8.5 USE OF VIRTUAL SCENARIOS FOR METEOROLOGICAL, DISPERSION, AND ATMOSPHERIC CHEMISTRY MODELING

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1. INTRODUCTION

Field experiments involving the release of reactive chemical species can be difficult and costly endeavors. As a way to plan for these exercises or to test operational readiness in case of an accidental release, exercises can be conducted that use virtual weather, dispersion, and chemistry scenarios. This paper describes a virtual weather scenario with realistic meteorological data that is input into transport, dispersion and atmospheric chemistry models. An Observing System Simulation Experiment (OSSE) was run to obtain the required meteorological data. OSSEs are designed to examine the impact of new and/or current observations on meteorological analyses and forecasts under differing and realistic virtual weather regimes (Arnold and Dey 1986; Rohaly and Krishnamurti 1993; Atlas 1997; De Pondeca and Zou 2001).

An OSSE includes a nature run to provide the assumed truth and extracted simulated observations. These simulated observations are then incorporated into another model using a data assimilation cycle to generate the subsequent analyses and forecasts. The impact of assimilating temperature, winds, etc. from the nature run into the other model simulation can be assessed using subjective and objective verification. Additionally, the three-dimensional gridded nature fields provide the plume truth from the transport and dispersion models which can then be compared with the results from the assimilation runs. These results determine what impact, if any, the simulated observations have on subsequent plume analyses and forecasts.

Wide ranging atmospheric chemistry release scenarios can be investigated that include different release rates and schedules, species, and locations with varying land use and topography. The atmospheric chemistry module is based on a puff model using Livermore Solver for Ordinary Differential Equations (LSODE) (Hindmarsh 2006) as a solver where chemistry compounds of interest are easily appended to different choices of background mechanisms such as Carbon Bond (Gery et al. 1988) or SAPRC (Carter 2000).

In this presentation, we will describe a virtual chemical release run during September 2006 over Albuquerque, New Mexico (Figure 1). Two different mesoscale models along with a dispersion model coupled with an atmospheric chemistry model provided the realistic scenarios.

1. Virtual scenario

The exercise described in this paper was set up with one team, Team A, running the virtual scenarios using a series of models that simulated an actual chemical release. Once Team A completed their modeling the data was given to Team B. The Team B data represents the data they would have during an actual chemical release. A block diagram of the each team's roles is shown in Figure 2. Team B was given sampler concentration data, limited meteorological observation data, and global gridded meteorological data. Team B performed their analyses using different models and techniques than Team A. Some of the models used by Teams A and B are shown in Figure 3.

The basic premise of the exercise was::

- A chemical monitor detects Diisopropyl Methylphosphonate (DIMP) at a sampler located in southeastern Albuquerque, NM
- Where did it originate?
- What and how much was released?
- What will emergency response be?

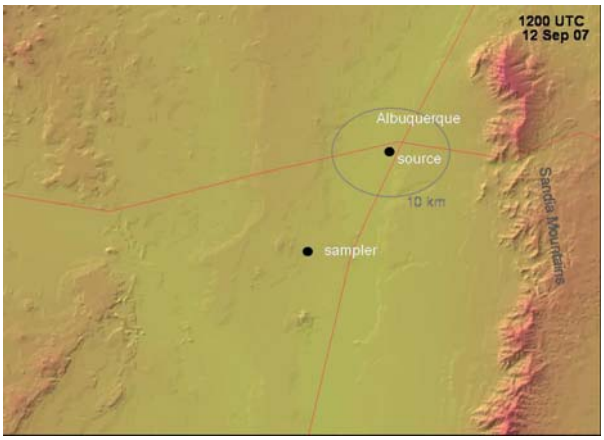

Figure 1. Topography of Albuquerque, NM, location of virtual exercise.

