

DRAFT FINAL REPORT FOR

Project: H23-2003-C2

MM5 Modeling for TexAQS 2000 with GOES Satellite Data Assimilation

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1 Introduction

The following report summarizes the activities and results for project *H23-2003-C2*, the assimilation of Geostationary Operational Environmental Satellite (GOES) data in MM5 (Pennsylvania State University/National Center for Atmospheric Research (PSU/NCAR) Mesoscale Model Version 5) at University of Alabama in Huntsville. While the utilization of GOES data has proven to be useful and demonstrates improvements in the performance of MM5, the report also points out the areas that need further attention. The study covers the period of August 23 through September 1, 2000, which coincides with Texas Air Quality Study 2000.

Some of the results from this project have been summarized in McNider et al. 2004, Biazar et al. 2004, Haines et al. 2004, and Han et al. 2004. The manuscripts will be attached as appendix to this report. In the following, after a short introduction we will proceed with a detailed description of the satellite assimilation technique used in this study. The description will detail the modifications we made to our techniques and also the addition of a new soil option in MM5 with improved numerical techniques. Then a short description of the satellite retrievals will be presented. Finally, the results from this study will be presented and will be followed by a discussion.

1.1 Scientific Background

There are two important but observationally uncertain parameters in the grid averaged surface energy budgets of mesoscale models – surface moisture availability and thermal heat capacity. Given the importance of surface heating in determination of boundary layer characteristics, the errors in the specification of these parameters have profound impact on the model predictions. We have been developing techniques (McNider et al. 1994, Lapenta et al. 1999) for assimilating Geostationary Operational Environmental Satellite (GOES) skin temperature tendencies during the mid-morning time frame to improve specification of surface moisture.

In the past surface moisture availability in models such as MM5 has been specified based on land use classification and climatological conditions or through land surface hydrology models. Use of the first technique leads to errors due to inaccuracies in relating land use types to moisture and due to deviations from climatological norms. The second technique – the use of a surface hydrological model while perhaps an improvement still requires specifications of difficult to quantify parameters such as root zone moisture, plant physiological characteristics such as root uptake, stomatal resistance, soil hydrologic conductivity, and antecedent precipitation.

Heat capacity of the surface in models such as MM5 has also been specified based on land use classification. While specification of heat capacity is relatively straight forward for single composition objects such as water, stone, concrete etc. The practical specification of heat capacity on a 4 km or 12 km grid where the surface is made up of everything from buildings, to streets, to grass, to trees to standing water is extremely

difficult. This is especially true in the highly heterogeneous urban and suburban environment.

In our techniques (discussed below) we have used satellite observations of surface skin temperature as an observational constraint to correct initial land use guesses of grid moisture availability and heat capacity. The satellite pixel radiative measurements also provide a natural averaging process needed for the grid average values in the model. In the past, satellite assimilation techniques for adjusting moisture availability have been tested in both case study modes (McNider et al. 1994, 1995) and operational modes (Lapenta et al 2000) and have shown to improve model performance. In this project, we have used satellite assimilation observational constraints, to greatly improve the characterization of the surface energy budget on fine spatial scales for the TEXAQS 2000.

1.2 Introduction to the Satellite Assimilation Technique

Early in the development of boundary layer mesoscale models (Deardorff 1978; Wetzel 1978; McCumber and Pielke 1981; Zhang and Anthes 1982) and later in global scale models (Dickinson 1984; Sellers et al. 1986) it was recognized that the correct specification and partitioning of surface fluxes were critical to the accurate characterization of boundary layer behavior. Additionally, spatial variations in surface fluxes and net radiation can lead to organized mesoscale circulations that often dominate the evolution of the regional atmospheric state affecting precipitation patterns and quantity (Koch et al. 1997; Lynn et al. 1998; Avissar and Pielke 1989; Rabin et al. 1990; Pielke et al. 1991). Additionally, the amount of radiation coming into the boundary layer and surface which is a function of cloud transmission and surface albedo is critical to boundary layer behavior and photochemical reactions.

In air quality simulations these boundary layer processes control mixing heights (impacting pollutant concentrations), temperatures (controlling thermal decomposition of PAN and other organic nitrates) and photolysis rates. Because of the importance of the surface energy budget and uncertainties in its implementation within models, we and other investigators have attempted to develop techniques to use satellite information to improve the fidelity of the land-surface models (Price 1982; Carlson et al. 1981; Wetzel et al. 1984; McNider et al. 1994; Gilles and Carlson 1995; McNider et al. 1995; Jiang and Islam 1999).

A prognostic equation for the surface skin temperature, based on the surface energy budget, can be written in the following form (Wetzel 1984; Pielke et al. 1991; Smirnova 1997),

$$C_b \left(\frac{dT_G}{dt} \right) = (R_N + H + G) + E \quad (1)$$

where dT_G/dt is the rate of change of the land surface temperature (LST), C_b the surface heat capacity, R_N is the net radiation (including incident shortwave, incoming

atmospheric longwave, and outgoing longwave), H is the sensible heat flux, G is the soil heat flux, and E is the latent heat flux.

In the actual application of such an energy budget in a regional model, either separate budgets must be developed for vegetative canopies (perhaps further decomposed into deep rooted and shallow rooted vegetation), bare soil and standing water (McCumber and Pielke 1981; Smirnova 1997). Or, a composite surface must be formed which reflects the aggregate effects of these distinct components (Wetzel et al. 1984). In this investigation we are taking the philosophy that the simpler composite approach is preferred.

