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MESOSCALE ATMOSPHERIC MODELING OF THE JULY 12, 1992 TRITIUM RELEASE FROM THE SAVANNAH RIVER SITE (U)

by J. D. Fast

Westinghouse Savannah River Company
Savannah River Site
Aiken, South Carolina 29808

Other Authors:

B. L. O'Steen
R. P. Addis

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Jerome D. Fast, B. Lance O'Steen, and Robert P. Addis
Westinghouse Savannah River Company
Savannah River Site
Aiken, South Carolina 29808

ABSTRACT

In August of 1991, the Environmental Transport Group (ETG) began the development of an advanced Emergency Response (ER) system based upon the Colorado State University Regional Atmospheric Modeling System (RAMS). This model simulates the three-dimensional, time-dependent, flow field and thermodynamic structure of the planetary boundary layer (PBL). A companion Lagrangian Particle Dispersion Model (LPDM) simulates contaminant transport based on the flow and turbulence fields generated by RAMS. This paper describes the performance of the advanced ER system in predicting transport and diffusion near the SRS when compared to meteorological and sampling data taken during the July 12, 1992 tritium release. Since PUFF/PLUME and 2DPUF are two Weather INformation and Display (WIND) System atmospheric models that were used to predict the transport and diffusion of the plume at the time of the release, the results from the advanced ER system are also compared to those produced by PUFF/PLUME and 2DPUF.

The integrated concentration of tritium predicted by the advanced ER system compared very well to the limited amount of data taken from three tritium monitors at the site boundary; however, care must be taken in evaluating the model from this data since the total amount of tritium released on July 12, 1992 was relatively small and the observed concentrations at the tritium monitors were very low. The advanced ER system was also able to predict the initial direction of the plume better than PUFF/PLUME and 2DPUF when the predicted plume centerline and width were compared to data taken from the tritium monitors. As expected, the plume direction and width 25 km downwind of the site produced by the advanced ER system and 2DPUF were substantially different because the advanced ER system takes into account a more complex wind field.

INTRODUCTION

Atmospheric transport and diffusion models have been developed for real-time calculations of the location and concentration of toxic or radioactive materials during an unplanned release at the Savannah River Site (SRS). These models employ one or two-dimensional measured wind characteristics to determine advection of air-borne contaminants and assume Gaussian distributions to represent turbulent diffusion. These models have been incorporated into an automated menu-driven program called the Weather INformation and Display (WIND) System (Hunter 1990). The assumptions employed by the WIND System atmospheric models allow the computations of the ground-level concentration of toxic or radioactive materials to be made quickly; however, Gaussian models suffer from limitations because of the simplifications made to the governing equations. Nevertheless, most commercial emergency response models in use today employ the Gaussian assumption.

The WIND System atmospheric models are unique in that they incorporate a forecasted wind field based on large-scale model results from the National Weather Service (NWS) Model Output Statistics (MOS) product. However, the MOS forecast wind field is only one-dimensional. Thus, even with MOS forecast capability, the WIND System atmospheric model results have limited real-time regional capability due to spatial inhomogeneity unaccounted for in the forecast meteorological fields. A more realistic forecast, at both local and regional scales, requires prognostic, three-dimensional fields that will be demonstrated in this paper.

Three-dimensional, coupled atmospheric-dispersion models, such as RAMS and LPDM are not limited by the simplifications of the Gaussian diffusion assumption. These two models have been used in the past to predict the transport of pollutants in a variety of complex atmospheric circulations (Pielke *et al.* 1987a,b) and the use of similar three-dimensional models in ER applications has been the subject of a recent symposium (OCDE 1991). Unfortunately, models such as RAMS require large amounts of computational time when run with high resolution for a regional forecast. Full utilization in such an operational capacity is still not practical at this time. However, advances in computer technology has made possible high-resolution, semi-diagnostic calculations for local contaminant transport, and low-resolution, fully-prognostic calculations for regional-scale contaminant transport (O'Steen and Fast 1992).

RAMS and LPDM were executed in two modes of operation including (1) a post-accident analysis mode, and (2) a semi-diagnostic mode to determine the local and regional transport and diffusion from the July 12, 1992 tritium release from H-area at the SRS. Three-dimensional wind, turbulence, and temperature fields were reconstructed for July 12 by assimilating the local meteorological data observed at the SRS and the National Weather Service (NWS) surface observations into the RAMS model. The second mode of operation was used to demonstrate the performance of the advanced ER system in an emergency response situation. The fully-prognostic capabilities of the advanced ER system based on RAMS and LPDM are not examined in this study, but will be investigated in the near future.

ADVANCED EMERGENCY RESPONSE MODELING SYSTEM

A schematic diagram showing the computational resources available for the advanced ER system, the individual codes, and the input and output data is depicted in Fig. 1. The configuration of RAMS and LPDM for the July 12 case are described below in more detail.

RAMS model

RAMS is a three-dimensional atmospheric model that predicts the time-dependent, flow field and thermodynamic structure within and above the PBL (Tripoli and Cotton 1982) All atmospheric models require input data for initial conditions and or lateral boundary conditions. The required input for RAMS consists of National Meteorological Center (NMC) Nested Grid Model (NGM) output and National Weather Service (NWS) surface and upper-air data (O'Steen and Fast 1992). The NGM is an atmospheric model used by the National Meteorological Center (NMC) to produce operational weather forecasts twice a day for North America. Over the U. S., the resolution of the NGM is approximately 90 km. Combining the NGM model output and the most recent NWS observations is one way of obtaining large-scale three-dimensional dynamic and thermodynamic fields. However, there may be instances in which the local wind characteristics at SRS can differ substantially from the large-scale wind field. Then, the initial conditions in RAMS would not adequately represent the wind field over SRS and may reduce the reliability of the subsequent dispersion forecasts.

Four-dimensional data assimilation (4DDA) techniques provide a method for incorporating meteorological observations (including high-resolution data such as those available from the SRS meteorological towers) into the model results over an extended period of time. 4DDA techniques have received a great deal of attention recently to not only improve the initial conditions of mesoscale forecast models, but to create high-quality four-dimensional mesoscale analysis fields that can be used as input to air-quality models. Several 4DDA techniques have been recently developed to incorporate high-resolution asynoptic observational data into atmospheric model forecasts (Harms *et al.* 1991). One of those techniques is Newtonian relaxation, in which the model variables are gradually driven, or nudged, toward the observations by extra forcing terms in the governing equations. Although it is less rigorous than state-of-the-art techniques such as Kalman-Bucy filtering or the adjoint method, Newtonian relaxation is more practical due to its simplicity and less demanding computational requirements which are important in ER applications. The results of recent studies (Kao and Yamada 1988; Stauffer and Seaman 1990; Stauffer and Seaman 1991; Yamada and Hermi 1991) have indicated that improved initial conditions and forecasts can be generated by this technique.

