8.5 **IMPACTS ON DISPERSION PREDICTION RESULTING FROM DIFFERENT TYPES OF NWP ENSEMBLES**

Jared A. Lee*
L. Joel Peltier
Sue Ellen Haupt
David R. Stauffer
John C. Wyngaard
Aijun Deng
The Pennsylvania State University, University Park, Pennsylvania

1. INTRODUCTION

For homeland and defense security and air quality applications it is necessary to model accurately the atmospheric transport and dispersion (AT&D) of chemical, biological, radiological or nuclear (CBRN) contaminants from accidental or deliberate releases. Accurate, reliable AT&D forecasts are difficult to make, however. Contaminant dispersion in the atmosphere is a complex process that is dictated by the properties of a turbulent, three-dimensional wind field. The wind field in the planetary boundary layer (PBL) is naturally turbulent. The details of such turbulent flows are, by nature, unpredictable. Even small perturbations to initial conditions or boundary conditions produce different realizations of the flow pattern and, thus, the contaminant dispersion.

Recognizing the limitations of forecasting with a single realization, contemporary numerical weather prediction (NWP) uses ensembles of simulations. The wind field from a single deterministic NWP run represents one member of this ensemble of possible realizations. Ensemble members typically differ by imposed initial and lateral boundary conditions (ICs and LBCs), underlying physics parameterization schemes, and often the choice of NWP modeling system. In addition, ensembles provide an estimate of the spread of possible outcomes of the future state of the atmosphere. Members of a dispersion ensemble can be generated by making a dispersion forecast for each member of a meteorological ensemble. This dispersion ensemble can then be averaged to obtain a mean prediction. The spread of the ensemble is correlated to the uncertainty (Grimit and Mass 2002). Largely due to computational expense, limited observations and the need for rapid response, however, AT&D models driven by single NWP model runs are preferred. The use of NWP ensembles in dispersion modeling applications is becoming more common (Warner *et al.* 2002; Galmarini *et al.* 2004a,b).

In one such study, Lee *et al.* (2009) modeled the observed plume and assessed the uncertainty in concentration predictions during the 1983 Cross-Appalachian Tracer Experiment (CAPTEX-83) (Ferber *et al.* 1986), by coupling The Pennsylvania State University-National Center for Atmospheric Research (PSU-NCAR) Fifth-generation Mesoscale Model (MM5) (Grell *et al.* 1994) with the Second-order Closure Integrated Puff (SCIPUFF) dispersion model (Sykes *et al.* 2004). The 19 MM5 experiments all used the same ICs and LBCs, but varied certain physics parameterizations and data assimilation (DA) schemes in an effort to obtain the best possible representation of the meteorology during the case. Their concentration predictions from SCIPUFF indicated that while much of the variability inherent to the meteorological conditions appeared to be represented, other sources of uncertainty, such as IC and LBC variability, should also be represented.

Thus we hypothesize that IC/LBC variability is important to AT&D modeling applications, but that a hybrid NWP ensemble modeling approach, *i.e.*, one which varies ICs, LBCs and physics parameterization schemes together, will result in more ensemble spread than one that varies only the ICs or LBCs. This requires us to study short-range mesoscale NWP forecasts in the planetary boundary layer (PBL). The purpose of this study is to evaluate best methods for constructing an NWP ensemble for the purpose of accurately predicting AT&D as well as for quantifying the uncertainty in those predictions.

2. TREATMENT OF UNCERTAINTY IN SCIPUFF

SCIPUFF provides a probabilistic treatment of dispersion with the capability of predicting concentration probability density functions as functions of time and space (Rao 2005). SCIPUFF's modeling accounts for the stochastic uncertainty that results from unresolved atmospheric turbulence. Modeling technology is also in place in SCIPUFF, through the ensemble uncertainty modeling, to account for the uncertainty that results from meteorological input data and parameter uncertainties or model physics errors; however, definitions for all of the modeling parameters are not complete. Uncertainty in the meteorological input data, especially horizontal wind variance, is the main source of total dispersion uncertainty (Rao 2005). Other large sources of dispersion uncertainty include transport over complex terrain, transport over long distances, and deep convection with cold pools and outflow boundaries (Deng *et al.* 2004).

