Numerical Weather Forecasting at the Savannah River Site

by

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Numerical Weather Forecasting at the Savannah River Site (U)

Robert L. Buckley

Savannah River Technology Center

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ABSTRACT

Facilities such as the Savannah River Site (SRS), which contain the potential for hazardous atmospheric releases, rely on the predictive capabilities of dispersion models to assess possible emergency response actions. Accurate and timely wind field input to these models is crucial. Steady-state (diagnostic) winds are commonly used because they can be obtained with minimal computational effort; however, they can be grossly inaccurate during changing weather conditions. Three-dimensional prognostic fields are created using recent advances in computing speed and a mesoscale numerical model. The operational design in relation to domain size and forecast time is presented, along with verification of model results over extended time periods with archived surface observations. Application of model output in two atmospheric transport models used at SRS is also discussed.

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1. INTRODUCTION

The Atmospheric Technologies Group (ATG) plays a major role in providing emergency response capabilities for the Savannah River Site (SRS). Meteorological data are used to drive atmospheric transport codes of varying complexity, which can be used to provide predictions of hazardous pollutant locations in the event of an accidental release. While these predictions have been routinely provided by the Savannah River Site (SRS) through the use of the Weather INformation and Display (WIND) System (Hunter 1990), ATG is expanding its forecasting capabilities by using a prognostic numerical model. The goal is to provide three-dimensional meteorological data in an operational capacity over various spatial and temporal scales as input for these atmospheric transport codes. This effort expands the geographical domain for these calculations to include a sizeable portion of the southeastern United States. In addition, it improves the existing capabilities by providing more accurate winds for input to the dispersion models. Although the prime utility would be for current releases in which meteorological observations are known at the initial time of calculation, the use of the prognostic model is also beneficial for near-current releases (< 24 hours old). The operational meteorological modeling effort at SRS serves as a ground truth for further model development as well as for use in other applications.

The prognostic numerical model used to generate the forecasts is the Regional Atmospheric Modeling System (RAMS) developed at Colorado State University (Pielke et al. 1992). Use of the mesoscale model allows for incorporation of mesoscale features such as the sea breeze which commonly affect local weather conditions (Kurzeja et al. 1991, Buckley and Kurzeja 1997a). Other efforts to use a prognostic model for operational purposes are discussed by McQueen et al. (1995) who examine the eastern United States, and by Manobianco et al. (1996) who use a model to provide forecasts for the Kennedy Space Center in Cape Canaveral, Florida.

The WIND system dispersion models at the SRS include Puff-Plume (PFPL, Garrett and Murphy 1981) which employs one-dimensional measured winds to advect atmospheric contaminants assuming Gaussian distributions, and 2DPUF, a two-dimensional version of PFPL (Addis and O'Steen 1990). If a release occurs at or near the SRS, these codes utilize observed winds from the current time in a persistence mode. Both codes require minimal computational time, but are inadequate in their current configuration for conditions with winds exhibiting high spatial and temporal variability (such as during frontal passage). Therefore, the prognostic numerical model provides these dispersion models with more physically justifiable windfields, especially in locations where no observations exist, or as a forecasting tool.

Also available is a stochastic Lagrangian particle dispersion model (LPDM, Uliasz 1993) which incorporates three-dimensional, time-varying conditions. A user-specified number of particles are released and subjected to the mean wind flow and turbulence fields

generated by the prognostic numerical model. Although more time-consuming than the Gaussian-based codes, LPDM should be used in highly time-dependent and spatially variable flows and where atmospheric vertical structure is important. In addition, a parallel version of LPDM has been written (Buckley and O'Steen 1997) which allows for better concentration resolution.

Two approaches to the prognostic forecasting based on domain size are considered in this study, as summarized in Table 1. The regional domain (SC/GA) encompasses the southeast United States and provides long-term forecast information for the two-state region of South Carolina and Georgia (see Fig. 1). Because parts of the Appalachian Mountains and Atlantic Ocean are included in the modeling domain, mesoscale features may be simulated. The other approach (SRS/LOC) uses RAMS at high resolution to supply short-term forecasts covering an area roughly 50 square miles centered on SRS.

The SC/GA simulations have been running operationally since April 1998, while the SRS/LOC simulations have been produced since August 1998. Because the SC/GA domain has been tested more extensively, more details are provided in this report regarding this forecast option. Section 2 of this report gives further details regarding the dispersion and prognostic models. Included are descriptions of the necessary modifications to RAMS to provide wind and turbulence input for the dispersion models, as well as alterations to 2DPUF to ingest the wind data. The operational design including timing aspects and RAMS simulation characteristics are outlined in Section 3. Section 4 discusses comparisons of the model results with archived observations over an extended period. Applications of the RAMS forecast to several hypothetical releases from SRS is covered in Section 5, while concluding remarks are addressed in Section 6.

2. MODEL DESCRIPTIONS AND MODIFICATIONS

2.1 Prognostic Model (RAMS)

The atmospheric mesoscale model used in this study is the Regional Atmospheric Modeling System (RAMS). Information regarding this versatile, primitive-equation finite-difference model may be found in Tripoli and Cotton (1982) and Pielke et al. (1992). A wide range of atmospheric motions may be studied with this model due to the use of a two-way nested grid system. Incorporation of topographic features occurs through the use of a terrain-following vertical coordinate system, while turbulence is parameterized using Mellor and Yamada's level 2.5 scheme (Mellor and Yamada 1982), as modified by Helfand and Labraga (1988) for growing turbulence.

The first step in performing the simulation is to create initialization files at a user-specified time containing the three-dimensional large-scale observational data (horizontal velocity components, potential temperature, pressure, moisture) interpolated to the RAMS (polar-stereographic) model grid. This interpolation is performed on isentropic

and terrain-following coordinate surfaces (Pielke et. al. 1992). The initialization file corresponding to the starting time in the simulation is then used to create an initial condition for the entire three-dimensional RAMS model grid. Subsequent files (i.e. 6-hr forecasts, 12-hr forecasts, etc.) are used for lateral boundary conditions using linear interpolation in time, based on the Davies relaxation assumption (Davies 1976).

These thermodynamic fields are generated from large-scale analyses developed by the National Oceanic and Atmospheric Administration (NOAA) National Centers for Environmental Prediction (NCEP, formerly the National Meteorological Center, NMC). The large-scale data used in the SC/GA simulation come from the NCEP Eta model (Black 1994). For simulations described in this report, the Eta version contains a horizontal grid spacing of 80 km (covering North America) with information available at vertical levels of constant pressure from the surface (1000 mb) up to 10 mb. Numerous meteorological fields (including winds, temperature, and moisture) are available every 12 hours (00 and 12 Greenwich Mean Time, GMT) with a forecast product generated at 6 hour intervals (out to 48 hours). If this large-scale information is not available, then the Aviation model (Sela 1980) is utilized with a grid spacing of roughly 190 km. For the SRS/LOC simulations, the Rapid Update Cycle (RUC) model is used (Benjamin et al. 1994). The RUC model is a subset of the Eta model and is available every three hours providing a 12-hr forecast of weather conditions for the contiguous 48-state region at a resolution of roughly 60 kilometers. Large-scale data are obtained from both the Air Resources Laboratory and Weather Services International (WSI, 1997).

A soil model developed by McCumber and Pielke (1981) and modified by Tremback and Kessler (1985) is used to determine surface temperatures from surface energy balances involving net radiation, turbulent latent and sensible heat flux, and soil heat flux. Sandy clay loam soil is assumed for the southeast United States with initial soil moisture between 20 and 50%. The Biosphere Atmosphere Transfer Scheme (BATS, Dickinson et al. 1986) is used for the vegetation parameterization, which further serves to modify surface fluxes. Variable fractional land coverage and sea-surface temperatures are also used for input to the model.

2.2 Modifications to RAMS

Applications of the RAMS model results to the operational atmospheric transport codes used at SRS required modifications to generate standard deviations of azimuth and elevation angle (σ_A, σ_E). These quantities are utilized in the dispersion calculations (e.g. see Pasquill 1983) within PFPL and 2DPUF. For the SC/GA simulations, the horizontal grid spacing (20 km) is too coarse to capture all turbulent activity. Thus, the subgrid-scale parameterization (Mellor and Yamada 1982) scheme must be used to determine turbulent moments. (This procedure is also performed for the SRS/LOC simulation). The standard deviations are comprised of a resolved and subgrid portion

$$\sigma_A = \sigma_{A_R} + \sigma_{A_S} \quad (1)$$

where the resolved portion accounts for deviations over a user-specified time at the resolvable scale (in this case, over the past hour). Ignoring cross-wind effects, the deviations are calculated for the horizontal plane from:

$$\sigma_{A_R} = \frac{\sqrt{\sigma_u^2 + \sigma_v^2}}{\bar{s}} \quad (2)$$

where the variance terms are expressed (for the u -component) as:

$$\sigma_u^2 = \overline{u'u'} = \frac{1}{N-1} \sum_{i=1}^N (u_i - \bar{u})^2 \quad (3)$$

and mean quantities denoted with overbars are calculated as:

$$\bar{u} = \frac{\sum_{i=1}^N u_i}{N} \quad (4)$$

for each individual timestep, i . The total averaging period accesses N timesteps. Note that the mean wind speed is calculated as a scalar quantity:

$$\bar{s} = \frac{\sum_{i=1}^N \sqrt{u_i^2 + v_i^2}}{N} \quad (5)$$

For the subgrid terms, the turbulence parameterization provides σ_u^2 and σ_v^2 directly. Typically, the resolved components are negligible compared with the subgrid terms for a grid spacing greater than 10 km. The standard deviation of elevation angle is similarly calculated with vertical velocity in the numerator:

$$\sigma_{E_R} = \frac{\sqrt{\sigma_w^2}}{\bar{s}} \text{ and } \sigma_w^2 = \overline{w'w'} = \frac{1}{N-1} \sum_{i=1}^N (w_i - \bar{w})^2.$$

Numerically generated deviations at 26 m (lowest model level in the SC/GA simulations) have been compared with measured values at the climatology facility near C-area at SRS (Parker and Addis, 1993). A typical forecast example is illustrated in Fig. 2. Shown in each panel are time-dependent meteorological quantities over the 24-hour forecast period.

