Modeling Protocol
(Version 1.1)

Annual Application of MM5 to the Continental United States

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1 INTRODUCTION

This document presents the protocol governing the application of the PSU/NCAR Mesoscale Model (MM5) to the continental U.S. This computationally intensive activity is aimed at developing the meteorological fields needed to operate a variety of regional-scale oxidant, fine particulate, and acid deposition models. A companion protocol being developed under this work assignment addresses MM5 application procedures to two (2) episodic simulations over the western and eastern U.S.

1.1 Background

Over the past half decade, emergent requirements for direct numerical simulation of urban and regional scale photochemical and secondary aerosol air quality—spawned largely by the new particulate matter ($PM_{2.5}$) and regional haze regulations—have led to intensified efforts to construct high-resolution emissions, meteorological and air quality data sets. The concomitant increase in computational throughput of low-cost modern scientific workstations has ushered in a new era of regional air quality modeling. It is now possible, for example, to exercise sophisticated mesoscale prognostic meteorological models and Eulerian photochemical/aerosol models for the full annual period, simulating ozone, sulfate and nitrate deposition, and secondary organic aerosols (SOA) across the entire United States (U.S.) or over discrete sub-regions.

1.2 Study objectives

Consistent with ongoing U.S. Environmental Protection Agency (EPA) programs, this work assignment is aimed at developing high-resolution, gridded meteorological data sets that can be used to support urban and regional scale air quality modeling over the continental United States. In this protocol, we lay out a technical approach for exercising and testing the model over the entire U.S. for a full year at 36 km horizontal grid scale.

1.3 Purpose of Protocol

This protocol documents the activities in performing the modeling required to support the development of the meteorological model outputs. These activities include: (a) selection of appropriate databases and modeling episodes, (b) evaluating the performance of the meteorological model, (c) sensitivity and performance testing of the meteorological modeling system, (d) delivery of the meteorological model outputs for subsequent use in air quality modeling, and (e) documentation of the meteorological modeling study findings. A companion report being developed under this work assignment will give an in-depth description of the MM5 model evaluation process for both episodic and annual average conditions.

2 Model Selection

The meteorological model selected for use in the study is non-hydrostatic Penn State University/National Center for Atmospheric Research (PSU/NCAR) mesoscale meteorological model (MM5) version 3.5. Described by Dudhia et al., 2001, the MM5 is perhaps the most technically advanced public-domain prognostic model available for operational use in preparing inputs to urban- and regional-scale photochemical air quality models.

The MM5 model is being continually updated. During the course this study the MM5 website will be monitored and if issues are discovered with this version of MM5, the implications for this study will be discussed with the client representative.

3 Episode Selection

The recommended annual episode for this study is the year 2001. This year is attractive because of the availability of observations for which to evaluate the meteorological and subsequent air quality modeling, the lack of any major climatic anomalies, and the opportunity of having an MM5 simulation completed in time for the 2000 to 2004 regional haze base planning period.

The full period to be modeled will extend from 16 Dec 2000 at 12Z to 15 January 2002 at 12Z. The model will be run in independent 5 day periods, with a new period starting every 5 days. This scheme will allow 12 hours of model initialization (i.e. spinup) before the model calculations are deemed suitable for use in air quality models. A sample simulation period is presented in Table 3.1. The purpose of the 5 day reinitialization is to eliminate the error growth in long term simulations.

The model output files (MMOUT) will be split into separate files every 48 hours to assure that the model output files do not exceed the 2 Gigabyte file size limit on certain computer systems.

Table 3-1: Model Simulation Initialization Schedule.

