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Project Summary

Evaluation and Sensitivity Analyses Results of the MESOPUFF II Model with CAPTEX Measurements

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The MESOPUFF II regional Lagrangian puff model has been evaluated and tested with the Cross-Appalachian Tracer Experiment (CAPTEX) data base. The model was applied to the six full-scale CAPTEX episodes in order to investigate its ability to transport and disperse the tracer plume formed from the 3-hour release of an inert, non-depositing perfluorocarbon tracer gas from either one of two selected sites. Model performance was quantitatively determined from traditional statistical measures of difference and correlation between modeled and observed tracer concentrations paired in time and location. Graphical maps displaying observed and modeled plume patterns were also employed to qualitatively assess spatial displacements, while analysis of plume centroid positions provided quantitative information about the amount of separation and difference in downwind distances between the respective plumes with time for each two day episode.

Diagnostic test results applying optional single level wind fields available in the model and certain optional dispersion methods are compared to results from the default model runs, which employed a mixed-layer averaged wind field and Gaussian dispersion parameters. Transport time and location of impact of the peak tracer concentration and its magnitude at the first sampling arc were examined for the various diagnostic test runs and compared against measured results.

Sensitivity test runs were also performed that focused on selected options and variations in key parameters in the model's dry deposition and chemical transformation mechanisms in order to assess their impact on 24-h mean and peak sulfur dioxide and sulfate concentrations using emissions from a realistic elevated point source.

This Project Summary was developed by the EPA's Atmospheric Research and Exposure Assessment Laboratory, Research Triangle Park, NC, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

The ability of a regional-scale air quality model to reproduce spatial pollutant concentration fields or deposition patterns on a short-term basis is strongly dependent upon its formulations for simulating the atmospheric transport and dispersion processes. Thus, an evaluation of these crucial model components against field measurements is an important element in establishing the credibility of any model.

Experimental field studies with certain tracer gases have provided valuable concentration measurements and meteorological data on regional scales, which have allowed assessments of the transport and dispersion methods in models. One of the most recent tracer data sets available for this purpose is from the Cross-Appalachian Tracer Experiment (CAPTEX). The CAPTEX data base has provided a challenging set of episodes for testing regional-scale transport and dispersion models. This intensive field study was specifically designed and conducted with the intention of acquiring accurate tracer data over an extensive surface sampling network and concurrent upper air meteorological measurements along with ancillary measurements on tower and airborne platforms.

The full report documents the results of an evaluation and testing effort of the MESOPUFF II model system with the CAPTEX data base. MESOPUFF II is a second generation Lagrangian puff model, which was designed to treat the transport, dispersion, chemical transformation for SO_x and NO_x, and the removal (dry and wet) processes influencing pollutant emissions from elevated point and/or area sources over regional scales for multiple-diurnal cycles. Any non-reacting, non-depositing gas may also be modeled by electing not to simulate transformation or deposition processes in the model runs. The MESOPUFF II (Version 4.3) model was executed and evaluated with the measurements obtained from the six full-scale experimental cases from CAPTEX.

Quantitative results are provided by traditional statistical measures of difference between modeled and observed mean and peak tracer concentrations in an effort to assess model performance. However, the analysis tools were not limited to statistical results of concentration pairs. Selected graphical maps of modeled/observed plume patterns were also produced to provide qualitative evidence to assist in the interpretation of model performance and to indicate where improvements might be needed. Plume centroid positions were analyzed to obtain quantitative measures of the difference in downwind distance and separation of the observed and modeled plumes as a function of time.

Diagnostic test runs were performed with alternate single level wind fields available from the meteorological processor and with variations in the dispersion method provided in the model. The results of the diagnostic model runs are compared to the default model runs and to actual values for the CAPTEX cases to investigate differences in transport and dispersion.

Since the model evaluation was limited to an assessment of the transport and dispersion components, a select group of model sensitivity runs was also undertaken to investigate the impact on 24-hour mean and peak SO_x concentrations due to changes in key technical parameters or the selection of options in the dry deposition and chemical transformation methods. The model base case run and sensitivity test runs were all performed using the same meteorological fields from a single CAPTEX episode and the emissions from a realistic, large elevated point source.