While the simulated quantities do not show the variability of the observations, the general trends are quite good.

2.3 Dispersion Models

The Puff/Plume model characterizes releases as Gaussian puffs or plumes that are simulated as a series of straight-line segments from the time of release (Garrett and Murphy 1981) out to a maximum period of 12 hours. Wind and turbulence components are generated for use in PFPL by the local tower network if available. Previously, a forecast of winds and turbulence for the local simulation could be obtained using the NWS Model Output Statistics (MOS) product tailored specifically for space-averaged winds within the SRS. Since this product is no longer available, persistence is currently used by PFPL if observational data do not exist. Therefore, available prognostic (RAMS) data can improve the forecasting capability of PFPL. Since PFPL requires input from a single location, wind and turbulence components are calculated in RAMS at an interpolated position corresponding to the SRS grid center (81.625 °W, 33.2514 °N) at three different model levels (26, 91, and 267 m). In addition, these values are calculated at center locations for 5 area counties (Richmond and Columbia counties in Georgia; Aiken, Barnwell and Allendale counties in South Carolina). The resulting county-specific wind and turbulence components may then be used as a forecast product by the respective counties in the event of an accidental release. Observational data are used if available, with simulated data being utilized only in forecast situations. Thus, no changes to the PFPL code are needed.

PFPL is appropriate for short-term releases, but its accuracy diminishes at distances far from SRS or many hours into the future if winds are variable. An extension of the model is 2DPUF (Addis and O'Steen, 1990), which was developed to alleviate some of the limitations of PFPL. The 2DPUF atmospheric transport model treats a release as a sequence of Gaussian puffs that are advected and dispersed by winds using multiple trajectories over a 24-hr period. Thus, a major improvement of this model over PFPL is that continuous releases over many hours may be modeled, as opposed to instantaneous releases.

Two types of release scenarios are assumed. The "local" option is chosen for SRS applications and relies extensively on local tower data, while the "regional" option covers the two-state area of Georgia and South Carolina and utilizes surface and upper-air observations. In order for the regional option to be performed, 24 hours of observations from the time of release must be available. During a forecast situation, the local 2DPUF simulation uses persistence (formerly the MOS product) from one location, while the regional simulation can not be performed. The benefits of providing forecasts for 2DPUF are evident: the prognostic RAMS forecasts may be used for the local simulations in a manner similar to that described for PFPL (i.e. use of a single point at the SRS center),

while the regional simulations may be run in forecast using fully three-dimensional wind and turbulence fields.

2.4 Modifications to 2DPUF

The required modifications to 2DPUF to ingest the RAMS fields were extensive and apply to the "regional" option. (Note that domain size and forecast time requirements prohibit use of the SRS/LOC simulations for this application). In the latest (unmodified) version of 2DPUF, a three-dimensional wind field grid is first established for the regional simulations. The grid has dimensions (17x19x11) for each hour of the 24-hr period with a horizontal grid spacing of 40 km (17x19) and vertical levels at 100 m and from 200 m to 2000 m in 200 m increments. The center of the grid is located at (33.2514°N, 81.6250°W) with a southwest corner of (30.01410°N, 85.05620°W) and appropriate constant latitude and longitude spacing. Observations are obtained from 66 surface aviation observations (SAO, hourly) and 12 radiosonde significant level data (SGL, twice daily) stations (available from WSI). An exponentially-weighted objective analysis of the observations is used to create the three-dimensional wind field, which is then vertically averaged to produce a two-dimensional horizontal wind field. The vertical averaging occurs only over those layers within the mixing height.

Puffs (which may consist of varying isotopes) are then released at 15-minute intervals. A transport grid is created by linearly interpolating the (17x19) wind fields to a (151x151) grid with 5 km node spacing and center coordinates as in the wind field grid. Output of dose or deposition for each isotope is then given on a polar grid (1 km x 1 deg) centered at the release and extending out to 300 km.

Along with the simulated wind fields, numerous parameters obtained from the RAMS simulation (i.e. grid coordinates and sizes) must be available for use in 2DPUF. Thus, a text file (described in Appendix A) is created with each RAMS simulation. The 'old' wind field grid (17x19x11) is replaced with the RAMS domain, with differing dimensions depending on the RAMS domain size. Although all vertical levels may be chosen, only 5 are currently taken to facilitate quicker solutions in 2DPUF. For compatibility with the vertical interpolation of soundings in 2DPUF, the RAMS model levels selected include the one nearest the surface (~26 m AGL), as well as levels near 150, 500, 1000, and 2000 m. Since the RAMS grid is on a polar-stereographic projection, the latitude and longitude values of each node in the RAMS grid must also be made available to 2DPUF.

The RAMS winds are then blended with available observations using the Barnes (1973) objective analysis technique. These observations are obtained for the same SAO and SGL previously discussed. The Barnes scheme is a Gaussian weighted-average method that assigns weights according to the distance between the observation location and the regular gridded data, specified as a wavelength. Generally, if the wavelength of influence

is large relative to the domain size, fields tend to be smooth, with the observational data heavily weighted in the analysed fields. Conversely, very small wavelengths allows RAMS winds to exert a strong influence in data-sparse regions. For the application to 2DPUF described in this report, the wavelength is assumed to be 500 km.

The blending procedure is complicated by the existence of only 36 hours of the latest RAMS simulations. Based on the release time and the current time, the availability of both simulated and observed data must be checked before creating the wind fields. A schematic representation of this effort is illustrated in Fig. 3.

There are actually two files with wind information saved for use in 2DPUF. RAMS simulations are run twice daily (initialized with large-scale 00 GMT and 12 GMT data). When the current simulation (beginning at time $t_{sc,i}$) is completed, the information from the previous simulation (12 hours prior) is retained (now with initial time $t_{sp,i}$), but renamed for use only in the event of earlier releases. Data files are overwritten every 12 hours. Thus, the maximum amount of RAMS wind information available to 2DPUF is 36 hours (12 hours before, and 24 hours after the large-scale time of 00 or 12 GMT). There are actually periods when, if a release occurs, less than 24 hours of forecast information is available (such as just prior to receiving information from the next simulation). If this occurs, then persistence using the latest available forecast time is used in determining plume movement. 2DPUF has thus been modified to determine when the release occurs relative to the availability of RAMS data ('old' or 'current') and uses the proper dataset.

Forecasts are generally available ~1 to 2 hours prior to $t_{sc,i}$ (see Fig. 3). Thus, most applications of 2DPUF for current emergency response (when $t_c = t_r$) are between $t_{sc,i}$ and $(t_{sc,i} + 12)$. Various scenarios are possible for a release time. For a given release time, 24 hours of wind data must be made available for use in 2DPUF. Referring to the time line of Fig. 3 and a particular time, $[t_r \leq t < (t_r + 24)]$:

- (1) $t < t_{sp,i}$: No RAMS data is available (only 36 hours is saved at any given time). Use the objective analysis technique already existing in 2DPUF (exponential weighting based on distance).
- (2) $t_{sp,i} \leq t < t_{sc,i}$: Use Barnes objective analysis technique to blend previous RAMS wind fields with observations. This is done on a given level of data above ground (i.e. for a two-dimensional plane) and repeated for successive vertical levels (as determined by the RAMS data). Full weighting is given to "good" observational data. If $t > t_c$, then no blending is required since no observations exist.

- (3) $t_{sc,i} \leq t \leq t_{sc,f}$: Use Barnes objective analysis technique to blend the current RAMS wind fields with observations for $t \leq t_c$. If $t > t_c$, no blending is required.
- (4) $t_{sc,f} < t$: Use persistence for winds at $t = t_{sc,f}$.

It should also be noted that during the transition time ($t = t_c$), a smoothing routine is implemented. Once the winds have been generated for the required 24-hr period, the wind field is interpolated to the (151x151) transport grid and calculations proceed as before. (Future work should involve eliminating this fixed transport grid and using the RAMS grid).

