11/3/78 release has 390 m reported BL height of all release (next lowest is 810 m).*
- *Including temperature in Operational Met. did not improve predictions noticeably*
- *Not clear at this point why Operational met outperforms Full met*

HPAC VERTICAL CONCENTRATION SLICES:
1000 NG/M^3, 7/6/79 RELEASE

The figure shows HPAC vertical concentration slices at 1000 ng/m^3 roughly down the plume centerline for several times after the start of the 7/6/79 release (for reference, the peak and mean observed concentrations on the first arc for this release are 2928 ng/m^3 and 965 ng/m^3 respectively). The 1 minute contour impacts the ground and extends to almost three times the release height, indicating a large vertical diffusivity. After 85 minutes (the length of the release) the downwind extent of the 1000 ng/m^3 contour at ground level does reach the first sampler arc. Similar behavior is observed in the HPAC vertical slice concentration histories for the other releases. It is reasonable to assume the unaccounted for mass in the HPAC simulations remains lofted or impacts the ground before the sampler grid. A large modeled vertical diffusivity relative to actual atmospheric conditions is one possible explanation for this.

HPAC Vertical Concentration Slices:
1000 ng/m³, 7/6/79 Release

First sampler arc observations
  Peak concentration = 2928 ng/m³
  Mean concentration = 965 ng/m³

After 1 minute, the HPAC 1000 ng/m³ contour impacts the ground and extends to ~ 3 times the release height

At 85 minutes (release duration) the 1000 ng/m³ contour at ground level does not extend to the first sampler arc (2 km downwind)

7/6/79 : HPAC Vertical Concentration Slices: 1000 ng/m³
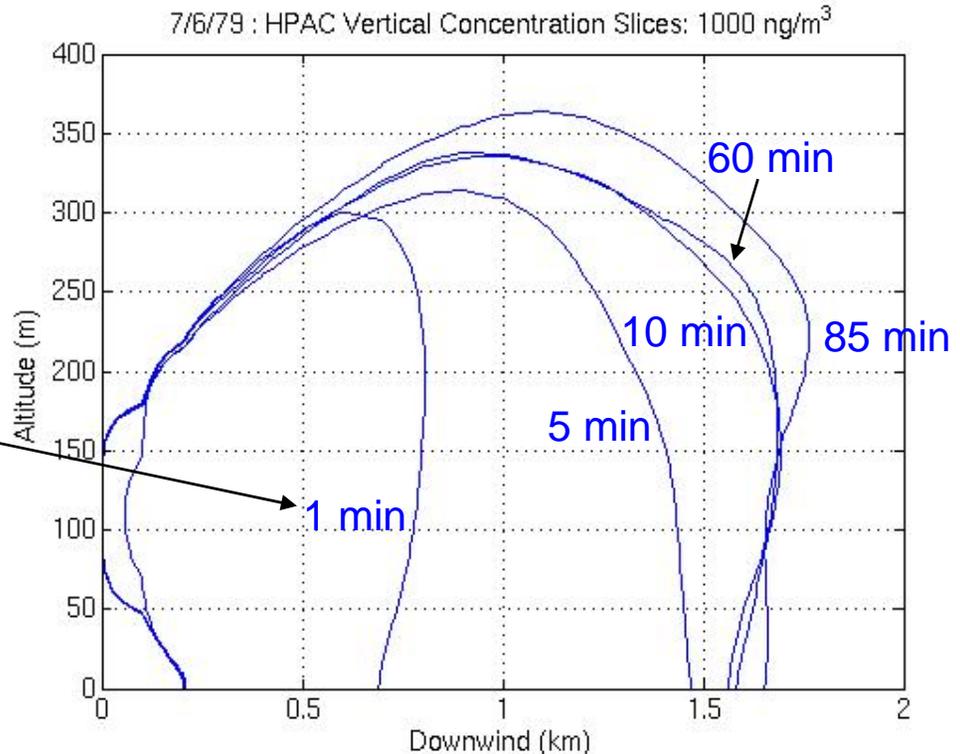
Reasonable to assume that unaccounted for mass in HPAC simulations is lofted or already on the ground before the sampler arcs - large modeled vertical diffusivity relative to atmospheric conditions is a possible explanation for this

Similar behavior is observed in the HPAC vertical slice concentration histories for the other releases

