Contract No:

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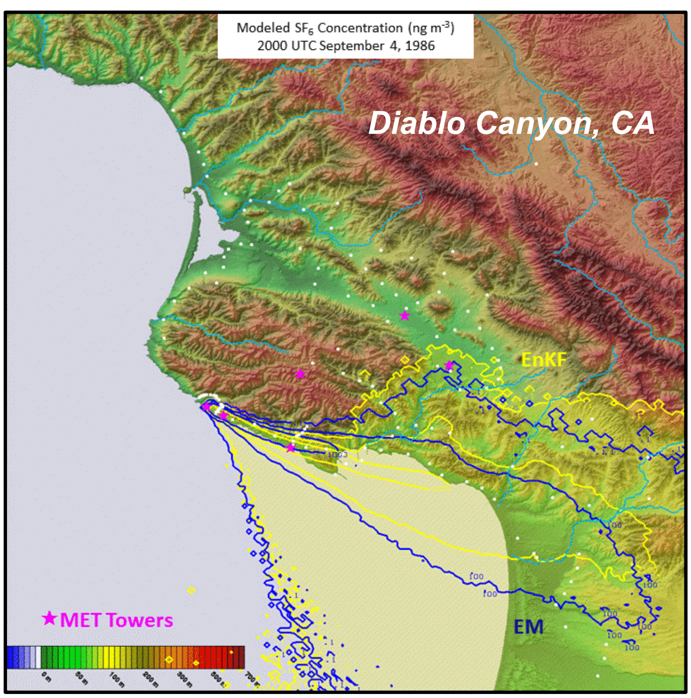
Advanced Atmospheric Ensemble Modeling Techniques

Ensemble modeling (EM), the creation of multiple atmospheric simulations for a given time period, has become an essential tool for characterizing uncertainties in model predictions. We explore two novel ensemble modeling techniques: (1) perturbation of model parameters (Adaptive Programming, AP), and (2) data assimilation (Ensemble Kalman Filter, EnKF). The current research is an extension to work from last year and examines transport on a small spatial scale (<100 km) in complex terrain, for more rigorous testing of the ensemble technique. Two different release cases were studied, a coastal release (SF_6) and an inland release (Freon) which consisted of two release times. Observations of tracer concentration and meteorology are used to judge the ensemble results. In addition, adaptive grid techniques have been developed to reduce required computing resources for transport calculations. Using a 20-member ensemble, the standard approach generated downwind transport that was quantitatively good for both releases; however, the EnKF method produced additional improvement for the coastal release where the spatial and temporal differences due to interior valley heating lead to the inland movement of the plume. The AP technique showed improvements for both release cases, with more improvement shown in the inland release. This research demonstrated that transport accuracy can be improved when models are adapted to a particular location/time or when important local data is assimilated into the simulation and enhances SRNL's capability in atmospheric transport modeling in support of its current customer base and local site missions, as well as our ability to attract new customers within the intelligence community.



This figure illustrates improvements in coastal release plume transport using the EnKF compared to the standard EM approach. Pink stars denote locations of Met towers providing data at 5 minute intervals. The yellow shaded area and contours represent the EnKF modeled plume 5 hours after the initial release time, while blue contours denote the EM simulation. White points show locations of tracer measurements during the experiment.

Model analysis shows that daytime warming of the interior valley area leads to the inland motion of the plume around the higher terrain of Diablo Canyon. Greatest modeled plume concentration differences result due to the plume movement northward toward the interior valley and into smaller canyon areas. Further offshore to the south, model simulations are more consistent due to the stable temperature and wind fields.

Awards and Recognition

This research was selected for presentation to the SRNS Board of Directors in October 2016.

Intellectual Property Review

This report has been reviewed by SRNL Legal Counsel for intellectual property considerations and is approved to be publically published in its current form.

SRNL Legal Signature

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Signature **Date**

Advanced Atmospheric Ensemble Modeling Techniques

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Thrust Area: NS

Project Type: Standard

Project Start Date: October 20, 2015
Project End Date: September 30, 2017

Ensemble modeling has become an essential tool for characterizing uncertainty in atmospheric model predictions. Airborne transport models are commonly driven by mesoscale atmospheric models, whose accuracy is reduced by model biases and limited available data. Ensemble modeling quantifies model uncertainty by providing a range of possible atmospheric end-states, but is still subject to underlying biases. In this extended LDRD, we have used the Diablo Canyon Tracer Experiment as a testbed to compare standard ensemble modeling with two novel techniques on a spatial scale of relevance to non-proliferation: (1) a physics-based ensemble, which adapts models to specific geographical locations and time frames, and (2) data assimilation with an Ensemble Kalman filter. This research has demonstrated that transport accuracy can be improved when a model is adapted to a particular location and time or when local data is assimilated rigorously into the simulation.