Model Description

The MESOPUFF II modeling system is composed of separate computer codes to process meteorological data (READ56, MESOPAC II), to compute pollutant concentrations (MESOPUFF II), and to perform various postprocessing operations on modeled concentrations from receptor sites or over a gridded domain (MESOFILE II). All of these model elements were exercised in this evaluation effort.

MESOPAC II is the primary processor program, which generates the hourly gridded fields of the horizontal wind components for two layers (default), mixing height (Z_i), surface friction velocity (U_*), convective velocity scale (w_*), Obukhov length (L), and PGT stability class (A-F) from National Weather Service (NWS) hourly surface observations, twice-daily upper air data, and land use categories. Precipitation measurements are optional and were not used in this effort because dry conditions generally prevailed during CAPTEX episodes.

The two operational (default) wind fields are: a mixed-layer averaged wind field to represent the flow between the surface and current Z_i and an upper layer averaged wind field for the region from Z_i to the 700 mb height. There are also alternative single level wind fields, which can be constructed if selected.

The MESOPUFF II model applies the puff superposition technique to simulate a continuous pollutant plume from either point and/or area sources. Each puff is horizontally symmetric with a Gaussian distribution. The puff release and sampling rates must be specified by the user in each application. The horizontal (σ_y) and vertical (σ_z) dispersion parameters govern puff growth out to 100 km (default). Values of the dispersion parameters are computed from power law formulas derived from curve fits to tl Turner dispersion curves for the differe stability classes. Puff dispersion follo\ time dependent relationships at great downwind distances. No puff splitting performed in the model. The height of puff center is automatically compared Z_i at each hour in order to determine tl appropriate layer-averaged wind field 1 transport. Puff dispersion above Z_i governed by E stability class.

Model Evaluation Data

The field study phase of CAPTE consisted of individual ground-lev releases of a perfluoromon methylcyclohexane (C_7H_{14}) tracer g over a 3-hour period on selected da during the period from mid-September late October 1983. The amount of trac emitted was accurately controlled and constant release rate was assumed o\ the release period. The desirab attributes for this tracer include extremely low background level and interference from other sources. T release sites were at Dayton, Ohio Sudbury, Ontario. There were four fu scale experimental releases (#1- conducted from Dayton during afterno periods, which assured strong verti mixing and the prevailing flo\ transported the tracer plume across t sampling region. Release #6 from Dayt was very brief and was not modele Releases #5 and #7 were conducted fr Sudbury under northwesterly win during two different nocturnal periods.

The tracer was accurately measu by automatic sequential samplers either 3- or 6-hour intervals at 87 si over an extensive surface netwc encompassing the northeastern Unit States and southeastern Canada. T network of sites was designed in a deployed at approximately 100 km int vals extending from 300 km to ab 1100 km downwind of Dayton.

The tracer measurements we provided in units of femtoliters/liter (fl with an ambient background of 3.4 fl removed from each concentration in data set. With a maximum of consecutive samples allowing m measurements to span up to 36 ho and a sampling strategy designed bring all sites on-line simultaneou along each arc prior to the expec arrival of the observed plume, the fi experiments encompassed about two days of travel across the region in m of the cases.

The domains for the meteorologi processor and model grids were defi to be the same size and encompas the CAPTEX sampling network. The model domain was defined by 30 E-W x 19 N-S grid squares for the Dayton cases and it was expanded to 24 N-S grid squares for the Sudbury cases. The grid spacing was set to 37 km for all cases. This value was partly selected due to the resolution of the land use data base. Land use types needed for the model domain were obtained from an in-house land use inventory, which contained the fractional coverage of 12 different land use categories at approximately twice the resolution of the model grid. Since the model allows only a single land use type to be specified for each grid square, the land use category covering the greatest fraction of the total area within each grid square was selected.

