

Development of a Land Surface Model. Part I: Application in a Mesoscale Meteorological Model

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(Manuscript received 29 May 1999, in final form 1 March 2000)

ABSTRACT

Parameterization of land surface processes and consideration of surface inhomogeneities are very important to mesoscale meteorological modeling applications, especially those that provide information for air quality modeling. To provide crucial, reliable information on the diurnal evolution of the planetary boundary layer (PBL) and its dynamic characteristics, it is necessary in a mesoscale model to include a land surface parameterization that simulates the essential physics processes and is computationally efficient.

A land surface model is developed and implemented in the Fifth-Generation Pennsylvania State University–National Center for Atmospheric Research Mesoscale Model (MM5) to enable MM5 to respond to changing soil moisture and vegetation conditions. This land surface model includes explicit soil moisture, which is based on the Interactions between Soil, Biosphere, and Atmosphere model and three pathways for evaporation, including soil evaporation, canopy evaporation, and vegetative evapotranspiration. The stomatal conductance, leaf-to-canopy scaling, and surface moisture parameterizations are newly developed based on a variety of sources in the current literature. Also, a processing procedure for gridding soil and vegetation parameters and simulating seasonal growth has been developed. MM5 with the land surface model is tested and evaluated against observations and the “standard” MM5, which uses a simple surface moisture availability scheme to estimate the soil wetness and then the latent heat flux, for two cases from the First International Satellite Land Surface Climatology Project Field Experiment. The evaluation analysis focuses primarily on surface fluxes of heat and moisture, near-surface temperature, soil temperature, PBL height, and vertical temperature profiles. A subsequent article will describe extensions of this model to simulate chemical dry deposition.

1. Introduction

Realistic simulation of surface fluxes of moisture and heat is critical for modeling of planetary boundary layer (PBL) development and surface level temperature and humidity in mesoscale meteorological models. Surface latent heat fluxes are largely controlled by soil moisture and evapotranspiration. Land surface heterogeneities, such as differences in soil texture, soil wetness, and vegetation, have significant effects on formation and distribution of shallow and deep cumulus clouds (An-

thes 1984; Chen and Avissar 1994; Avissar and Liu 1996; Wetzal et al. 1996). Furthermore, accurate air quality modeling requires a meteorological model to provide reliable information on PBL height and its diurnal evolution, surface temperature, cloud coverage, and profiles of temperature, humidity, and wind (Anthes and Warner 1978). All the physical processes relevant to this information are wholly or partially dependent on surface wetness and vegetation characteristics that control the partitioning of the available net radiation into sensible and latent heat fluxes. Therefore, it is extremely important to parameterize land surface processes adequately in mesoscale meteorological models in support of air quality modeling.

The Fifth-Generation Pennsylvania State University–National Center for Atmospheric Research Mesoscale Model (MM5) (Grell et al. 1994) currently uses a simple surface moisture availability scheme to compute the relative amount of latent heat flux. The moisture availability is the ratio of actual evaporation to the potential

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evaporation from the surface. In the standard version of MM5, moisture availability is specified according to land use category and season but does not vary from hour to hour or day to day. Sensitivity experiments by Zhang and Anthes (1982) showed that changes in moisture availability can result in significant differences in the PBL parameters. For example, when the fractional moisture availability was increased from 0.0 to 0.5, the peak surface potential temperature decreased from 42° to 34°C because more of the available radiation at the ground was used for evaporation. Their results also showed that the maximum PBL height is strongly dependent on the moisture availability. Because the moisture availability in MM5 is fixed in time, the model cannot respond to changing surface moisture conditions resulting from greater or less than average precipitation. Evaluations and assessments of PBL characteristics from MM5 simulations have also shown these problems in air quality modeling applications (Pleim and Ching 1993). To improve these aspects of MM5, we have developed a more advanced land surface and PBL model that includes explicit simulation of soil moisture in two soil layers and parameterization of evapotranspiration. This model was first developed in a one-dimensional mode and tested against several field studies (Pleim and Xiu 1995), including the Wangara boundary layer experiment (Clarke et al. 1971), which took place in an arid part of Australia, and the First International Satellite Land Surface Climatology Project Field Experiment (FIFE) (Sellers et al. 1992), which took place in a moderately moist grassland. It was also implemented in the previous version (widely known as MM4) of MM5 (Xiu and Pleim 1995) and was tested against FIFE observations. The agreement between model simulations and observations encouraged us to implement this advanced land surface and PBL model in the MM5 modeling system. Because the surface fluxes of many gaseous chemicals (dry depositions) are dependent on stomatal processes in a way similar to evapotranspiration, we developed compatible techniques for modeling chemical fluxes in air quality models (Pleim et al. 1996), which will be further described in Part II of this paper.

Ever since Deardorff's (1978) pioneering work on parameterizations for both soil and vegetation, many sophisticated land surface models have been developed for climate modeling and mesoscale modeling (e.g., Dickinson et al. 1993; Xue et al. 1991; Liang et al. 1994; Mahrt and Pan 1984; Noilhan and Planton 1989; Wetzel and Boone 1995). Among these models, the Interactions between Soil, Biosphere, and Atmosphere (ISBA) model, developed by Noilhan and Planton (1989), hereinafter referred to as NP89, and then described in more detail by Jacquemin and Noilhan (1990) and Mahfouf (1991), is specifically designed for mesoscale modeling. The ISBA model requires a minimal number of input parameters for representing the land surface and surface-atmosphere exchange processes most essential to mesoscale meteorology. This land surface model has