The Newtonian relaxation technique has been incorporated in RAMS to generate better initial conditions for a forecast and to provide a meshing of model results with the observations taken from the SRS meteorological towers for optimal diagnostic fields for ER purposes. The code has been evaluated using data taken from one experiment of the Atmospheric Studies in COmplex Terrain (ASCOT) program (sponsored by the DOE Office of Health and Environmental Research) along the front range of the Rockies in Colorado (Fast and O'Steen 1992a). The dispersion of non-buoyant particles and the predicted surface concentrations were also compared to tracer data taken from the 1991 Winter Validation Study conducted by EG&G Rocky Flats personnel (Fast and O'Steen 1992b). One of the reasons the ASCOT program was established was to develop techniques for predicting transport and diffusion of pollutants in complex terrain for emergency response needs. The results of the study indicated that 4DDA was able to produce high-resolution mesoscale analysis fields that could be used to predict the transport and diffusion of pollutants.

LPDM model

The advanced ER system employs a Lagrangian Particle Dispersion Model (LPDM) to simulate contaminant transport based on the flow and turbulence fields generated by RAMS (McNider *et al.* 1988). The mean-wind components produced by RAMS are used to advect non-buoyant particles, and the turbulent velocity fluctuations of the particles are determined by the turbulence fields in RAMS and a finite difference analog to the Langevin stochastic differential equation. Dosimetry calculations have been added to LPDM so that the transport and diffusion of radionuclides can be determined. Deposition and more complex dosimetry will be incorporated into LPDM at a later date. LPDM employs a three-dimensional grid to calculate the particle concentration in individual cells. The results of the model can be compared to observed values by interpolating the predicted surface concentrations to specific locations.

METEOROLOGICAL CONDITIONS

A pronounced ridge of high pressure was off the southeast coast of the U. S. on July 12, 1992 as shown in Fig. 2. At the time of the release, the weather was partly cloudy with a temperature of 92° F. The wind measurements averaged over a 15-minute period during the time of the release of tritium are depicted in Fig. 3a. At the H-area meteorological tower, the average winds were from the west-southwest at 2.3 m s^{-1} (5.3 mph). The average winds were from the south between 1.5 - 2.5 m s^{-1} (3.5 - 5.8 mph) for the meteorological towers south of H-area. The observations at this time indicated that convergence of the flow could be particularly important in determining the transport of the plume from H-area shortly after the release time. During the next several hours wind directions were observed to become more southwesterly, then southerly throughout the site as seen in Figs. 3b - 3d. The specific wind field characteristics can be found in Table 1.

Shortly after 1300 EDT, thunderstorms developed rapidly along a line extending from central Georgia into central South Carolina to the northeast of SRS. The strongest storm in the area developed around 1400 EDT in northeast Aiken County, and moved slowly eastward into western Orangeburg County during the next few hours. The wind observations at the meteorological towers indicated thunderstorm activity on the site after 1800 EDT (not shown). All of the thunderstorm activity diminished by the early evening hours.

EXPERIMENTAL DESIGN

Three simulations were performed for the July 12, 1992 tritium release including:

case 1: fully diagnostic post-accident analysis mode
case 2: semi-diagnostic operational system (O'Steen and Fast 1992) assuming knowledge of release at 1230 EDT
case 3: same as case 2, except knowledge of release at 1330 EDT

In case 1, RAMS was executed with all of the available meteorological data as if a post-accident analysis was to be made. The model was initialized at 0800 EDT on July 12, 1992 with the initial and boundary conditions specified using the large-scale results from the NGM model. A 24-hour forecast of the wind field was made in which the data from the meteorological towers were assimilated every 15 minutes during the entire forecast using the 4DDA technique.

Cases 2 and 3 are what would be predicted by the advanced ER system if it was executed in a semi-diagnostic operational mode. Case 2 assumes that the modeling system is run at the time of the release; therefore, a constant, three-dimensional wind field based on the latest winds at 1230 EDT are used. Over short periods of time, the constant wind field assumption is a relatively good assumption (Hunter 1989) over the SRS that can be used for local transport on the site. This assumption also reduces the computational time required to produce a dispersion forecasts so that the RAMS and LPDM models can be used in ER applications. Case 3 assumes that the modeling system is run one hour after the release time. In this situation, meteorological information is available between 1230 EDT and 1330 EDT and is assimilated into the wind fields produced by RAMS. Then, a constant wind field is used after 1330 EDT.

Prognostic forecasts of the wind field could also be made based on the initial conditions produced by cases 2 or 3; however, the relatively extensive computational time required for such as calculation would make it impractical for ER applications at this time unless the system was operating on a supercomputer. In addition, concentrations measured at several locations downwind of the SRS in South Carolina were extremely low and it would be difficult to evaluate the prognostic capability of the advanced ER system for this particular tritium release. For both of these reasons, prognostic forecasts are not examined in this report, but will be investigated in the near future.

For all three cases, a plume was produced by assuming a release between 1215 and 1217 EDT, 61 m above the surface at the H-area location. 9600 particles were released by LPDM to simulate the observed plume. Surface concentrations were calculated and interpolated to the observed tritium monitor locations at Windsor, Williston, and Dark Horse Gates near the site perimeter, as well as several off-site locations where mobile sampling took place.

NUMERICAL RESULTS

The observed southwesterly and southerly flow that persisted over SRS for most of the afternoon was also produced by RAMS in the local wind field for case 1 at 1230, 1330, 1430 and 1730 EDT as shown in Fig. 4. A moderate amount of spatial inhomogeneity in the local wind observations were assimilated into the three-dimensional wind field produced by RAMS. 4DDA was able to produce a wind field that was consistent with the observations; however, the model was not overwhelmed by them.

A statistical comparison of the model results produced by RAMS for case 1 is shown in Fig. 5 in which the Root-

Mean-Squared (RMS) error was calculated for wind speed, wind direction, and temperature. Most of the wind speed errors were less than 1 m s^{-1} and were as low as 0.5 m s^{-1} at the time of the tritium release. These errors could have been reduced even further if the observations were weighted more in the 4DDA technique; however, it was decided to employ weights that were the same order of magnitude as those found in other similar studies (Kao and Yamada 1988; Stauffer and Seaman 1990; Stauffer and Seaman 1991; Yamada and Hermi 1991). Relatively large errors occurred between 1800 and 2000 EDT when thunderstorm activity produced large spatial and temporal variability in the wind field over the site. These errors were produced because the cloud microphysics in RAMS was not activated. Relatively large RMS errors also occurred for the temperature during this time as seen in Fig. 5c. Since the release occurred at 1230 EDT, the errors in the wind field from 1800 pm to 2000 EDT did not impact the predicted plume path near the site.

Thunderstorms occur an average of 56 days out the year at Augusta (Hunter 1989) and their duration is usually a few hours; therefore, large variabilities in the wind field due to thunderstorms, such as those on July 12, probably occur for only a small fraction of the time over the site. Nevertheless, the performance of the 4DDA technique in these situations needs to be investigated further.

In addition to 4DDA, another advantage of running RAMS in a semi-diagnostic mode is that a realistic development of the thermodynamic boundary layer can be produced. The boundary-layer depth is an important parameter in determining the amount of dispersion near the surface. The predicted boundary-layer height determined by RAMS and 2DPUF is shown in Fig. 6. The boundary-layer height in 2DPUF is based on a climatological value with the maximum value of 1 km above the ground. RAMS predicted a boundary layer height of nearly 1.5 km by the late afternoon. Given that the weather that day was very hot with partly cloudy skies, the results from RAMS are probably more realistic. Unfortunately, observations of the boundary-layer height measured by an acoustic sodar were not available that day to confirm the model calculations.