This is based on three considerations:

1. For short-term weather predictions or after the fact air pollution case studies the critical partitioning of processes which allow long-term unadjusted runs that conserve water and energy are not needed. On the other hand GCM's must accurately keep track of water over many months or years of simulation; thus, it is imperative that they have detailed soil moisture models, hydrology and vegetative models.
2. The radiatively resolved pixels from satellite imaging sensors provide a natural integration consistent with a grid average composite.
3. It makes analytical manipulation and inversion of surface energy budget equations easier (see McNider et al. 1994) facilitating use of satellite data.

Previous investigators (see Carlson 1986 and Wetzel et al. 1984) have looked at a combination of a range of uncertainty in parameters affecting terms in the surface energy budget and sensitivity to this range of uncertainty. For the clear sky case, where net radiation can be adequately specified, Fig. 1 (taken from Carlson 1986) shows uncertainties in moisture availability and thermal inertia represent the largest potential errors in the behavior of the energy budget. For example, the likelihood of missing the wind speed by 10 m s^{-1} is much less than missing the specification of moisture availability and thermal inertia over the ranges shown in Fig. 1. Carlson et al. (1981) in an important early remote sensing study attempted to use two pieces of information (a polar orbiter daytime and nighttime IR measurement of temperature) to solve for moisture availability and thermal inertia. Wetzel et al. (1994) used the sensitivity to moisture availability to hypothesize that mid-morning LST tendencies could be used to infer moisture availability. We utilized a similar approach to formulate a satellite assimilation technique (McNider et al. 1994) that assigns all of the difference between a satellite (GOES) LST tendency and a model tendency to errors in the evaporative flux and subsequently inverted surface similarity relations to adjust moisture availability. This assimilation technique has been shown in case study tests and in a semi-operational environment to improve surface energy budget performance (Lapenta et al. 1999). Diak and Whipple (1995) also showed that LST tendencies from GOES could be used to estimate the partitioning of latent and sensible fluxes.

Just as Wetzel (1984) and Carlson (1986) in their sensitivity studies showed that moisture was most important in the mid-morning time frame, they also showed that LST tendencies were most sensitive to thermal inertia during the evening (Fig. 1). As part of this study, in a manner analogous to our utilization of GOES data to recover moisture

availability in the morning time frame, we have used GOES evening LST tendencies to adjust the bulk heat capacity in the surface energy budget.

1.3 Application to TexAQS2000 Period

In this project we utilized the approach taken by McNider et al. 1994 (hereafter referred to as McN94), for a case study during Texas Air Quality Study 2000 (TexAQS2000). We further refined and improved the technique for the recovery of moisture availability, and we also used the evening tendencies to recover the surface heat capacity. In the following a detailed description of the method used in this study will be offered.

2 Methodology

McN94 described a procedure that takes a practical approach towards assimilating land skin temperatures (LST) by recognizing that adjustments in this parameter must be consistent with other components of the surface energy budget. The technique requires the use of GOES derived IR LST *tendencies* and GOES derived net solar radiation over the time period of interest. It is based upon adjusting the model's bulk moisture availability so that the model's *rate of change* of LST agrees more closely with that observed from the satellite. Therefore, the simulated latent heat flux, which is highly correlated with surface moisture availability during this time period, is adjusted based upon differences between the modeled and satellite-derived LST tendencies.

Following McN94, we first define the surface energy budgets for the model and satellite as in (1) by assigning subscripts m and s to all terms, respectively. Since we are now considering a composite surface representing the characteristics of vegetation, soil etc. rather than bare soil, C_b is no longer simply a heat capacity. It is more like a combination of heat capacity and thermal transfe and as a result represents a resistance to forcing (see McN94). Next, we invoke the critical assumption that all of the terms in the model's surface energy budget are the same as for the actual energy budget observed by the satellite except for the latent energy term E . This is consistent with the ideas discussed above that we know the least about evapotranspiration and that in the mid-morning the energy budget is most sensitive to moisture availability (Wetzel et al. 1984). With this assumption we take the difference of the surface energy budgets for the model and satellite to obtain

$$E_s = C_b \left[\left(\frac{dT_G}{dt} \right)_s - \left(\frac{dT_G}{dt} \right)_m \right] + E_m \quad (2)$$

where $\left(\frac{dT_G}{dt} \right)_s$ is calculated from hourly GOES-derived LST products retrieved at model grid points.

The way in which the moisture flux is adjusted within the model is dependent upon the flux formulation used. In McN94, the surface specific humidity was analytically recovered from similarity theory using this satellite-inferred evapotranspiration (E_s). In MM5, surface specific humidity is not a prognostic variable. Therefore, we adjust what

is called the moisture availability parameter (M) which represents the *fraction* of possible evaporation for a saturated surface (equal to 1 over open water and 0 over a non-evaporating surface). The latent heat flux in the Blackadar boundary layer scheme in MM5 (Blackadar 1979; Zhang and Anthes 1982) is given by

$$E_m = \frac{M\rho(q_{sat}(T_g) - q_a)ku_*}{\ln\left(\frac{ku_*z_a}{k_a} + \frac{z_a}{z_l}\right) - \varphi_h}, \quad (3)$$

where $q_{sat}(T_g)$ is the saturation mixing ratio of the surface, q_a is the mixing ratio of the air immediately above the surface, k is the von Karman constant, u_* is the frictional velocity, z_a the height of the lowest model layer, z_l the depth of the molecular layer, k_a is a background molecular diffusivity, and φ_h is a non-dimensional stability parameter for heat and water vapor. To obtain the satellite-inferred moisture availability, we solve (3) for M using the satellite-inferred latent flux as derived from (2) and get the satellite inferred moisture availability

$$M_s = E_s \frac{\ln\left(\frac{ku_*z_a}{k_a} + \frac{z_a}{z_l}\right) - \varphi_h}{\rho ku_* (q_{sfc}(T_g) - q_a)}. \quad (4)$$

In addition to the recovery of moisture availability, the GOES derived net solar radiation is also assimilated into the models surface energy budget via direct insertion.