been demonstrated in a one-dimensional version (NP89; Jacquemin and Noilhan 1990) and a three-dimensional meso- β -scale meteorological model (Bougeault et al. 1999a,b; Noilhan et al. 1991) in which results compared favorably with the Hydrological Atmospheric Pilot Experiment-Modélisation du Bilan Hydrique (HAPEX-MOBILHY) observations (André et al. 1986). In addition, the ISBA model has been compared to other simpler and more complicated models as part of the World Climate Research Programme Project for Intercomparison of Land Surface Parameterization Schemes (PILPS) (Henderson-Sellers et al. 1993, 1995). The PILPS studies have shown the ISBA model's capabilities to simulate realistically the surface energy budget with partitioning of available energy between sensible and latent heat fluxes and the water budget with partitioning of precipitation between evaporation and runoff plus drainage (Shao and Henderson-Sellers 1996; Mahfouf et al. 1996). The ISBA model is relatively computationally efficient and needs only four extra parameters [i.e., soil texture classification, leaf area index (LAI), fractional vegetative coverage, and minimum stomatal resistance] to be incorporated into a mesoscale modeling system.

Another land surface model developed specifically for mesoscale meteorological models has recently been implemented in the National Centers for Environmental Prediction (NCEP) Eta Model (Chen et al. 1996) and is implemented also in MM5. The MM5 implementation has created an opportunity for synergistic development efforts including geophysical data processing, which will be used by both land surface schemes within the MM5 system. Also, intercomparisons of different schemes within the same mesoscale model will further advance development and evaluation.

From an atmospheric modeling point of view, the most important component in the land surface model is the parameterization of surface moisture flux, which includes evaporation from bare soil and evapotranspiration through vegetation. Therefore, we have made many substantial improvements to the stomatal resistance and surface moisture parameterizations from the original ISBA model. Although our land surface modeling began with implementation of the ISBA model we now consider the land surface model described here to be a related but distinct model. Therefore, the model description in section 2 focuses on the aspects of this model that differ from ISBA and especially on developments since the description presented in Pleim and Xiu (1995). Section 3 briefly describes the processing of soil and vegetation parameters for mesoscale application. Model simulations and comparisons are presented in section 4, and conclusions are in section 5.

2. Model description

Pleim and Xiu (1995) (hereinafter referred to as PX95) and Xiu and Pleim (1995) describe the devel-

opment and initial testing of a land surface and PBL model for use in mesoscale models. Since those papers, we have continued developing this model and applied it in a modified version of MM5. The land surface model's key elements include soil moisture based on the ISBA model, surface fluxes including parameterization of vegetation, and a nonlocal closure PBL model developed by Pleim and Chang (1992). The surface model includes a two-layer soil model with a 1-cm surface layer and a 1-m root zone layer. Evaporation has three pathways: direct soil surface evaporation, vegetative evapotranspiration, and evaporation from wet canopies. Ground surface (1 cm) temperature is computed from the surface energy balance using a force-restore algorithm for heat exchange within the soil. Stomatal conductance is parameterized according to root zone soil moisture, air temperature and air humidity, photosynthetically active radiation (PAR), and several vegetation parameters such as LAI and minimum stomatal resistance. Although originally based on the ISBA model, the stomatal and canopy parameterizations are almost entirely new. New features include a canopy shelter factor to account for shading within denser canopies, new stomatal functions with respect to environmental parameters, and inclusion of a data assimilation scheme similar to the technique described by Bouttier et al. (1993). A simple parameterization for describing seasonal growth of vegetation, including leaf-out of deciduous trees, has also been developed and tested. The data assimilation scheme and seasonal vegetation model will be described in detail in Part II.

a. Land surface model

The land surface model is based on a set of five partial differential equations for prognostic integration of soil temperature in two layers, soil moisture in two layers, and canopy liquid water as shown in PX95. Local changes in soil surface temperature result from the residual of the surface energy balance among net radiation (R_n), surface heat flux (H), latent heat flux (LE), and soil heat flux, which is parameterized as a restoring force back toward the deep soil temperature with a time constant of 1 day. The only difference from Eqs. (2)–(5) as presented in PX95 is in the expression for deep soil temperature T_2 where the timescale of variation τ is defined as 10 days rather than 1 day. This definition eliminates the diurnal signal from T_2 but allows longer-term changes including seasonal and synoptic variations. This scheme also differs from the standard MM5 (MM5STD) model for which the deep soil temperature is initialized as the diurnal average of the previous day of simulation and then is held constant for the duration of the run. The new model has the capability of continuous simulation of soil temperature and moisture across a series of runs. Seasonal evaluation runs of the deciduous leaf-out algorithm, which is based on T_2 ,

show that the model simulates seasonal trends in deep soil temperature well (to be shown in Part II).

The soil model is essentially unchanged from ISBA as described by NP89. Soil moisture coefficients used in the prognostic soil moisture equations are formulated in terms of basic soil parameters, such as field capacity (w_{fc}), wilting point (w_{wlt}), saturation (w_{sat}), and various other thermal and hydraulic properties of the soil as described in the appendix of Jacquemin and Noilhan (1990). All soil properties are specified according to the 11 soil types of the U.S. Department of Agriculture (USDA) soil textural classification (Clapp and Hornberger 1978). Therefore, the only soil data required for this model are the soil texture types. In our version the prognostic equations are integrated using a semi-implicit Crank–Nicolson technique.