The instantaneous concentration of tritium oxide predicted at two time periods for case 1 are shown in Fig. 7. The plume moved to the northeast and the leading edge intersected the site boundary at 1330 EDT and the maximum concentration moved over the site boundary by 1430 EDT. Since it is roughly 10 km from H-area to the site boundary, an average transport speed of approximately 2.2 m s^{-1} would be required for the predicted plume to intersect the site boundary. The average wind speed at H-area from 1215 to 1330 EDT was 1.9 m s^{-1}. Gaussian models, such as PUFF/PLUME and 2DPUF, which use the meteorological tower information in a post-accident analysis mode would have predicted the plume arrival time to be roughly 15 minutes later than the advanced ER system. Unfortunately, the arrival time of the plume could not be obtained from the perimeter monitors. The predicted plumes for cases 2 and 3 were similar to those in Fig. 7 and are not shown.

The integrated concentration of tritium oxide predicted for case 1 is shown in Fig. 8 to illustrate the path of the plume during the afternoon. The predicted plume centerline passed just to the northwest of Williston gate at the site boundary with the western edge passing over Windsor Gate. Observations taken at the three tritium monitors at the site boundary are listed in Table 2 and appear to confirm that the predicted plume path was correct. Both the observations and the model predictions had the highest concentrations at Williston Gate, slightly lower values at Dark Horse Gate, and relatively low values at the Windsor Gate monitor. The magnitudes of the integrated concentrations (and therefore the dose) for both the model and the observations are the same. It is interesting to note that the results from cases 2 and 3 are sometimes better than those from case 1; however, care must be taken in interpreting the observed integrated concentrations in Table 2 since the values are relatively low and the value at Windsor Gate was just above the background level.

A time history of the concentration at the tritium monitor locations was also calculated by the advanced ER system as shown in Fig 9. The concentrations depicted in Fig. 9a were determined on a fine grid mesh, while those in Fig. 9b were determined on a slightly coarser mesh; therefore, the plots in Fig. 9b are artificially smoother than those in Fig. 9a. The edge of the plume was also found to pass near Aiken State Park 4 - 5 hours after the release (Fig. 9c); however ,the concentrations were predicted to be very low as shown in Fig. 10c. Sampling was done at Aiken State Park 19 miles from SRS between 1715 and 1545 EDT, but the predicted concentrations were much higher than those observed (Dunn 1992). The time history of the concentrations produced by cases 2 and 3 were similar to those in Fig. 9.

The vertical distribution of the plume is shown in Fig. 10 at the same time periods as the surface concentrations in Fig. 7. The simulated plume was mixed throughout convective boundary layer, although the maximum concentration still occurred near the surface. Two hours after the release of the plume, the upper portion of the plume was advected at a greater speed because of the vertical wind shear. Vertical wind shear is an important feature of the three-dimensional wind field that convectional Gaussian dispersion models cannot simulate.

The output of the advanced ER system was also compared to the existing operational WIND System dispersion models PUFF/PLUME and 2DPUF. PUFF/PLUME was used initially on July 12 to predict the path of the plume (Dunn 1992) (Fig. 11a) and 2DPUF was executed later in a post-accident analysis mode (Fig. 11b). PUFF/PLUME's and 2DPUF's centerline was further west, passing close to Windsor Gate. If the tritium monitor observations are correct, it appeared that the advanced ER system predicted the trajectory more accurately. PUFF/PLUME does incorporate a time-dependent wind field; however, it does not vary in space and is based on the winds at H-Area and the MOS forecast that is only valid at a single location. The small amount of variability in the wind field shown in Fig. 3 was probably very important in transporting the plume in this case. The plume width produced by 2DPUF was also similar to the one produced by the advanced ER system. Figure 11 also demonstrates the kind of differences one can expect between the various models. On July 12, the weather conditions were such that Gaussian models should perform adequately. There are obviously other weather conditions in which three-dimensional wind fields can have even a greater impact on the transport and diffusion around SRS.

CONCLUSION

The ability to execute the RAMS and LPDM codes for post-accident analysis and semi-diagnostic modes of operation for local contaminant transport has been demonstrated. Large-scale, regional and local (SRS towers) data were all included in this analysis through initial conditions, time-dependent boundary conditions, and periodic data assimilation. The integrated concentration of tritium predicted by the advanced ER system compared very well to the limited amount of data taken from three tritium monitors at the site boundary. The advanced ER system was also able to predict the initial direction of the plume better than PUFF/PLUME and 2DPUF. The software for executing the advanced ER system in an operational mode is currently being developed. Extensive testing of the system will be done in the near future, and implementation will follow.

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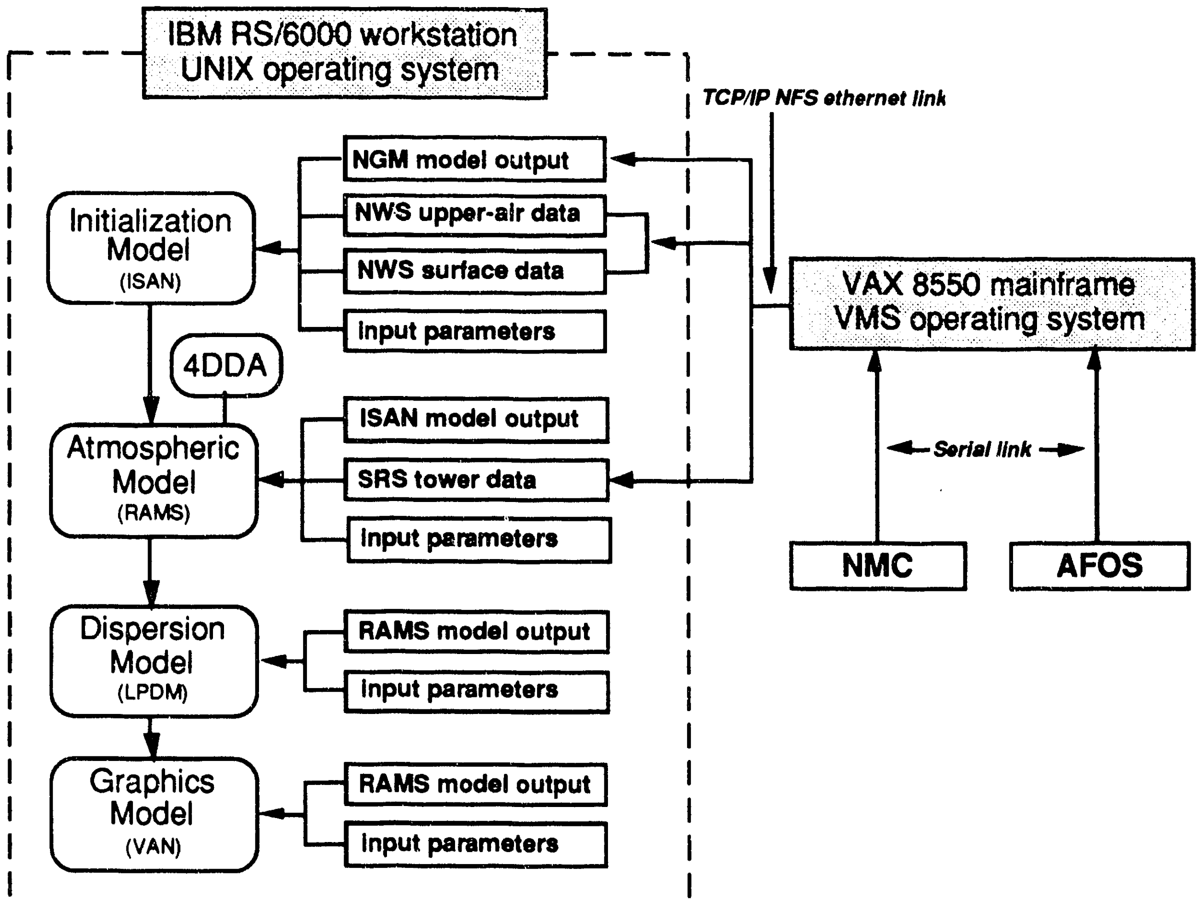