FY2017 Objectives

- Obtain data (meteorological and tracer) from the Diablo Canyon (DC) tracer experiment for September 04, 1986, for testing of the ensemble techniques.
- Apply three sets of ensemble simulations to the DC tracer releases: standard ensemble, Adaptive Programming, and Ensemble Kalman-filter techniques.
- Modify existing statistical tools to evaluate each ensemble dataset by comparing it to the DC measurements. This includes both the meteorological and tracer concentration components.
- Develop adaptive grid technology to enhance transport modeling (provide better resolution in regions of interest, such as near the source, or in steep gradient topography).

Introduction

The assessment of emissions from known or suspected weapons facilities that release radionuclide, chemical, or biological materials is of great interest. Source emission estimates are often obtained by scaling downwind effluent measurements by atmospheric dilution rates estimated from airborne dispersion models. The latter are often forced by mesoscale meteorological models, which are of limited accuracy. A more robust solution is to use an 'ensemble' of model simulations, with a range of solutions. We seek to improve the standard ensemble approach through the development of two novel methods: (1) minimization of model error using adaptive (physics-based) programming techniques (AP, Roebber, 2015) and (2) application of a Kalman filter for assimilation of key local observations into the model prediction (EnKF, Evenson, 2003). Transport accuracy can be substantially improved when a model is adapted to a particular location and time and through a utilization of available local data.

Ensemble modeling (EM) – the running of multiple simulations of the same event – has become the standard for quantifying uncertainties in atmospheric forecasts (Figure 1). Typically, agreement between simulations will decrease with longer forecast times and longer downwind distance from the source. EM accounts for uncertainty due to limited input data and for non-linearities inherent in the Navier-Stokes equations, and has been shown to increase model forecast skill compared to single deterministic simulations (Galmarini et al., 2004). Unfortunately, ensembles based on a biased model will retain those biases, and the current practice is to perform EM with minimal consideration for the suitability or completeness of the ensemble (Stensrud et al., 2009).

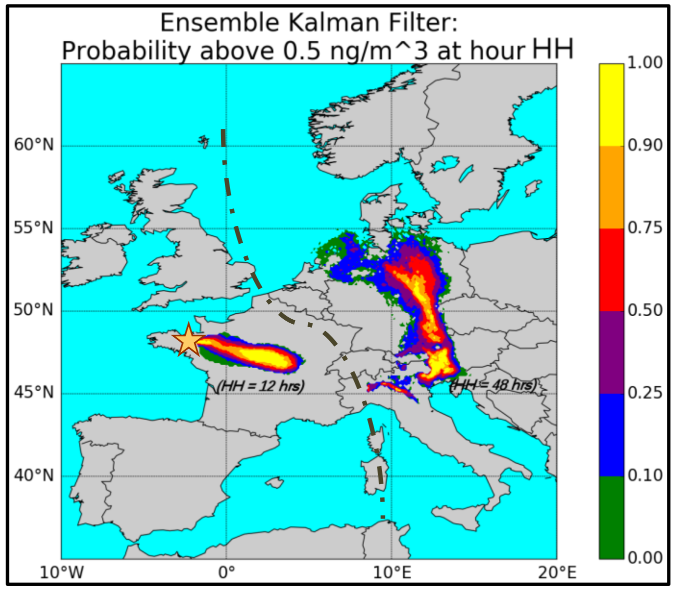

Figure 1. *Confidence levels for ensembles run in Europe where contours represent the fraction of models agreeing on exceedance of a specified concentration threshold. Two times (12, 48 hrs) after release are shown.*

Improvements in ensemble modeling are important in applications related to atmospheric transport and dispersion, such as emergency response and non-proliferation. In the first year of the project, focus was on simulating the European Tracer Experiment (ETEX, Girardi et al., 1998) to evaluate the quality of two novel ensemble modeling techniques. Improvement in modeling of both methods was illustrated. The current research uses meteorological and concentration data collected during the Diablo Canyon Nuclear Power Plant Tracer Experiment (DOPPTEX) at Diablo Canyon, California in September 1986 (Thuiller, 1992). The terrain is more complex and the experiment covers a much smaller spatial domain (<100 km) than ETEX (>2000 km), and is thus a more representative non-proliferation problem. The experiment also includes two different types of releases, a coastal release of SF_6 over an eight hour period, and an inland release of Freon that consisted of two separate releases (two hours and three hours) separated by a three hour period.