Date	Period 1	Period2
16 Dec. 12Z		
17 Dec. 0Z		
17 Dec. 12Z		
18 Dec. 0Z		
18 Dec. 12Z		
19 Dec. 0Z		
19 Dec. 12Z		
20 Dec. 0Z		
20 Dec. 12Z		
21 Dec. 0Z		
21 Dec. 12Z		
22 Dec. 0Z		
22 Dec. 12Z		
23 Dec. 0Z		
23 Dec. 12Z		
24 Dec. 0Z		
24 Dec. 12Z		
25 Dec. 0Z		
25 Dec. 12Z		
26 Dec. 0Z		
26 Dec. 12Z		
27 Dec. 0Z		

4 Modeling Domain and Data Availability

4.1 Modeling Domain

Horizontal Domain Definition: The computational domain for this application is presented in Figure 4-1. The domain consists of an array of 165 x 129 grid cells with 36km horizontal spacing. This grid was selected to maximize the coverage of the ETA analysis region. This domain uses the recently selected "national Regional Planning Organization (RPO)" grid projection which has a pole of 40^0, -97^0 with true latitudes of 33^0 and 45^0. This domain is identical to the national emissions modeling surrogate grid being prepared for the Lake Michigan Air Directors Consortium (LADCO) and the RPO sensitivity modeling study grid (Baker, et al. 2002).

Vertical Domain Definition: MM5 will be exercised with 34 vertical layers with an approximately 38 meter deep surface layer. The MM5 vertical domain is presented in both sigma and height coordinates in Table 4-1.

4.2 Data Availability

The data to be used in the annual MM5 application consists of meteorological model derived inputs, geographic inputs and observed data. These data are used both for running the MM5 model and for evaluating the results. The major datasets to be used in this study, along with the availability for 2001 are presented in Table 4-2.

All major datasets have been downloaded from NCAR. The only documented data issues are for the ETA initialization fields from 12Z 14 October to 6Z 17 October. For this period the data may be contaminated by erroneous precipitation assimilation and suspect greenness fraction. Special attention will be paid to the MM5 initialization and data assimilation files during this period.

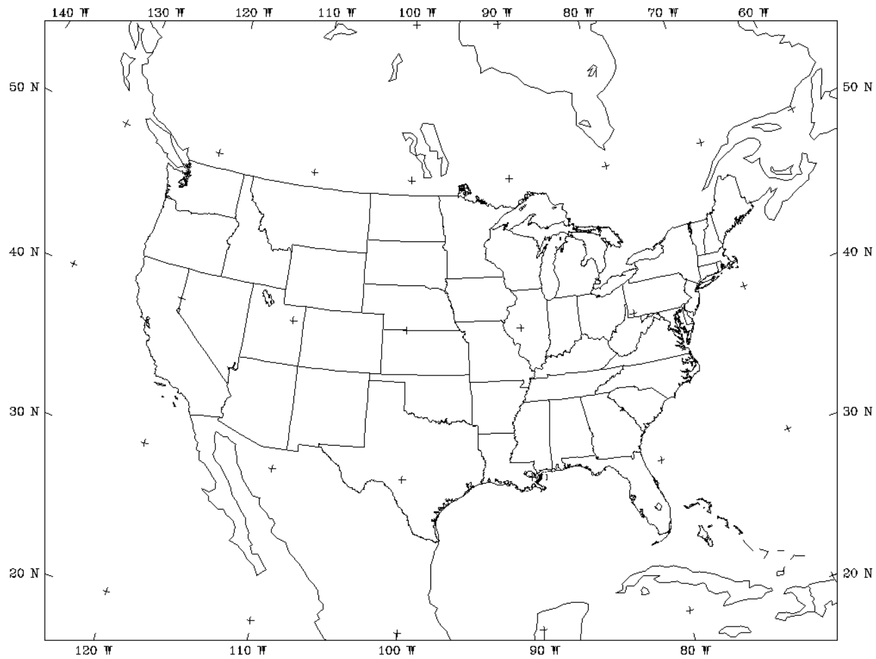
Table 4-1: MM5 Vertical Domain Specification.