Fig. 1 Schematic diagram of the computational environment and individual modules of the three-dimensional advanced ER system

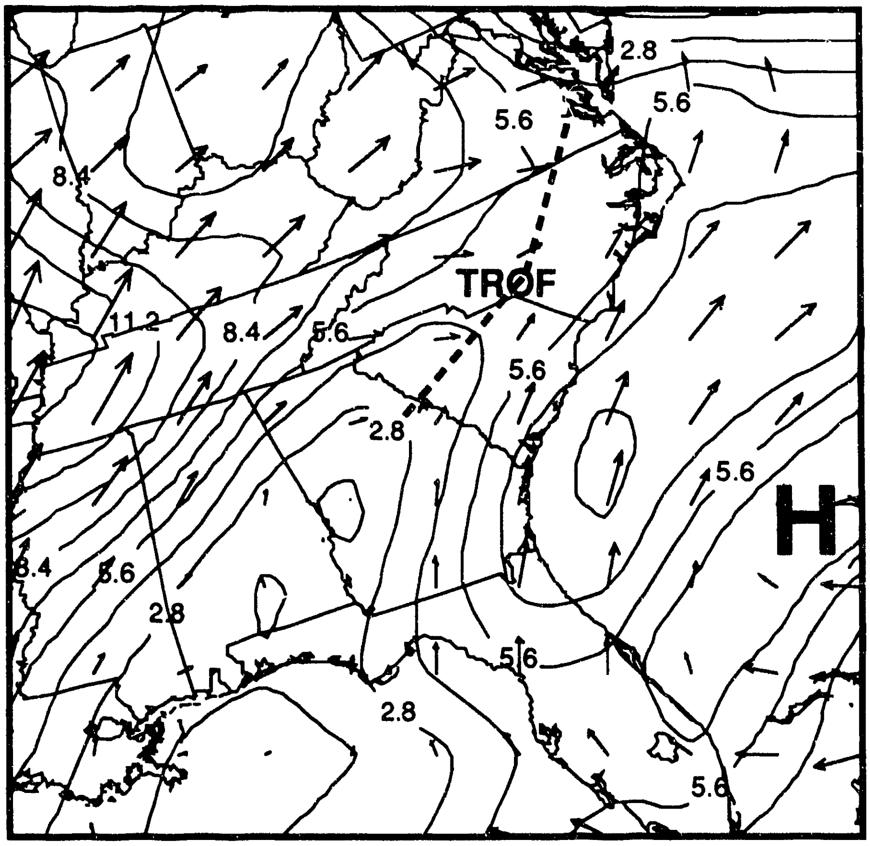


Fig. 2 Surface weather map at 0800 EDT, July 12, 1992, with NGM surface analysis of wind direction (arrows) and wind speed (contours) in m s^{-1}

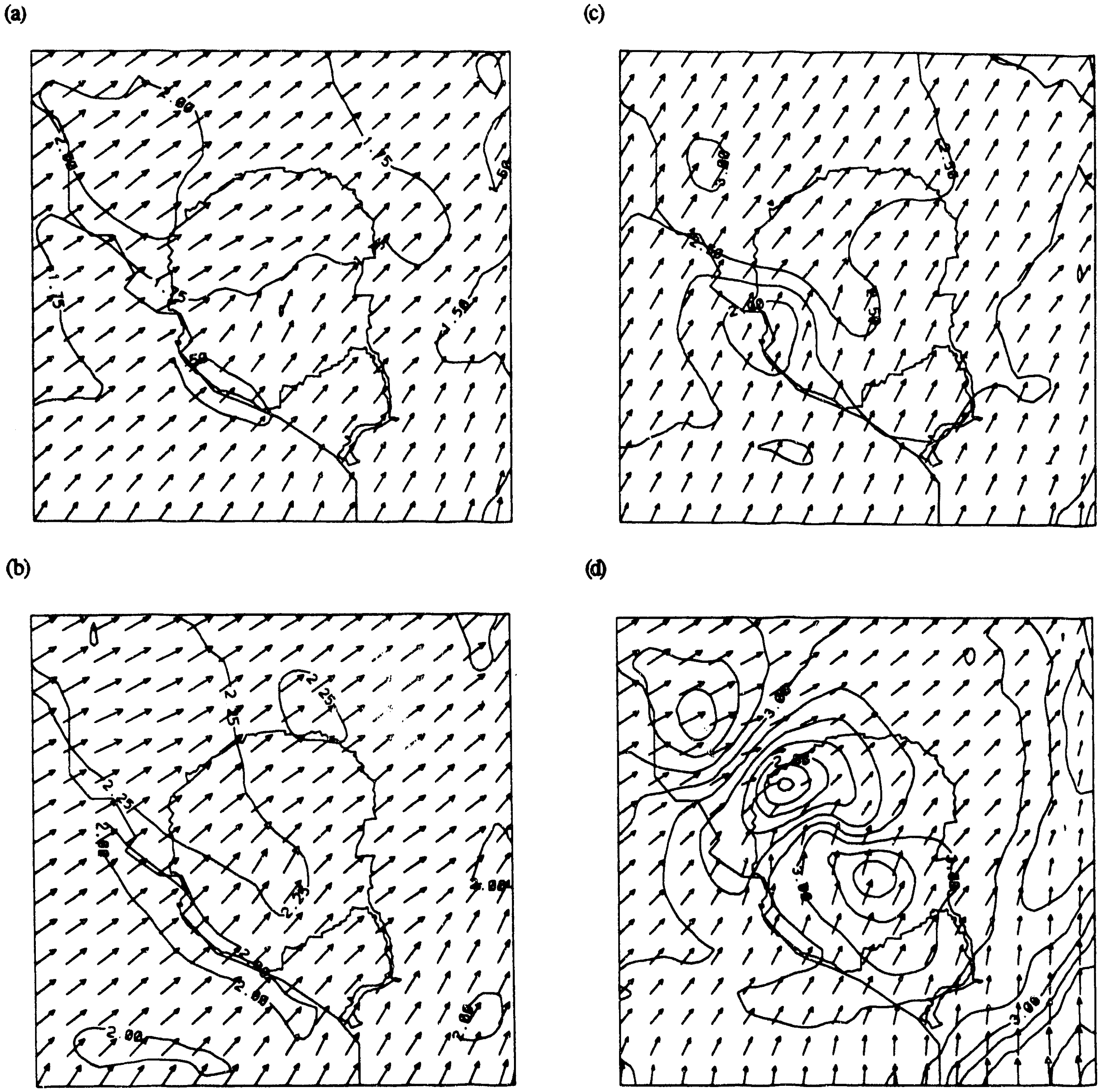


Fig. 4 Local wind field determined by RAMS valid at (a) 1230, (b) 1330, (c) 1430, and (d) 1730 EDT July 12, 1992, where the contours are wind speed in m s^{-1}