The most important part of the land surface model in terms of its capability to simulate realistically the partitioning of sensible and latent heat fluxes is the parameterization of evaporation. Evaporation is computed using an electrical analog ($I = V/R$) such that evaporative flux E is analogous to electrical current I , humidity differences Δq are analogous to potential differences or voltage V , and the combined coefficients represent conductance, or inverse of resistance ($E = \Delta q/R$). The total evaporation is the sum of evaporation from the soil (E_g), wet canopies (E_r), and evapotranspiration (E_{tr}):

$$E_g = \rho_a(1 - \text{veg}) \frac{\beta}{R_a + R_{bw}} [q_{sat}(T_s) - q_a], \quad (1)$$

$$E_r = \rho_a \text{veg} \frac{\delta}{R_a + R_{bw}} [q_{sat}(T_s) - q_a], \quad \text{and} \quad (2)$$

$$E_{tr} = \rho_a \text{veg} \frac{1 - \delta}{R_a + R_{bw} + R_c} [q_{sat}(T_s) - q_a], \quad (3)$$

where ρ_a is air density, veg is the fractional area covered by vegetation, β is the availability factor of water from wet soil, R_a is the aerodynamic resistance, R_{bw} is the quasi-laminar boundary layer resistance for water vapor, R_c is the canopy resistance, $q_{sat}(T_s)$ is the saturated mixing ratio at the soil surface temperature T_s , q_a is the atmospheric mixing ratio in the lowest model layer, and δ is the fraction of leaf area that is covered with water. An important difference from the equations presented in NP89 and Jacquemin and Noilhan (1990) is the use of the β factor in Eq. (1) to account for soil moisture availability rather than the previously used α factor. For both approaches the factor ranges from 0 to 1 as surface soil moisture varies from zero to field capacity. The difference is that the β factor multiplies the mixing ratio deficit ($q_{sat} - q_a$) and the α factor multiplies the surface saturation mixing ratio q_{sat} . Mahfouf and Noilhan (1991) showed that, with silty clay loam soil, the α methods and β methods are comparable during the daytime but different at night. However, when we implemented the original ISBA model, which uses the α method, in MM5, the surface soil moisture had a tendency to os-

cillate during the daytime in the more arid regions of the modeling domain. This is because when soil is very dry, especially with sandy soil in desert areas, the difference ($\alpha q_{\text{sat}} - q_a$) can become negative when α is very small, thereby resulting in a negative (downward) E_g . Small increases in soil moisture can then cause α to increase enough to reverse the flux, resulting in oscillations. While this phenomenon may be realistic, where the soil is so dry that it essentially removes moisture from the air, the oscillations caused by the α form of the evaporation equation are clearly unrealistic and undesirable. Therefore, we considered the β method in which the sign of E_g does not depend on the magnitude of the soil moisture. Lee and Pielke (1992) and Ye and Pielke (1993) studied the many methods used to parameterize evaporation from bare soil. Their analysis indicates that the α method always overestimates daytime evaporation where the soil is subsaturated and the β method provides a good estimate of daytime evaporation but could be significantly inaccurate at night, particularly where soil is dry. After carefully evaluating those methods, we chose to adopt the Lee and Pielke (1992) β formulation:

$$\beta = \frac{1}{4} \left[1 - \cos \left(\frac{w_g}{w_{\text{fc}}} \pi \right) \right]^2, \quad (4)$$

where $\beta = 1$ when $w_g = w_{\text{fc}}$, and w_{fc} is the soil field capacity. We chose it as much for its better numerical behavior as for its greater daytime accuracy.

The aerodynamic resistance R_a is computed assuming similarity with heat flux such that

$$R_a = \frac{1}{ku_*} \left(\ln \frac{z_1}{z_0} + \psi_h \right), \quad (5)$$

where z_1 is the height of model layer 1, z_0 is the roughness length, u_* is surface friction velocity, and k is the von Kármán constant. The stability function ψ_h is estimated as in the Blackadar high-resolution PBL model in the MM5 system (Grell et al. 1994). The quasi-laminar boundary layer resistance for either heat or water vapor is defined as $R_b = (5/u_*) \text{Sc}^{2/3}$, where the Schmidt number Sc for heat is the kinematic viscosity of air γ divided by the molecular thermal diffusivity (γ_θ). Similarly, for water vapor, $\text{Sc} = \gamma/D_w$, where D_w is the molecular diffusivity of water vapor.

In highly vegetated areas, surface moisture flux is generally dominated by evapotranspiration E_{tr} . The key parameter for realistic simulation of evapotranspiration is the canopy resistance R_c . Most parameterizations of canopy resistance have two parts: the leaf-based stomatal resistance R_{st} and the aggregation of leaf resistance to bulk canopy resistance. In both of these we have made substantial changes from the original ISBA model. Canopy resistance is

$$R_c = \frac{P_s}{\text{LAI}} R_{\text{st}} \quad (6)$$

and stomatal resistance is

$$R_{\text{st}} = \frac{R_{\text{stmin}}}{F_1(\text{PAR})F_2(w_2)F_3(\text{RH}_s)F_4(T_a)}, \quad (7)$$

where RH_s is the relative humidity at the leaf surface and T_a is the temperature in the lowest model layer. Equation (6) represents the aggregate effect of all leaves on the total canopy resistance to evapotranspiration. From a strictly areal point of view, the ratio of R_{st}/R_c should be equal to LAI, as in the ISBA model. However, many experiments have shown that this ratio is usually less than LAI because of the effects of some leaves shading other leaves in dense canopies (Saugier and Katerji 1991; Rochette et al. 1991; Kelliher et al. 1995). Therefore it is useful to define a shelter factor as $P_s = \text{LAI}/(R_{\text{st}}/R_c)$ to account for the diminishing effect of increased leaf area in dense canopies. Mascart et al. (1991) suggest a function for the shelter factor of $P_s = 0.3\text{LAI} + 1.2$. However, we have applied $P_s = 0.3\text{LAI} + 0.7$ so that $P_s = 1$ at $\text{LAI} = 1$. Figure 1 shows our shelter factor as a function of LAI along with shelter factors derived from several measurement studies. Note that the few measurements of this sort that are available do not collapse very well to a simple function of LAI even for the same species.