85

MAJOR FINDINGS

The slide highlights the major findings of this study. The main finding is that both HPAC and NARAC underpredict the 1-hour average ground concentrations of the elevated Copenhagen releases, with the HPAC underpredictions being much more pronounced than those of NARAC. With respect to the statistics FB, NAD, NMSE, and BNMSE, the differences between HPAC and NARAC are statistically significant at the 2 percent level. Multivariate ANOVA hypothesis applied to FB, NAD, BNMSE, Fac2, Fac5, and Fac10 shows that HPAC and NARAC differ at the 1% level of significance. Resampled HPAC and NARAC summed concentration MOEs are also well separated. The 4 HPAC terrain /landcover modes and the 3 met options do not "fix" the severe HPAC underpredictions. Finally, the HPAC vertical slice concentration contours suggest that the modeled HPAC vertical diffusivity is larger than what was present during the releases.

MAJOR FINDINGS

- **HPAC** and **NARAC** tend to underpredict these elevated releases at the sampler locations, with HPAC underpredictions being more pronounced

Ratio	NARAC	HPAC
$<Obs>/<Pred>$	1.22	2.44
$\mathrm{med}(Obs)/\mathrm{med}(Pred)$	1.01	1.90

- **HPAC** and **NARAC** differences are statistically significant at the 2% level with respect to FB, NAD, NMSE, and BNMSE (under MANOVA, HPAC and NARAC differences are significant at the 1 % level)

- Resampled (0.99 confidence regions) **HPAC** and **NARAC** summed concentration MOEs are completely separated (implying statistically significant differences)

- HPAC Mode and Met options do not "fix" the HPAC underpredictions

- HPAC vertical concentration slice contours suggest modeled vertical diffusivity is larger than atmospheric conditions during the releases

SECONDARY FINDINGS

The secondary findings of this study are listed in the slide.

SECONDARY FINDINGS

- **At at low threshold (20 ng/m^3 ~ 2 times minimum detectable concentration), the MOE performance of HPAC and NARAC are both favorable and nearly the same (slight false positive)**

- **At thresholds well above the instrument noise (> 10x instrument limit), differences in the models relative and absolute accuracy are more evident**

- **HPAC predictions conducted with constant surface roughness outperformed those conducted with landcover enabled; In general, "Terrain on", SR=0.6 m performed the best**

  - **Nonintuitive result: perhaps current landcover database does not represent the 1978-1979 Copenhagen area landcover**

- **Operational weather profiles (wind, speed and direction only or with temperature) yielded better HPAC predictions than those with full meteorological inputs, except for one of the 9 releases - not clear why this is happening.**