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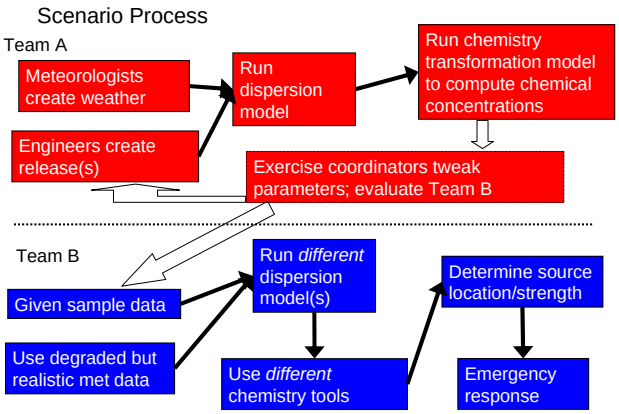

Figure 2. Block diagram of virtual scenario process.

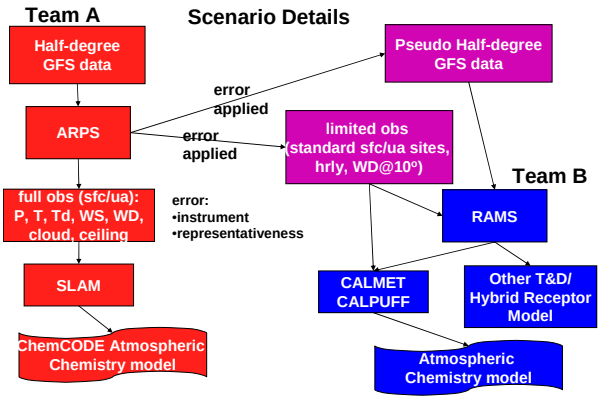

Figure 3. Block diagram of virtual scenario details.

2. MODELS AND MODELING METHODOLOGY

For this experiment, the location chosen was Albuquerque, NM. Albuquerque, NM presents numerous challenges from a numerical weather prediction (NWP) modeling point-of-view due to its varying land-use, arid climate, and very complex topography. A two-week period, from 0000 UTC 01 through 0000 UTC 16 September 2006 was selected to run the virtual weather scenario. The first week was characterized by a broad low-level south-easterly flow typical of a late summer monsoon pattern over the area of interest; however the second weak was dominated by subtle low-level wind shifts (mostly from the south and west) as several synoptic-scale systems passed by to the north of the region.

2. ARPS

The NWP model used for the nature run (truth) was the Advanced Regional Prediction System (ARPS; Xue et al. 2000; Xue et al. 2001). The ARPS is a complete, fully automated, stand-alone system designed to forecast storm- and regional-scale weather phenomena. Table 1 provides a brief summary of the major dynamical and physical features of the ARPS used for this study. All terrain data sets used in the ARPS are based on Digital Elevation Model data available from the U.S. Geological Survey sites, which are also used by the National Imagery and Mapping Agency. The ARPS pre-processors perform additional adjustments to the elevation data for oceans and lakes to ensure that terrain, soil and vegetation data are consistent. Global sea-surface temperatures were interpolated from the Navy Operational Global Atmospheric Prediction System (NOGAPS) model initial conditions at 1^{o} x 1^{o} grid spacing, whereas soil moisture was initialized using fixed values based on climatological soil types.

An ARPS 50-km nature run (domain A, Figure 4) covering much of North America, and the Pacific and Atlantic Ocean was initialized using National Centers for Environmental Prediction Global Forecast System (GFS) final analysis fields from 0000 UTC 1 September 2006 and run for 15 days. The GFS grids were also used to provide lateral boundary conditions at 6-h intervals throughout the model run. The ARPS 50-km nature (truth) fields were also supplied to Team B to simulate the typical ½ degree GFS fields used to initialize and run analyses cycles using meteorological models. Ideally, a hemispheric or even global model should be used to truly mimic the ½ degree GFS analyses (global model). However, due to computational and time constraints a smaller subset grid was used; but was made large enough to limit the impact of the 50-km ARPS lateral boundary conditions on the inner domains.

