P1.23 REAL-TIME SIMULTANEOUS PREDICTION OF AIR POLLUTION AND WEATHER DURING THE HOUSTON 2000 FIELD EXPERIMENT

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1 INTRODUCTION

The complexity of accurately forecasting changes in the large number of three-dimensional, non-linear variables needed for weather prediction has challenged meteorologists for decades. Even more difficult is the prediction of air quality, as this requires not only an accurate weather forecast, but also knowledge and prediction of emissions, deposition, and chemical reactions of the compounds that are envolved. In addition, three-dimensional observed meteorological fields are used to initialize and verify meteorological models on a daily basis. No such option exists for air pollution applications, where three-dimensional observations are mostly restricted to field experiments. Only some surface observations of a few compunds are taken on a regular basis. Hence, the Houston 2000 field experiment was a great opportunity to not only apply complex modeling systems in real time, but also to verify results and evaluate the quality of the forecasts.

Since the relevant processes contributing to photochemical air pollution are highly complex, non-linear and coupled, numerical simulation models are indispensable tool for diagnostic and prognostic analyses, and can therefore serve other scientists (such as observationalists or chemists) in diagnosing and analysing observations.

Most of the 'state of the art' modeling systems that are being used consist of several parts, including horizontal and vertical advection of tracers, physical processes that effect the tracers (such as turbulent mixing, convection, clouds, and radiation), and a chemical mechanism that describes the gas phase chemical interactions. The chemical processes are usually treated independently of the meteorological model, except that the transport is driven by output from a meteorological model. Due to this separation of meteorology and chemistry there is a loss of possibly important information of atmospheric processes that quite often have a time scale of much less than one hour, e.g. wind speed and direction, rainfall and cloud formation. Especially on the regional scale with gridsizes down to 1 km, the wind field and other meteorological parameters are highly variable and neglecting these variances may introduce certain errors.

The modeling system that was used in this study does not separate the meteorology and chemistry, but integrates the meteorological and chemical processes simultaneously ('online'). It represents the most consistent way to couple the meteorology and chemistry.

2 Model description

Here we will only give a summary of the modeling system used during the experiment. For a more detailed description the reader is referred to Grell et al. (2000).

The fifth-generation Penn State/NCAR Mesoscale Model (MM5, Grell et al. 1994) was used as the cornerstone of this modeling system. All MM5 capabilities (based currently

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[¶] NOAA Aeronomy Laboratory, Boulder, Colorado on Version 3) were retained. It can be used in nonhydrostatic mode (Dudhia 1993), and it has the capabilities for four-dimensional data assimilation (FDDA) of analysis and observations data (synoptic and asynoptic, Stauffer and Seaman 1994). In addition to the original capabilities it also includes a soil/vegetation/snow parameterization developed by Smirnova et al. (2000).

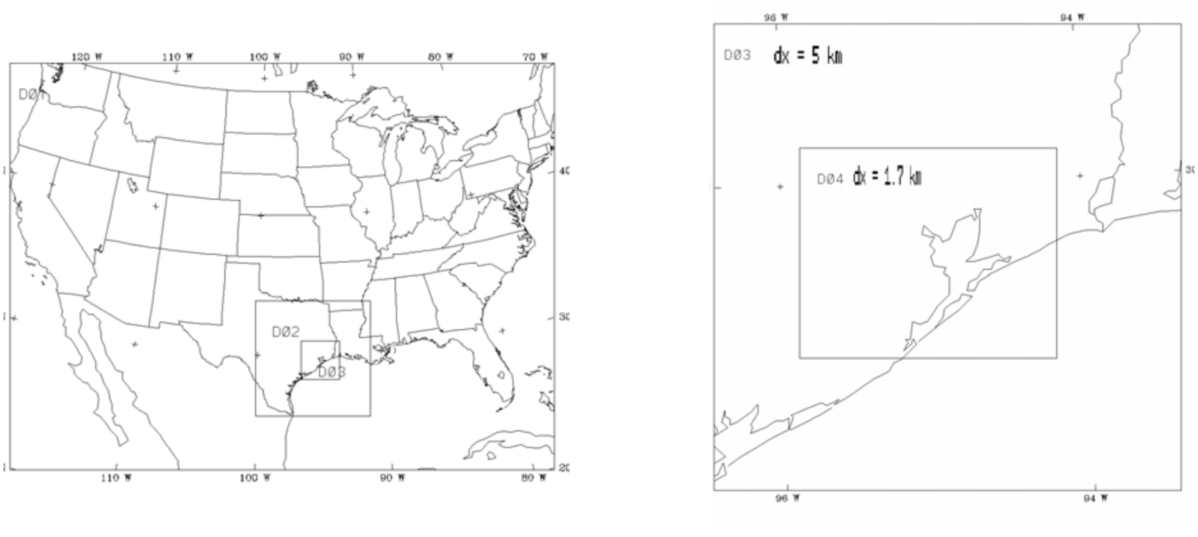
Gridscale and sub-gridscale transport of species is treated within the meteorological model ('online'). The advective transport of tracers in MM5 was changed by implementing a three-dimensional positive definite advection scheme developed by Smolarkiewicz and Grabowski (1990). The RADM2 gas-phase chemical mechanism (Stockwell et al. 1990), originally developed for the Regional Acid Deposition Model version 2 (RADM2) (Chang et al. 1989), is used to treat the interaction of the chemical species with each other. The Madronich (1987) photolysis scheme provides the photolysis rates ('online'). Deposition is calculated as in the 'flux-resistance' analogy (Wesley 1989), and is directly tied to the turbulence and soil/veg/snow parameterization. Sulfate is present in the form of aerosol particles, its deposition is described according to Erisman et al. (1994). Biogenic emissions are also calculated 'online', following Simpson et al. (1995) and Guenther et al. (1993, 1994).