Descriptions of various subroutines in 2DPUF are available in Addis and O'Steen (1990). Required changes to these routines to ingest the RAMS data and perform the necessary blending or interpolation are documented in Appendix B.

3. OPERATIONAL DESIGN

The operational scheme uses RAMS to generate meteorological fields. Model domain selection is important to ensure inclusion of topographic features relevant to the wind-field generation. The simulation region for the SC/GA case (Fig. 4a) is centered about the Savannah River Site and includes a portion of the Appalachian Mountains and the Atlantic Ocean to allow for the development of such mesoscale features as mountain slope flow and sea breezes. By utilizing 20-km horizontal grid spacing and detailed surface input, mesoscale effects may be captured by RAMS, which are not available with large-scale models. Research at the SRS on sea-breeze development (Buckley and Kurzeja 1997a, b) guided domain selection. Further input characteristics for the simulation are given in Table 2a. For the SRS/LOC simulation (Fig. 4b), the region is selected so that both SRS and Augusta are included. Characteristics for this simulation (Table 2b) are similar to the regional case, except convective parameterization can not be used due to small horizontal grid spacing (Tremback 1990).

The lateral and initial boundary conditions for RAMS are first created. Files containing land-surface characteristics (i.e. vegetation and sea-surface temperature) are generated monthly and used throughout that period. Other meteorological conditions are generated each time new large-scale data become available. This first requires verification of the existence of the large-scale Eta or RUC data. For the SC/GA simulation, if the Eta model data are not transmitted within a specified time period (usually 2 hours from initial attempts to acquire the data), then large-scale Aviation model data are utilized. For the SRS/LOC simulations, RUC data generally becomes available 2 hours from the time of analysis.

The input file to RAMS is modified when the data are known to exist so that variables denoting the starting simulation time and forecast times are reflected by the current analysis time of the latest available large-scale data. The large-scale data and input file are then sent to the SRS Cray Supercomputing System using the file transfer protocol (ftp). The Cray is used to perform the simulations because it can complete the task more quickly than the other available computing platforms.

Automation of this procedure at regularly scheduled times is performed using the local 'cron' daemon (AIX Version 3.2 1993) to run scripts containing a series of shell commands. The modification to the RAMS input file is performed using the Interactive Data Language (IDL [version 4.0.1 1995]), which is currently available only on IBM workstations and personal computers. The IDL software is used in this instance due to its relative ease and flexibility in manipulating strings when compared with the Fortran programming language. Once the information has been sent to the Cray, a series of shell commands are executed in the background (i.e. batch mode), again at regularly scheduled times.

Note that the mesoscale model requires a 'spinup' time to create proper boundary layer and thermal structure within the atmosphere; the 'spinup' time is usually taken to be at least 12 hours. Due to time limitations for the operational model, a 6-hr 'spinup' period is used in these simulations. An option exists in which the information from the previous simulation (corresponding to the starting time of the current simulation) is blended with the large-scale data before beginning the simulation. Thus, important smaller-scale features not present in the large-scale (Eta or RUC) model data may be transferred to the next simulation. *However, if conditions from the previous RAMS simulation deviate significantly from the initial conditions of the current simulation, then the blending mechanism may be counterproductive.* If large-scale data are not present for a given simulation time and the simulation has to be abandoned, then the next simulation will be performed without any prior archived data (i.e. 'spinup' occurs during the simulation). Blending in the manner described above is not used in any of the work discussed here.

A separate script is executed once the initialization process is complete, causing the atmospheric model simulation to commence. The meteorological information created as the simulation proceeds is archived in 'analysis' files at a specified time interval (generally one hour in this application). Once the atmospheric simulation is complete, another script is executed which creates graphical output from the archived analysis files. Examples of useful graphical displays created include streamline flow fields and contour plots of various meteorological variables in two-dimensional space at a given time and variable plots in time for a given profile in space. These plots may be used to quickly examine the model results from a variety of perspectives.

Once the RAMS model simulation is complete, the data are available for use in the atmospheric dispersion codes. The data file containing a 24-hour (or 6-hr) forecast of

winds and turbulence (deviations of azimuth and elevation angle) is also generated. The horizontal wind components (at specified vertical levels) are saved when 'analysis' files in RAMS are generated. With 2DPUF and the SC/GA simulation, the latitude/longitude coordinates for each grid point must also be saved.

In a situation where three-dimensional dispersion modeling is required, LPDM may be used to generate particle and concentration plots for a variety of situations. This code directly reads the archived meteorological data (winds and turbulence) created by RAMS. As LPDM is computationally expensive relative to PFPL or 2DPUF, its use in an operational capacity is limited.

The procedure is illustrated by timelines for each simulation domain in Fig. 5. As shown in Fig. 5a for the SC/GA domain, the 00 and 12 GMT Eta model datasets generally become available between 4 and 6 hours later (i.e. 05 and 17 GMT). Processing the data to obtain the initialization and lateral boundary conditions for the RAMS simulations takes several minutes, while the simulation itself takes roughly 3 to 4 hours. At this point, blending of archived meteorological data from the previous simulation and current large-scale data fields (6 hours after the initial analysis time) is performed if desired. Thus, the simulation results are available between 10 and 12 hours after the initial time of the Eta model output, allowing for 24 hours of forecast.

For the SRS/LOC domain (Fig. 5b), the RUC dataset becomes available roughly 2 hours after the valid analysis time. The simulation begins at the valid analysis time and continues for a 12-hr period. Allowing for a 6-hr 'spinup' period, this leaves a 6-hr forecast product, which is usually available 1 to 2 hours prior to the forecast time.

It is important to consider the reliability of the RAMS simulations in creating a forecast product. Table 3 shows the results for an 8-month period for the SC/GA domain. Of the 58 failures, ~70% are the result of either the Cray or Andrew File Sharing (AFS, on which the IBM workstation resides) systems being down. The other 30% relate to missing large-scale data. This has been partially rectified by considering various sources of large-scale data (i.e. Eta, Aviation).

For the SRS/LOC domain, 81 out of 976 possible simulations for August through November 1998 failed (~8%). Of these failures, roughly 40% are related to computer failure, and 60% related to faulty data transmission. It should be possible to perform the simulations on a separate machine if the Cray supercomputing system is inoperative. However, generating the forecast within the allotted timeframe will then be difficult.

4. MODEL VERIFICATION WITH OBSERVATIONS

Several iterations of the model input parameters were explored before settling on the current configuration. Among the variables explored were the horizontal grid spacing, timestep, minimum allowable turbulent kinetic energy for use in Mellor-Yamada 2.5, and

the strength of nudging. Of particular significance is the roughness length, z_0 , a parameter specified for the soil model and used in the determination of surface fluxes of momentum, heat, and moisture. Smaller values (~ 0.01 m) imply smooth surfaces and generally larger wind speeds in the lower atmosphere, whereas larger values (~ 1.0 m) imply very rough surfaces and slower wind speeds due to increased friction effects (Thom 1976). Values of $z_0 \approx 0.01$ m were found to produce surface wind speeds larger than observed. Thus, this parameter was increased roughly an order of magnitude to produce satisfactory results.

The other parameter of major significance is the initial soil moisture assumed throughout the model domain. Because the exchange of sensible heat and water vapor between the land and atmosphere is largely controlled by the soil moisture, it has been shown in numerous studies to affect surface temperatures (for example, Wilson et al. 1987, Mahfouf et al. 1987, Bouttier et al. 1992). The initial setting used here is constant throughout the model domain (between 20 and 50% saturation by total volume). The Eta and Aviation numerical models produce forecasts of volumetric soil moisture, which have only recently been accessed by the ATG. This information can be used in RAMS, but further testing is still required.

Comparison of simulations with observations has been automated using scripts and batch jobs similar to those previously described. To avoid problems with lateral boundaries of the model domain (Davies 1983, Warner et al. 1997), comparisons are limited to a region spanning ~ 500 km in each horizontal direction for the SC/GA simulations and centered about the pole (center) position of the RAMS grid. Simulated and observed values of wind direction, speed, temperature and dew point temperature are averaged over all of the surface observing stations in the domain ($NOBS \sim 21$) at a given time for the 24-hr forecast period. An example of this output is shown in Fig. 6 for a 00 GMT, 21 January 1998 simulation. This particular example shows a positive wind speed bias (~ 0.5 to 1.0 m s^{-1}), with the largest errors occurring after dark when the average wind direction backs from east-southeasterly to east-northeasterly. Temperatures are underestimated before this time, but agree with observations after dark, while dew point biases are $\sim 2^\circ\text{C}$ throughout the period. Note that wind and turbulence comparisons at a single point near C-area as discussed in Fig. 2 are also generated for each forecast period.

Vertical profiles may be compared at specific times by utilizing WSI upper-air data that is reported twice daily (00 and 12 GMT). Figure 7 illustrates differences in temperature and dew point at Atlanta, Georgia (top) and Charleston, South Carolina (bottom) at times 6, 18, and 30 hours into the simulation up to 500 mb. Wind speed and direction for the same times and locations are illustrated in Fig. 8. While direct comparison is difficult for a given spatial location due to modeled averaging effects, general trends in model effectiveness can be seen. The smoothing effect of the vertical grid on simulated values is evident in this example from examination of the dew point (i.e. Fig. 7, Atlanta, 12 GMT, 21 and 22 January 1998, or Charleston, 12 GMT, 22 January). Although the

strength of the model-predicted low-level jets are high (Fig. 8, especially Atlanta, 00 GMT, 22 January), wind direction varies by no more than 45° at any location and time.