k(MM5)	sigma	press.(mb)	height(m)	depth(m)
34	0.000	10000	15674	2004
33	0.050	14500	13670	1585
32	0.100	19000	12085	1321
31	0.150	23500	10764	1139
30	0.200	28000	9625	1004
29	0.250	32500	8621	900
28	0.300	37000	7720	817
27	0.350	41500	6903	750
26	0.400	46000	6153	693
25	0.450	50500	5461	645
24	0.500	55000	4816	604
23	0.550	59500	4212	568
22	0.600	64000	3644	536
21	0.650	68500	3108	508
20	0.700	73000	2600	388
19	0.740	76600	2212	282
18	0.770	79300	1930	274
17	0.800	82000	1657	178
16	0.820	83800	1478	175
15	0.840	85600	1303	172
14	0.860	87400	1130	169
13	0.880	89200	961	167
12	0.900	91000	794	82
11	0.910	91900	712	82
10	0.920	92800	631	81
9	0.930	93700	550	80
8	0.940	94600	469	80
7	0.950	95500	389	79
6	0.960	96400	310	78
5	0.970	97300	232	78
4	0.980	98200	154	39
3	0.985	98650	115	39
2	0.990	99100	77	38
1	0.995	99550	38	38
0	1.000	100000	0	0

Table 4-2: Meteorological Databases and Availability.

Dataset	Use	Identifier	Availability
NCEP ETA Archives	"First-guess" field for MM5 initialization and FDDA	ETA	Thru Dec '02
NCEP ADP Global Upper Air Observation Subsets	Objective analysis into MM5 initial, boundary and FDDA fields	DS353.4	Thru Feb '02
NCEP ADP Global Surface Observations	Used for objective analysis into MM5 initial, boundary and FDDA fields	DS464.0	Thru Feb '02
Reynolds, Stoke and Smith Global SST Analyses (weekly IO2)	Sea surface temperatures	DS277.0	Thru Mar '02
TDL Surface Hourly Observations	Model Evaluation	DS472.0	Thru Feb'02
FSL/NCDC Radiosonde Archive	Model Evaluation	RAOBS	Thru Dec '02
NCDC 3240 Hourly Precipitation	Model Evaluation	RAIN	Thru Dec '02

Figure 4-1: Annual MM5 Computational Domain.



5 Input Data Preparation Procedures

5.1 Fixed Data Inputs

Topography Topographic information will be developed using the National Center for Atmospheric Research (NCAR) terrain databases. The grid will be based on the 5 min (~9 km) Geophysical Data Center global data. Terrain data are interpolated to the model grid using a Cressman-type objective analysis scheme. To avoid interpolating elevated terrain over water, after the terrain databases are interpolated onto the MM5 grid, the NCAR graphic water body database will be used to correct elevations over water bodies. The terrain elevations are presented in Figure 5-1.

Vegetation Type and Land Use: Vegetation type and land use information is developed using the most recently released 2 min. (~ 4 km) PSU/NCAR databases provided with the MM5 distribution. Standard MM5 surface characteristics corresponding to each land use category will be employed.

5.2 Variable Data Input

Atmospheric Data: Initial conditions to the MM5 will be developed from operationally-analyzed fields derived from the National Centers for Environmental Prediction (NCEP) ETA model following the procedures outlined by Stauffer and Seaman (1990). The synoptic-scale data to be used for this initialization (and in the analysis nudging discussed below) will be obtained from the conventional National Weather Service (NWS) twice-daily radiosondes and 3-hr NWS surface observations. These data include the horizontal wind components (u and v), temperature (T), and relative humidity (RH) at the standard pressure levels, plus sea-level pressure (SLP) and ground temperature (T_g). Here, T_g represents surface temperature over land and sea-surface temperature over water. The so-called "first guess" NMC-analyzed fields will be interpolated to several supplemental analysis levels (950, 925, 900, 800, 750, 650, 600, 550, 450 and 350 mb) and then modified by blending in the NWS standard rawinsonde data using a successive-correlation type of objective analysis that accounts for enhanced along-wind correlation of variables in strongly curved flow (Benjamin and Seaman, 1985). Subsequently, the three-dimensional variable fields will be interpolated onto the MM5's sigma vertical coordinate system.