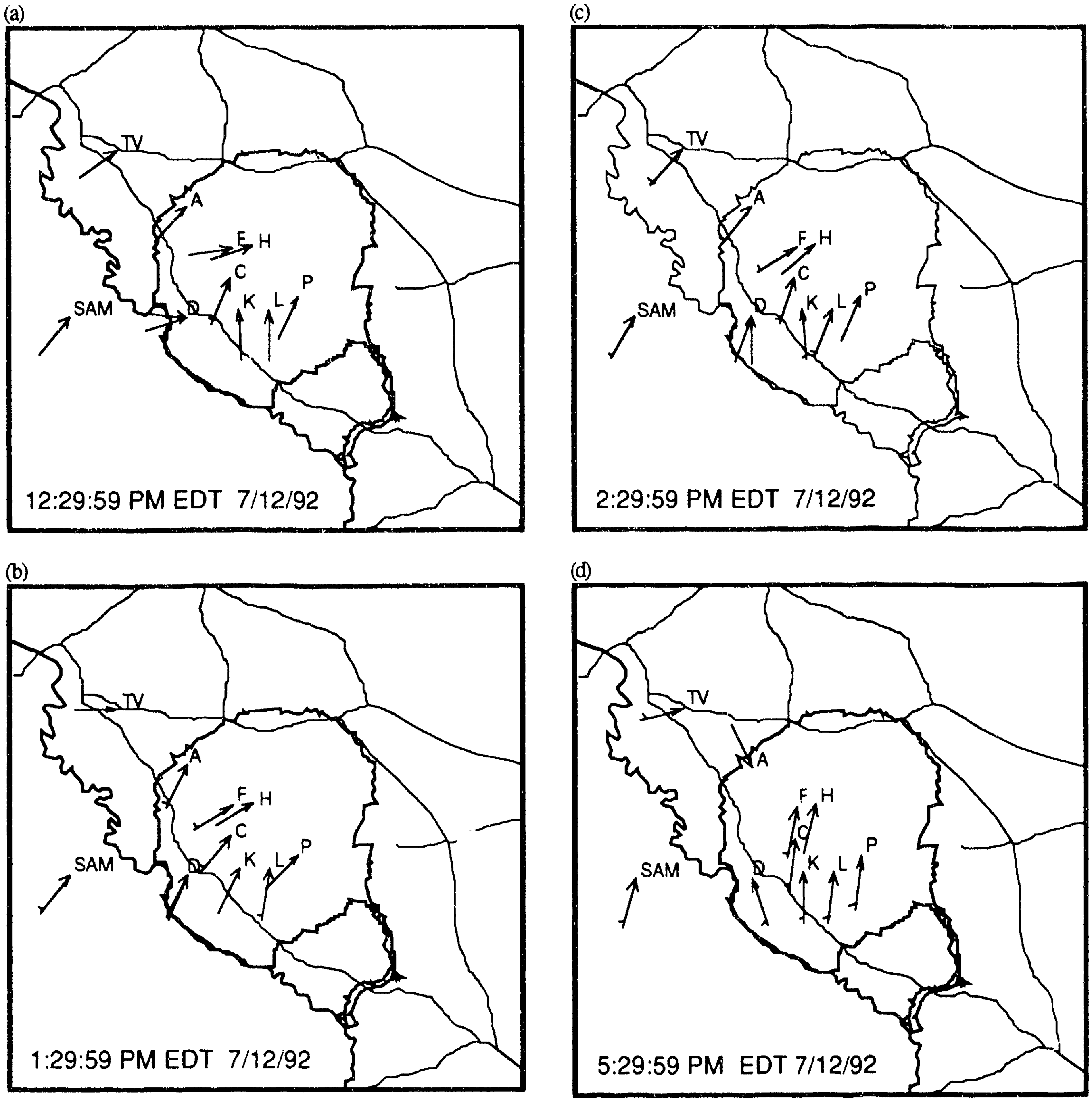
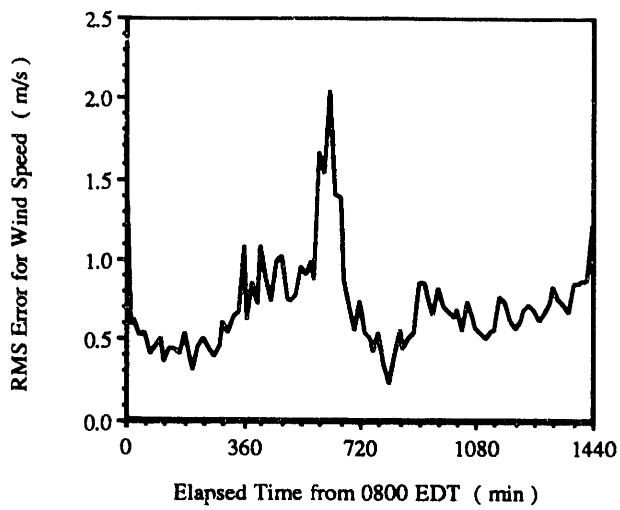


Fig. 3 Observed wind field at (a) 1230, (b) 1330, (c) 1430, and (d) 1730 EDT, July 12, 1992 where the letters denote individual SRS meteorological towers and SAM is the Spatial Averaged Mean wind

(a)



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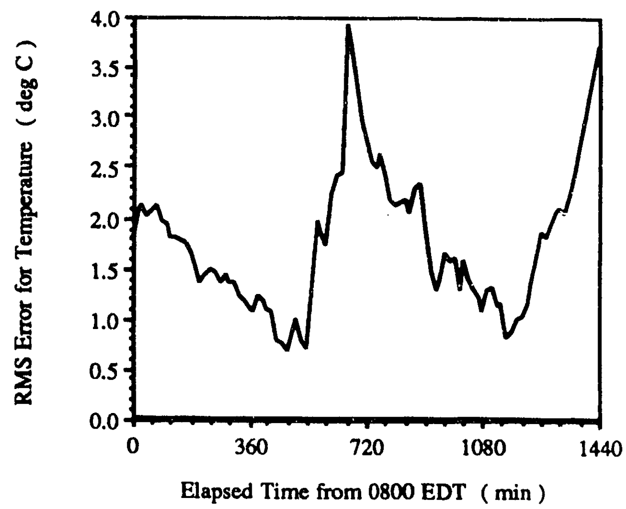

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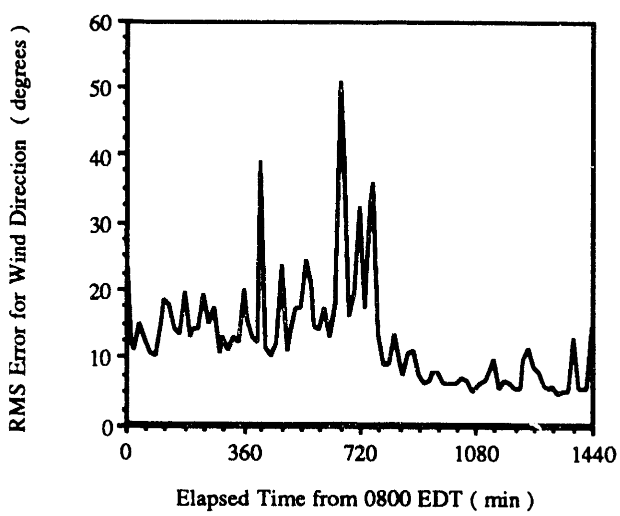