A possible alternative to using LAI to estimate the relationship between stomatal and canopy conductance is to use remote sensing data such as the normalized difference vegetation index (NDVI), which can be derived directly from satellite data. This idea is attractive for two reasons: 1) NDVI accounts for the shading effects in dense canopies better than LAI does with an empirical shelter factor because NDVI is derived from a “bird’s-eye” view of the canopy; and 2) NDVI gives a realistic estimate of seasonal changes in vegetative cover, thereby obviating the need for seasonal vegetation parameterizations. The main difficulty, however, is calibration of the scaling functions of NDVI by plant species. Much work is being done to define the relationships between NDVI and LAI for many vegetation types (e.g., Gao and Wesely 1995; Gao 1995). However, using NDVI to define LAI exploits only the second of the benefits described above. Therefore, we have future ambitions to define R_c/R_{st} directly from NDVI since this seems to be a much stronger relationship and LAI is not needed at all.

Leaf-scale stomatal resistance R_{st} , computed as in Eq. (7), depends on four stress functions (F_1 – F_4) of environmental factors that influence stomatal function, and the minimum stomatal resistance (R_{stmin}), which depends on vegetative species. The minimum stomatal resistance is a bulk parameter that reflects the maximum conductance of a leaf per unit area under unstressed conditions (well watered, full sunlight, and optimal temperature and humidity). This parameter is specified in

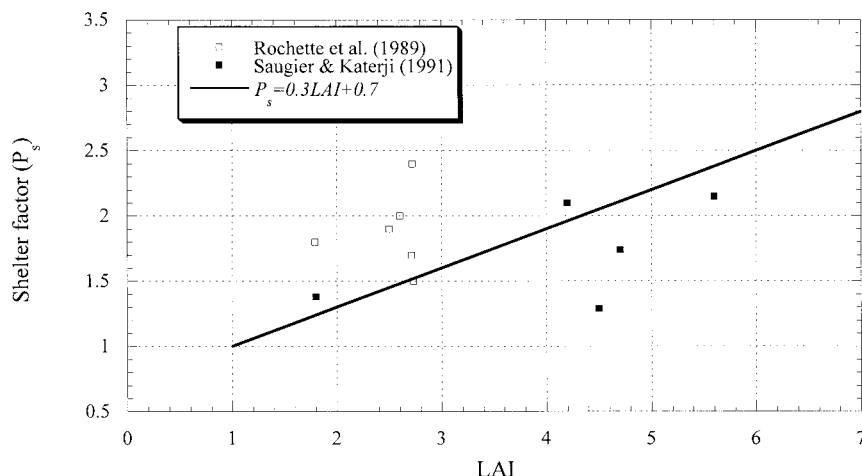


FIG. 1. Shelter factor $P_s = LAI/(R_s/R_c)$. The open squares are for maize (Rochette et al. 1989) and filled squares are for various crops and trees (Saugier and Katerji 1991). The line is the P_s suggested in this paper.

the land surface model according to vegetation type as described in section 3b.

The keys to the model's ability to simulate transpiration in real-world conditions are the four environmental stress functions [F_1 – F_4 in Eq. (7)]. It has been realized that realistic parameterizations of these functions are crucial in the transpiration calculation, especially in reducing overestimation (underestimation) of evaporation during wet (dry) periods (Chen et al. 1996). Therefore, all four functions have been updated from NP89 both to smooth their effects and to give better results. The radiative stress function is

$$F_1 = \frac{1 + f}{f + R_{stmin}/R_{stmax}}, \quad (8)$$

with

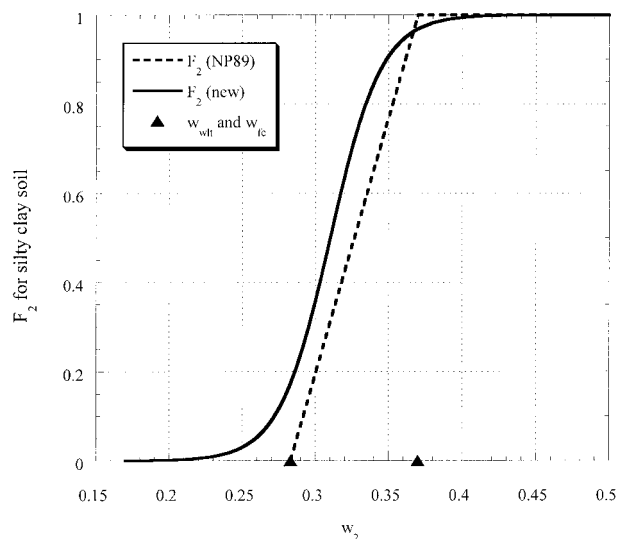


FIG. 2. Stress function F_2 as a function of w_2 for silty clay soil.

$$f = 0.55 \frac{2R_G}{R_{GL}},$$

where R_{stmax} is maximum stomatal resistance, which is an arbitrarily large number (5000 s m^{-1}); R_G is solar radiation at the surface, and the 0.55 factor is an approximation for the photosynthetically active portion; and R_{GL} is a limit value of 30 W m^{-2} for forest and 100 W m^{-2} for crops according to NP89. The only difference from the F_1 in NP89 is that the dependence on LAI has been removed because the effects of leaf shading within the canopy are now accounted for by the shelter factor P_s . Therefore, the F_1 defined here represents the effects of sunlight on an individual leaf rather than the integrated effect on a canopy.