For the SRS/LOC simulations, WIND tower data is utilized along with WSI surface observations from Bush Field in Augusta, Georgia in 6-hr periods, which are generated every 3 hours. Hourly comparisons of wind direction, wind speed, temperature, and dew point temperature at 61-m as averaged over the 8 area-tower locations (A, C, D, F, H, K, L, and P, see Fig. 4b) are generated. An example for a 00 GMT, 28 July 1998 simulation (comparison between 06 and 12 GMT) is illustrated in Fig. 9. In addition, temperature measurements at the same locations at 2-m are averaged and compared with the lowest RAMS model level (10-m) averages (Fig. 10). Finally, comparison of meteorological values at the Augusta location is generated and shown in Fig. 11.

It is also useful to assess the impact of using 2-km grid spacing (SRS/LOC) rather than 20-km grid spacing (SC/GA) near the CSRA. Wind and turbulence values at SRS near the surface (as calculated for input to PFPL or 2DPUF) for a 24-hr forecast period from the SC/GA simulation are compared with 4 separate 6-hr forecasts generated from the SRS/LOC simulations. Both are compared with the observations as obtained from the climatology facility near C-area at 18-m. An example plot is illustrated in Fig. 12 for the 24-hr forecast period beginning at 00 GMT, 05 September 1998. It is difficult to see improvement in predicted wind direction by increasing the grid resolution, except for the first 8 hours. In fact, the SC/GA simulation does better during the final 8 hours. This implies that increased grid resolution does not automatically result in better predictions. There is a definite improvement in wind speed predictions using the 2-km simulation, with similar characteristics seen for the turbulence quantities. Further quantification of the differences exhibited by the two simulations is needed.

Validation of model results is required over an extended period. Verification of the SC/GA model configuration has been performed using simulations performed for nine full months (January 1998, April to November 1998). Details of this comparison are given in Appendix C. A relative comparison of the 20-km simulations and 2-km simulations with observations near the SRS for the months of September and October 1998 is also discussed.

5. APPLICATIONS TO TRANSPORT MODELS USED AT SRS

Since a maximum 12-hr forecast is required by PFPL (and 24 needed for 2DPUF), the SC/GA model simulation is used in the following analyses. Future applications might involve using the SRS/LOC simulation for the initial 6-hr forecast period, and SC/GA simulation for the latter time frames.

The following illustrations show the impact of using RAMS forecast data in the atmospheric dispersion models. Depending on the accuracy of the wind input and length of the forecast period, results may improve over the use of simple persistence.

5.1 PFPL

The first case involves an instantaneous release of 1.0 Ci of Pu^{239} from H-area (61 m AGL) at 12 LST, 20 May 1998. Plume transport for three different simulations is shown in Fig. 13. Solid circles denote the use of observed data, and open circles denote forecast data. Larger puffs denote more widespread dispersion. This simulation was actually performed 4 hours after the assumed release time (16 LST) for the footprints labeled PRST and SIML. These simulations use available observations up to 16 LST, and persistence (PRST) or RAMS forecast data (SIML) afterward. The footprint labeled OBSV represents results in a retrospective simulation in which observations are available at all times. The use of persistence over the final 8 hours results in a northeasterly trajectory out to an area between Florence and Myrtle Beach, South Carolina. Addition of the RAMS data results in a plume direction which shifts to east-northeast after crossing I-95, slows down after 10 hours, then turns back to northeasterly for the final 2 hours. Use of observational data alone indicates a footprint splitting the two forecast simulations. In this instance, the use of persistence is actually better than the use of RAMS winds. However, it is evident the turbulent quantities (σ_A, σ_E) predicted by RAMS are an improvement over those assumed in persistence, as puff sizes are in better agreement between OBSV and SIML by the end of the 12-hr forecast period.

Figure 14 illustrates a similar set of PFPL simulations, but for a release time of 08 LST, 2 June 1998 that is performed 4 hours later (12 LST). The release initially heads to the northeast as indicated by the small puff just west of Williston, SC. Over the next two hours, winds shift to north-northeast (puff located in the northeast section of SRS), then to the northeast, resulting in a puff which is essentially on top of the release location 4 hours after release. The "observed" footprint (OBSV) shows a continued veering of winds over the next 4 hours before settling on a northeasterly trajectory. The persisted track (PRST) remains on a heading toward the southwest, eventually crossing Louisville, GA, in the opposite direction of observed winds. The use of RAMS forecasted winds (SIML) results in a footprint tracking to the east-northeast crossing through Bamberg, SC. In this case, the prognostic model is an improvement over persistence, but high wind variability during the simulation still leads to widely varying footprints.

The final case is for a release at 08 LST, 06 August 1998, again performed 4 hours later (12 LST). As illustrated in Fig. 15, the assumption of persistence over the final 8 hours produces a south-southwesterly trajectory (PRST). Addition of the RAMS data results in a plume (SIML) which veers toward the west. Use of observational data after they become available (OBSV) reveals plume movement similar to the RAMS forecast product. In this instance, the RAMS forecast was quite good. It is clear from these

simulations, that highly variable winds in both time and space can result in very poor transport predictions.

5.2 2DPUF

Due to the variability in PFPL results for 2 June 1998 (Fig. 14), a simulation using 2DPUF for this time period is examined. Notification of the release is assumed to occur at ~16:30 LST, 2 June 1998 for a continuous 10-hr release of tritium oxide (1000 Ci per hour) from F area (61 m AGL) beginning at 06:00 LST. Thus, the latest upper-air and surface information is valid at 08:00 (12 GMT) and 16:00 LST, respectively, and the latest RAMS forecast information is valid from 08:00 LST, 2 June to 08:00 LST, 3 June. Since the release occurred prior to 08:00 LST, 2 June, the previous RAMS simulation results (generated 12 hours prior) were utilized as well.

Results are presented in the form of dose contours on a map covering South Carolina and part of Georgia (Fig. 16). The first illustration (PRST) uses the previous version of 2DPUF in a forecast mode, which requires the use of spatially-constant winds and turbulence information from the SRS center for simulation times preceding 16:00 LST, and persistence thereafter. This is essentially the same information used by PFPL in assessing pollutant transport. The predicted plume covers a wide area surrounding the SRS extending clockwise from south-southwest to northeast of the release location. An examination of the hourly SRS winds used in the calculations (Fig. 17) reveals a change in direction during the time of the release from southwesterly to northeasterly, then back to southwesterly before persisting. This also explains the circular route taken by the puffs in Fig. 14. Persistence used by the model is evidenced by the straight-line trajectory beginning roughly 60 km northeast of SRS as the plume passes through Florence, South Carolina and into North Carolina. Lower wind speeds throughout the time period of the release result in more concentrated plume doses near SRS.

Results using the modified version of 2DPUF with the blended RAMS wind fields and available observations are also illustrated (SIML). Intense plume doses are seen by the irregularity of the innermost contour to the east-northeast of SRS. When the contaminant is released at 06:00 LST, winds are from the southwest. However, wind changes as predicted by RAMS and blended with observations do not experience the drastic 180° wind shift indicated in Fig. 17, since no plume contours exist west of the release point. These differences are not surprising since the vertically averaged winds used to advect the plume incorporate westerly winds aloft. Differences in plume location also arise from horizontal spatial-dependence of the winds. Effluent released at 06:00 LST certainly experienced different winds as it moved away from the source (i.e. to the northeast), and did not necessarily encounter the wind patterns of (PRST), when spatially uniform winds are assumed. Nevertheless, a wider plume footprint in the closest 100 kilometers to the source implies slower wind speeds and higher variability in wind directions, in agreement

with conditions at SRS during this period. The latter part of the simulation indicates the plume is subjected to winds from the west-southwest, as Myrtle Beach is impacted.

A retrospective simulation using the previous version of 2DPUF and all observations over the same time period is also shown (OBSV). In this case, the objectively analyzed (17x19x11) wind field grid is used, and a more uniform plume footprint directed to the east-northeast is indicated. Again, vertical averaging of the winds likely accounts for the lack of a plume footprint to the west of SRS. The plume footprint exits South Carolina between Myrtle Beach and Charleston, indicating more westerly winds than predicted by RAMS.

These examples illustrate the application of temporally and spatially-dependent wind and turbulence input for use in atmospheric transport models. Although precise plume location will also depend on averaging techniques (i.e. Barnes input parameters, vertical wind averaging), the use of these winds instead of persistence enhances the hazardous release assessment capabilities of the SRS.

6. SUMMARY/CONCLUSIONS

The operational predictive capabilities of the ATG dispersion codes benefit from use of regional or local data fields created with a prognostic mesoscale model. Spatially, this provides meteorological information in data-sparse regions, while temporally, it supplies forecast winds. While the local WINDS tower data have been useful for transport modeling at SRS, diagnostic predictions of effluent releases or transport for a source many kilometers from the site will necessarily suffer as a result of assuming improper winds for input into the dispersion models. The operational schemes described in this report are applicable to both the SRS and the regional surroundings.