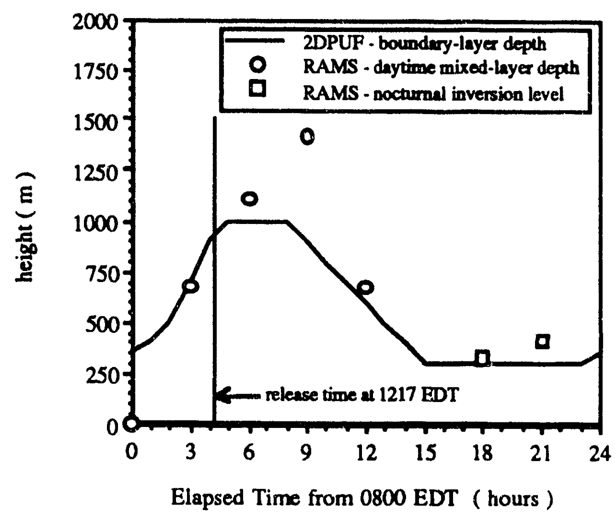

Fig. 5 Root Mean Square (RMS) error for (a) wind speed, (b) wind direction, and (c) temperature for case 1

Fig. 6 Boundary layer height used by 2DPUF and predicted by RAMS for July 12, 1992

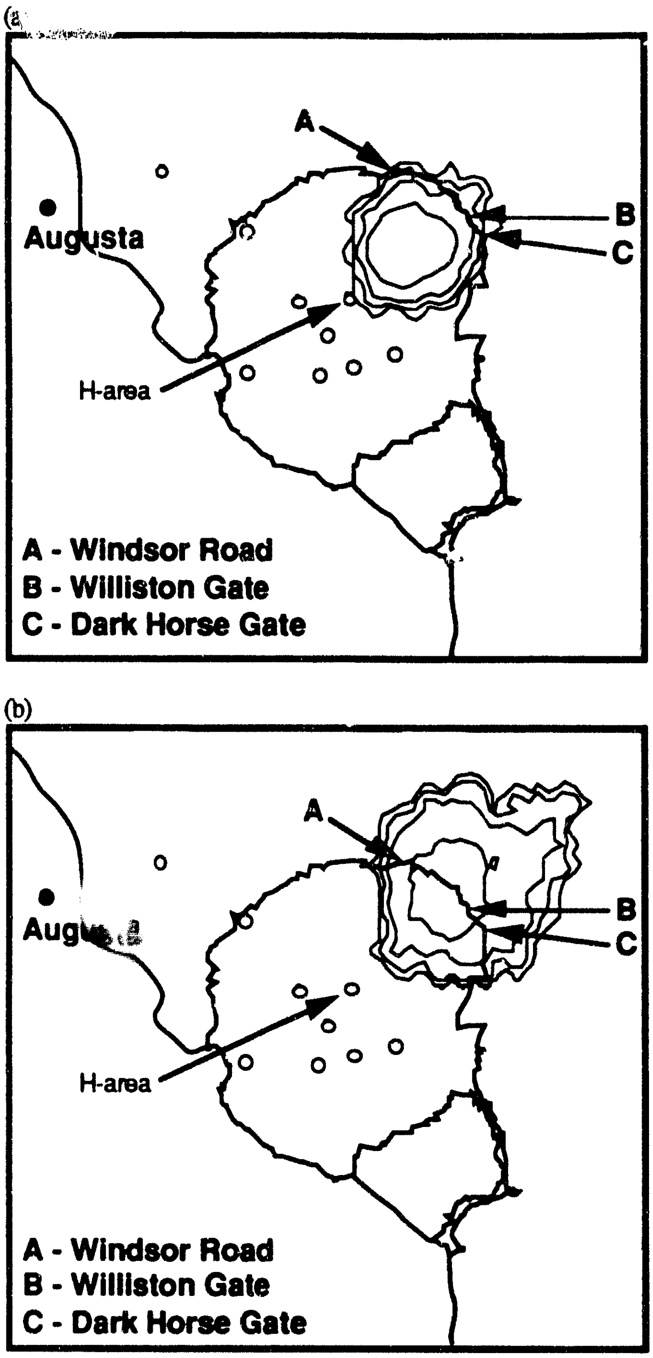

Fig. 7 Instantaneous concentration of tritium oxide from a release at H-area predicted by LPDM at (a) 1330 EDT and (b) 1430 EDT, July 12, 1992 (contours from 1.7e-2 to 1.7e-5 pCi ml^{-1} by a factor of 10)

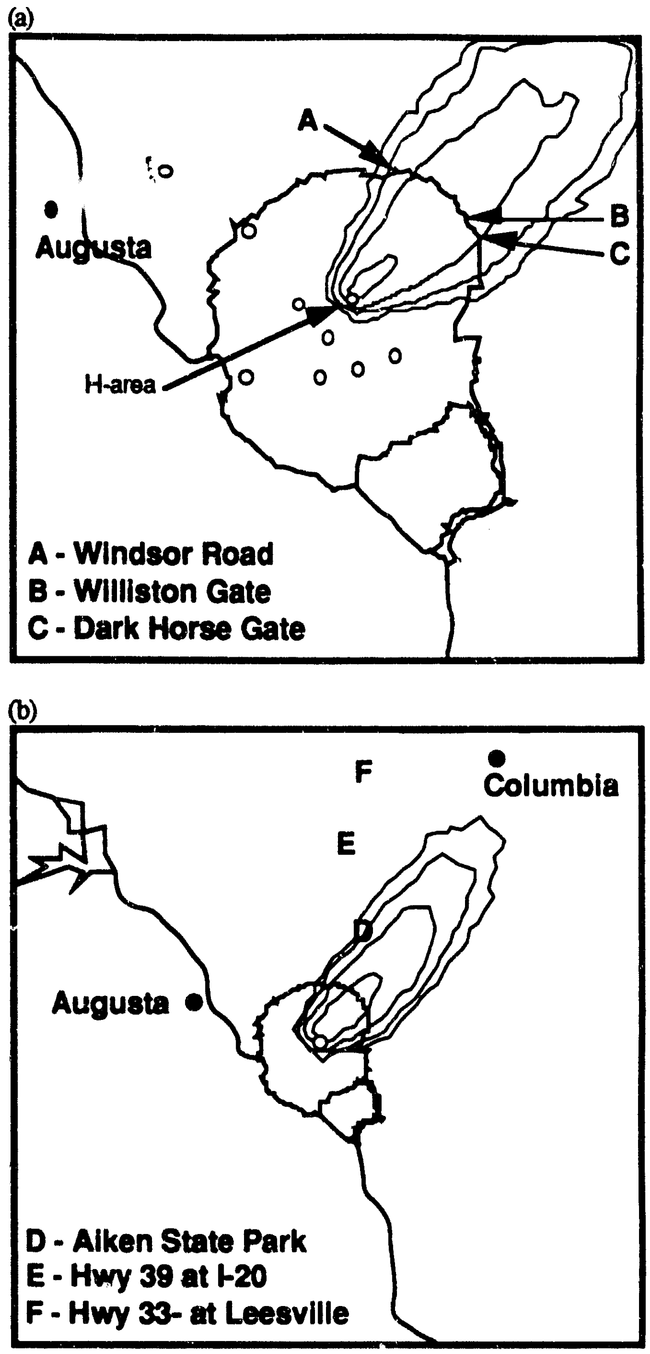

Fig. 8 Integrated concentration of tritium oxide from a release at H-area predicted by LPDM at (a) 1730 EDT on the local grid and (b) 1830 EDT on the regional grid, July 12, 1992 (contours from 4.1e-1 to 4.2e-4 pCi ml^{-1} by a factor of 10)