Approach

The approach used in this research is similar to the prior year's efforts: Select a suitable modeling scenario and compare the standard EM approach with two novel ensemble techniques. Adaptive Programming (AP) accounts for errors due to the formulation of the model physics. Mesoscale models employ parameterizations to describe unresolved physical processes such as turbulence and cloud formation. A variety of parameterization settings are possible, each with a range of plausible values. Determining the appropriate parameter set is typically performed by trial and error, which is slow and less efficient due to the many simulations required to sample the entire parameter 'space'. AP is a more robust, iterative process by which we perturb the model parameters to generate an ensemble of members. The individual ensemble members are then run, and the best performing member according to available observations is selected to serve as the 'parent' of the next generation. After a number of iterations, the simulations should converge to an ensemble that is best suited (adapted) to the prevailing atmospheric conditions. The second novel approach uses an ensemble Kalman filter (EnKF) to examine the impact of assimilating selected observations into the simulation. The EnKF improves upon existing methods of data assimilation. Standard data assimilation affords equal weight to surface and above-ground winds, but the latter are much more representative of regional air flow, and should force a much broader scale adjustment to the model fields. The EnKF technique combines the model prediction and the calculated error variance of each observation in order to determine the optimal weighting for observations at every step. Meteorological data from the ensemble techniques were ingested into the Lagrangian Particle Dispersion Model (LPDM, Uliasz 1993) to create three-dimensional, time-varying concentration fields. LPDM is also modified to use an adaptive grid (AG) technique that changes the uniform grid mesh to use finer resolution in regions of interest. Additional analysis of vertical plume structure was conducted using HYSPLIT (Draxler et al., 1998) in order to analyze performance of LPDM.

The research described here uses data from the Diablo Canyon tracer experiment (DOPPTEX) conducted in 1986 (Thuiller, 1992). Access to collections of both meteorological data and tracer measurements permits rigorous comparison of these approaches. Statistical techniques developed in the first of the study were used once again for the model evaluation (Mosca et al., 1998). Since time is critical during emergency response situations, research into use of adapted grids was also explored. The technique modifies grid spacing to provide better resolution at points of interest, and coarser resolution in less-critical areas (Srivasta et al., 2001; Khan et al., 2005). Such techniques may result in more rapid results, or provide better accuracy due to improved resolution at the source.

Results/Discussion

Model simulations for transport were conducted for transport from two locations where tracers were released. The first release comprised a continuous 8 hour SF_6 release from the Diablo canyon power plant location immediately adjacent to the pacific coast, while the second release comprised a transient release of Freon for durations of 2 and 3 hours from an interior valley location. The standard ensemble modeling (EM) approach is to perturb the initial meteorological conditions (fields of wind, temperature, etc.), assuming inherent uncertainty in the measurements used to develop them, and generate an ensemble of forecast solutions whose spread about the mean quantifies the forecast uncertainty. This is the baseline standard for comparing the two novel methods of EM. Twenty members were generated with the Weather

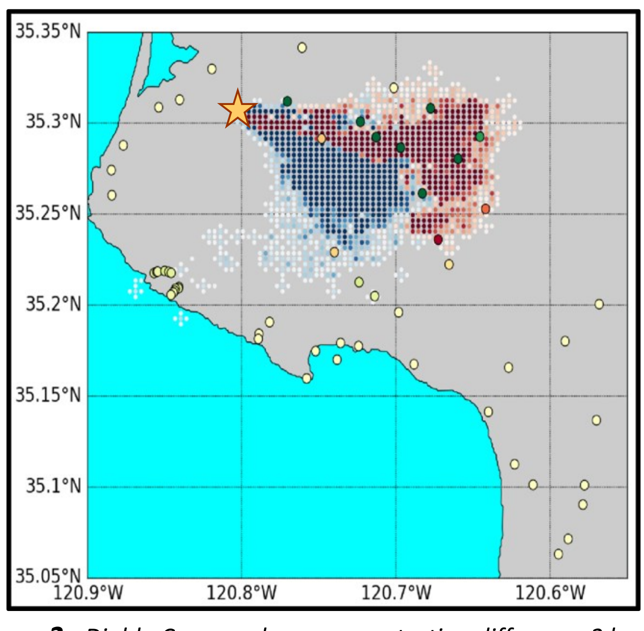

Figure 2. *Diablo Canyon plume concentration difference 2 hours after release between the AP Base case and AP Generation 40. Red shading indicates a drop in concentration, while blue shading shows increased concentration. Circles denote tracer observation locations. The green circles indicate improved model results, while red circles indicate a decline in model results relative to observations.*

Research and Forecast (WRF, Skamarock et al., 2008) model using a technique described in Berner et al. (2011) involving stochastic perturbation to the WRF simulations. In general, the EM runs exhibited less variation for the inland release than for the coastal location due to the observed difference of nearly 20 degrees Fahrenheit between land and ocean temperatures.