The functions of root-zone soil moisture and air temperature (F_2 and F_4) were modified to follow the form of logistic curves as suggested by Avissar et al. (1985). Logistic curves are S shaped and therefore good for representing a smooth transition from one state to another. Also, logistic curves can be defined with varying degrees of abruptness, from an almost linear transition to an almost threshold behavior, which can be altered while maintaining differentiability. The function of root-zone soil moisture is

$$F_2 = 1/\{1 + \exp[-5.0(w_{af} - b_w)]\}, \quad (9)$$

where the available soil moisture fraction is

$$w_{af} = \frac{w_2 - w_{wlt}}{w_{fc} - w_{wlt}},$$

and the half point of the function (where $F_2 = 0.5$) is

$$b_w = (w_{fc} - w_{wlt})/3 + w_{wlt},$$

where w_{wlt} is the wilting point. Figure 2 shows the new F_2 and the one from NP89 as a function of w_2 for silty clay soil.

In many previous land surface models, including NP89, Jacquemin and Noilhan (1990), Wetzal and Chang (1987), Mihailovic et al. (1993), Sellers et al. (1986), and Avissar et al. (1985), the function of air humidity, F_3 , is expressed in terms of vapor pressure deficit (vpd) between the inside of the leaf, assumed to be saturated (vapor pressure e_s) at leaf temperature, and ambient air humidity (vapor pressure e_a) [$\text{vpd} = e_s(T_s) - e_a$]. Meanwhile, recent advances in plant physiology research have led to a new generation of stomatal models based on leaf photosynthesis (Sellers et al. 1997) in which stomatal conductance ($g_{st} = 1/R_{st}$) is directly related to the carbon dioxide assimilation rate. These models often represent stomatal dependence on humidity as a linear function of RH_s (Ball et al. 1987; Collatz et al. 1991):

$$g_{st} = g'_{st} \text{RH}_s + g_{st \min} \quad (10)$$

where g'_{st} is the stomatal conductance at $\text{RH}_s = 1$, and $g_{st \min}$ is the minimum stomatal conductance at $\text{RH}_s = 0$. Clearly, it makes more sense that stomata react to the humidity at the surface of the leaf rather than the ambient air humidity at some height above the canopy. Although a physical mechanism for this linear relationship to leaf surface relative humidity has not been determined, experimental data show it to be a very good fit (Ball et al. 1987). Recently, however, analyses of other laboratory experiments indicate that a linear relationship between stomatal conductance g_{st} and evapotranspiration E_{tr} best fits the data (Mott and Parkhurst 1991; Leuning 1995; Monteith 1995). Pleim (1999) has analyzed the stomatal response of these different humidity functions to changes in ambient humidity, temperature, and aerodynamic resistance, and concluded that for application in a mesoscale meteorological model, using an empirical model of stomatal conductance, the leaf surface relative humidity function is most suitable.

Because leaf surface relative humidity is not an easily measured or modeled quantity, it must be computed from other parameters. According to the electrical analog, the humidity at the leaf surface q_l is an intermediate potential between the ambient air humidity q_a and the leaf interior humidity $q_s(T_s)$. With an assumption of constant flux from the ambient air to the leaf interior, the relative humidity at the leaf surface [$\text{RH}_s = q_l/q_s(T_s)$] can be represented as

$$\text{RH}_s = \frac{q_a g_a + q_s g_{st}}{(g_{st} + g_a) q_s}, \quad (11)$$

where g_a is the air conductance [$1/(R_a + R_b)$], and q_s is shorthand for $q_s(T_s)$. If we assume that $g_{st \min}$ in Eq. (10) is small in comparison with g_{st} , which will be true in all but the driest conditions, and that g'_{st} is the result of Eq. (7) without the effect of humidity ($g'_{st} = F_3/R_{st}$), then RH_s is the solution of a quadratic equation that can be computed, once all the other components of Eq. (7) have been determined. In this land surface model, F_3 is

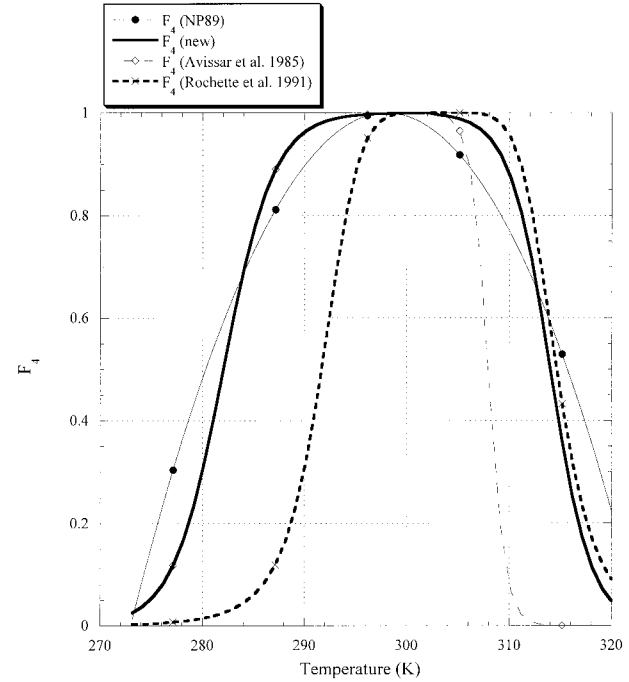


FIG. 3. Stress function F_4 as a function of temperature (K).

equal to RH_s but with a minimum imposed at 0.25 as suggested in Jacquemin and Noilhan (1990).