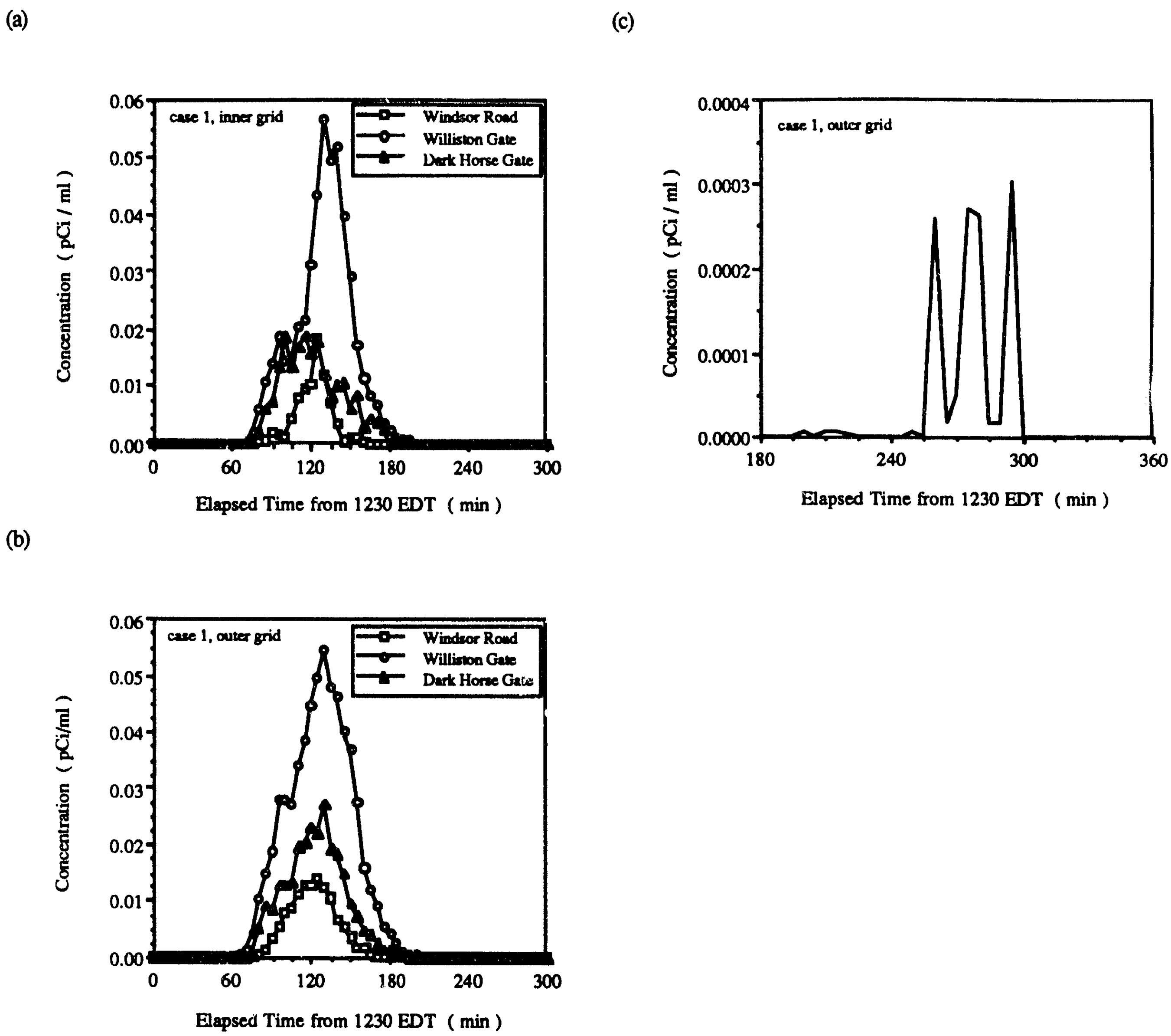

Fig. 9 Instantaneous concentration predicted by LPDM at (a) three perimeter monitor locations on the fine concentration grid, (b) three perimeter monitor location on the coarse concentration grid, and (c) one off-site location at Aiken State Park on the coarse concentration grid for case 1

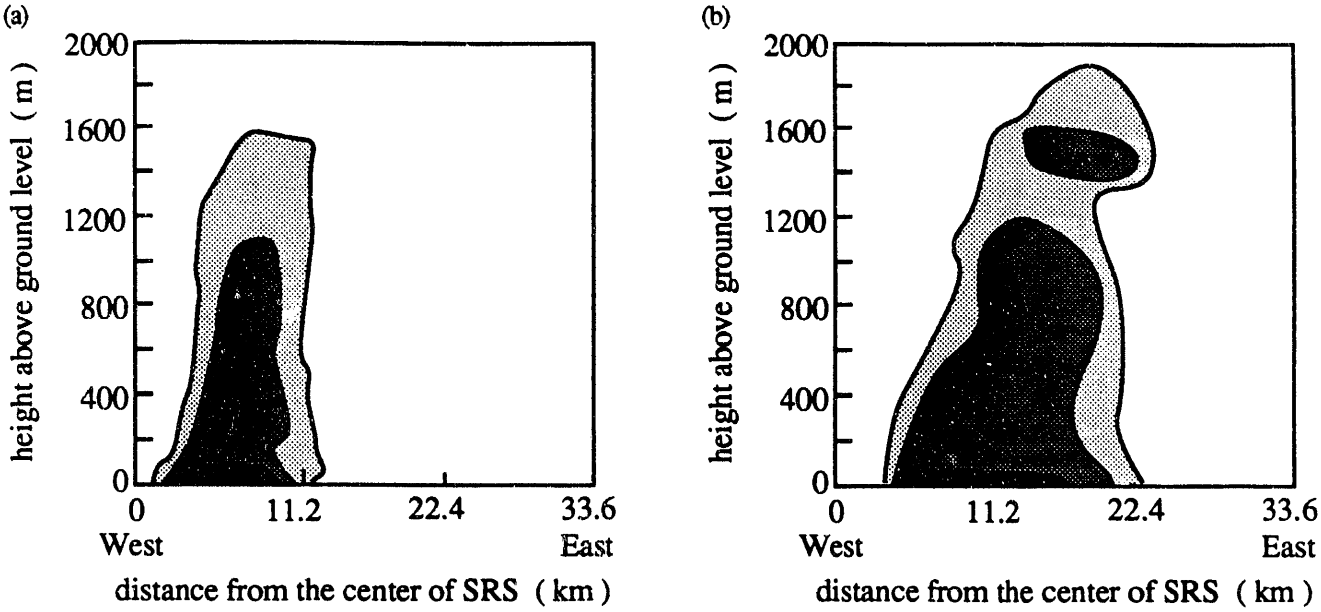

Fig. 10 Vertical distribution of particles predicted by LPDM at (a) 1330 EDT and (b) 1430 EDT, July 12, 1992 where shading indicates relative concentration of particles