Two different operational schemes have been devised based on spatial domain size, and available forecast time. This report focuses on the regional two-state simulation (SC/GA) using RAMS, since it has been in operation longer. Statistical comparisons of model output with surface observations over both spatially-averaged domain sizes and individual locations for extended time periods reveal good model predictions. Application of the time and space-dependent wind fields in hypothetical release situations using two Gaussian dispersion codes to model the transport, revealed the possibility of significant differences in the predicted plume location using the RAMS fields. Improvements in predicted plume location relative to calculations using persistence depend upon the accuracy of the input wind fields.

Future work can be directed in several areas. The fine resolution (SRS/LOC) simulations should be utilized. This entails further statistical verification when compared with the coarser RAMS grid runs, as well as with available observations. Use of the particle model (LPDM) in an operational sense should also be examined. The three-dimensional

and temporal nature of winds has been shown to create problems for the simpler Gaussian models, and use of LPDM is restricted only by computational considerations.

As the NWS large-scale models become more refined (the new Meso-ETA model contains a horizontal grid spacing of 29-km and will be available from WSI late next year), the need for using a mesoscale model at regional scales such as discussed here becomes less important. This implies that in future applications, RAMS and LPDM will be used primarily for local simulations and near-source predictions (i.e. horizontal resolutions ~ 1 km). In other words, as large-scale model grid-spacing decreases, the RAMS simulations whose boundary conditions are driven by these models can also be refined to provide more information at smaller length scales.

One final consideration is to improve the reliability of the RAMS simulations in creating a forecast product. As discussed previously, the current operational design provides forecast information roughly 90% of the time. It is important to remember that the work discussed here is still in the research and development phase, and improvements are being addressed. A forecast available 90% of the time is better than no forecast product at all. Although there are no requirements for forecasting availability, it is prudent to provide the information as often as possible.

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Table 1: Operational Forecast Options

Case	SC/GA	SRS/LOC
Purpose	<ul style="list-style-type: none"> •Typical tritium release impacting two-state area •Inclusion of mesoscale effects 	<ul style="list-style-type: none"> •Provide local wind field at very high resolution
Domain	Georgia/South Carolina	CSRA ^a
Forecast Time (hr)	24	6
Update Frequency (hr)	12	3
Approximate Range (km)	800	100
Δx^b (km)	20	2

a: Central Savannah River area.

b: Horizontal resolution available in the model.

Table 2a: Characteristics for the SC/GA Simulation

Spatial and Temporal Characteristics			
Simulation Time	30 hr	Timestep	30 s
Horizontal Grid Points (x,y)	41 × 39	Grid Spacing	20 km
Vertical Grid Points	31	Model Top	16189 m
Vertical Spacing: Surface	46 m	Vertical Spacing: Top	1033 m
Pole Latitude	33.25 °N	Pole Longitude	81.625 °W
Surface Input			
Topography	30'' USGS (~1 km resolution)		
Vegetation	1 km NDVI derived from AVHRR		
Sea Surface Temperature	Global 1° horizontal resolution obtained monthly		
Other			
Lateral Boundary Condition	Davies relaxation (1976) toward large scale; $f=300$ s		
Radiation (short and long)	Chen and Cotton (1983); $f=1800$ s		
Convective Parameterization	Modified Kuo cumulus (Tremback 1990); $f=1800$ s		
Turbulence Parameterization	Modified Mellor-Yamada 2.5 (Helfand and Labraga 1988)		

Table 2b: Characteristics for the SRS/LOC Simulation

Spatial and Temporal Characteristics			
Simulation Time	12 hr	Timestep	15 s
Horizontal Grid Points (x,y)	51×47	Grid Spacing	2 km
Vertical Grid Points	22	Model Top	6589 m
Vertical Spacing: Surface	21 m	Vertical Spacing: Top	1033 m
Pole Latitude	33.256 °N	Pole Longitude	81.75 °W
Surface Input			
Topography	30'' USGS (~1 km resolution)		
Vegetation	1 km NDVI derived from AVHRR		
Sea Surface Temperature	Not applicable		
Other			
Lateral Boundary Condition	Davies relaxation (1976) toward large scale; $f=150$ s		
Radiation (short and long)	Chen and Cotton (1983); $f=1800$ s		
Convective Parameterization	None		
Turbulence Parameterization	Modified Mellor-Yamada 2.5 (Helfand and Labraga 1988)		

Table 3: RAMS Simulation Reliability for the SC/GA Domain

MONTH	POSSIBLE	SUCCESSFUL	PERCENTAGE
April 1998	60	49	82
May 1998	62	59	95
June 1998	60	48	80
July 1998	62	57	92
August 1998	62	46	74
September 1998	60	60	100
October 1998	62	57	92
November 1998	60	54	90
<i>Total</i>	<i>488</i>	<i>430</i>	<i>88</i>

Figure 1: Geographical coverage for the various domains.

Figure 2: Comparison of winds and turbulence for the RAMS simulation (SC/GA domain, solid lines) and observations (dashed lines) as a function of time. The 24-hr period begins at 00:00 GMT, 18 May 1998. Simulated values are taken at 26 m AGL from a horizontally interpolated geographic position at SRS center, while observed values are taken from the climatology facility near C-area at 36 m. The quantities are: (a) Meteorological wind direction ($^{\circ}$), (b) wind speed (m s^{-1}), (c) azimuth angle deviation ($^{\circ}$), (d) elevation angle deviation ($^{\circ}$).

Figure 3: Schematic timeline detailing the use of RAMS wind components and available surface and upper-air observations in 2DPUF. The variables denoted in the illustration represent:

- t_R : Time of release
- t_C : Current time
- $t_{sp,i}$: Initial time of the previous RAMS simulation (either 00 GMT or 12 GMT)
- $t_{sc,i}$: Initial time of the current RAMS simulation (either 12 GMT or 00 GMT)
- $t_{sc,f}$: Final time of the current RAMS simulation ($t_{sc,i} + 24$)

Figure 4a: SC/GA domain showing major cities, state outlines, and contours of topography (m).

Figure 4b: SRS/LOC domain showing an outline of the SRS, location of area towers, and contours of topography (m).

Figure 5a: Timing aspects for the SC/GA simulation.

Figure 5b: Timing aspects for the SRS/LOC simulation.

Surface Comparisons (Spatially-Averaged) for the 00 GMT, 21 January 1998 Simulation

Figure 6: Comparison of (a) wind direction ($^{\circ}$), (b) wind speed (m s^{-1}), (c) temperature ($^{\circ}\text{C}$), and (d) dew point temperature ($^{\circ}\text{C}$) for simulations using the SC/GA domain and observations. This comparison is for the simulation of 00 GMT, 21 January 1998 and takes into account all available observations at the given time in the inner 500 km of the domain (a maximum of 21 stations). Observation averages are given by the broken line marked with '+', while the simulation averages are denoted by the solid lines.

Upper-Air Comparisons for the 00 GMT, 21 January 1998 Simulation

Figure 7: Upper-air comparisons of temperature and dew point temperature (SC/GA domain) at selected times and locations. The top 3 panels are for Atlanta, GA in 12-hr increments beginning on the left at 12 GMT, 21 January 1998. Line representations given in the legend. The lower 3 panels are for the same times, but at Charleston, SC. The vertical scale is atmospheric pressure (mb), while the horizontal scale is temperature (°C).

Upper-Air Comparisons for the 00 GMT, 21 January 1998 Simulation

Figure 8: Upper-air comparisons of wind speed (top half) and wind direction (bottom half) for different times and locations. Wind speeds comparisons between RAMS simulations (SC/GA domain) and observations at Atlanta, GA, beginning at 12 GMT, 21 January 1998 and continuing across the figure at 12-hour increments are given by the top row. The next row represents the same times, but for Charleston, SC. Comparisons of wind direction at Atlanta are given by the third row, while the bottom row illustrates comparisons of wind direction in Charleston.

Figure 9: Comparison of (a) wind direction ($^{\circ}$), (b) wind speed (m s^{-1}), (c) temperature ($^{\circ}\text{C}$), and (d) dew point temperature ($^{\circ}\text{C}$) for simulations (SRS/LOC domain) and observations for a 6-hr forecast period. This comparison is for the simulation of 00 GMT, 28 July 1998 (forecast period beginning 06 GMT) and takes into account the 8 tower locations at 61-m AGL at the given forecast. Observation averages are given by the broken line marked with '+', while the simulation averages are denoted by the solid lines.

Figure 10: (a) Comparison of temperature ($^{\circ}\text{C}$) for simulations (SRS/LOC domain) and observations as in Fig. 9c, except observations are at 2 m. Simulated temperatures taken from the lowest model level of 10-m AGL. Values of temperature are depicted in the top panel, while bias is shown in the bottom panel. Positive bias denotes a prediction that was too high when compared with the observation.