The AP ensemble technique perturbed 9 different model parameter inputs (including surface temperature, soil moisture, and turbulence length scale) of the Regional Atmospheric Modeling System (RAMS, Cotton et al., 2001). RAMS is used due to prior experience with AP at SRNL (O'Steen and Werth, 2009). The scoring of each AP ensemble member was based on upper-air observations at X locations both upwind and downwind of the tracer release locations, with the best result from a given "generation" saved for use in the next iteration. This was repeated for 40 generations. An example of improved simulation results is given in Figure 2, showing the difference in concentration between the Base Case simulation and the Generation 40 result. The AP technique showed improvements in both release cases, with more improvements showing in the inland release scenario. The coastal release did show an improvement in the timing of the downwind movement of the plume, the direction of plume movement was still slightly off shore. Results from the AP work from the first year of research are the subject of a drafted peer-review journal article.

The EnKF technique used the WRF-Data Assimilation Research Testbed (DART) software (Anderson et al., 2009) and the original EM members as the starting point. The EnKF technique showed better overall improvement than the AP technique for DOPPTEX, especially for the coastal release (Figure 1) where land and ocean temperatures provided significant spatial differences, while the diurnal warming of the interior valley induced an inland plume motion which curved around the higher coastal terrain of Diablo Canyon downwind of the release point. EnKF assimilation utilized both surface based meteorology tower measurements at 5 minute intervals and upper air measurements from SODAR at 30 minute intervals. Since the radiational heating of the interior valley demonstrated significant forcing effects on the plume motion, the surface measurements contributed most to forecast improvement.

The adaptive grid technology was developed in a general sense for use at SRNL, and specifically applied to Diablo Canyon. Figure 3 shows an example of the modification to grid mesh where only 4% of the grid points were used compared to our standard modeling techniques. Due to the adaptive nature of the grid, these points were concentrated in regions of higher concentration gradients, leading to similar resolution at points of greatest interest compared to our original simulations. This technique showed better results for the coastal release. The inland release consisted of two separate releases which were both in the domain at the same time, causing some issues with the adaptive grid converging on the areas of interest In

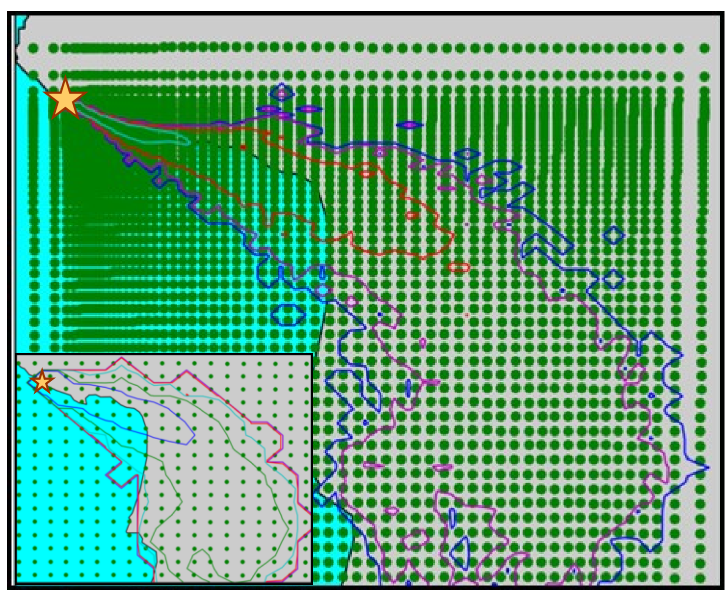

Figure 3. *Modified transport grid mesh using adaptive grid (AG) technique. Note the higher density of grid points near the source location, given by the star. Inset shows an initial uniform grid mesh before application of the AG technique.*

practice, the process does not necessarily improve simulation speed as hoped, but does provide improved resolution around the regions of interest.