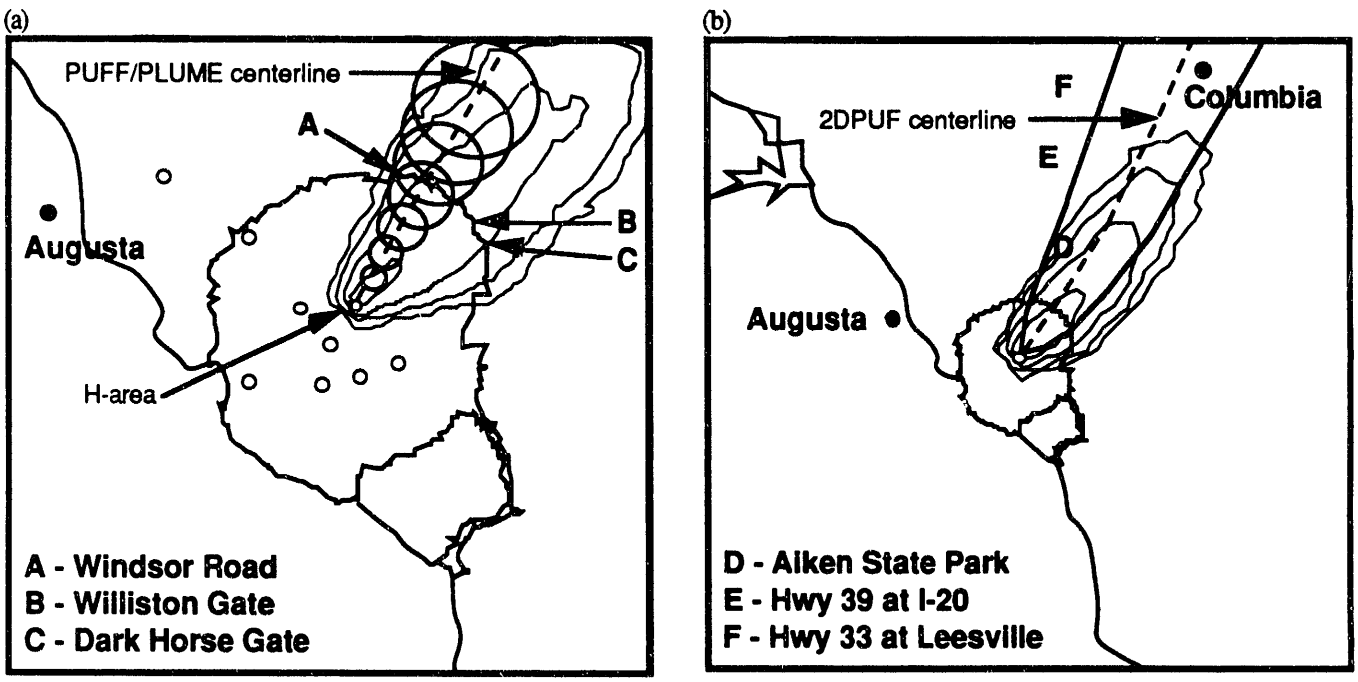

Fig. 11 Comparision of the plume direction and width predicted by (a) the initial calculation by PUFF/PLUME shortly after the time of the release (dark circles) and LPDM (light contours) and (b) the regional wind calculation of 2DPUF (dark contour) and LPDM (light contours)

Table 1 15 minute average data from the SRS meteorological towers at (a) 1230, (b) 1330, (c) 1430, and (d) 1730 EDT, July 12, 1992 cooresponding to the plots in Fig. 3, where θ is the azimuth, V the wind speed, V_{gust} the maximum wind gust, σ_a the horizontal fluctuation of the wind, and σ_e the vertical flucutation of the wind

(a)

AREA	θ deg	V m s^{-1}	V_{gust} m s^{-1}	σ_a	σ_e
A	226	1.8	4.1	42.4	23.2
C	205	2.5	4.9	21.0	21.3
D1	274	1.7	3.3	22.1	14.6
D2	253	1.8	3.6	20.7	14.2
F	261	2.1	4.4	35.1	22.8
H	255	2.3	3.9	17.0	18.5
K	176	1.9	4.3	32.3	25.1
P	211	1.5	3.5	37.6	25.7
L	182	2.3	4.0	19.0	20.1
TV	229	2.2	5.4	22.7	17.4
SAM	222	2.1	5.4	27.5	20.9

(c)

AREA	θ deg	V m s^{-1}	V_{gust} m s^{-1}	σ_a	σ_e
A	223	3.4	6.9	22.3	17.6
C	202	3.0	5.6	17.9	17.8
D1	204	0.8	3.7	65.2	19.8
D2	181	0.8	5.6	86.2	23.9
F	241	3.8	6.5	19.7	15.6
H	236	2.0	5.4	35.5	20.0
K	172	2.8	5.4	24.7	17.7
P	210	2.3	5.1	33.3	21.8
L	204	2.9	5.8	17.1	19.2
TV	214	3.2	6.8	21.4	16.9
SAM	213	2.7	6.9	30.9	18.9

(b)

AREA	θ deg	V m s^{-1}	V_{gust} m s^{-1}	σ_a	σ_e
A	209	2.8	5.5	33.2	22.4
C	225	2.9	6.1	22.6	19.2
D1	209	1.5	4.6	49.4	18.1
D2	213	2.0	5.4	35.1	18.7
F	241	2.7	4.7	17.7	16.9
H	245	2.1	4.8	27.6	26.1
K	213	2.3	5.5	35.2	20
P	230	2.5	5.1	26.8	19.9
L	192	3.3	5.4	14.8	12.2
TV	261	2.3	6.0	32.3	22.2
SAM	224	2.5	6.1	27.3	19.7

(d)

AREA	θ deg	V m s^{-1}	V_{gust} m s^{-1}	σ_a	σ_e
A	328	1.6	7.5	49.9	9.9
C	189	3.8	7.0	19.7	12.2
D1	159	2.7	4.8	15.1	13.8
D2	160	3.7	5.0	9.4	10.8
F	192	3.5	5.4	15.6	7.4
H	201	1.8	3.5	23.9	10.9
K	182	3.4	6.0	19.2	11.6
P	192	4.2	6.3	10.5	7.6
L	189	4.6	6.5	11.0	6.7
TV	252	4.2	7.3	9.3	7.6
SAM	196	3.4	7.5	18.7	9.4

Table 2. Integrated concentration of tritium observed at three perimeter monitors and predicted by LPDM

Location	observed pCi ml^{-1}	case 1 pCi ml^{-1}	case 2 pCi ml^{-1}	case 3 pCi ml^{-1}
Windsor Road	0.056	0.081	0.050	0.026
Williston Gate	0.768	0.474	0.583	0.571
Dark Horse Gate	0.600	0.200	0.128	0.313

END

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