The fourth environmental stress function is related to ambient temperature. Again, we deviated from the NP89 formulation, which used a quadratic function peaking at the optimal temperature of 298 K. Instead, we followed the method of Avissar et al. (1985), which results in a function with a plateau over a range of optimal temperatures. The idea is that temperature inhibits stomatal function only at extremes of heat or cold. Here, F_4 is defined as

$$F_4 = 1/\{1 + \exp[a_T(T_a - b_T)]\}, \quad (12)$$

where $a_T = -0.41$ and $b_T = 282.05$ for $T_a < 302.15$ K, and $a_T = 1.18$ and $b_T = 314$ for $T_a > 302.15$ K. Note that the high side of the function extends into higher temperatures than those suggested by Avissar et al. (1985), who used $b_T = 307.95$. The current function is very similar to the function used by Rochette et al. (1991) and is close to the high side of the NP89 F_4 function. Figure 3 illustrates F_4 as a function of air temperature as defined in Eq. (12) and from the literature (NP89; Avissar et al. 1985; Rochette et al. 1991).

b. The data assimilation scheme for soil moisture and temperature

The new land surface model includes an indirect data assimilation scheme similar to the technique described by Bouttier et al. (1993). The assimilation scheme uses the errors in the modeled values of temperature and relative humidity for the lowest model layer as com-

pared with gridded analyses of surface-based observations. These errors are used to nudge root-zone and upper-layer soil moisture. The concept is that errors in low-level temperature and humidity may be due to erroneous partitioning of latent and sensible heat surface fluxes, which, in turn, may be caused by unrealistic soil moisture conditions. We recognize that soil moisture, while critically important to surface exchange processes, is very difficult to initialize accurately and is very crudely modeled. Therefore, it is an obvious target for dynamic adjustment, but not by direct 4D data assimilation (4DDA), given that widespread operational measurements of soil moisture are not available. Indirect nudging depends on strong coupling between near-surface temperature and humidity, and soil moisture through evaporation and evapotranspiration. Thus, nudging coefficients must be carefully prescribed to act only when and where this coupling is strong so that soil moisture nudging is not employed when model errors have other causes. Bouttier et al. (1993) used statistical analyses of a 1D model to derive assimilation coefficients. However, we reason that statistical analyses of the behavior of a deterministic model should not be necessary. Therefore, we prescribe assimilation coefficients as functions of model parameters such as solar insolation, air temperature, leaf area, soil texture, vegetation coverage, and aerodynamic resistance, in order to nudge most strongly when surface–atmosphere coupling is greatest.

This assimilation technique is far from flawless since it may cause changes in soil moisture when atmospheric errors have nothing to do with surface fluxes. Therefore, the magnitude of the assimilation coefficients is small compared to physical forcings and takes several days to produce a significant change in soil moisture. Thus, short-term errors due to unrelated phenomena, such as mistiming of frontal passages or erroneous predictions of cloud cover, have minimal impact on soil moisture adjustment. The details of this scheme and evaluation of its performance will be presented in Part II.

c. PBL model

The PBL model, based on the Asymmetric Convective Model (ACM) developed by Pleim and Chang (1992), is coupled with the land surface model through heat fluxes and other surface variables. The PBL height is calculated using the bulk Richardson number as suggested by Holtslag et al. (1990) and described in PX95. When the Blackadar PBL scheme is used, MM5STD calculates PBL height only under convective conditions, when Blackadar's convective PBL scheme (Blackadar 1978) defines the top of the PBL as the limit of free convection plus a 20% buoyancy overshoot (Grell et al. 1994; Zhang and Anthes 1982). Even though ACM is used here as the PBL model, the land surface model could be coupled with any other PBL model available in the MM5 system, such as the Blackadar PBL scheme (Blackadar 1976, 1978, 1979; Zhang and Anthes 1982),

the Medium Range Forecast model scheme (Hong and Pan 1996), and the Burk–Thompson turbulent kinetic energy scheme (Burk and Thompson 1989).

3. Soil and vegetation parameters

There are several soil and vegetation parameters needed to run the land surface model in MM5. Among them, the essential parameters are soil type, leaf area index, minimum stomatal resistance, and vegetation coverage. In this section, we describe the data sources and the methodology used to aggregate these data into MM5 grids.

a. Soil parameters

Currently the soil texture data are based on the conterminous U.S. 1-km soil texture datasets for the area within the lower 48 states in the United States, and the Digital Soil Map of the World for other areas. The base datasets are the USDA State Soil Geographic Database, and the soil maps are generated from detailed soil survey data. The conterminous U.S. 1-km soil texture datasets are in the public domain (Miller and White 1998) and at the time of writing their information can be found at <http://EarthInteractions.org/>. The data contain soil texture type according to the USDA soil textural classification (Clapp and Hornberger 1978) in 11 vertical layers. For the current model, the data from layer 5 (30–40-cm depth) were chosen to be representative of root-zone soil texture. The Digital Soil Map of the World is generated by the Food and Agriculture Organization of the United Nations Educational, Scientific, and Culture Organization. This dataset has three textural classes (coarse, medium, and fine) for map unit polygons of approximately 1° resolution, which we translate into the USDA soil texture classification. Soil texture-related parameters such as saturation w_{sat} , field capacity w_{fc} , and wilting point w_{wit} are defined according to the USDA classification following the ISBA model (Jacquemin and Noilhan 1990).

b. Vegetation parameters

We derived land use-related parameters from the North American Land Cover Characteristics Database available from the U.S. Geological Survey (USGS), which is based on 1-km Advanced Very High Resolution Radiometer data spanning April 1992–March 1993. These data are available in several thematic classification schemes from which we selected the USGS Land Use–Land Cover (LULC) System (Anderson et al. 1976), often referred to as Anderson level 2, which is composed of 24 vegetation/land use types. This dataset has better resolution and more detailed land use categories than the one used in MM5 (appendix 4 of Grell et al. 1994). The 1-km USGS LULC data were aggregated to the 36-km MM5 grid (described in section 4)

TABLE 1. Land use-related parameters as specified for 25 vegetation/land use types.