Water Temperature: Water temperatures will be derived from the global ETA skin surface temperature database. It is recognized that these skin temperatures can lead to temperature errors along coastlines. However, for this sort of analysis focusing on bulk continental scale transport, this issue is likely not important. One of the proposed sensitivity and diagnostic simulations presented in section 7 is aimed at addressing this issue.

Clouds and Precipitation: While the non-hydrostatic MM5 treats cloud formation and precipitation directly through explicit resolved-scale and parameterized sub-grid scale processes, the model does not require precipitation or cloud inputs. The potential for precipitation and cloud formation enters through the thermodynamic and cloud processes formulations in the model. The only precipitation-related input required is the initial mixing ratio field that will be developed from the NCEP and NMC data sets previously discussed.

5.3 Multi-scale FDDA

The multi-scale Four Dimensional Data Assimilation (FDDA) technique developed at Penn State (Stauffer and Seaman, 1990, 1994) and used in MM5 is based on Newtonian relaxation, or nudging, which is a continuous assimilation method that relaxes the model state toward the observed state by adding to one or more of the prognostic equations artificial tendency terms based on the difference between the two states. It is said to be a form of continuous data assimilation because the nudging term is applied at every time step, thereby minimizing "shock" to the model solutions that may occur in intermittent assimilation schemes.

The multi-scale FDDA technique was developed by Stauffer and Seaman (1994) and includes simultaneous use of two approaches outlined in Stauffer and Seaman (1990) and Stauffer et al. (1991): (a) nudging toward gridded analyses which are interpolated to the model's current time step, and (b) nudging directly toward individual observations within a time-and-space "window" surrounding the data. These two approaches are referred to as "analysis nudging" and "obs nudging", respectively. Analysis nudging is ideal for assimilating synoptic data that cover most or all of a model domain at discrete times. Obs nudging does not require gridded analyses of observations and is better suited for assimilating high-frequency asynoptic data that may be distributed non-uniformly in space and time (e.g., the intensive studies data). The routine observational networks to be used in this study are not sufficiently dense enough to support obs nudging.

It is critically important to understand the influence FDDA is having on the model simulation. Properly applied, FDDA is a guide for the model, gently moving the model estimates towards the analyzed synoptic fields. Improperly applied, FDDA is a sledgehammer that forces the model towards observations in data rich areas while degrading the model field away from the observations.

The nudging coefficients to be applied in this study are 2.5×10^{-4} sec^{-1} for winds and temperature and 1×10^{-5} sec^{-1} for mixing ratio. These nudging coefficients are relatively weak and should not have an undesirably large impact on the model simulation. Only 3D analysis nudging will be performed and thermodynamic variables will not be nudged within the boundary layer. Several of the sensitivity and diagnostic simulations proposed in Section 7 are designed to better understand FDDA.

As a sensitivity test, the "ZFAC mods" will be applied to the MM5 model source code. These modifications exclude all data assimilation below a user specified level. The lowest layer to be used in this study is 850 Mbar. The ZFAC mods were developed to correct a deficiency in the MM5 model where nocturnal jets were suppressed at night because the FDDA analysis field was not able to resolve the feature. If the ZFAC mods do not degrade the bias and error statistics of the model, the mods will be used in the base configuration.

5.4 Physics Options

This section presents physics options to be used in the meteorological modeling.

5.4.1 Cumulus Parameterization

The Kain-Fritsch (1993) cumulus parameterization will be used for this application. This scheme uses a sophisticated cloud mixing scheme to determine entrainment/detrainment and removing all available buoyant energy in the relaxation time. This scheme also predicts both updraft and downdraft properties.