Figure 11: Comparison of (a) wind direction ($^{\circ}$), (b) wind speed (m s^{-1}), (c) temperature ($^{\circ}\text{C}$), and (d) dew point temperature ($^{\circ}\text{C}$) for simulations from the SRS/LOC domain and observations from Bush Field in Augusta, Georgia for a 6-hr forecast period. Observed values are given by the broken line marked with '+', while the simulated values are denoted by the solid lines.

Figure 12: Comparison of (a) wind direction ($^{\circ}$), (b) wind speed (m s^{-1}), (c) deviation in azimuth angle ($^{\circ}$), and (d) deviation in elevation angle ($^{\circ}$) for simulations from the SC/GA domain (20-km), SRS/LOC domain (2-km), and observations. This comparison is for the SC/GA simulation of 12 GMT, 04 September 1998 and 4 SRS/LOC simulations (18 GMT, 04 September; 00, 06, and 12 GMT, 05 September) at the lowest model level. The values for the 20-km simulation (solid lines) are at 26-m, while the values for the 2-km simulation (dashed lines) are at 10-m. Observations are denoted with asterisks and are taken from the climatology facility near C-area at 18 m.

Figure 13: Sample output from PFPL for a transport simulation beginning at 12:00 LST, 20 May 1998. An instantaneous 1.0 Ci release of Pu^{239} is assumed. Successive circles denote puff locations in hourly increments over a 12-hr period from the time of release. Circles with dark shading indicate times when observations are known, while the lighter shading denotes the use of forecast information. The three footprints (from north to south) represent the use of persistence after 4 hours of simulation (PRST), the use of observations at all times when they later became available (OBSV), and the use of RAMS-generated winds and turbulence at SRS after 4 hours of simulation (SIML).

Figure 14: As in Fig. 13, except for a release at 08:00 LST, 02 June 1998 and observations available until 12:00 LST, 02 June 1998.

Figure 16: Sample output from 2DPUF for a transport simulation beginning at 06:00 LST, 02 June 1998. A continuous 10-hr release (1000 Ci per hour) of tritium oxide from F-area (61 m AGL) is assumed. Contours represent varying dose levels (mrem). Simulations using forecast information are performed ~16:30 LST, allowing for RAMS wind and turbulence input starting at 08:00 LST, 02 June 1998. The three footprints represent the use of persistence (utilizing SRS winds, labeled PRST), the use of blended RAMS and observation fields during the forecast period (SIML), and the use of the previous 2DPUF version at a later time when all observational information is available (OBSV).

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Figure 17: SRS winds between 06:00 LST and 21:00 LST, 02 June 1998, used in the 2DPUF simulation results shown in Fig. 16. Wind direction is given by the solid line with scale to the left, while wind speed is given by the dashed line with scale to the right.

APPENDIX A: Input Parameters to 2DPUF as Generated in RAMS

In a text file, the following are RAMS grid characteristics that are used in 2DPUF:

POLELAT, POLELON: latitude and longitude of the RAMS grid polepoint from which winds data is taken. The RAMS grid is polar-stereographic and this is considered the origin of the grid.

SWX, SWY: southwest coordinate of the RAMS grid from which winds data is taken. The numbers represent the distance (meters) from the grid center, with negative numbers indicating west and south of center.

DELX, DELY: grid spacing between horizontal adjacent nodes in the RAMS model (meters)

NX, NY, NZ: number of grid points in the east-west, north-south, and vertical direction of the three-dimensional RAMS grid. NZ is actually only a subset of values that could be taken.

ZT_RAM: array of size NZ containing the level above ground (meters) in which wind data is being supplied from the RAMS model.

TOPO_RAM, LAT_RAM, LON_RAM: arrays of size (NX by NY) containing the topographic height (meters), latitude (deg N), and longitude (deg E) of each of the RAMS grid points in the horizontal plane. Note that in RAMS, an Arakawa-C staggered grid system is implemented in which the u , v wind components do not lie on these grid points. Thus, adjustments have been made in RAMS to interpolate the winds to the given locations contained within these arrays. Although the topographic information is not currently used, the locations are needed for objective analysis weighting schemes, as well as in the determination of the puff locations in the 2DPUF grid.

TIME_STRING: time stamp of the dataset to be read in to 2DPUF created in RAMS. It is in the form "dd-mmm-yy-hhz" where 'dd' is the day, 'mmm' is the month (3-letter abbreviation), 'yy' is the year (last two digits, but can quite easily be made 'year-2000 compliant' by considering an extra 2 digits), and 'hh' is the hour in Greenwich Mean (Zulu) Time. RAMS outputs the wind data in specified time increments (hourly here) from the start of the simulation. The simulation is actually run for 30 hours, with only the final 24 hours (25 times) used in 2DPUF. The first six hours is allotted to model 'spin up' in generating realistic boundary layers and clouds.

APPENDIX B: Modifications to 2DPUF Source Code

2DPUF_MAIN.FOR: This is the main driver for the model. It has been modified to read in RAMS grid array sizes for defining wind components and location arrays.

BLEND.FOR: This routine has been written to perform the blending of observations with RAMS winds. After first checking to see if 'good' observed data exists, a two-pass Barnes analysis scheme (1973) is used to create the blended fields with results placed on the RAMS latitude/longitude locations. Note that this blending is not performed for the deviations (σ_A, σ_E).

GWINDS.FOR: This is the main routine for the gridded wind analysis. Most of the modifications are contained within this subroutine and those that it calls. More RAMS characteristics as well as the Barnes objective analysis parameters are ingested here (see Appendix A). The subroutine READ_BINARY has been created to read in a binary file created during the RAMS simulation, which contains arrays of the u , v wind components and the turbulent deviations, σ_A, σ_E . Time stamps are determined for the previous wind dataset, the current wind dataset, as well as for the puff release based on the Julian hour ($24 \times \text{Julian day} + \text{hour of current day}$). Winds and turbulence from RAMS are saved accordingly in the arrays U_RAM, V_RAM, SA_RAM, and SE_RAM of dimension (NT, NZ, NX, NY) where NT is the number of times (24 hours).

GWINDS2.FOR: Called from GWINDS.FOR, this routine generates the objectively analyzed gridded wind fields. Based on release times, observations are blended with simulated values if necessary, calling a new subroutine BLEND.FOR. Observed upper-air and surface data are read in for the proper times based on the time of release. For the observed surface data, a check is made of the wind components to ensure a miscoded data value is not used. An average of wind speeds is taken for the given time at all reporting stations, and standard deviations are calculated. If the observed wind speed differs from the average by more than 3 standard deviations, it is discarded.

Regarding the deviations (σ_A, σ_E), if the release time is before the earliest available simulated RAMS time, turbulent quantities are assumed constant throughout the domain using the site average calculated for that hour. If RAMS data exists, then these spatially-dependent values are used. As in the case of the wind components, persistence is used if the 2DPUF simulation time exceeds the final RAMS simulation time ($t > t_{sc,f}$ in Fig. 3). A smoothing routine is also implemented within GWINDS2 for the transition from observed data to forecast data ($t > t_C$, Fig. 3) as used in the previously existing procedure SMTH.FOR (Addis and O'Steen 1990).

Finally, vertical averaging of the different horizontal levels is performed (TPORT.FOR), based on the maximum depth as determined by the mixing height. The levels over which to average will differ since RAMS gridded levels are not defined at the same heights as in the older version of 2DPUF. This results in time-dependent wind and turbulence components in two-dimensions that are ready for use by the dispersion portion of 2DPUF.

INTERP.FOR: This routine has been modified to interpolate from the RAMS latitude/longitude nodes to the (151x151) transport grid of 5 km resolution centered at SRS (rather than from the (17x19) grid used previously). This interpolation is performed for the wind and turbulence components, and should eventually be changed to accommodate variable grid dimensions and locations.

OBJ.FOR: The original objective analysis routine has been modified to account for RAMS grid dimensions in (km), rather than assuming a constant value.

READ_INPUT.FOR: This routine now accepts as input the RAMS horizontal grid dimensions and spatial latitude/longitude locations, as well as the spatially-dependent wind and turbulence values.

RGNL_CENTERLOCS.FOR: This routine now passes in the RAMS grid dimensions and spatial latitude/longitude locations.

SAM.FOR: The routine which creates, advects, and disperses puffs has been modified to pass in turbulence and wind components for regional simulations which are now a function of the RAMS x and y node numbers (NX, NY). In addition, bounds are placed on the turbulent deviations (σ_A, σ_E) to be between 0.1 and 90°.

SFCDAT.FOR: This reads in observed regional surface data and has been modified to calculate the Julian hour of the latest available surface observations. This is used along with the Julian hour of the release to determine when blending with simulated RAMS data is necessary.

SGLDAT.FOR: This read in observed regional upper-air data and has been modified to calculate the Julian hour of the latest available upper-air observations. This is used along with the Julian hour of the release to determine when blending with simulated RAMS data is necessary.

TIMINT.FOR: This routine performs the time interpolation between existing sounding observations (12-hr increments). This has been modified to perform linear interpolation between observed datasets if only two exist over the given release and calculation period, while the previous quadratic interpolation is used if all three times are available for the 24-hr 2DPUF simulation period. Note that if the release time is

after the latest available upper-air time, then upper-air wind data from the RAMS simulations is used.