Upper air profiles from the regular National Weather Service (NWS) rawinsonde sites and 10 supplemental locations were obtained at 6-hour intervals during each experimental period. However, profile data for only the 00 and 12 GMT launches were required for model input. The upper air data from the six NWS upper air stations in the region were applied in the model evaluation runs.

Hourly surface observations from 25 regular reporting NWS surface stations (model limit) distributed over the model domain were also prepared for the model runs for each CAPTEX study period. Missing observations were interpolated with data from adjacent hours because MESOPAC II requires continuous surface measurements of cloud cover, ceiling height, wind speed, wind direction, temperature, pressure, and relative humidity on an hourly basis.

Model Evaluation Procedures and Results

The model was executed in order to simulate the tracer release for the six full-scale CAPTEX experiments. The model simulated the neutrally buoyant ground-level tracer releases by emitting puffs from a 1-m stack height with no plume rise for a 3-hour period with the actual emission rate (g s^{-1}) for each case. The puff release rate and puff sampling rate were both set to 4 h^{-1} as tests revealed negligible concentration differences at greater rates for this application. The chemical transformation and deposition processes were not simulated. Model execution time was greatly reduced by specifying that hourly concentrations be calculated only at the grid coordinates of the surface sampling sites. The default methods and features specified in the user's guide were applied in these operational model runs. The modeled results were averaged to obtain concentrations at 3- or 6-hour intervals by the MESOFILE II postprocessor program in order to correspond with the time periods of the tracer measurements.

Concentration pairs with both values exhibiting zero were excluded from statistical analysis since neither observed nor modeled plume impacted these points. This eliminated 1088 out of the 1895 total pairs. Additionally, a relatively few tracer concentrations of 1-2 fl l^{-1} obtained at sites separated from the observed plume pattern were screened out of the data base because they were deemed to be anomalous. The final data set contained 734 modeled and observed concentration pairs.

Statistical results from analysis of observed (O) and model predicted (P) concentrations paired in time and space were computed for each experiment and the overall data set. MESOPUFF II overpredicted mean concentrations, although model values were within a factor of two of the observed means in experiments #2,#4,#7, and for the full data set. The greatest overprediction occurred in CAPTEX #3, which also exhibited the most complicated vertical wind shear pattern among these episodes. The values of various statistics for residuals (O_i - P_i) were larger than the observed mean concentrations and correlations were generally low. These results from the statistical measures are similar to those obtained with other regional model evaluations with tracer data sets. Spatial displacements between the respective plumes were attributed for the considerable scatter and low correlations in the statistical results. The results revealed the difficulty that the regional models have in accurately replicating the plume trajectory and plume spread over long distances.

Graphical maps of modeled and observed values over the study region provided valuable evidence for interpreting the amount of overlap of the respective plumes. The plume patterns were depicted by symbols at the locations of sampling sites where nonzero observed and modeled concentrations occurred. The model simulated the actual path and pattern of the tracer plume quite well for the relatively strong, steady westerly flow situation during CAPTEX #4 when wind direction shear was small. Nevertheless, differences between the modeled and actual transport speeds produced variations in the time of impact of the modeled plume, which assisted in explaining the low correlation for this experiment. More notable spatial differences were found in the positions and extents of the observed and modeled plume patterns during CAPTEX #3 where vertical direction shear was significant in the mixed layer. Similar maps of plume patterns for individual event periods gave useful qualitative evidence about the relative plume overlap during the course of each episode. The maps of plume patterns certainly verified the existence of notable plume separations particularly during the late periods of each CAPTEX case.

A valuable analysis technique that emerged to assess spatial displacements between modeled and observed plume patterns was the determination of plume centroid positions. The centroid location of a plume was defined to be the density-weighted maximum concentration location. Therefore, quantitative measures were computed as the downwind distance difference and separation distance between observed and modeled plumes at each time period. Analyses of these results revealed that the observed tracer was often found farther downwind than the modeled results after the first night in each Dayton case. The actual plume was likely transported by faster winds aloft and was also directed along a different path than the modeled plume, which was transported by slower winds derived over a shallow lower layer.