5.4.2 Planetary Boundary Layer Scheme

The high resolution Blackadar PBL will be used. Several studies in the past few years have focused on the impact of the PBL scheme for air quality related MM5 modeling, with no one scheme being clearly preferred. One of the proposed diagnostic and sensitivity test simulations outlined in Section 7 is designed to help address this issue.

5.4.3 Explicit Moisture Scheme

The Dudhia Simple Ice scheme will be used. The simple ice scheme predicts both cloud, rain water, and ice phases. No supercooled water is allowed and immediate melting of water above freezing is assumed.

5.4.4 Radiation Scheme

The Rapid Radiative Transfer Model (RRTM) (Mlawer et al. 1997) radiation scheme will be used. This longwave radiation scheme is a new, highly accurate, and efficient method that uses a correlated-k model to represent the effects of the detailed absorption spectrum. The model accounts for water vapor, carbon dioxide and ozone.

5.4.5 Ground Temperature Scheme

The multilayer soil temperature model will be employed. This model predicts temperature in 1, 2, 4, 8, and 16 cm. layers with fixed substrate below using the vertical diffusion equation. Thermal inertia is based on a force/restore scheme and includes vertically resolved temperature variation. This scheme allows for more rapid response of surface temperature than a simple slab model.

6 Model Performance Evaluation

The specific procedures to be used in the model performance evaluation are being prepared under Task A of this work assignment. This section presents an overview of the evaluation process.

6.1 Operational Evaluation

The *operational evaluation* refers to an assessment of the model's ability to estimate correctly the atmospheric observations whether or not the process descriptions in the model are accurate (Tesche, 1991). It is an examination of how well the model reproduces the observed meteorological fields in time and space consistent with the needs of air quality models. The operational evaluation gives little, if any, information about whether the results are correct from a scientific perspective or whether they are simply the fortuitous product of compensating errors. Therefore, a "successful" operational evaluation is a necessary but insufficient condition for achieving a sound, reliable modeling exercise.

It is difficult to identify the specific performance metrics that will be applied. The goal of Task A of this work assignment is to identify new performance tests for long-term simulation models. Metrics that have been previously applied to episodic meteorological model applications for air quality planning are presented in Table 6-1.

A challenge in evaluating large-scale models it to determine the appropriate scale for evaluation. It is very possible, even likely, to have regional performance issues masked in statistical evaluations because the signal is masked by different model behavior in other parts of the domain. In performing the model performance evaluation it is also important to understand the political environment in which the science is conducted. For these reasons the performance metrics will be conducted on a statewide basis, an RPO basis, and a national level.

6.1.1 Scientific Evaluation

The *scientific evaluation* addresses the realism of the basic meteorological processes simulated by the model. This involves testing the model as an entire system as well as its component parts. The scientific evaluation seeks to determine whether the model's behavior, in the aggregate and in its component modules, is consistent with prevailing theory, knowledge of physical processes, and observations. The main objective is to reveal the presence of bias and internal (compensating) errors in the model that, unless discovered and rectified, or at least quantified, may lead to erroneous or fundamentally incorrect policy decisions based on model usage.

The scientific evaluation ideally consists of a series of diagnostic and mechanistic tests aimed at: (a) examining the existence of compensatory errors, (b) determining the causes of failure of a flawed model, (c) stressing a model to ensure failure if indeed the model is flawed, (d) provide additional insight into model performance beyond that supplied through routine, operational evaluation procedures.

Table 6-1: Possible Statistical Measures and Graphical Displays to be Used in the MM5 Operational Evaluation.