A one-way nested 15-km domain covering a large portion of the western United States (domain B, Figure 4 was initialized at 0000 UTC 2 September 2006 and run for 14 days. For the 15-km ARPS simulation, lateral boundary conditions were supplied by the ARPS 50-km simulations at 6-h intervals. Simulated measurements were extracted from standard conventional surface stations (1-h intervals) and rawinsondes (12-h intervals) during each 15-km ARPS simulation. The locations of these observations represented observation density over the southwest United States.

Table 1. Summary of dynamical and physical features of the ARPS.

Feature	Description
Equations	Nonhydrostatic and fully compressible
Coordinate system	Generalized terrain-following height coordinate (sigma-z) with stretching
Geometry	Full three-dimensional configuration
Prognostic variables	u, v, and w wind components, Potential temperature and pressure, Subgrid-scale turbulent kinetic energy (TKE), Mixing ratios for water vapor, cloud and rainwater, and ice species
Initial condition	Global Forecast System (GFS)
Lateral boundary conditions	Global Forecast System (GFS) ARPS
Top / bottom boundary conditions	Radiation condition and rigid boundary with Rayleigh sponge layer
Nesting	1-way interactive mode
Subgrid scale turbulence	1.5-order closure TKE-based scheme, fully three-dimensional in sigma-z
PBL turbulence parameteri-zation	1.5-order TKE based non-local mixing
Cloud micro-physics	Lin/Tao five-category ice microphysics
Cumulus parameteri-zation	Kain / Fritsch with shallow convection
Soil model	Two-layer soil-vegetation model with surface energy budget
Radiation	Full shortwave / longwave schemes with cloud-radiation interaction

The ARPS was configured for a high-resolution domain covering New Mexico with 3-km grid spacing (domain C, Figure 4). The ARPS 3-km simulation was initialized at 0000 UTC 2 September 2006 and integrated for 14 days to 0000 UTC 16 September 2006. The 3-km nature simulation obtained initial conditions and boundary conditions at 3-h intervals from the 14-day ARPS 15-km simulation. The convective parameterization scheme was deactivated so only explicit microphysics was used to model precipitation processes. Ideally the nature run (inner nest) should be run at the finest possible grid spacing to simulate the small-scale motions that actually occur in the atmosphere, especially in areas with varying topography (i.e. simulate a realistic truth). For this study, 3-km grid spacing provided the best possible compromise in obtaining a high-resolution truth yet being able to complete the entire 2 week simulation in the reasonable amount of time. All of the remaining dynamical and physical features of the ARPS remained unchanged from the simulations conducted for the 50-km and 15-km nature simulations. Simulated measurements from surface networks and upper-air sites were extracted at selected locations throughout the simulation.

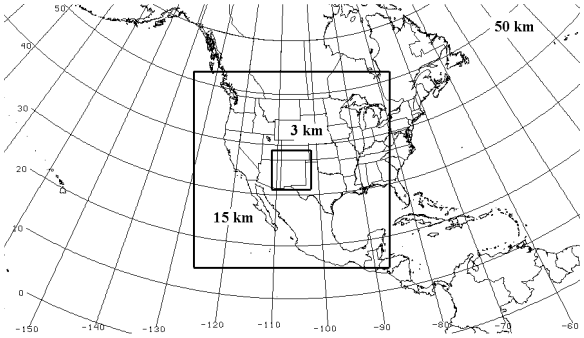

Figure 4. Grid configuration for ARPS simulations. Grid A represents the outer domain, grid B denotes the middle domain, and grid C represents the inner domain with grid configuration attributes summarized in Table 2.

Table 2. Summary of ARPS grid configuration for the nature (truth) simulations. The number of grid points in the east-west, north-south, and vertical directions is given by NX, NY, and NZ respectively.