Diagnostic and Sensitivity Test Results

Model test runs with different wind fields and dispersion features in the model provided interesting differences from the default methods applied in the operational evaluation. This effort was undertaken to investigate differences in plume transport between the mixed-layer averaged winds and optional single level wind fields available from the meteorological processor and to examine variations in peak concentrations by changes in the dispersion method in the model.

Results at the first arc at 300 km revealed that the mixed-layer averaged wind field provided a better representation of actual plume transport speed and direction than single-level wind fields generated for the surface or 850 mb height. The comparative results indicated the modeled plumes traveled much slower and to the left (counter-clockwise) with a surface wind field, while 850 mb winds transported the modeled plumes more rapidly and to the right (clockwise) of the observed tracer plume.

Modeled peak concentrations from the default model runs in the evaluation overpredicted observed peak values whether unpaired in time or location. For the high-25 concentrations, the modeled peak value of 1010±436 fl l^{-1} can be compared to the observed peak of 637±436 fl l^{-1}. The highest concentrations were also found at the 300 km arc sites during the initial day of each Dayton experiment. Overprediction of the peak values certainly was a strong reason why the overall mean concentrations values were also overpredicted for these cases. Examination of the meteorological processor output fields indicated that stability class 4 (neutral) was often specified during the afternoon hours of the release periods due to the strong winds in these cases. It appeared that vertical dispersion was underestimated for the neutral stability cases with the current formulation for the Gaussian dispersion coefficient at the short-range distances. In diagnostic test runs with the uniform vertical mixing option, where puffs are immediately distributed over the entire depth of the mixing layer, results showed modeled peak concentrations were more comparable to the observed peak values for the Dayton cases. While observed plumes had become vertically well-mixed, evidence indicated the vertical dispersion coefficient in the model had not increased rapidly enough under neutral conditions to disperse the puffs through the entire depth of the afternoon mixing layer before reaching the 300 km arc. Results from other model test runs indicated that a reduction of the cross-over distance between distance-dependent and the time-dependent dispersion schemes to 50 km and 10 km generally produced even higher peak concentrations than with the default value of 100 km for this application.

The purpose of the model sensitivity runs was to investigate the impact on 24-h mean and peak SO_x concentrations from select variations in certain key parameters in the dry deposition and chemical transformation modules. The emissions in all model test runs were continuous from a single elevated point source. The base case run included the default features for deposition and chemical conversion of SO_2 to SO_4. Each test case run involved the variation of a single parameter or option. All model runs utilized the same meteorological fields from a CAPTEX episode and the simulation period was 48 hours.

The dry deposition method incorporated into MESOPUFF II is based on the deposition velocity concept, which is computed from the sum of aerodynamic and surface resistances. The transformation rate of SO_2 is determined from a regression expression which contains the dominant variables controlling this process as derived from analyses of photochemical model simulations.

Results were obtained by computing the 24-h plume average concentration and peak concentration from each model run. The select group of model sensitivity run cases included: no dry deposition, no chemical transformation, immediate uniform vertical mixing to Z_i, changes to the SO_2 or SO_4 surface resistance, and a plus or minus 50% variation in background ozone concentrations. Generally, peak SO_2 concentrations were much less sensitive than peak sulfate concentrations in the model runs when either deposition or chemical transformation were not simulated. Peak SO_4 values were affected more by the selected variations in these model components because high sulfate concentrations occurred at much greater distances downwind that peak SO_2 values. Tables of results contain the actual percentage differences from the base case run for both 24-h periods.

Conclusions

The results of the evaluation revealed that the model overpredicted both mean and peak concentrations. The overpredictions were most pronounced for the Dayton releases at the first two sampling arcs. Since differences in horizontal plume spread were not evident during the first day of transport, it was concluded that the primary cause for the model overpredictions was an underestimation of vertical plume growth for neutral stability, which was the stability class most often specified during the afternoon release periods. A different dispersion formula for the Gaussian vertical dispersion parameter for neutral conditions fitted to the Pasquill D1 curve should be incorporated and tested within the current framework of the model. This revision would provide for more rapid vertical plume spread with the default Gaussian dispersion distance-dependent scheme under neutral conditions.