While sub-grid variability is often parameterized, grid-resolved variability is usually not parameterized by

* *Corresponding author address:* Jared Lee, The Pennsylvania State University, Department of Meteorology, 503 Walker Building, University Park, PA 16802, USA. Email: jal488@meteo.psu.edu.

AT&D models. SCIPUFF, however, treats grid-resolved variability as a process that augments diffusion. The model introduces additional metrics to describe this variability in terms of ensemble variability. The parameters are the ensemble velocity variances and covariance, UUE, VVE and UVE, respectively, and a characteristic length scale, SLE (Sykes *et al.* 2004). Because the ensemble variability model within SCIPUFF is intended to parameterize the effects of ensemble wind-field variability, the formulation of models for these outer variability parameters is an important step toward improved dispersion predictions. Such models are assessed in a previous study by Lee *et al.* (2009).

3. CASE STUDY: CAPTEX-83

Episode 1 of CAPTEX-83 took place on 18-19 September 1983. Over a three-hour period, from 1700 UTC to 2000 UTC on 18 September 1983, 208 kg of a perfluorocarbon tracer gas (perfluoro-monomethyl-cyclohexane, C_7F_{14}) were released at ground level at Wright-Patterson Air Force Base (39.80°N, -84.05°E) near Dayton, Ohio. The tracer gas was released in the middle of the day (1200-1500 local standard time). Downwind of the tracer release, a network of 86 monitoring stations in the northeastern United States and southeastern Canada, located in arcs approximately 300 km to 1100 km from the release, recorded surface concentrations of the tracer.

The region of the experiment stretches from the eastern Great Lakes region to New England over a time period 1200 UTC on 18 September 1983 to 1800 UTC on 19 September 1983. A large high-pressure system centered over the Mid-Atlantic coast influenced the case at first, with a broad southwesterly wind flow in the Midwest and Northeast. Warm and cold fronts associated with a 982-hPa low in south-central Canada were moving quickly through the western Great Lakes. A low-level jet played a large role in transporting the tracer, and was a prominent night-time feature associated with this frontal system. For a more complete description of the meteorology during this episode of CAPTEX-83, including analysis maps, see Deng *et al.* (2004) and Deng and Stauffer (2006).

This is a challenging meteorological case in which to study long-range transport and dispersion, due to the propagating mid-latitude cyclone and its front-driven convection. With an unstable PBL, the tracer mixed rapidly throughout the entire depth of the boundary layer (Deng *et al.* 2004). At the starting time of the tracer release, southwesterly winds were prevalent across Ohio ahead of the advancing cold front and transported the tracer northeastward. The front later became stationary as the low-pressure system occluded, and continued to have a large impact on the transport of the tracer. The complex terrain in the experimental domain, including the Appalachians and Adirondacks, adds yet another challenge for both NWP and AT&D models.

4. EXPERIMENTAL DESIGN

In this study we coupled version 2.2.1 of the Weather Research & Forecasting Advanced Research WRF (WRF-ARW) model (Skamarock *et al.* 2005) with SCIPUFF. Four nested-grid WRF-ARW experiments were created to study the impacts of varying ICs/LBCs and physics parameterization schemes, as detailed in Table 1. Two of the experiments used the 32-km horizontal resolution North American Regional Reanalysis (NARR) (Mesinger *et al.* 2006) for the ICs/LBCs, and the other two used the Office Note 84-formatted ICs/LBCs supplemented with MM5 RAWINS analysis (ON84+RAWINS). ON84+RAWINS is the same IC dataset that was used in the MM5 experiments in Deng *et al.* (2004), Deng and Stauffer (2006), and Lee *et al.* (2009). For physics variability, two of the experiments used the default Mellor-Yamada-Janjic (MYJ) PBL scheme that is found in WRF-ARW v2.2.1 (“old MYJ”), and the other two used a version of the MYJ PBL scheme that had been modified to diagnose the PBL height differently (“new MYJ”).

The inner horizontal grid resolution for all four WRF-ARW experiments is 4 km. There are 32 levels in the vertical, from the surface up to 100 hPa, with 16 levels below 850 mb. No four-dimensional data assimilation (FDDA) was used on any of the domains.