Horiz. Resolu-tion (km)	Av, Vertical Resolu-tion (m)	NX	NY	NZ	Domain Size (km)
50	425	259	147	45	12,950 x 7,350 x 19
15	425	291	291	45	4,365 x 4,365 x 19
3	425	291	291	45	873 x 873 x 19

2. Simulated "Truth" Observations

Conventional in situ surface and upper air observations were extracted from the ARPS simulations. These simulated observations from ARPS were supplied to Team B to be used for

analysis in their meteorological modeling process. To simulate measurements obtained from surface and rawinsonde instrumentation, three-dimensional position data of surface and upper-air stations were used to extract measurements from the ARPS simulations.

The locations for the surface observations were determined by first obtaining locations of typical surface observations at both synoptic and non-synoptic times. The data were then extracted from the ARPS data at hourly intervals for the locations matching the synoptic and non-synoptic times. The locations for the upper air observations were obtained in a similar way using upper air locations from the region as the baseline before applying the latitude/longitude offset.

The simulated rawinsonde data were only extracted at 12-h intervals (0000 UTC and 1200 UTC) similar to the observation frequency of current operational rawinsonde networks. Each simulated rawinsonde observation contained 26 levels of data in order to emulate the significant and mandatory levels reported by current rawinsonde measurements.

To simulate observation error, a random component was added to each of the observations based on typical errors in the region. The actual magnitudes of the simulated random errors are given in Table 3. Note that the random errors applied to the u and v components of the wind were dependent on simulated wind speed. Additionally, in order to address the current reporting accuracy of observations in the region, simulated wind direction for surface stations was reported to the nearest 5 degrees while simulated wind direction for upper air stations was reported to the nearest 10 degrees (ENSCO; Dr. Steve Masters, personal communication). Finally, it is important to note that for this study, error of representativeness, in which an observation is measuring a localized phenomenon rather than the average condition around a single point, were not added to any of the simulated data types.

The ARPS 3-km nature simulation was used as input into SLAM to run the truth transport and dispersion. It is important to note that SLAM could not directly read in the ARPS 3-km gridded fields. In order to overcome this significant issue the simulated four-dimensional fields from ARPS were instead extracted at latitude/longitude locations that matched the grid spacing of the 3-km ARPS run similar to the technique used to simulate surface and upper-air observations (see above). The major difference is that the ARPS surface observations were extracted at 3 km intervals and the upper air observations were extracted at 6 km intervals. Of course no latitude/longitude offset was needed for the region of interest since these observations were used for the truth transport and dispersion. The domain of the truth observations was subset of the complete ARPS grid (domain C, Figure 4). Additionally, these observations did not include any error since they were used to drive the truth transport and dispersion.

Table 3. Observations simulated from ARPS. For each observation reported, the variables and random errors are given. The actual random errors applied to the u and v component winds were dependent on the wind speed of each observation.

Observation Type	Variables	Random Error
Rawinsonde	Temperature	$\pm$ 0.5 K
	Dew point	$\pm$ 2 K
	Pressure	$\pm$ 1 hPa
	u- / v- winds	
	Speed > 3.74 m s^{-1}	$\pm$ 1 m s^{-1}
	Speed < 3.74	$\pm$ 0.95 m s^{-1}
	Speed < 1 and > 0 m s^{-1}	$\pm$ 0.80 m s^{-1}
Surface	Temperature	$\pm$ 0.5 K
	Dew point	$\pm$ 2 K
	Pressure	$\pm$ 1 hPa
	u- / v- winds	
	Speed > 3.74 m s^{-1}	$\pm$ 1 m s^{-1}
	Speed < 3.74 m s^{-1}	$\pm$ 0.95 m s^{-1}
	Speed < 1.0 and > 0 m s^{-1}	$\pm$ 0.80 m s^{-1}

Modifications were made to the ARPS source code to calculate “truth” cloud cover at each simulated surface observation that was used as input to SLAM. The cloud cover was important since it was later used in the chemistry calculations. The algorithm is a vertical profile of relative humidity to estimate the simulated cloud fraction at each model grid point. In a real-world scenario an actual observed cloud cover value is reported across the sky; whereas for this study simulated relative humidity at a single model vertical grid point was used to represent reality. Therefore, it is entirely possible that any moisture biases within the model could have

directly lead to slight under or over-estimates of the cloud cover input into the chemistry calculations. However, as stated above within the OSSE methodology above, the goal here was to create a realistic/typical weather scenario using a high-resolution model not to duplicate the actual weather regime during this period. The translation we used to convert the ARPS cloud cover determination into the WMO format data is shown in Table 4.