TWODPUF.FOR: The main subroutine for the dispersion analysis, this has been modified to pass along the RAMS grid characteristics (NX, NY, NZ), along with the number of times (NT).

VINT.FOR: This performs the vertical interpolation of observed sounding data to the specified vertical levels above ground. This has been modified to perform the interpolation to the vertical RAMS grid levels (rather than the previously defined levels of 100 (m), 200, 400, etc.).

APPENDIX C: Statistical Comparison of Observed and Simulated Data

C.1 Background

A statistical comparison of observed and (SC/GA) simulated meteorological values is performed by first examining all valid data at all times and locations, N_{TOT} . Values of wind speed, temperature and dew point temperature were obtained from the model simulation using horizontal interpolation to locations where surface observations exist. Precise agreement should not be expected, since the surface observations are time-averaged local values ~10 m above ground, while simulated winds represent a spatial average over the grid box. For the SC/GA operational runs, there is a maximum of 21 stations within the inner portion of the domain. (Note that the lowest model level (26-m AGL) was used in this interpolation for comparison with station data. Although similarity theory could have been used to interpolate to a lower level (i.e. 10-m), this was not performed here). Surface observations are obtained by first decoding the WSI data for the various stations and filtering out those stations with missing data. A simple average of all 'good' observational data is taken for each variable as in the following:

$$\bar{A}_{OBS} = \frac{\sum_{i=1}^{N_{TOT}} a_{OBS_i}}{N_{TOT}} \quad (C.1)$$

where a_{OBS_i} are the individual observed values. The standard deviation may then be calculated from (CRC 1974):

$$\sigma_{OBS} = \left(\frac{\sum_{i=1}^{N_{TOT}} [a_{OBS_i} - \bar{A}_{OBS}]^2}{N_{TOT} - 1} \right)^{\frac{1}{2}} \quad (C.2)$$

Similar expressions are used to obtain the simulated average and standard deviation over the same N_{TOT} times and locations. The total number of data points is determined using the standard deviation of the observations for a given time over the entire domain, averaging the results together, and throwing out those values which do not fit within 3 to 4 standard deviations of the mean value for the given time. Note also that zero wind speed or variable wind direction measurements were eliminated as well. In this way, possibly erroneous observed data is discarded.

Another means of exploring simulation results is to examine absolute biases as a function of the time of day. One may examine biases at a single location, or over the spatial domain by performing an average on the variables. For each time of a given simulation,

the total number of available surface observations for a given meteorological variable is compared with its corresponding simulated value by first averaging the quantity in space (or considering an individual point if interested in only a single location). One must ensure a sufficient number of observations exist for meaningful spatial averages. Therefore, those times during a given simulation which do not contain at least 5 observations within the spatial domain, are filtered out. The average absolute bias, $|\overline{B}_{h,d}|$, for a given hour, h , of a simulation "day", d , over the i station locations is calculated using

$$|\overline{B}_{h,d}| = |\overline{a}_{S_i} - \overline{a}_{O_i}| \quad (C.3)$$

where the spatial averages are calculated from

$$\overline{a}_{S_i} = \frac{\sum_{i=1}^{N_{STA_{h,d}}} a_{S_{i,h,d}}}{N_{STA_{h,d}}} \text{ and } \overline{a}_{O_i} = \frac{\sum_{i=1}^{N_{STA_{h,d}}} a_{O_{i,h,d}}}{N_{STA_{h,d}}}.$$

The individual meteorological value for simulation and observation is given by $a_{S_{i,h,d}}$ and $a_{O_{i,h,d}}$, respectively, and $N_{STA_{h,d}} (\geq 5)$ is the number of valid observations. The total absolute bias over all times and days of simulation may then be found from

$$|\overline{B}_{TOT}| = \frac{1}{N_d} \sum_{d=1}^{N_d} \left[\frac{1}{N_{h,d}} \sum_{h=1}^{N_{h,d}} |\overline{B}_{h,d}| \right] \quad (C.4)$$

where N_d is the number of days of simulation and $N_{h,d}$ is the number of hours during a simulation day in which at least 5 good observations exist. For the 24-hr forecast period, results are taken at 2-hr intervals, implying $\max(N_{h,d}) = 13$. The root-mean-square (RMS) difference error is calculated using

$$RMS_{TOT} = \left(\frac{1}{N_d} \sum_{d=1}^{N_d} \left[\frac{1}{N_{h,d}} \sum_{h=1}^{N_{h,d}} \overline{B}_{h,d}^2 \right] \right)^{\frac{1}{2}}. \quad (C.5)$$

Note that for an individual location, the bias is calculated by replacing Eqn. (C.3) with

$$|\overline{B}_{h,d}| = |a_{S_{i,h,d}} - a_{O_{i,h,d}}| \quad (C.6)$$

C.2 Spatially Averaged Results as a Function of Time

The values for the various statistical quantities (Eqns. (C.1), (C.2), (C.4), and (C.5)) are given in Table C.1. In the table, the number of available observing times, N_{AO} , is simply the sum of $N_{h,d}$ over all N_d . (Thus, if $N_d = 34$ and $\max(N_{h,d}) = 13$, the maximum total number of observing times is 442). Note that a maximum of two simulations may be performed per day. Total simulations for each month are as follows: $N_{d,JAN98} = 34$, $N_{d,APR98} = 47$, $N_{d,MAY98} = 55$, $N_{d,JUN98} = 42$, $N_{d,JUL98} = 56$, $N_{d,AUG98} = 46$, $N_{d,SEP98} = 60$, $N_{d,OCT98} = 57$, $N_{d,NOV98} = 54$.

The average simulated values ($\bar{A}$) for each variable are generally within 10% of the observed average. A positive wind speed bias exists at all times of the year, while simulated temperatures tend to be low during the winter and high in the summer. Deviations (σ) are higher for the winter conditions, indicating greater variability in the weather patterns, which is typical of the southeastern United States for these time periods, especially for the temperature and dew point. The simulated deviations are higher than the observed deviations for most times and variables, with the exception of temperatures during the warmer months. This indicates more uniformity in simulated fields during the summer months than observed. The average absolute errors ($\bar{B}$) indicate better agreement in temperature and wind speed during the warmer months. It is interesting to note that RMS and absolute errors in wind direction are best during April 1998, while the wind speed errors are largest.

Examination of the biases as a function of time of day (Eqn. (C.3)) reveal further information. Figures C.1 and C.2 show average temperature biases for each day of a cool winter period (January 1998) and a warm summer period (July 1998). Separate plots for the given time of day are shown in the figure, with the horizontal axis denoting the particular day of the simulation, and the vertical axis representing the temperature bias. Note that where less than 5 observations existed over the domain, results were not tabulated, as denoted by 'M' in the figures. Similar figures for scalar wind speed are given in Figs. C.3, C.4.

The general trend for both extended data sets is to underestimate temperatures during the late morning (09 to 12 LST, Figs. C.1 and C.2), and to slightly overestimate temperature during the late evening (19 to 00 LST). The negative bias is more evident during January 1998. No discernable pattern in bias can be seen for wind speed, except that errors tend to be larger in the afternoon hours when winds are generally stronger. The overall positive bias in wind speed for the winter simulations is largely due to overestimates during the late night period (01 to 07 LST, Fig. C.3).

In general, temperature differences affect surface fluxes of sensible heat, momentum and moisture, leading to changes in surface wind speeds. Overestimates in temperature such

as on days 7 and 14 of the winter simulation (see 01 to 07 LST, Fig. C.1), result in higher heat and momentum fluxes leading to higher wind speeds (Fig. C.3, for the same time periods). Likewise, a similar trend toward lower speeds results from underestimates in temperature (12 to 14 LST, Figs. C.2, C.4). The results shown here are for the simulations utilizing the 00 GMT large-scale data. Similar trends are seen for the 12 GMT large-scale data simulations (i.e. decreased accuracy in temperatures during the early and late-morning hours) and for other time periods.

Of course, other factors lead to model inconsistency, such as the large-scale driving conditions (in this case, the Eta model). If the forecast accuracy of the Eta model is poor, then nudging lateral boundary conditions of the RAMS model to these values will create errors. An example of this is seen in the spike of wind speed on day 7 for the winter simulation in the early morning hours (05 and 07 LST, respectively 28 and 30 hours forecast from the beginning of the simulation, Fig. C.3). The original 36-hour forecast from 00 GMT, 15 January which was used for this particular simulation, predicted wind speeds through South Carolina to be between 6 and 10 m s^{-1} by 12 GMT, 16 January. However, actual wind speeds were between 1 and 4 m s^{-1} .

C.3 Results at Specific Locations as a Function of Time

One may also examine particular locations within the simulation region. Since the spatial averaging performed in Eqn. (C.3) is replaced with Eqn. (C.6), larger errors may arise. By examining different locations within the region, an indication of the spatial variability in error may be discerned. Five separate locations have been chosen: Atlanta, GA (33.650°N, 84.417°W), Augusta, GA (33.367°N, 81.967°W), Alma, GA (31.533°N, 82.517°W), Charlotte, NC (35.217°N, 80.933°W), and Charleston, SC (32.900°N, 80.033°W).