Carlson (1986) showed that while moisture availability was the most sensitive variable in the mid-morning time frame in the surface energy budget, heat capacity was shown to be the most sensitive parameter in the early evening.

Consider that the model bulk heat capacity (C_{bm}) may be different from what can be retrieved from satellite observations (C_{bs}). This means that use of C_{bs} in the surface energy budget (equation 1) will yield the observed skin temperature tendency. We assume that the moisture availability has been correctly specified (or surface evaporation is negligible late in the day when stomata have closed), and there is negligible difference in net radiation, sensible, latent, and soil heat fluxes. Then we can subtract the model and satellite energy budget equations and solve for C_{bs} to get:

$$C_{bs} = C_{bm} \left(\frac{dT_G}{dt} \right)_m / \left(\frac{dT_G}{dt} \right)_s \quad (5)$$

The initial value for the model C_{bm} would be determined in the normal fashion via a simple lookup table. The new C_{bs} would be subsequently used as the model value.

2.1 Nudging for Moisture Availability Adjustments

Equation (4) describes how the moisture availability can be recovered so that the model skin temperature tendency agrees with the satellite observation. However, in the implementation of this technique we encounter several problems. Basically, for this technique to be successful our assumptions must hold. That is, all the error causing a disagreement between the satellite observation and the model prediction is due to the error in the latent heat flux. Therefore if there are errors in the other terms of the equation 1, errors in the retrievals, or numerical errors, we may over-/under-adjust moisture availability. The other factor at work is the feedback that propagates in the other terms of the equation as the result of such adjustment.

A crucial component of equation (1) during the mid-morning period is the incident short-wave radiation (insolation). Insolation is the main forcing term in the equation that causes the skin temperature increase. To be consistent with the satellite observation, we must use the retrieved insolation. Since the satellite retrieved insolation is provided hourly, use of a constant insolation for one hour during the period that this forcing term is changing rapidly will introduce large errors in our computations. The assimilation technique was modified to resolve these problems. In the following a detailed description of the modifications is offered.

2.1.1 Detailed Description of Moisture Availability Adjustment

We allow

$$h = \frac{C_b}{E_m} \left[\left(\frac{dT_G}{dt} \right)_m - \left(\frac{dT_G}{dt} \right)_s \right] \quad (6)$$

represent the adjustment needed to bring the model moisture flux in agreement with the satellite inferred flux; the recovered latent heat flux (equation 2) then can be expressed as:

$$E_s = (1 + h) E_m \quad (7)$$

Now equation (4) can be expressed as:

$$M_s = E_s \frac{\ln \left(\frac{k u_* z_a}{k_a z_l} + \frac{z_a}{z_l} \right) - \varphi_h}{\rho k u_* (q_{sfc}(T_g) - q_a)} = (1 + h) M_m \quad (8)$$

Where $q_{sfc}(T_g)$ is the saturation mixing ratio of the surface, q_a is the mixing ratio of the air immediately above the surface, k is the von Karman constant, u_* is the frictional velocity, z_a the height of the lowest model layer, z_l the depth of the molecular layer, k_a is a background molecular diffusivity, and φ_h is a non-dimensional stability parameter for heat and water vapor.

As mentioned above, in addition to the recovery of moisture availability the GOES derived net solar radiation also is assimilated into the MM5 surface energy budget via direct insertion. This is critical in getting the variation in surface insolation correct and to meet the assumptions of the moisture recovery technique. In order for the insolation to be consistent with the satellite retrieved LST and also satisfy the required temporal resolution, at each model time step, the observed insolations are interpolated to the current model time.

In our case studies we found out that this method introduces a warm/dry bias in long simulations used for air quality case studies. One of the problems is that equation 1 is extremely sensitive to moisture availability changes and can become unstable. This high sensitivity/instability causes oscillation in the model LST tendency and produces large disagreements between the model and the satellite tendencies. At times the disagreement is so large that the adjustment term (h) causes the adjusted moisture availability to become negative or exceeds its upper limit, 1. In order to minimize the error and to insure that the model tendency converges to the satellite tendency, we have modified our method to constrain h by nudging the model moisture availability to its satellite inferred value. The nudging factor δ_M is expressed as:

$$\delta_M = G(\Delta t_m, \Delta t_s) H(\Delta x_m, \Delta x_s) R(M) S(h) \approx \frac{.06 h}{h^2 + 25}. \quad (9)$$

Where G is the time step nudging factor that accounts for the fact that satellite tendencies are hourly while the model tendencies are calculated at each time step ($G \sim \Delta t_m / \Delta t_s$). H accounts for higher spatial variation of GOES skin temperature retrievals ($\sim 4\text{km}$ grid) vs. the model grid resolution ($G \sim \Delta x_s / \Delta x_m$). R is the response factor adjusted based on the duration of assimilation. And S is defined as a function of h to insure that the adjustment to moisture availability is only performed when our assumptions are valid and the difference between satellite observed tendencies and that of the model are reasonable and can be ascribed to the latent heat flux term.