Table 4. Cloud cover definitions from WMO code 2700

Code as entered into standard format data	WMO definition	Numerical definition	ARPS cloud cover determination
/	Cloud is indiscernible for reasons other than fog or other meteorological phenomena, or observation not made		
0	Sky clear	0/10	$\leq$ 0.05
1	1 oktas	1/10 – 2/10	>0.05 and <0.25
2	2 oktas	2/10 – 3/10	$\geq$0.25 and <0.35
3	3 oktas	4/10	$\geq$0.35 and <0.45
4	4 oktas	5/10	$\geq$0.45 and <0.55
5	5 oktas	6/10	$\geq$0.55 and <0.65
6	6 oktas	7/10 – 8/10	$\geq$0.65 and <0.85
7	7 oktas or more but not 8 oktas	9/10 or more, but not 10/10	$\geq$0.85 and <0.95
8	8 oktas	10/10	$\geq$0.95
9	Sky obscured by fog or other meteorological phenenomena		

3. SLAM

The Short-range Layered Atmospheric Model (SLAM) is a multiple layer, Gaussian puff modeling system for the simulation of transport, diffusion, dry and wet deposition, and radioactive or biological decay of tracers released from a point, line, or area source at short range to mesoscale distances. The model may be applied to simulate the dispersion of tracers forward in time from a source to calculate airborne concentrations at a sampler, or motion backward in time from a given receptor location in order to determine contributions from potential sources. (Atchison and Kienzle 2002, ENSCO 2007)

When using the ARPS model output, the SLAM model was run in an upper-air and/or surface data mode. Trajectories were started at 10 minute intervals with a 1 minute model step size. A duration of 24 hours was used for all trajectory calculations.

4. RAMS

The pollutant release was modeled by first generating meteorological data using the Modeling to simulate the analyses that Team B would be conducting was performed with the Regional Atmospheric Modeling System (RAMS) (Pielke et al. 1992). The RAMS configuration used in this study was:

- 3 nested grids (25, 5, 2.5 km)
- Initialized with 1-degree GFS at 6-hr intervals
- Simulation duration: Sep 12-15, 2006
- Fine domain grid centered over Albuquerque, NM
- Observational Data Assimilation (ODA) using extracted surface/upper air obs from ARPS runs at routine weather station spacing

5. ChemCode

Chemical Concentrations by Ordinary Differential Equation (ChemCODE) is a suite of applications that predicts the atmospheric fate of chemicals within Transport and Dispersion (T&D) models. The “Ambient” portion of the model simulates the reactivity of the environment through which a pollutant is transported. The plume portion of ChemCODE requires input from standard puff models (i.e., SLAM, CALPUFF), meteorological inputs (e.g., temperature, cloud cover, radiation), and chemical mechanism inputs (reaction mechanism). The model uses a set of ordinary differential equations to predict changes in pollutant concentration based on diffusion, chemistry, and physical processes (e.g., deposition). ChemCODE uses the Livermore Solver for Ordinary Differential Equation (LSODE) as a solver.

Ambient: The ambient of ChemCODE simulates the “reactivity” of the environment for a specific geographical location/region. It uses an emissions file to release material from man-made and biological sources into the simulated “environment”. It then uses a mechanism

(series of chemical reactions) to define how these released chemicals will interact with each other. By solving the equation below, Ambient predicts how the concentrations of those materials will change over time.

$$\frac{\delta C_i}{\delta t_{reaction}} = k_i * C_i \quad (1)$$

The change in concentration c of a material i is driven by the reaction rate constant k. The term rate "constant" can be misleading since k will often vary with temperature, pressure, and/or sunlight. An Ambient "run" will simulate concentration profiles that might be expected throughout a 24 hour period in the particular location. This is the reactive environment through which released chemicals might travel.