FY2017 Accomplishments

- DOPPTEX data were collected and organized for use in the ensemble modeling. This included assembling input gridded and observed meteorological data, as well as measured tracer concentrations.
- Statistical metrics and software were modified from last year's development for ETEX and applied to DOPPTEX collections to assess ensemble model skill. Metrics can be applied to both meteorological results as well as the tracer data. However, the lack of meteorological observations for this study prevents an independent data set for statistical analysis.
- A 20-member standard ensemble (using the WRF mesoscale model and running LPDM for transport) was generated for DOPPTEX.
- A 20-member EnKF ensemble (using WRF-DART platform and running LPDM for transport) was generated for DOPPTEX. Software developed to allow for specific input of surface and upper-air meteorological data for ETEX was used here as well. The results showed improved statistics most pronounced in the flow interaction between the complex terrain and the land-ocean radiational heating differences. The close proximity of measurements provided at 5 minute intervals provided the ability to allow for local radiational forcing to impact the plume motion.
- A 10-member AP ensemble (using RAMS mesoscale model and running LPDM for transport) was generated for DOPPTEX. The results showed modest improvement in tracer plume statistics, but with a clear shift of the plume away from an area to which it did not extend based on tracer measurements.
- Adaptive grid techniques were developed with assistance from Georgia Tech and applied to DOPPTEX. Statistical improvement in simulated tracer concentrations relative to the original uniform mesh was found.

Future Directions

- Analysis of the AP parameter adjustments. Which parameter settings provide the best results?
- Further testing of the EnKF technique: What specific observations should be used? How much weight should be given to various observations?
- Further testing of the AG to transport simulations to reduce computational burden, or improve plume accuracy in regions of interest.
- Application of AG techniques for both site-related emergency response and Strategic Partnership Projects (SPP) supporting numerous intelligence community sponsors.
- Explore and explain the differences in novel ensemble technique improvement (AP, EnKF) over standard EM as applied to large-scale problems (ETEX) versus a small-scale problem (DOPPTEX).

FY 2017 Publications/Presentations

1. SRNS Board of Directors poster presentation (18 October 2016).
2. Buckley, R. L., S. R. Chiswell, R. J. Kurzeja, G. M. Maze, B. J. Viner, and D. W. Werth, 2017: Novel Atmospheric Ensemble Modeling Techniques Applied to Long-Range Transport. 97th American Meteorological Society Annual Meeting, *28th Conference on Weather Analysis and Forecasting/24th Conference on Numerical Weather Prediction* (Seattle, WA on 25 January, 2017).

3. Buckley, R. L., S. R. Chiswell, R. J. Kurzeja, G. M. Maze, B. J. Viner, and D. W. Werth, 2017: Novel Atmospheric Ensemble Modeling Techniques Applied to Long-Range Transport, Palmetto Chapter of the American Meteorological Society *21st Annual Mini-Technical Meeting* (Columbia, SC on 02 March 2017).
4. SRNL External Review Committee (08 May, 2017).
5. Buckley, R. L., S. R. Chiswell, R. J. Kurzeja, G. M. Maze, B. J. Viner, and D. W. Werth, 2017: Ensemble Atmospheric Modeling Techniques Applied to Mesoscale Dispersion. *21st Annual George Mason University Conference on Atmospheric Transport and Dispersion* (Fairfax, VW on 13 June, 2017).
6. Werth et al. Draft of paper discussing AP technique applied to ETEX (1st year results), to be submitted to *Atmos Env*ir.
7. Buckley R. L., S. R. Chiswell, R. J. Kurzeja, G. M. Maze, B. J. Viner, and D. W. Werth, 2017: Advanced Atmospheric Ensemble Modeling Techniques – draft site report.

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Acronyms
AG: Adaptive Grid
AP: Adaptive Programming
DOPPTEX: Diablo Canyon tracer experiment
EM: Ensemble modeling
EnKF: Ensemble Kalman Filter
ETEX: European Tracer Experiment
HYSPLIT: Hybrid Single Particle Lagrangian Trajectory model
IC: Intelligence community
LDRD: Laboratory Directed Research and Development
LPDM: Lagrangian Particle Dispersion Model
RAMS: Regional Atmospheric Modeling System
SRNL: Savannah River National Laboratory
WRF: Weather Research and Forecast model
WRF-DART: Weather Research and Forecast-Data Assimilation Research Testbed

Intellectual Property
None to date.

Total Number of Post-Doctoral Researchers
Dr. Grace M. Maze served as a post-doctoral researcher on this project for much of the first year (FY2016), as directed by the Oak Ridge Associated Universities (ORAU), before being hired on permanently in August 2016.