$$S(h) = \frac{10 h}{h^2 + 25}. \quad (10)$$

The function varies between 0 and 1 and insures that the largest adjustment only will take place when h is within a reasonable range. The factor affecting h and causing large variations in its value is the high sensitivity of the surface energy budget to radiation forcing in the mid-morning period and also to the changes in moisture availability. The function S also insures that there is minimal adjustment to M at lower values of h . This is an artificial solution to a real problem that arises from the fact that the surface heat capacity also needs to be adjusted in conjunction with the adjustment in M . Using the new adjustment term, the moisture availability is adjusted accordingly.

$$M_s = (1 + \delta)M_m \quad (11)$$

The results with the new adjustment term indicated improvements in the model results compared to the observations. Figure 2 shows the skin temperatures as observed by satellite for August 30, 2000, at 19:45 GMT. The figure also shows the skin temperatures from control simulation and the simulation with satellite assimilation at 20:00 GMT. It is obvious that the assimilation technique is making notable improvement in the skin temperatures compared to the control run. The temperatures in the western part of the domain, while showing an improvement over the control simulation, are still cooler than the satellite observations. This is due to the fact that the western part of the domain is initially dry and therefore our method of adjusting the moisture availability is not as effective as it is in the center of the domain. It should be noted that in this simulation heat capacity was not adjusted. Panel (d) in figure 2 shows the corresponding adjusted moisture availability. As it can be seen, most of the domain, with the exception of northern-northeastern part of the domain, dries out for this period. This is in agreement with the surface analysis chart for this period.

2.2 Improved Numeric and Nudging for Heat Capacity Adjustments

Equation 5 described the method used for adjusting model heat capacity for the satellite retrieved skin temperature tendencies. However, in the implementation of this technique in addition to some of the same considerations as for adjusting moisture availability, there are other factors that need to be taken into account.

In the initial implementation of this technique within MM5 we realized that we could only infer the heat capacity for the grids in which our assumptions hold. This means that the adjustments to the heat capacity is only performed for the grids where:

- 1) Both the satellite-observed tendency and the model tendency are negative.
- 2) Both model and the satellite indicate clear sky.

The reason for excluding the grids where the model predicts clouds while it is clear is the increasing importance of atmospheric longwave radiation in the evening period. This is to ensure that our assumption with respect to the radiation forcing is not violated. According to Carlson (1986) the evening period for which the largest drop in the skin temperature is most sensitive to the surface heat capacity is from 15:00 to 18:00 LST. After this period the decrease in the skin temperature is still sensitive to the heat capacity, but the decrease is not as pronounced. During the time period for the first phase (similar to mid-morning period) the surface energy budget adjusts quickly to the reduction in short-wave radiation. But toward the end of the period (18:00 LST) as the short-wave radiation diminishes, long-wave radiation become more important in the energy budget. Therefore, a discrepancy between model and observation with respect to clouds become important. To avoid inappropriate adjustment of heat capacity, we do not adjust heat capacity for the grid cells in which MM5 predicts cloud. Even by limiting the adjustment to the grids that satisfy the above constraints, the inferred heat capacities exhibited large spatial and temporal variations.

Analyzing the results we realized that we needed to take an approach similar to the moisture availability adjustment. That is to nudge the heat capacity toward the inferred value rather than forcing it so strongly. This will allow for the surface energy budget

equation to gradually approach a new balance and for the model heat capacity to converge to that of the inferred value. It also allows for a feedback caused by the adjustment to the energy budget equation.

There are several unique complexities involved in the evening period during which the adjustments are done. During the mid-morning period, shortwave radiation is the dominant forcing for surface heating, while the sensible heat flux (for our dry period) is the dominant mechanism for loss of surface heat. In the evening period, as the insolation decreases, longwave radiation becomes more important. Meaning that its frequent update becomes imperative. Also, the timing of the evening transition period from daytime boundary layer to the nocturnal boundary layer becomes an issue if we want our assumptions to hold.

We devised a nudging approach to ensure the convergence of heat capacity to its inferred value and made several simulations implementing the followings:

- 1) Nudging the heat capacity toward the hourly inferred value.
- 2) Nudging the heat capacity toward the average evening inferred value.
- 3) Choice of the evening period for adjustments (for example, 15:00-18:00 vs 15:00-21:00 local standard time).

The nudging approach allows time for model feedback and gradual convergence of the solution. The first set of simulations was less than satisfactory. Observed skin temperature tendencies (for some areas) exhibited large variations from hour to hour that was absent in the model predictions. This could be due to both cloud contamination and the fact that the insolation forcing is decreasing while the atmospheric effects on the surface become more pronounced for the evening period. Since adjusting heat capacity was more sensitive to cloud contamination in the observations than moisture availability, averaging the observed tendencies for 15:00-18:00 period produced better results. Therefore we picked the second nudging approach over the first approach.

Another issue to be addressed was the choice of the period for performing the adjustment. Carlson sensitivity study suggests that the skin temperature during the early evening period is most sensitive to the changes in heat capacity. However, in this period, the rapid reduction of solar insolation is also important and cloud contamination of satellite retrievals is of more concern. Prolonging the time window to late evening also poses other problems such as a mismatch between the observed transition time (collapse of boundary layer) and that of the model. Our sensitivity study indicated that the choice of early evening period is a better selection if several constraints are applied. An important constraint is a more rapid update of the atmospheric radiation field. This considerably increases the computational cost, but due to the importance of the longwave radiation in the evening it is unavoidable. A less costly approach is to calculate the radiation field for a longer period and then use interpolation at each model step. Due to other priorities this approach was not implemented.