Plume: The plume mode of ChemCODE releases a chemical into a particular environment that was simulated by Ambient and predicts how its concentration will change as a result of several fate processes as it travels from a release location. The equation below describes these processes

$$\frac{\delta C}{\delta t_{total}} = \frac{\delta C}{\delta t_{Diffusion}} + \frac{\delta C}{\delta t_{\mathrm{Re}\,action}} + \frac{\delta C}{\delta t_{Deposition}} + \frac{\delta C}{\delta t_{Het}} + \frac{\delta C}{\delta t_{Other}} \quad (2)$$

where $\frac{\delta C_i}{\delta t_x} = k_{i,x} * C_i$ (3)

Similar to Ambient, the rate constant k describes how quickly a particular process will change the concentration (C) of the release chemical. In the plume mode, these processes include diffusion, reaction, wet and dry deposition, uptake onto particulate matter or heterogeneous chemistry (het) and any other process that might alter the amount of the chemical that remains airborne during transport. The Plume mode uses a parent transport and dispersion model selected by the user to define the "path" and dimensions of a puff during transport. The Plume simply calculates changes in concentration for material in the puff as they move along the defined trajectory.

For the virtual exercise, the material chosen to release in the simulation was DIMP (Diisopropyl Methylphosphonate, $C_7H_{17}O_3P$). DIMP, which is often used as a simulant, degrades rapidly in ultraviolet sunlight. For the exercise DIMP was released at a rate of 1500 g/hr for three hours

Ambient concentrations of O3, NOx, and OH for the two day period of this exercise are shown in Figure 5.

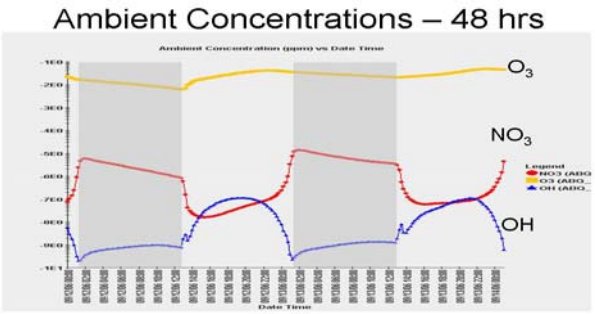

Figure 5. Ambient concentration profiles for Albuquerque for 48 hour period.

3. RESULTS

The modeling performed by Team A to create the virtual chemical release scenario resulted in a surface cloud of DIMP that was released as a single puff and advected southwest of the source.

A comparison of the dispersion of DIMP with a nonreactive inert tracer for three times is shown in Figure 6 through 8. The DIMP is shown to decrease rapidly after 1500 UTC once the solar radiation increases after sunrise. Figure 9 depicts changes in concentration of DIMP (diffusion and chemistry) with respected to non-reactive tracer compound (diffusion only) which demonstrates the important of chemistry in atmospheric transport and diffusion.

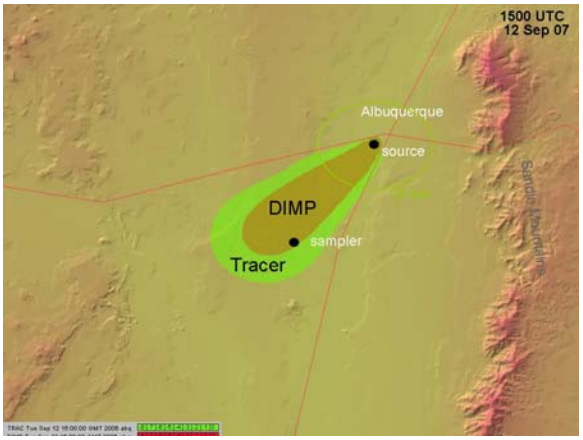

Figure 6 Comparison of concentrations of DIMP vs. non-reactive tracer at 1500 UTC 12 Sep 2006.