  - **Further investigation is required to understand this result**
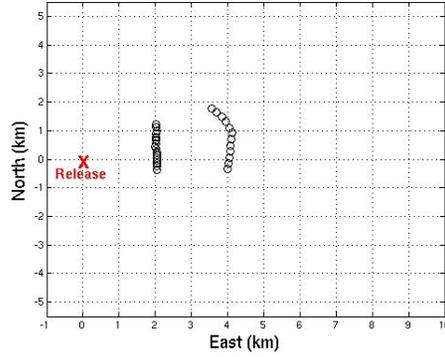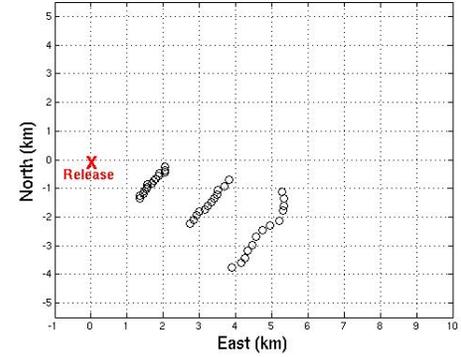
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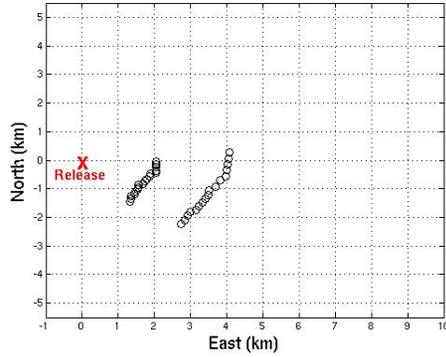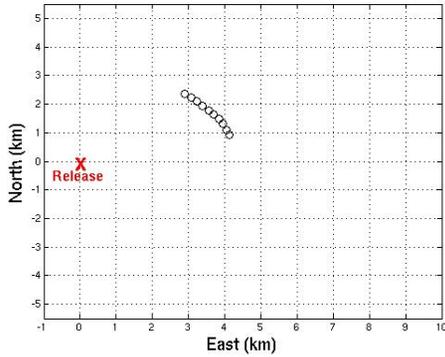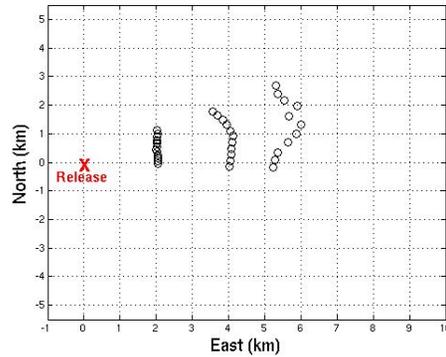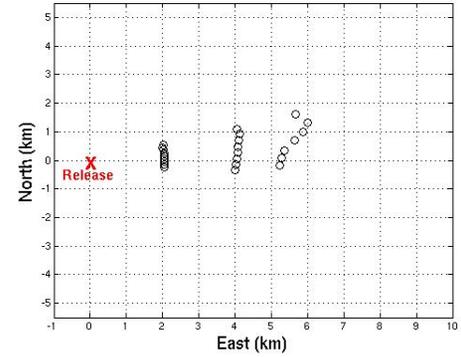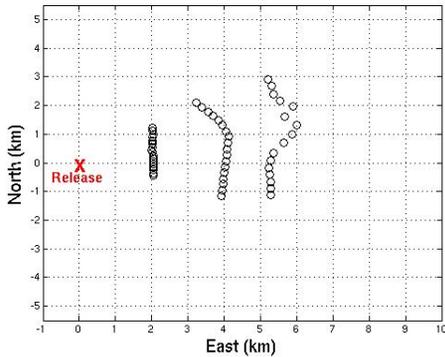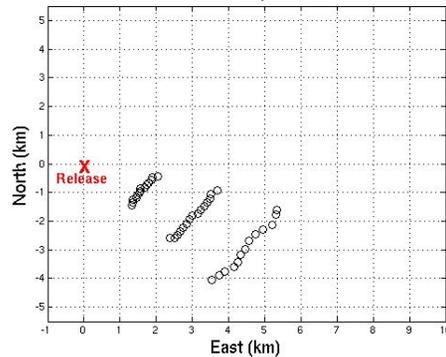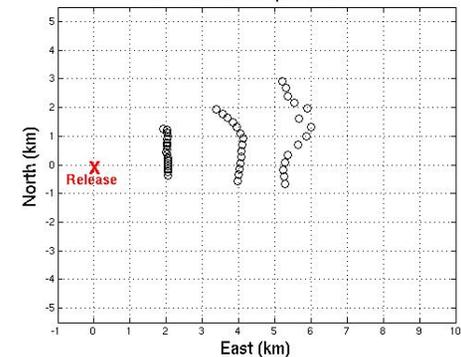
Arc 1