Land use name	$R_{\text{st min}}$ (s m^{-1})	z_0 (cm)	Mxfr (%)	Mnfr (%)	MxLA	MnLA
Urban or built-up land	150.0	50.0	40.0	20.0	2.0	0.5
Dryland cropland and pasture	70.0	10.0	95.0	15.0	3.0	0.5
Irrigated cropland and pasture	60.0	10.0	95.0	10.0	3.0	0.5
Mixed cropland and pasture	70.0	10.0	95.0	15.0	3.0	0.5
Grassland/cropland mosaic	80.0	10.0	95.0	35.0	2.5	1.0
Woodland/cropland mosaic	180.0	40.0	95.0	40.0	4.0	1.5
Grassland	83.0	10.0	95.0	70.0	2.0	1.0
Shrubland	200.0	20.0	70.0	50.0	3.0	1.0
Mixed shrubland/grassland	150.0	20.0	85.0	60.0	3.0	1.0
Savanna	120.0	20.0	80.0	60.0	2.0	1.0
Broadleaf deciduous forest	200.0	50.0	95.0	50.0	5.0	1.0
Evergreen coniferous	175.0	50.0	90.0	80.0	6.0	4.0
Mixed forest	200.0	50.0	95.0	60.0	5.0	2.0
Deciduous/coniferous forest	175.0	50.0	95.0	50.0	5.0	1.0
Evergreen broadleaf forest	120.0	40.0	95.0	85.0	5.0	4.0
Water	9999.0	0.01	00.0	00.0	0.0	0.0
Herbaceous wetland	164.0	15.0	60.0	40.0	2.0	1.0
Forested wetlands	200.0	45.0	90.0	80.0	5.0	3.0
Barren or sparsely vegetated	100.0	5.0	10.0	5.0	0.5	0.2
Herbaceous tundra	150.0	10.0	20.0	10.0	1.0	0.5
Bare ground tundra	100.0	5.0	5.0	2.0	0.1	0.1
Wet tundra	100.0	5.0	10.0	5.0	1.0	0.5
Mixed tundra	150.0	5.0	20.0	5.0	1.0	0.5
Perennial snowfields or glaciers	300.0	5.0	5.0	2.0	0.1	0.1
Southern pine	154.0	50.0	95.0	85.0	3.0	2.5

while retaining the fractional coverage of each vegetation/land use type. Gridcell values of each parameter were then computed using appropriately weighted aggregation techniques. LAI and vegetation coverage are linearly averaged, roughness length is logarithmically averaged, and minimum stomatal resistance is inversely averaged weighted by LAI. In addition to the 24 Anderson level-2 categories, we have added a customized category for the southeastern United States to account for southern pine trees. Wherever the Evergreen Coniferous category occurs south of 38°N latitude, it is reclassified as Southern Pine, because the pine trees in the southeastern states, such as loblolly pine, have very different characteristics from the spruce and fir trees of the boreal forest in the north. In particular, LAI is considerably lower for southern pines.

Table 1 shows the values of six land use-related parameters specified for each of the 25 vegetation/land use types in our land surface model: minimum stomatal resistance $R_{\text{st min}}$, roughness length z_0 , maximum vegetation fraction Mxfr, minimum vegetation fraction Mnfr, maximum LAI MxLA, and minimum LAI MnLA. Estimates of minimum stomatal resistance were made through review of published studies, including Körner (1994), Saugier and Katerji (1991), Hunt et al. (1991), Kelliher et al. (1995), Rochette et al. (1991), Turner (1991), and Körner et al. (1979). Because the vegetation classes are general, we estimated minimum stomatal resistance primarily as combinations of the values for broadleaf woody plants, coniferous woody plants, agricultural plants, and grasses. In this table, number 9999.0 means no data. The maximum and minimum LAI and vegetation fraction values are used as the limits of

the seasonal range of these parameters. A detailed description and evaluation of the seasonal vegetation algorithms will be presented in Part II.

4. Model simulation and results

The modified version of MM5 including the land surface model (referred to as MM5PX in the text and plots hereinafter) was applied to the FIFE field study, which is summarized by Sellers et al. (1988, 1992). The field study was conducted near Manhattan, Kansas, covering a 15 km $\times$ 15 km area of mainly tall grass prairie. This extensive observation program involved satellite, meteorological, biophysical, and hydrological measurements during the growing seasons of 1987 and 1989. We revisited the 11 July 1987 case and the 6 June 1987 case that were simulated using the one-dimensional prototype of the land surface model (PX95). For these studies we ran the three-dimensional model for two 12-day periods leading up to 11 July and 6 June. For the July case, the weather was gradually clearing in the FIFE area during the period of comparison, from rain on 7 July to dry but partly cloudy sky on 9 July to mostly clear sky on 11 July, until late afternoon [1600 local time (LT)] when significant cloud cover developed. It was very windy during the daytime for these three days at the surface and aloft, with surface wind around 10 m s⁻¹ and low-level wind speed up to 20 m s⁻¹. For the June case, the weather was cloudless during the daytime for the last three days (4–6 June 1987) of the simulation. The winds were more moderate than the July case at about 10–12 m s⁻¹ from the south in the PBL.