Another practical limitation in our approach was that we do not have surface insolation retrievals beyond 23:45 GMT. At this time there is still considerable short wave

radiation present at the western part of the domain. Since MM5 calculated radiation field may not be consistent with the GOES retrieved values, to stop the direct insertion of the GOES radiation field after this time and to use MM5 radiation field will shock the system and will cause numerical instability. Our remedy to this problem was to allow for a smooth transition from satellite retrieved surface insolation to the MM5 calculated radiation field for the western part of the domain.

Figure 4 shows thermal capacity for standard MM5 and that of inferred from satellite observations of skin temperature. While there is no independent way of confirming these results for heat capacity, the general pattern seems to agree with the rainfall pattern for this period and partly with the landuse map. Also encouraging is that while the simulations for each domain (resolution) is independent of the others, the general pattern over the 4-km domain remains the same but with more detail in higher resolution simulations.

Since we were interested in the impact of these adjustments on reducing the model warm bias, we compared the results with NWS stations. Figure 5 shows our first attempt at comparing the new results (assim-HC) with the previous assimilation run where only moisture availability was adjusted (assim_old). It is obvious that the new results are far superior to the previous run. But we could not ascribe all of the improvement to the heat capacity adjustment, since we did not observe a dramatic change in the moisture availability field.

We had long realized that the explicit solver for the soil diffusion equation for the 5-layer soil model within the slab model is a problem. But short of writing our own code, we always dealt with it by reducing the soil time step (during the assimilation period) and increasing the computational expense. In implementing the heat capacity adjustments we had to drastically decrease the soil time step even outside the assimilation period. This apparently fixed the undetected computational error that we were getting during the day.

It seems that in the previous run, due to the computational error emanating from the explicit solver in the MM5 5-layer soil model, soil sublayer temperature inappropriately increases and causes an excessive soil heat flux to the surface layer during the night. This has been the main cause of the nighttime warming in the previous assimilation runs.

We made another simulation with only adjusting moisture availability (satellite assimilation during mid-morning period only) with decreased soil time step for the 12-km domain. The results are presented in Figure 6. While satellite assimilation simulations reduce the MM5 daytime cold bias, their prediction of the nighttime temperature is still warmer than the control.

Interestingly for the range of changes we were making to the heat capacity, model did not show much sensitivity. We attempted to reduce our lower limit for the heat capacity to allow it to approach a more sensitive value. These attempts failed again due to the poor solver within the slab model.

Therefore, we realized that the explicit solver within MM5 slab model is not adequate for our study. The warm bias in the previous assimilation runs was due to the errors originating from the solver in the 5-layer soil model. The model uses Euler's method for solving the ODE, and an explicit method for solving the PDE describing heat diffusion through soil. If the energy balance equation exhibit sensitivity to a change in temperature or a parameter in the equation, the error in the forward Euler method could be large. In our case this error was exacerbated and propagated to the soil temperatures through the explicit PDE solver. This was causing the soil sub-layer to store excessive energy and gradually release it to the surface layer over time.

A temporary solution for this problem was to force the model to take much smaller sub-time steps for the soil ODE solver. Doing this resolved the problem with the artificial warm bias that was observed in the earlier simulations. However, it was not adequate for the adjustments we were making to the heat capacity.

In MM5, the volumetric heat capacity is allowed to vary from $1.2E6$ to $3.5E6 \text{ Jm}^{-3}\text{K}^{-1}$ (equivalent to a variation of $6.6E4$ to $19E4 \text{ Jm}^{-2}\text{K}^{-1}$ for slab). When we confined our adjustments to this range of values, we could not observe much of difference between the results from assimilation simulations with and without heat capacity adjustment. Allowing the heat capacity to reach and surpass the lower limit was not successful because again the solvers in MM5 could not handle it and the model would crash.

To rectify part of the problem we introduced a new option (soil option 4) for soil option in MM5. This option is similar to the 5-layer soil model. It uses Crank-Nicolson method for solving ground heat diffusion equation. Use of a stable PDE solver has a damping effect on the error over time. Also a new method was devised to calculate the appropriate time step (soil time step) for calculating ground temperature. Now at each location soil time step is calculated based on the local ground temperature gradient. This means that if the balance of the surface heat fluxes is large, much smaller time steps will be taken to solve the ODE. We also increased the depth of the last soil layer (reservoir layer) to reduce its impact on the higher frequency changes in the upper layer's temperature.

It should be noted however, that even the above modifications are not adequate for all situations. Since the real cause of the problem is the inadequate ODE solver, a permanent solution would be a complete overhaul of the ODE solver. But the modifications above allowed us to complete the simulations for our heat capacity adjustments.

2.3 Satellite retrievals

Currently, the following remotely-sensed data products, all of which are based on Geostationary Operational Environmental Satellite (GOES) visible and infrared channels are available:

(1) Clear Sky Composite – an intermediate product used for estimation of both albedo and insolation. It consists of the minimum albedo observed at a particular time over a twenty-day period in the GOES visible band.