Sampler Number	x (m)	y (m)	UTM-East (m)	UTM-North (m)
Arc1-1	866	-1545	343387	6178033
Arc1-2	952	-1546	343473	6178029
Arc1-3	1038	-1532	343559	6178040
Arc1-4	1141	-1563	343661	6178005
Arc1-5	1233	-1586	343752	6177978
Arc1-6	1323	-1558	343843	6178003
Arc1-7	1345	-1486	343868	6178074
Arc1-8	1371	-1403	343897	6178156
Arc1-9	1398	-1312	343927	6178246
Arc1-10	1404	-1214	343937	6178343
Arc1-11	1492	-1131	344028	6178423
Arc1-12	1516	-1044	344055	6178509
Arc1-13	1582	-964	344124	6178587
Arc1-14	1592	-884	344137	6178666
Arc1-15	1602	-798	344150	6178752
Arc1-16	1703	-767	344253	6178779
Arc1-17	1766	-681	344319	6178862
Arc1-18	1800	-593	344356	6178949
Arc1-19	1877	-485	344437	6179054
Arc1-20	1921	-405	344484	6179132
Arc1-21	2067	-371	344631	6179161
Arc1-22	2061	-284	344629	6179248
Arc1-23	2055	-180	344627	6179352
Arc1-24	2050	-82	344625	6179450
Arc1-25	2044	20	344623	6179552
Arc1-26	2038	119	344621	6179651
Arc1-27	2032	225	344619	6179758
Arc1-28	2026	329	344617	6179862
Arc1-29	2000	434	344595	6179968
Arc1-30	1978	524	344577	6180058
Arc1-31	2008	626	344610	6180159
Arc1-32	2002	758	344609	6180291
Arc1-33	1996	854	344607	6180387
Arc1-34	1991	956	344606	6180490
Arc1-35	1995	1081	344615	6180614
Arc1-36	1986	1187	344610	6180721
Arc1-37	1969	1287	344597	6180821
Arc1-38	1880	1333	344509	6180871
Arc1-39	1829	1407	344461	6180946
Arc1-40	1750	1480	344385	6181022
Arc1-41	1697	1566	344335	6181110
Arc1-42	1594	1657	344236	6181205
Arc1-43	1507	1708	344151	6181259
Arc1-44	1440	1742	344085	6181296
Arc1-17A	2094	-761	344644	6178770
Arc1-18A	2087	-638	344641	6178893
Arc1-19A	2078	-538	344636	6178993
Arc1-20A	2071	-446	344633	6179086

Arc 2

Sampler Number	x (m)	y (m)	UTM-East (m)	UTM-North (m)
Arc2-1	1548	-2681	344025	6176872
Arc2-2	1690	-2603	344170	6176945
Arc2-3	1841	-2578	344322	6176964
Arc2-4	1998	-2554	344479	6176982
Arc2-5	2155	-2529	344637	6177001
Arc2-6	2313	-2505	344796	6177019
Arc2-7	2469	-2480	344953	6177038
Arc2-8	2616	-2492	345099	6177020
Arc2-9	2691	-2388	345178	6177121
Arc2-10	2747	-2258	345239	6177249
Arc2-11	2818	-2134	345315	6177370
Arc2-12	2920	-1987	345422	6177513
Arc2-13	3002	-1830	345510	6177667
Arc2-14	3075	-1704	345588	6177790
Arc2-15	3204	-1629	345720	6177860
Arc2-16	3299	-1498	345820	6177988
Arc2-17	3380	-1367	345906	6178115
Arc2-18	3448	-1231	345979	6178249
Arc2-19	3518	-1093	346054	6178384
Arc2-20	3558	-919	346100	6178556
Arc2-21	3729	-787	346276	6178682
Arc2-22	3837	-550	346393	6178914
Arc2-23	3998	-418	346559	6179040
Arc2-24	4012	-196	346582	6179262
Arc2-25	4026	9	346603	6179466
Arc2-26	4038	208	346623	6179664
Arc2-27	4053	431	346646	6179887
Arc2-28	4066	638	346667	6180093
Arc2-29	4083	865	346693	6180319
Arc2-30	4094	1083	346712	6180536
Arc2-31	3999	1255	346624	6180712
Arc2-32	3891	1459	346524	6180920
Arc2-33	3773	1615	346412	6181080
Arc2-34	3635	1772	346280	6181242
Arc2-35	3486	1922	346137	6181398
Arc2-36	3304	2079	345961	6181562
Arc2-37	3152	2230	345815	6181718
Arc2-38	2987	2353	345654	6181848
Arc2-39	2805	2462	345477	6181964
Arc2-40	2628	2543	345303	6182051
Arc2-41	2432	2671	345112	6182187
Arc2-42	2275	2811	344960	6182332
Arc2-43	2153	2963	344844	6182489
Arc2-20A	3960	-1009	346499	6178451
Arc2-21A	3972	-818	346518	6178642
Arc2-22A	3987	-586	346542	6178873