The ability to scale to high performance and large problem sizes has been demonstrated with the distributed-memory parallel MM5 (Michalakes, 2000). The additional complexity of this code and the additional storage requirements of the large number of new prognostic variables makes distributed memory parallel computers even more attractive for running coupled atmosphere-chemistry models.

3 Experimental setup

During the summer of 2000 this model was run in real time over four domains. Fig. 1 shows the locations of the covered areas. Horizontal resolutions for the three domains are 60 km (D1, covering continental US), 15km (D2, covering large parts of Texas and Louisiana), 5 km (D3, covering the southeast corner of Texas, and 1.67 km (D4, centered on the Galveston Bay area). The vertical resolution employs 27 terrain-following height levels, which are stretched in the vertical. The highest resolution was near the ground with a surface layer thickness of approximately 15 m. To get meteorological input data for D1, the 40 km RUC analysis was interpolated both horizontally and vertically to the 60 km grid. Three-hourly boundary conditions were provided by NCEP's ETA model. The model was then integrated in its full physics/chemistry version to provide two 48-hour forecasts per day. The 3-hourly output was used to initalize meteorological fields for domain D2, as well as to provide meteorological and chemical boundary conditions. The same procedure was implemented to provide initial and boundary conditions for D3 and D4, where each time the coarser domain served as the provider of input for meteorological fields, and boundary conditions for meteorological as well as chemical fields. Domains D2, D3, and D4 were only integrated for 24 hours. The chemical fields on all domains are initialized with the previous 12-hour forecast fields. A mixed phase microphysics scheme was used for explicit treatment of precipitation on all domains. The highest resolution domain was run without a convective parameterization, all other domains allowed for both, explixit and implicit treatment of convection.

Anthropogenic emissions data are derived primarly from the U.S. EPA county-wide emissions for a base year of 1996, (EPA NET-96, version 3.12, ozone season day; U.S. EPA, 2000). One important modification is the incorporation of commercial shipping emissions from the Texas Natural Resource Conservation Commission (TNRCC), which are a factor of 9 lower than the EPA estimates for the Houston region and are apportioned along major shipping lanes. Highway fractions from 2 km resolution land-use data of Texas (Wiedinmyer et al., 2001) are used to allocate mobile area source emissions as well as the petroleum product storage, industrial, and solvent sectors of the nonmobile area emissions within each Texas county. For both point and area sources, the hourly allocation factors, and hydrocarbon speciation of the VOC from the EPA (U.S. EPA, 1989) are used. For regions outside of Texas, the spatial partitioning of the mobile and nonmobile area sources within a county is also taken from the 1/4 degree longitude by 1/6 degree latitude EPA emissions in-



(a) (b)

Figure 1: Geographical view of the four domains for the real-time prediction experiment. Domain D1 (a) is integrated with 60 km horizontal resolution, domain D2 (a) with 15 km, D3 (a and b) with 5 km, and D4 (b) with 1.67km.

ventory (U.S. EPA, 1989). U.S. county boundary data, coastline and water body boundaries from the NCAR graphics libraries, and a unique application of the AREAS package of NCAR graphics, are used to confine emissions to land, and provide a consistent normalization between county totals and the various emission and model grid systems. The sensitivity of the photochemical results to the emissions inventory, particularly the VOC emissions from various industrial sources in the Houston-Galveston region, will be a primary focus of model post-analysis studies (see also McKeen et al. 2002).

The real time runs were integrated on the Forecast Systems Laboratory (FSL)'s supercomputer, a massively parallel cluster of Alpha Ev667 processors with Linux operating systems. All runs used 36 processors. domain D4 was the costliest, using about 1 hour of wall clock time for 10 hour of simulatiom time. Atmospheric models such as MM5 entail a high ratio of computation to communication. The addition of atmospheric chemistry processes further improves this ratio, with the result that scalability to large numbers of processors is further improved so that the availability of additional processors would have lead to a further significant decrease in wall clock time.