- (2) Infrared Cloud Mask – a cloud mask computed from the GOES 3.7 and 10.7 micron channels, using thresholding and spatial coherence to identify clouds using cloud-land differences in solar reflectance (daytime) and emissivity (nighttime).
- (3) Albedo and Insolation – computed following Gautier et al., (1980) and Diak and Gautier (1983) from GOES visible channel observations. Albedo is determined using the Clear Sky Composite, and Insolation is estimated as total insolation from direct and diffuse sources, including cloud attenuation.
- (4) Skin Temperature and Total Precipitable Water – retrieved simultaneously using a physical split window technique (Jedlovec 1987; Suggs et al. 1998) with at least two longwave window GOES channels. The technique is based on perturbation of the radiative transfer equation, using first-guess profiles of temperature and moisture from the mesoscale model forecasts and an assumed emissivity of 0.98. Retrievals can be made at model resolution, with pixel averaging of the observed radiances, or at pixel resolution.

The Infrared Measurement and Processing Group (hereafter IR Group) at the National Space Science and Technology Center performed the satellite retrievals for this study. Currently, the IR group uses GOES Product Generation System (GPGS) to provide routine real-time retrievals of skin temperature, total precipitable water, cloud top pressure, cloud albedo, surface albedo and surface insolation for the use of meteorological and air quality models [Haines et al., 2003]. As input, GPGS needs a first-guess field for its retrievals and the model grid information if the product is to be used in a grid model. For this study, the MM5 simulation that was utilized for the CMAQ runs provided the required information to GPGS and the retrievals reflected the MM5 grid cell values.

The algorithm used for the retrieval of albedo and surface insolation is the implementation of Gautier et al. (1980) method complemented by the improvements from Diak and Gautier (1983). The method uses the information from GOES Imager visible channel (.52-.72 μm) at 1-km resolution, and employs a clear and a cloudy atmosphere to explain the observed upwelling radiant energy. The model applies the effects of Rayleigh scattering, ozone absorption, water vapor absorption, cloud absorption, and cloud reflection. The effects of Rayleigh scattering are modeled after Coulson (1959) and Allen (1963) for the GOES visible band (radiant flux as viewed by the satellite) and for the bulk solar flux incident at the surface. Ozone absorption is modeled after Lacis and Hansen (1974). Water vapor absorption is assumed to be negligible in both the surface and cloud albedo calculations (explaining the observed radiance in the GOES visible band), but accounted for when applying the total solar flux in the surface insolation calculation. Water vapor absorption coefficients are obtained from Paltridge (1973), and total column water vapor is assumed to be 25 mm and adjusted for solar zenith angle. Cloud absorption is assumed to be a constant 7% of the incident flux at the top of the cloud [Diak and Gautier, 1983].

The first step in calculating cloud albedo is the retrieval of surface albedo. The surface albedo for the entire domain is calculated by using the clear-sky composite image. For the current study, a 20-day composite centered on the period of the case study was used

to generate the clear-sky composite image. The single composite image records the minimum albedo value for each pixel for a given hour. Assuming that for any given hour during the day (for the entire month) each pixel experiences clear-sky at least once, then the minimum value represents the clear-sky value for that pixel.

The model formulates the physical processes that describe the radiant energy observed at the satellite. This radiation transfer formulation can then be set equal to the radiance measured by the satellite. Since the absorption and scattering processes are estimated, the radiation equation is then solved for the only unknown (i.e., the surface albedo). This formulation also assumes that the visible channel surface albedo does not vary significantly within the time period of composite.

The insolation is calculated as the sum of solar radiation incident at the surface from both direct and diffuse sources and also includes the effect of attenuation by clouds. For the clear-sky case, the incident short-wave radiation at the surface is 1) the incident solar flux that is attenuated by Rayleigh scattering, ozone and water vapor absorption, and 2) the surface reflected flux scattered back to the surface by Rayleigh scattering. With the surface albedo known and the absorption and scattering processes estimated, the surface insolation is calculated directly.

For the cloudy-sky, the radiance observed by the satellite is assumed to be a function of the incident solar flux undergoing several processes. The satellite observed radiant energy is the sum of atmospheric backscatter, reflection of the incident solar flux from the cloud surface, backscatter within the cloud by Rayleigh scattering, and the amount of surface reflection that reaches satellite after attenuation. Since the radiance at the satellite, the surface albedo, and estimates of the scattering and absorption are known, the radiation formulation can then be solved for the cloud albedo. In practice, the algorithm calculates a surface insolation using both the clear-sky and cloudy-sky formulations for a given scene. If the cloudy-sky calculation is greater than or equal to the clear-sky value, then the clear-sky value is used and the scene is assumed clear. This is consistent with the cloud albedo being near zero for clear-sky conditions. For thick clouds, a bulk solar cloud absorption of 7% of the incident flux at the cloud top is assumed [Diak and Gautier, 1983]. Since the effect of cloud albedo dominates in the insolation calculation, uncertainties in cloud thickness have shown to produce only small effects on the surface insolation calculation. See Haines et al., 2003, for more information on the retrievals.

2.4 Model (MM5) configuration

The configuration for the control MM5 simulation was provided by John Nielsen-Gammon. This was done for consistency with other TexAQS2000 modeling studies. The control configuration use FDDA gridded nudging, Dudhia moisture scheme, Grell convective parameterization, Medium Range Forecast (MRF) PBL scheme, RRTM radiation scheme, shallow convection scheme, and 5-layer soil model. Grell cumulus parameterization has proven to be useful for smaller grid sizes (10-30 km). It tends to allow a balance between resolved scale rainfall and convective rainfall. For the assimilation runs, no FDDA nudging is used. For moisture availability adjustments the

assimilation period is between 7:00 and 10:30 AM local time. Satellite retrieved insolation is assimilated for the entire daytime period. As mentioned above, we examined different evening periods that were suitable for heat capacity adjustment. Our final simulations were configured to assimilate satellite skin temperature retrievals from 15:00 to 18:00 local time for heat capacity adjustments.