5. RESULTS

Each of the four experiments showed small differences in the wind fields, with more noticeable differences between the experiments with different ICs/LBCs than the experiments with different PBL schemes (not shown). There were great differences in the diagnosed PBL height among the four experiments, however (Fig. 1). The experiments with different PBL schemes exhibited substantially larger differences in the PBL depth than the two experiments with different ICs/LBCs, though there were also notable differences between the experiments with different ICs/LBCs. Typically the default MYJ scheme diagnoses PBL depths up to 50% greater than the modified MYJ scheme.

Large differences in the diagnosed or predicted PBL depth would be expected to lead to substantial differences in contaminant concentration predictions, because the top of the PBL tends to act like a “lid” on contaminants in the boundary layer. Therefore, due to conservation of mass, one would expect to see higher concentrations in a shallower PBL, and lower concentrations in a deeper PBL.

Figure 2 shows the concentration predictions for the four experiments at one time. The plume footprints are markedly different for the experiments with different ICs/LBCs, and the concentrations are also generally greater for the experiments with the modified MYJ scheme than with the default MYJ scheme. The results from the WRF-SCIPUFF system in this study indicate that the choice of both the IC/LBC datasets and certain physics parameterization schemes can have a substantial impact on concentration predictions and the potential hazard area.

6. SUMMARY AND CONCLUSIONS

As mentioned above, there are several options that can be varied to create an ensemble of NWP model runs, including the initial conditions, lateral boundary conditions, and physics parameterizations. Varying each of these options generally increases the spread and uncertainty representation of the ensemble. There are also several different approaches to defining perturbations for the ensemble ICs, including the use of singular vectors, bred modes, and various ensemble Kalman filtering techniques (Descamps and Talagrand 2007). The best ensemble modeling approach may be application-dependent, however. For instance, singular vectors and bred modes are likely not the best approaches for generating IC/LBC perturbations in short-range or limited-area ensemble modeling, due to the initial linear growth of large-scale errors (Eckel and Mass 2005). It is also expected that varying certain options, such as land-surface or soil-moisture options, may increase spread in AT&D predictions, but not necessarily for quantitative precipitation forecasts (QPF). Therefore, the ensemble configuration that might be best for one application may very well not be best for a different application.

From the four experiments in this study, we conclude that IC/LBC variability can affect concentration predictions substantially. We also conclude that varying physics parameterizations, especially schemes that have a direct impact on predicted PBL depths, can have a substantial impact on concentration predictions. Therefore, we conclude that a hybrid NWP ensemble modeling approach, one that varies both ICs/LBCs and physics parameterizations, is likely the best approach for the purposes of AT&D forecasting. Further testing is necessary with a larger, perhaps multi-model, ensemble that has greater model option diversity, over a wide range of synoptic and mesoscale conditions.

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TABLES AND FIGURES

TABLE 1. Summary of the IC/LBC dataset and the version of the MYJ PBL scheme used for each of the four experiments in this study.

Experiment	IC/LBC	MYJ PBL
A	ON84+RAWINS	Default
B	NARR	Default
C	ON84+RAWINS	Modified
D	NARR	Modified