Statistical Measure	Graphical Display
Surface Winds (m/s)	
Vector mean observed wind speed	Vector mean modeled and observed wind speeds as a function of time
Vector mean predicted wind speed	Scalar mean modeled and observed wind speeds as a function of time
Scalar mean observed wind speed	Modeled and observed mean wind directions as a function of time
Scalar mean predicted wind speed	Modeled and observed standard deviations in wind speed as a function of time
Mean observed wind direction	RMSE, $RMSE_s$, and $RMSE_u$ errors as a function of time
Mean predicted wind direction	Index of Agreement as a function of time
Standard deviation of observed wind speeds	Surface wind vector plots of modeled and observed winds every 3-hrs
Standard deviation of predicted wind speeds	Upper level wind vector plots every 3-hrs
Standard deviation of observed wind directions	
Standard deviation of predicted wind directions	
Total RMSE error in wind speeds	
Systematic RMSE error in wind speeds	
Unsystematic RMSE error in wind speeds	
Index of Agreement (I) in wind speeds	
$SKILL_E$ skill scores for surface wind speeds	
SKILLvar skill scores for surface wind speeds	

Surface Temperatures (Deg-C)	
Maximum region-wide observed surface temperature	Normalized bias in surface temperature estimates as a function of time
Maximum region-wide predicted surface temperature	Normalized error in surface temperature estimates as a function of time
Normalized bias in hourly surface temperature	Scatterplot of hourly observed and modeled surface temperatures
Mean bias in hourly surface temperature	Scatterplot of daily maximum observed and modeled surface temperatures
Normalized gross error in hourly surface temperature	Standard deviation of modeled and observed surface temperatures as a function of time
Mean gross error in hourly surface temperature	Spatial mean of hourly modeled and observed surface temperatures as a function of time
Average accuracy of daily maximum temperature estimates over all stations	Isopleths of hourly ground level temperatures every 3-hr
Variance in hourly temperature estimates	Time series of modeled and observed hourly temperatures as selected stations
Surface Mixing Ratio (G/kg)	
Maximum region-wide observed mixing ratio	Normalized bias in surface mixing ratio estimates as a function of time
Maximum region-wide predicted mixing ratio	Normalized error in surface mixing ratio estimates as a function of time
Normalized bias in hourly mixing ratio	Scatterplot of hourly observed and modeled surface mixing ratios
Mean bias in hourly mixing ratio	Scatterplot of daily maximum observed and modeled surface mixing ratios
Normalized gross error in hourly mixing ratio	Standard deviation of modeled and observed surface mixing ratios as a function of time
Mean gross error in hourly mixing ratio	Spatial mean of hourly modeled and

	observed surface mixing ratios as a function of time
Average accuracy of daily maximum mixing ratio	Isopleths of hourly ground level mixing ratios every 3-hr
Variance in hourly mixing ratio estimates	Time series of modeled and observed hourly mixing ratios at selected stations

7 Diagnostic Simulations

Determining the optimal configuration of the MM5 model for a specific application requires performing multiple experiments to identify the suite of physics and configuration options giving the "best" output fields. Unguided by diagnostic/sensitivity simulations, this effort quickly exhausts available time and resources. Our proposed approach, based on experience with both RAMS and MM5, is designed to quickly and efficiently identify a suitable model configuration.

Notwithstanding prodigious increases in processing speeds on today's computers, MM5 is still CPU-intensive. Based on our test simulations over the national grid, MM5 will take several computer weeks to simulate the full year of 2001. Thus, a concerted effort is needed to minimize the overall computational burden.

To optimize the resources available for this study, the model sensitivity testing will first focus on episodic modeling of winter and summer cases. February will be used for wintertime cases and July will be used for the summertime cases. Once the episodic simulations are complete, two annual simulations will be performed using the two episodic configurations judged by the study team and client representative to have the most promise.

Table 7-1: Proposed Episodic Sensitivity and Diagnostic Simulations.