3 Results

In the following we only present our final results that show much improvement over the earlier attempts. Our attempt at implementing satellite assimilation techniques for the Texas Air Quality Study has gone through an iterative process. At each step results exhibited some improvements over the control simulation but also pointed out some of the problems that needed to be corrected. What is promising is that after each iteration the performance of the model has improved.

All the modifications we have made so far have addressed either the numerical issues or have improved our techniques. We have not made any fine-tuning to the model or its input to make the results more agreeable with the observations. This means that conceptually the current version of the model with assimilation should perform well if applied to any other domain or any other period during the summer.

The inferred moisture availability exhibits the overall drying of the surface during the period of study for the Texas-2000 study period. Compared to the control simulations the assimilation runs improve the model predictions of temperature where the control exhibits cool bias, but exacerbate the warm bias in the control run. The assimilation runs also show improvement over the control runs as the model resolution increases (since the impact of land-use inhomogeneity become more pronounced and comparable to the satellite pixel area).

3.1 Verification of results

3.1.1 Model vs. satellite retrievals

Figure 2 shows the skin temperatures as observed by satellite for August 30, 2000, at 19:45 GMT for the 36-km domain. The figure also shows the skin temperatures from control simulation and the simulation with satellite assimilation at 20:00 GMT. It is obvious that the assimilation technique is making notable improvement in the skin temperatures compared to the control run. The temperatures in the western part of the domain, while showing an improvement over the control simulation are still cooler than the satellite observations. This is due to the fact that the western part of the domain is initially dry and therefore our method of adjusting the moisture availability is not as effective as it is in the center of the domain. This feature also points out the necessity for recovering surface heat capacity. Panel (d) in figure 2 shows the corresponding adjusted

moisture availability. As it can be seen, most of the domain, with the exception of northern-northeastern part of the domain, dries out for this period. This is in agreement with the surface analysis chart for this period.

Figures 7 and 8 exhibit the scatter plots for all four domains in the study (108-, 36-, 12-, and 4-km domains). The results indicate that as MM5 grid spacing decreases in high-resolution simulations, MM5 performance in capturing the spatial/temporal variation in skin temperature degrades. In the 12- and 4-km resolution domains, there is no skill in the control MM5 simulation. On the other hand, the satellite assimilation seems to be improving the model performance in explaining some of this variation. However, the scatter in the data is still substantial. There are several factors that could be contributing to this scatter. These factors include the errors in wind fields, the non-uniformity of bias in the retrievals, surface heat capacity, and/or the limitation of our technique (where the soil is extremely dry and the model is still unable to reproduce the satellite observed tendency).

These comparisons also point out that the satellite retrievals can be used for verification of the results. While the surface stations are sparse and pose some uncertainty when they are used for model verification, the satellite retrievals offer a spatial coverage that is comparable to the model grid structure. It should also be noted that there are uncertainties associated with the retrievals that should be taken into account.

3.1.2 Model vs. NWS surface observations

After performing all the corrections (as described above), a set of simulations for 36-, 12-, and 4-km domains for the period of August 23 to September 2, 2000, were performed. These simulations included two sets of assimilation runs. One only adjusting the moisture availability during the mid-morning periods and one in which both moisture availability and heat capacity are adjusted.

Overall, adjusting heat capacity has improved model predictions of near-surface air temperature in all the domains. We have used all the available NWS stations in each domain for the analysis. In the calculation of bias we have used either level-1 or 2-M temperatures from MM5 output. However, we have to take a closer look at the 2-M temperatures and how they are being calculated within MM5. They are very sensitive to the adjustments we make to the model and exhibit a large diurnal variation that is questionable. Figure 9 shows the difference between level-1 and 2-M temperatures for each simulation. While the diurnal variation for the control simulation does not change much for the entire period of simulation, the assimilation results exhibit an increased diurnal variation with nighttime instabilities. In our previous simulations (before the improved numerics) these differences were unreasonably increasing after the first day of the simulation meaning the model was experiencing an unreasonably sharp temperature gradient in the lower layer. With the improved numerics, while the gradient has decreased (but still is high), it shows a consistency from day to day. This is another indication of the numerical stability of the new runs.

Figure 10 shows the averaged 2-m temperature bias over the 4-km domain. As evident in the figure, assimilation improves the daytime temperature predictions. The impact is more pronounced after the 2nd day into the simulation, as more grid cells experience a change in moisture availability and heat capacity. The adjustment to the heat capacity reduces the nighttime warm bias seen in the previous simulations. It also reduces the daytime warm bias and even toward the end of the simulation introduces cold bias.

For the 12-km domain overall results are similar to the 4-km simulations and the same behavior is observed. Figure 11 exhibits the bias for this domain similar to figure 10. Interestingly, for this domain the latest assimilation run (assim-hc) the diurnal variation in the bias is less pronounced. There is also a gradual transition from warm bias to cold bias. It is possible that toward the end of the simulation there is an over-adjustment of the heat capacity. Also while the results from the two assimilation runs are notably different, the vertical temperature gradients in the two simulations are consistent (contrary to the 4-km results).

Figure 12 presents 2-M temperature and specific humidity bias and Root Mean Square Error for the 36-km domain over the entire period of the simulation. In the past we had presented these quantities for the period of 15- to 22-GMT, where the assimilation produced substantial improvements. Changing the heat capacity however seems to have improved the nighttime temperatures, but has degraded the daytime predictions slightly. There are still problems closer to the domain boundaries that could be due to the boundary effects. Some of the detailed features like the warm bias in the eastern part of Oklahoma extending to the western Arkansas need further examination.