The statistical results also showed that large scatter and low correlations occurred between modeled and observed concentrations paired in time and space for both mean and peak values. This reflected the inability of this model, as with other similar models, to accurate replicate the speed and/or direction of th tracer plume. Thus, the larg concentration differences where observe and modeled plumes did not overla were primarily attributed to trajector errors. However, the statistical analyse did not provide sufficient information fo an assessment of the causes for mod errors in transport.

Graphical displays and a technique t determine plume centroid position which indicated the size of the spati plume differences, greatly assisted i characterizing model trajectory error Spatial displacements of varying amount were evident from graphical maps o modeled and observed plume pattern with time. Plume centroid position derived as the concentration-weighte locations from non-zero values at 6-hou intervals, were used in quantifying di ferences in the downwind distance an the separation distance betwee observed and modeled plume Specifically, results from MESOPUFF indicated that the observed plume move faster and/or along a different path durin the nocturnal period and was generall found further downwind of the modele plume by the second daytime period i these episodes. The plume separatio distance, the difference in centroi locations between the observed an modeled plumes, ranged from 100-30 km during these cases at downwin distances of 500-1000 km. The mos rapid increase in plume separation als occurred during the nocturnal periods.

The CAPTEX tracer emission consisted of non-buoyant, ground-leve releases. For this source type, pu heights in MESOPUFF II were alway less than the mixing height, which cause modeled plumes to be continuall transported by the lower layer wind fiel This feature is believed to be shortcoming of the model desig especially during the nocturnal perio when greater vertical shears in speed an direction often prevail. It was conclude from analyses of the plume centroi positions that the modeled plumes mus have been advected by slower wind derived over the shallow mixed layer a night, while observed plumes had bee transported along a different trajectory b faster winds at higher levels. In the cas of an elevated source emitting a buoyan plume which rises to even higher level the model would have switched th plume transport at night to the uppe layer wind field when the mixing heigh dropped below the height of the pu center. Based on these results, mode applications for multi-day simulations of round-level, non-buoyant point emissions are not recommended. The model's treatment for this source type could be improved if the height of the puff center after release was redefined to be one-half of its vertical dimension and this revised puff center height reached a limit when vertical puff growth extended up to the mixing height.

Diagnostic tests of optional features in the model provided distinct differences in plume transport and dispersion from the default methods. The mixed-layer averaged wind field (i.e., default lower level wind field) was found to be superior to single level wind fields at the surface or 850 mb height in simulating the impact time and location of the tracer plume at the 300 km arc. Results suggested that it should remain as the preferred wind field for representing boundary layer transport when applying this model. Model test run results with the uniform vertical mixing option indicated that peak concentrations were much closer to observed values than those from the default Gaussian dispersion parameter methods. With the uniform vertical mixing method, puffs are completely dispersed through the entire extent of the boundary layer after release. These test results gave more evidence that modeled plumes required greater vertical mixing during the afternoon release periods. In lieu of the suggested revision to the Gaussian dispersion scheme noted earlier, the selection of this optional dispersion method appears to be an attractive alternative since it produces the desired vertical dispersion when neutral conditions are prevalent.

A limited group of model sensitivity runs was also performed in an effort to examine the impact on 24-h peak and plume average SO_2 and sulfate concentrations from variations in certain key parameters and changes in methods in the dry deposition and chemical transformation components of the model. The model base case and test case runs were exercised with the same meteorological fields from CAPTEX #1 and the same emission rates from a large, elevated point source. Results showed that sulfate concentrations were more sensitive to the selected variation in a parameter or method. In particular, sensitivity run results with differences in the surface SO_4 resistance or $\pm 50\%$ differences in background ozone concentration produced negligible variations in SO_2 peak and mean concentrations; however, the impact on sulfate concentrations was from 15-20%. This finding is particularly relevant to regional model applications since the higher concentration levels of sulfate were found at much greater downwind distances than was SO_2. It follows that SO_4 is influenced to a greater extent by transformation and deposition processes. A more extensive evaluation of these modules is advocated with suitable experimental data.