Arc 3

Sampler Number	x (m)	y (m)	UTM-East (m)	UTM-North (m)
Arc3-2	2898	-4900	345290	6174603
Arc3-3	3002	-4842	345396	6174657
Arc3-4	3139	-4614	345541	6174880
Arc3-5	3342	-4276	345757	6175210
Arc3-6	3541	-4118	345962	6175360
Arc3-7	3693	-3919	346121	6175553
Arc3-8	3883	-3752	346317	6175713
Arc3-9	4027	-3616	346467	6175843
Arc3-10	4283	-3447	346729	6176003
Arc3-11	4390	-3277	346842	6176168
Arc3-12	4459	-3010	346921	6176433
Arc3-13	4572	-2795	347042	6176643
Arc3-14	4668	-2514	347149	6176920
Arc3-15	4824	-2260	347315	6177168
Arc3-16	5029	-2108	347525	6177312
Arc3-17	5286	-1939	347788	6177471
Arc3-18	5378	-1570	347894	6177837
Arc3-19	5395	-1399	347918	6178007
Arc3-20	5375	-1139	347908	6178267
Arc3-21	5323	-913	347864	6178495
Arc3-22	5305	-690	347855	6178719
Arc3-23	5314	-456	347873	6178952
Arc3-24	5264	-218	347832	6179192
Arc3-25	5229	35	347807	6179446
Arc3-26	5268	277	347855	6179686
Arc3-27	5354	558	347951	6179964
Arc3-28	5618	914	348229	6180310
Arc3-29	5829	1208	348451	6180595
Arc3-30	5952	1544	348586	6180926
Arc3-31	5608	1827	348253	6181222
Arc3-32	5809	2176	348468	6181563
Arc3-33	5451	2381	348118	6181782
Arc3-34	5259	2601	347934	6182009
Arc3-35	5213	2880	347899	6182290
Arc3-36	5097	3112	347792	6182526
Arc3-37	4986	3363	347690	6182781
Arc3-38	4772	3545	347483	6182971
Arc3-39	4602	3754	347321	6183186
Arc3-40	4361	3821	347083	6183262
Arc3-41	4135	3950	346862	6183400
Arc3-42	4030	4115	346764	6183569
Arc3-43	3781	4138	346516	6183601
Arc3-44	3535	4269	346275	6183741

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Appendix A

GLOSSARY

Appendix A
GLOSSARY

ADAPT   Atmospheric Data and Parameterization Tool

AGL   above ground level

ARAC   Atmospheric Release Advisory Center

BNMSE   Bounded Normalized Mean Square Error

CBRN   Chemical, Biological, Radiological, and Nuclear

DHS   Department of Homeland Security

DOE   Department of Energy

DTRA   Defense Threat Reduction Agency

FB   Fractional Bias

HPAC   Hazard Prediction and Assessment Capability

IDA   Institute for Defense Analyses

IMAAC   Interagency Modeling and Atmospheric Assessment Center

LLNL   Lawrence Livermore National Laboratory

LODI   Lagrangian Operational Dispersion Integrator

MANOVA   multivariate analysis of variance
MLOD   method level of detection
MOE   Measure of Effectiveness

NAD   Normalized Absolute Difference
NARAC   National Atmospheric Release Advisory Center
NGA   National Geospatial Intelligence Agency
NMSE   Normalized Mean Square Error

OLAD   Over-Land Wind Dispersion

SCIPUFF   Second-Order Closure Integrated Puff Model
SF6   Sulfur Hexafluoride
SWIFT   Stationary Wind Fit and Turbulence
SWIM   SCIPUFF Weather Input Model

T&D   transport and dispersion

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13. SUPPLEMENTARY NOTES

14. ABSTRACT

The U.S. Government has invested in sophisticated computer models to predict the transport and dispersion (T&D) and the ensuing human effects of Chemical, Biological, Radiological, and Nuclear (CBRN) agents and materials. As new modeling capabilities are added, there is a continuing need to verify and validate T&D models through rigorous comparisons to field trial data. Since 2000, IDA has taken part in verification and validation activities connected with the Hazard Prediction and Assessment Capability (HPAC) model developed by the Defense Threat Reduction Agency (DTRA). In past studies we have compared the predictions of HPAC to several field trial data sets, covering a broad range of release conditions, terrain, and weather conditions. IDA has also conducted comparative evaluation studies involving the National Atmospheric Release Advisory Center (NARAC) emergency response model developed by Lawrence Livermore National Laboratory. Additional insight into model performance and capabilities can be gleaned by comparing the model predictions of two or more models to field trial data and to one another, which is the approach taken in the present study.

15. SUBJECT TERMS

transport and dispersion; chemical, biological, radiological, and nuclear; CBRN; Hazard Prediction and Assessment Capability; HPAC; National Atmospheric Release Advisory Center; NARAC

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