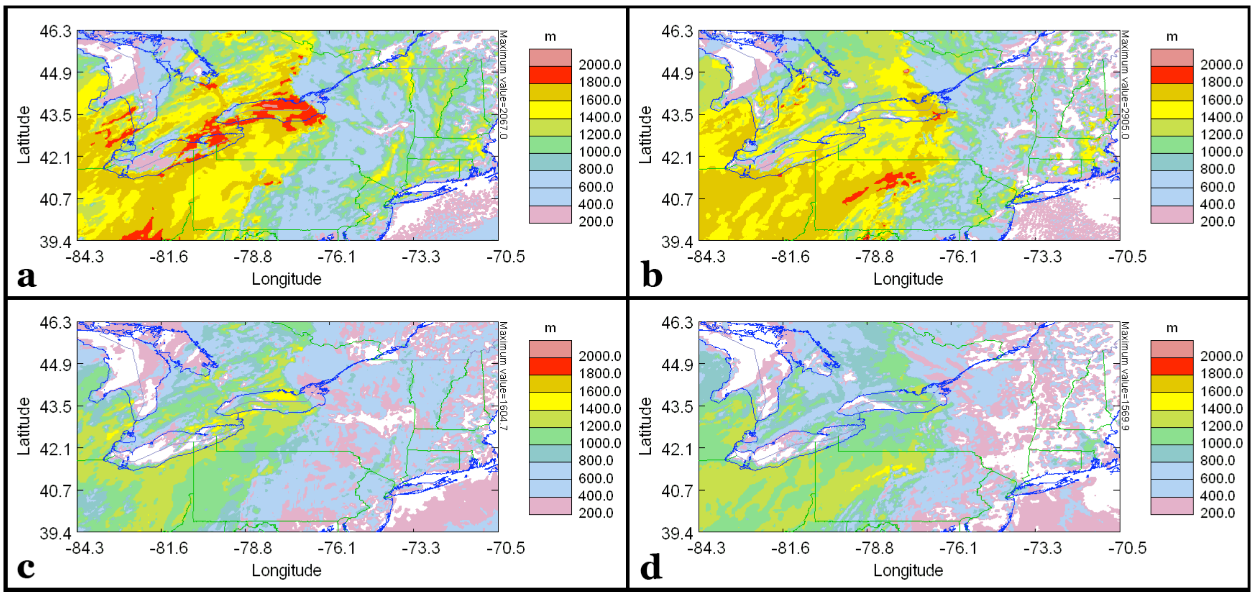

FIG. 1. PBL depths (m) at 2200 UTC on 18 Sep 1983, 5 h after the start of the tracer release. (a)-(d) correspond to Experiments A-D as listed in Table 1.

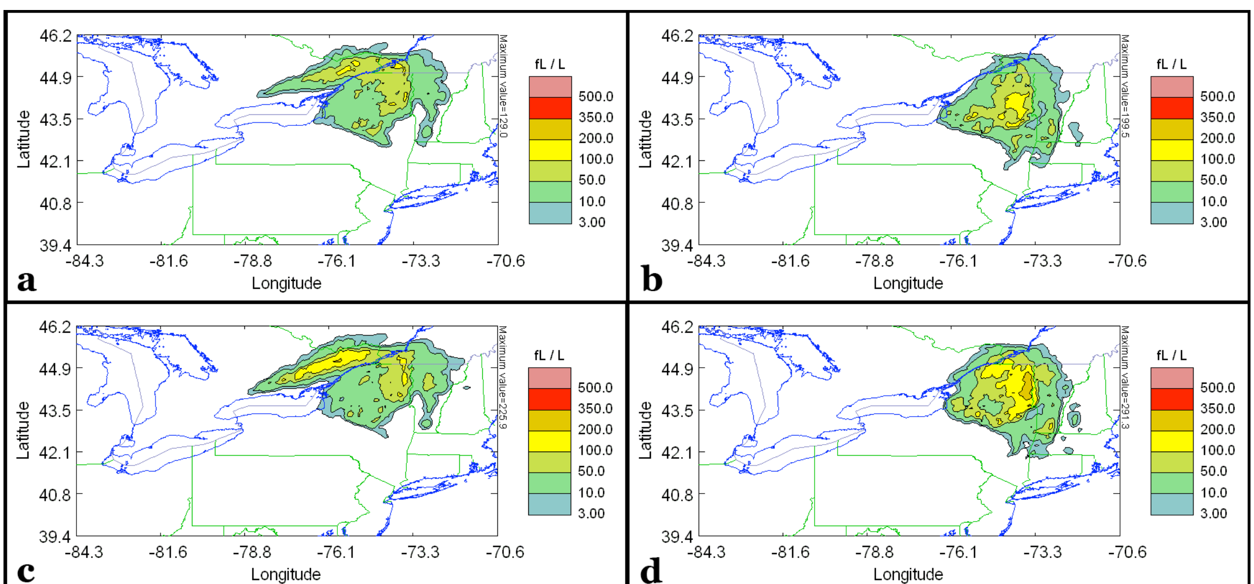

FIG. 2. Surface-level concentrations (fL L^{-1}) at 1000 UTC on 19 Sep 1983, 17 h after the start of the tracer release. (a)-(d) correspond to Experiments A-D as listed in Table 1.