Since MM5 2-M mixing ratios were not reliable, we used level-1 values for comparison. This is to evaluate the direction of the change over the control simulation. Over Texas and central part of the domain we see some improvements both in the bias and RMSE. But the area starting from south of Illinois/east of Missouri and extending north/northwest into the south of Iowa and into the east of Nebraska has a larger dry bias than the control. It should be noted that in the control simulation while we used FDDA option, the same area exhibited dry bias. Another factor to keep in mind is that for the period of this study the domain boundary regions to the north and northeast were cloudy for most of the time. This is shown in figure 13 where the percentage of time that a grid cell was cloudy according to GOES observation is depicted.

We also made comparisons of individual station observations to the results from the grid cell containing the station. In most cases the assimilation results show improvement, but there are several stations in the 4-km domain that are problematic. This could explain the higher variation of bias in Figure 10 (4-km domain) that is absent in Figure 11 (12-km domain). The 4-km domain is a subset of 12-km domain. Therefore as the number of stations used in the 4-km domain is limited, few problematic stations exert more influence. Their influence is diminished in the average as the 12-km domain covers a larger area and contains more stations. The model prediction for some of the individual stations performs exceptionally well toward the end of the simulation period.

We have also made simulations by recycling the retrieved moisture availability and heat capacity in our efforts to find the ideal configuration for doing satellite assimilation. The results from all the simulations indicated that the period of best performance for the assimilation runs are from August 27, to August 30. Since no adjustment is performed in the presence of clouds, it is understandable that it will take few days for all the grid cells to be affected by the assimilation. But, the reason for the degradation after August 30 should be further investigated.

3.1.3 Model vs. TexAQS2000 data - impact on boundary layer height

Comparing the model predicted boundary layer (BL) heights to that of observed during TexAQS-2000 revealed that the control simulation generally was predicting a lower ceiling for the boundary layer. Some of our earlier assimilation runs (before heat capacity adjustments) performed very well with respect to predicting the BL heights. But our recent simulations show some over-prediction in this respect. This could be due to the fact that the sensible heat flux in the assimilation runs is too high and during the day it is the dominant balancing term to the insolation. Perhaps in the future, the partitioning of the flux terms need to be examined in detail.

We compared the model predictions to the observations detailed in Sneff et al. (Final report for TCEQ project F-20: Spatial and Temporal Variations in Mixing Height in Houston). Figure 14 shows the observed BL heights for the evening of August 25. Comparing the heights to the model predictions exhibited in Figure 15 shows considerable improvements over the control simulation. The control simulation greatly under-predicted the heights. The satellite assimilation performed better than the control throughout the study period. Another example is demonstrated in Figures 16 and 17. Of course this evaluation is qualitative. While the observation spans over few hours and is a collection of point measurements at different times, model predictions have been averaged for the entire period of observation. Nevertheless, the improvement over the control simulation is evident.

4 Discussion & Recommendations

In this project we implemented satellite assimilation techniques in MM5 to recover grid-scale moisture availability and heat capacity for the TexAQS-2000 modeling period of August 23 through September 1, 2000. We modified our techniques and some of the numerics within MM5 to achieve optimum model performance. The results are promising and have shown improvements over the standard use of MM5.

By moisture availability adjustment we improved the model prediction of daytime temperatures. Both skin-temperature predictions and 2-m temperature predictions show better agreement with the observations. It also improved the prediction of BL heights. By adjusting the moisture availability alone, while the daytime temperature predictions were improved, the nighttime cooling of the surface was not adequate. Recovering the heat capacity from the afternoon skin-temperature observations seems to remedy this problem and our final results (adjusting both moisture availability and bulk heat capacity) exhibited good agreement with the observation. However, heat capacity adjustment

considerably adds to the computational cost. During the time period when heat capacity is adjusted the atmospheric radiation calculation has to be performed more frequently. Also during this period many smaller soil time steps is needed to avoid numerical errors. In the final simulations, however, the BL height predictions seem to have suffered. In our final simulations the model over-predicted the BL heights in general.

The early satellite retrievals we used had lower albedo and higher insolation value for the cloudy regions. This problem was caused by the lack of correction for GOES sensor degradation in the retrievals. In our latest simulations we have used the reprocessed data which corrects for this. The correction is causing higher values for albedo products and lower values for the insolation over the cloudy regions. This could be one of the causes for faster drying of the surface, as in general less energy is reaching the surface over the entire region. Cloud contamination in the retrievals is also an issue that needs to be aware of. Therefore, on days where there are patchy sub-pixel scale clouds over the region this technique is not recommended.

While our technique is only applied to grids with clear sky, the use of it under complete clear sky is recommended. We also recommend the use of recycling with respect to the recovered heat capacities. Since the surface heat capacity does not exhibit large variations from day to day, the model can be initialized with the recovered values from a previous run. This will eliminate the high computational cost associated with the heat capacity retrieval. A recycling option has been added to MM5 for both moisture availability and heat capacity.

One area that needs more attention is the examination of the surface fluxes in these results. As a matter of fact by examining the fluxes we found out about the numerical errors propagating through ground heat flux and causing the extreme nighttime warm bias in the early results. This led to introducing a new soil option with improved numerics in MM5. We are planning a re-examination of the partitioning of the flux terms within the surface energy budget.

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APPENDIX A

FIGURES

APPENDIX B

Relevant Manuscripts