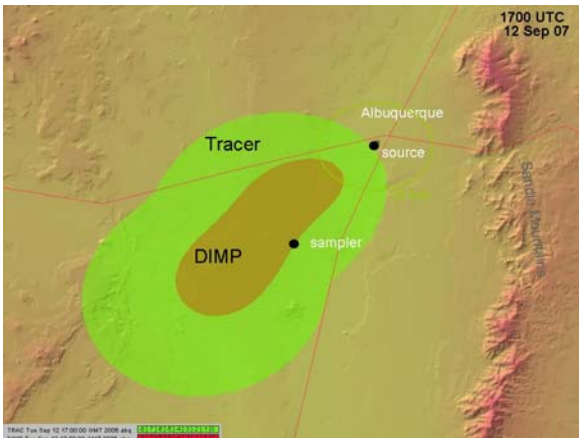

Figure 7. Comparison of concentrations of DIMP vs. non-reactive tracer at 1700 UTC 12 Sep 2006.

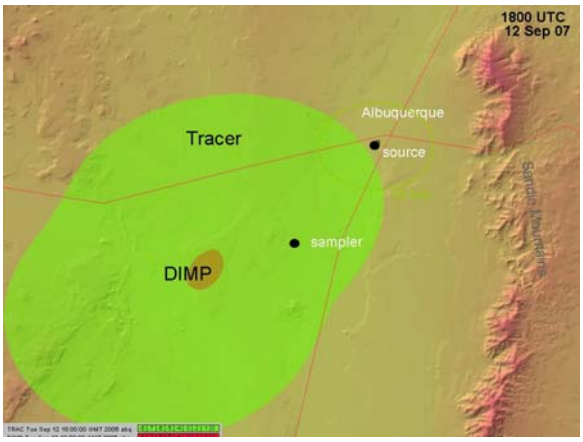

Figure 8. Comparison of concentrations of DIMP vs. non-reactive tracer at 1800 UTC 12 Sep 2006.

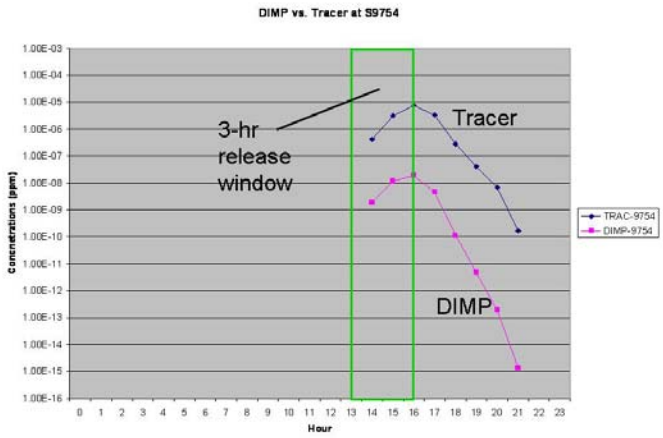

Figure 9. Times series of concentrations of DIMP vs. non-reactive tracer for 12 Sep 2006

4. CONCLUSIONS

Virtual exercises provided a cost-effective means of exploring range of parameters such as:

- Variety of chemical species
- Continuous vs. instantaneous releases
- Logistics of sampler locations
- Meteorological variations e.g. clouds, winds, stability

OSSEs allowed for multiple and complex dispersion situations with virtual weather over long duration. Some issues that were uncovered were:

- Slight differences in wind direction at source leads to different effluent travel paths
- Verification required at fine scales for both meteorology and concentration data
- Finer scales are different but are they better?

Atmospheric chemistry added increasing level of complexity and allowed for a variety of test exercise scenarios.

Future work using virtual scenarios will involve:

- Using in situ data for data assimilation/verification at fine scales
- Using ensemble methodology of analysis

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