Simulation	Period	Description	Purpose
Baseline	1-20 Feb. 2001 1-20 July 2001	Simulation with the baseline model options presented in this protocol	Provide a basis of comparison.
NNRP	1-20 Feb. 2001 1-20 July 2001	Use NCAR/NCEP Reanalysis Project (NNRP) initialization field with larger computational domain	Examine the differences in model estimation skill with different initialization datasets.
ZFAC	1-20 Feb. 2001 1-20 July 2001	Include the "ZFAC mods".	Examine the potential for nighttime jet suppression from low level FDDA.
No FDDA	1-20 Feb. 2001 1-20 July 2001	Remove all FDDA from simulation	To test that FDDA is no having an inordinately large impact on model results
High FDDA	1-20 Feb. 2001 1-20 July 2001	Double the FDDA nudging coefficient	Examine models sensitivity to the nudging coefficient
Soil Moisture	1-20 July 2001	Adjust soil moisture to reflect precipitation anomalies in 2001.	Examine impact of soil moisture parameters
Reisner Microphysics	1-20 Feb. 2001 1-20 July 2001	Use the more advanced Reisner microphysics option instead of simple ice	Examine impact on precipitation skill from more advanced moisture microphysics
Reynolds SST[1]	1-20 Feb. 2001 1-20 July 2001	Include higher resolution sea-surface temperature data	Examine the influence of coarse resolution earth skin temperature.
PBL Scheme[1]	1-20 Feb. 2001 1-20 July 2001	Employ alternative PBL scheme	Examine sensitivity of model to PBL scheme
Land Surface Model[1]	1-20 Feb. 2001 1-20 July 2001	Employ Land Surface Model	Explore ability of LSM model to improve model skill

[1]Project resources preclude this diagnostic and sensitivity simulation from being performed by the contractor team. The simulation will be performed by USEPA staff on a time available basis. It is possible that specification of the annual simulations may have to be decided before these simulations are completed.

8 Data Base and Reporting Submittal Procedures

Documents, technical memorandums, and data bases developed in this study will be submitted to the project sponsors for review and approval during the course of the modeling work.

A final technical report summarizing the entire meteorological modeling effort, including data base development, model application and model performance evaluation will be submitted to the project sponsors for review. In addition, all modeling input and output data bases and model codes used in this study will be transferred via media in the standard big-endian IEEE MM5 binary format to the project sponsors to allow for proper, independent review of the modeling assumptions, inputs, and outputs.

9 References

Baker, K., et. al. 2002: "Draft Meteorological and Photochemical Model Performance Sensitivity Project.", Lake Michigan Air Directors Consortium, Des Plaines IL.

Dudhia, J, D. Gill, Y-R Gou, K. Manning and W. Wang, 2001: PSU/NCAR Mesoscale Modeling System User's Guide (MM5 Modeling System Verion 3).

Kain, J.S. and J.M. Fritsch, 1993: Convective parameterization for mesoscale models: The Kain-Fritsch scheme. The representation of cumulus parameterization in mumerical models, K.A. Emanuel and D.J. Raymond, Eds., Amer. Meteor. Soc., 246 pp.

Mlawer, E.J., S.J. Taubman, P.D. Brown, M.J. Iacono and S.A. Clough, 1997: Radiative transfer for inhomogeneous atmosphere: RRTM, a validated correlated-k model for the longware. J. Geophys. Res., 102, 16663-16682.

Stauffer, D.R. and N.L. Seaman, 1990: Use of four-dimensional data assimilation in a limited-area mesoscale model. Part I: Experiments with synoptic data. Mon. Wea. Rev., 118, 1250-1277.

Stauffer, D.R., N.L. Seaman and F.S. Binkowski, 1991: Use of four-dimensional data assimilation in a limited-area mesoscale model. Part II: Effects of data assimilation within the planetary boundary layer. Mon. Wea. Rev., 119, 734-754.

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

Tesche, T. W., 1991. Evaluation Procedures for Using Numerical Meteorological Models as Input to Photochemical Models", 7th Joint Conference on Applications of Air Pollution Meteorology, American Meteorological Society, 14-18 January, New Orleans, LA.