4 Results

The Houston 2000 field experiment was a unique opportunity to not only apply complex modeling systems in real time, but also to verify results and evaluate the quality of the forecasts. During this talk we will give information about the overall performance of the model. A more detailed comparison of meteorology will be given by Bao et al. (2002), while Stu McKeen et al. (2002) concentrate on a comparison of ozone and ozone precursors as observed by aircraft and predicted by the model.

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6 REFERENCES

Bao, J.-W., S. McKeen, G. A. Grell, M. Trainer, and E.-Y. Hsie, 2002: A comparison of meteorological observations with the output of a real-time weather-chemistry forecasting model during the TEXAS AQS 2000 field experiment. *4th Conf. on Atmospheric CHemistry*, AMS, Orlando.

Chang, J. S., F.S. Binkowski, N.L. Seaman, J.N. McHenry, P.J. Samson, W.R. Stockwell, C.J. Walcek, S. Madronich, P.B. Middleton, J.E. Pleim and H.H. Lansford, 1989: The regional acid deposition model and engineering model. State-of-Science/Technology, Report 4, National Acid Precipitation Assessment Program, Washington D.C..

Dudhia, J., 1993: A nonhydrostatic version of the Penn State/NCAR mesoscale model: Validation tests and simulation of an Atlantic cyclone and cold front. *Mon. Wea. Rev.*, **121**, 1493-1513.

Erisman, J. W., A. van Pul, and P. Wyers, 1994: Parameterization of surface resistance for the quantification of atmospheric deposition of acidifying pollutants and ozone. *Atmos. Env.*, **28**, 2595-2607.

Grell, G. A., J. Dudhia, and D. R. Stauffer, 1994: a description of the Fifth-generation Penn State/NCAR Mesoscale Model (MM5). *NCAR Tech Note TN-398 + STR*, 122pp.

Grell, G. A., S. Emeis, W. R. Stockwell, T. Schoenemeyer, R. Forkel, J. Michalakes, R. Knoche, W. Seidl, 2000: Application of a multiscale, coupled MM5/chemistry model to the complex terrain of the VOTALP valley campaign. *Atmos. Env.*, **34**, 1435-1453.

Guenther, A. B., P. R. Zimmerman, P. C. Harley, R. K. Monson, and R. Fall, 1993: Isoprene and monoterpene emission rate variability: model evaluations and sensitivity analyses. *J. Geophys. Res.*, **98D**, 12609-12617.

Guenther, A., P. Zimmerman, and M. Wildermuth, 1994: Natural volatile organic compound emission rate estimates for U.S. woodland landscapes. *Atmos. Environ.*, **28**, 1197-1210.

Madronich, S., 1987: Photodissociation in the atmosphere, 1, Actinic flux and the effects of ground reflections and clouds, *J. Geophys. Res.* **92**, 9740-9752.

Michalakes, J., 2000: The Same-Source Parallel MM5. *Journal of Scientific Programming*, **8**, IOS Press, pp. 5-12.

McKeen, S., G. A. Grell, J.-W. Bao, M. Trainer, and E.-Y. Hsie, 2002: Results from the NOAA, FSL photochemical forecast model: Comparisons to aircraft and surface data during TEXAS-2000. *4th Conf. on Atmospheric CHemistry*, AMS, Orlando.

Simpson, D., A. Guenther, C. N. Hewitt, and R. Steinbrecher, 1995: Biogenic emissions in Europe. 1. estimates and uncertainties. *J. Geophys. Res.*, **100D**, 22875-22890.

Smirnova, T. G., J. M. Brown, and S. G. Benjamin, and O. Kim, 2000: Parameterization of cold season processes in the MAPS land-surface scheme. *J. Geophys. Res.*, **105**, 4077-4086.

Smolarkiewicz, P., and W. W. Grabowski, 1990: The multidimensional positive definite advection transport algorithm: nonoscillatory option. *J. comp. Phys.*,**86**, 355-375.

Stauffer, D.R. and N.L. Seaman, 1994: Multiscale four-dimensional data assimilation. *J. Appl. Meteor.*, 33, 416-434.

Stockwell, W. R., P. Middleton, J. S. Chang, and X. Tang, 1990: The second generation regional acid deposition model chemical mechanism for regional air quality modeling. *J. Geophys. Res.*, **95**, 16343-16367.

U.S. EPA, The 1985 NAPAP emissions inventory (version 2): Development of the annual data and modelers? tapes, Re. EPA-600/7-89-012a, 692 pp., Natl. Tech. Info. Serv., Springfield, VA., 1989.

U.S. EPA, National air pollutant emission trends, 1990-1998, EPA-45/R-00 002, Off. of Air Qual. Plann. and Stand., Research Triange Park, N.C., 2000.

Wesley, M. L., 1989: Parameterization of surface resistance to gaseous dry deposition in regional numerical models. *Atmos. Env.*, **16**, 1293-1304.

Wiedinmyer, C., Guenther, A., Estes, M., Strange,I.W., Yarwood, Greg, Allen, D.T., 2001: A landuse database and examples of biogenic isoprene emission estimates for the state of Texas, accepted for publication in *Atmos. Env.*.