A summary of the results is shown in Fig. C.5. Averages are taken in time over a month period for the four meteorological variables. For each city, between 2400 and 6000 data points have been used for comparison over the total time period.

Errors in wind direction (Fig. C.5a) are generally within 50°, although larger errors are exhibited for Charlotte, NC at all times of the year. This may be due to the proximity of Charlotte to the Appalachian mountain range, and the presence of local slope flows not generated by the model. Absolute wind speed biases at all locations range between 1 and 2 (m s^{-1}), with a maximum at Alma, GA. This is because the Alma station does not provide data at night when wind speeds are typically lower. The larger wind speed errors for April 1998 are directly correlated to the higher overall magnitude of winds during this month. The uniformity of the higher wind speeds during this month is also reflected by the generally minimized wind direction errors.

Overall temperature and dew point errors range between 1 and 3.5°C, but seem to be minimized along the coast (i.e. Charleston, SC), while moisture errors are worse during the cooler months near the domain center (i.e. Alma and Augusta, GA). This would indicate possible problems with surface budgets in the model, which could be linked to a variety of factors, including soil moisture, radiation and soil parameterizations. The large negative temperature bias found during the winter month during the late morning hours (Fig. C.2) is certainly reflected in the generally higher errors in temperature seen in Fig. C.5c.

C.4 Comparisons between Forecast Options

Meteorological forecast wind speed data, interpolated to the SRS climatology area, were collected for the months of September and October 1998 for the 20-km regional (SC/GA) simulations and the 2-km local (SRS/LOC) simulations and compared with WINDS tower observations. The lowest vertical model level for the 2-km local simulations is 10 m, which was used as the reference level. (Note that the lowest model level for the SC/GA simulations (26 m) was again used, as discussed in Section C.1). The climatology tower contains instrumentation at 4 levels, including 2 and 18 m. These two levels were used to interpolate to the 10-m level in these comparisons. Results are depicted in the form of scatter plots for two months (Fig. C.6). Data were taken at 2-hour intervals, utilizing the first 12 hours of the SC/GA (00 and 12 GMT) forecast simulations, and the 6-hr forecasts (00, 06, 12, and 18 GMT) from the SRS/LOC simulations.

Relative biases (B) and standard deviations (S) are calculated for each simulation set based on the total number of data points (N). Whenever data for any of the three cases does not exist, comparisons are not made. Clearly, wind speeds near the site using the SRS/LOC domain are more representative of observations. The positive wind speed bias discussed previously for the SC/GA simulations is also evident. Note that at higher wind speeds ($> 4 \text{ m s}^{-1}$), this bias is more prevalent. The increased vertical resolution (10-m surface rather than 26-m) for the 2-km domain is the primary reason for this improvement. Similar comparisons at the Bush Field airport in Augusta, GA (not shown) also indicate wind speed improvements using the finer grid.

A comparison of wind direction in the form of histograms is given in Fig. C.7 for the same two months illustrated in Fig. C.6. The wind direction is broken up into 22.5° sectors (degrees *from* which the wind is blowing) for each of the three data types. For September, the predominant wind direction is from the east, while for October, it shifts to the northeast. The local simulation appears to perform better than the regional case for the earlier month, while a distinction is unclear for the latter month. Further quantification of the differences exhibited by the two simulation domains is needed.

The results described in this appendix indicate generally good agreement between model and observation for either simulation domain, lending validity to use of the prognostic

model as a source of winds in the dispersion models. However, improvements to the model, such as the initialization of soil moisture or refined grid spacing, are needed in the future to create a more accurate forecast product.

Table C.1: Statistical Comparison of Observations and Simulations (SC/GA)

Variable	Time	N_{TOT}	$\bar{A}_{OBS}$	$\bar{A}_{SIM}$	σ_{OBS}	σ_{SIM}	N_{AO}	$ \bar{B}_{TOT} $	RMS_{TOT}
	01/98	6506	3.80	3.98	1.74	2.19	429	0.616	0.768
	04/98	9757	4.08	4.60	1.92	2.10	624	0.791	1.02
	05/98	10103	3.48	3.62	1.54	1.74	707	0.521	0.671
	06/98	7760	3.67	3.82	1.65	1.82	538	0.568	0.739
Wind Speed	07/98	10416	3.42	3.44	1.43	1.48	726	0.517	0.657
(m s ⁻¹)	08/98	7690	3.16	3.22	1.50	1.69	592	0.500	0.658
	09/98	9787	3.22	3.43	1.52	1.66	740	0.645	0.929
	10/98	9152	3.18	3.33	1.40	1.48	702	0.496	0.642
	11/98	9025	3.18	3.31	1.42	1.61	677	0.537	0.684
	Total	80196	3.46	3.63	1.60	1.80	5735	0.574	0.762
	01/98	6506	---	---	---	---	429	31.7	43.1
	04/98	9757	---	---	---	---	624	22.4	33.8
	05/98	10103	---	---	---	---	707	28.8	40.5
	06/98	7760	---	---	---	---	538	26.1	35.6
Direction	07/98	10416	---	---	---	---	726	25.0	34.3
(deg)	08/98	7690	---	---	---	---	592	32.2	43.1
	09/98	9787	---	---	---	---	740	32.6	47.4
	10/98	9152	---	---	---	---	702	46.4	62.1
	11/98	9025	---	---	---	---	677	41.2	55.2
	Total	80196	---	---	---	---	5735	32.0	45.2

Table C.1: Statistical Comparison of Observations and Simulations (cont)

Variable	Time	N_{TOT}	$\bar{A}_{OBS}$	$\bar{A}_{SIM}$	σ_{OBS}	σ_{SIM}	N_{AO}	$ \bar{B}_{TOT} $	RMS_{TOT}
	01/98	8363	8.17	7.73	5.17	5.90	440	1.60	1.94
	04/98	11704	16.7	17.3	5.06	5.18	624	1.53	1.48
	05/98	13513	22.8	23.4	5.14	5.26	711	1.19	1.48
	06/98	10161	27.5	28.5	5.01	4.48	538	1.37	1.84
Temperature	07/98	13803	27.2	28.1	3.95	3.66	726	1.08	1.39
(°C)	08/98	11377	26.2	27.1	4.21	3.86	597	1.26	1.55
	09/98	14527	24.0	24.7	4.50	4.39	768	1.49	1.83
	10/98	13905	18.2	18.0	6.11	5.68	737	2.00	2.55
	11/98	13249	14.3	14.3	5.71	5.87	702	2.20	2.75
	Total	110602	21.0	21.4	7.69	7.97	5843	1.53	2.00
	01/98	8351	4.17	4.18	5.43	5.80	440	1.24	1.57
	04/98	11600	11.0	11.1	5.18	5.16	624	1.45	1.84
	05/98	13323	17.4	16.6	3.97	3.84	711	1.55	1.96
	06/98	10190	20.8	20.1	2.51	2.89	538	1.54	1.92
Dew Point	07/98	13822	21.6	20.9	2.64	2.51	726	1.38	1.73
(°C)	08/98	11390	21.2	20.1	2.79	2.93	597	1.68	2.06
	09/98	14556	19.2	18.6	4.05	4.42	768	1.44	1.83
	10/98	13891	12.5	13.1	6.05	5.48	737	1.59	1.92
	11/98	13243	9.55	10.7	6.32	6.05	702	1.67	2.12
	Total	110366	15.7	15.4	7.12	6.68	5843	1.51	1.90

Figure C.1: Temperature biases ($^{\circ}\text{C}$) for January 1998 (00 GMT SC/GA simulations) for differing times of day. Observed average temperatures given by the dotted lines marked with '+', while biases given by solid lines. Each frame represents a different time of the day throughout the 24-hr forecast simulation period.

Figure C.2: As in Fig. C.1, except for July 1998 (00 GMT SC/GA simulations) temperatures biases.

Figure C.3: As in Fig. C.1, except for January 1998 (00 GMT SC/GA simulations) wind speed biases (m s⁻¹).

Figure C.4: As in Fig. C.3, except for July 1998 (00 GMT SC/GA simulations) wind speed biases.

Figure C.5: Average absolute biases for (a) wind direction ($^{\circ}$), (b) wind speed (m s^{-1}), (c) temperature ($^{\circ}\text{C}$), and dew point temperature ($^{\circ}\text{C}$) for five different surface locations. Averaged are based on results over an entire month using the 24-hr SC/GA simulations.

Figure C.6: Scatter plots comparing simulated and observed wind speeds (m/s) at climatology at SRS (10-m) at 2-hr intervals for September 1998 (top) and October 1998 (bottom). The SC/GA simulation is denoted with diamonds, while the SRS/LOC simulation is given by '+'. The number of data points is given by N, while the relative bias (B) and standard deviation (S) for each simulation is also given in the legend.

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Figure C.7: Histogram of wind direction in 22.5° sectors for the conditions of Fig. C.6. LOC is for the 2-km simulations, while REG denotes the 20-km simulations.