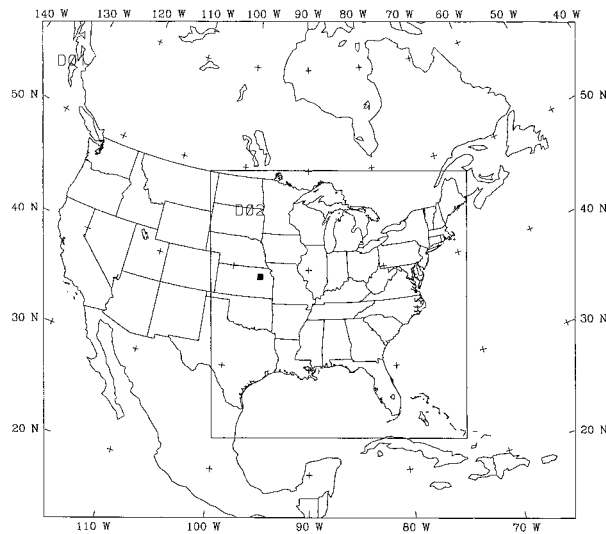


FIG. 4. Simulation domains with the coarse domain (D01) at 108-km grid spacing and the nested domain (D02) at 36-km grid spacing. The grid point at 39.00°N, 96.35°W is marked as a black square.

a. Model configuration

The MM5PX model was run in nonhydrostatic mode with 30 vertical layers up to 100 hPa using a terrain following sigma- p coordinate system on a Lambert conformal map projection. A one-way nesting technique was applied so that a coarse domain with horizontal resolution of 108 km was used to provide hourly boundary conditions for a nested fine domain with a horizontal resolution of 36 km. Both domains are shown in Fig. 4; however, we mainly analyze the model results from the nested domain (D02) with 36-km horizontal grid spacing. By using the data assimilation scheme for soil moisture, the initialization of soil moisture at the beginning of the modeling period is not very critical if the model is run for a long enough period to allow the soil hydrological mechanism to adjust to precipitation and other environmental conditions. Therefore, the model was run in three 5-day sections overlapping by 12 h for initialization from 0000 UTC 28 June to 0000 UTC 12 July 1987 and from 0000 UTC 24 May to 0000 UTC 7 June 1987. Soil temperature and soil moisture in both layers (top 1 cm and 1 m) were initialized in each section from the previous run to provide a continuous simulation of these parameters. At the start of the first 5-day run, soil moisture was initialized according to climatological rainfall patterns while accounting for

soil texture. In addition to the soil moisture assimilation scheme, an analysis-nudging 4DDA scheme (Stauffer and Seaman 1990) was used throughout the simulation for winds at all levels, and for temperature and humidity above the PBL (Stauffer et al. 1991). The Anthes–Kuo convective parameterization scheme (Anthes 1977) was used at the 108-km grid spacing, and the Kain–Fritsch scheme (Kain and Fritsch 1990, 1993) was used at 36-km spacing. Resolved-scale mixed-phase microphysics was enabled on both grids.

For comparison, we also ran MM5STD for the same period and domains with the same FDDA and physics options as in the MM5PX model, except for the land surface and PBL schemes. In MM5STD, the land surface process is parameterized with a simple scheme using the moisture availability (Grell et al. 1994), and Blackadar's PBL model is used.

The analysis and evaluation of the model outputs focus on surface and PBL parameters that are critical for air quality applications. The surface fluxes, PBL height, surface air temperature, and temperature profiles are examined for the last three days (0000 UTC 9–0000 UTC 12 July 1987 and 0000 UTC 4–0000 UTC 7 June 1987) of both simulation periods. The observation data are from one specific FIFE site that includes collocated Automatic Meteorological Stations site 11, eddy flux site 16, and Bowen ratio site 18. The mesoscale model results are retrieved from the MM5 grid point at 39.00°N, 96.35°W, where most FIFE observation sites are located. One point worth mentioning here is that no special treatment was applied to the soil and vegetation properties at this grid cell except the generic methodologies described in section 3. This will demonstrate the accuracy and generality of the modeling methodologies as applied to the whole domain. Table 2 shows several important soil and vegetation parameters used for the one-dimensional (PX95) and the three-dimensional simulations. The data used in the one-dimensional simulations are based on observations (all the relevant references were listed in PX95) but are suitable only for the 15 km $\times$ 15 km area where the field study took place. The data for the three-dimensional simulations were processed with the generic methodologies described in section 3 and are for the 36 km $\times$ 36 km grid cell surrounding the FIFE sites. The most significant difference between the 1D and 3D models is the value of the minimum stomatal resistance $R_{st\ min}$. For the 1D model we followed the ISBA's approach in which $R_{st\ min} = 40\ s\ m^{-1}$ is used for grassland, but for the 3D model the $R_{st\ min}$ is a gridcell

TABLE 2. Soil and vegetation parameters used for the one-dimensional (PX95) and the three-dimensional simulations of the FIFE field study.

Case	Model type	Soil type	LAI	veg (%)	$R_{st\ min}$	z_0 (cm)
Jul 1987	1D model	Silty clay loam	2.8	99	40	6.5
	3D model	Silty clay	2.46	94.7	82	10.7
Jun 1987	1D model	Silty clay loam	1.9	99	40	4.5
	3D model	Silty clay	2.10	91.7	82	8.7

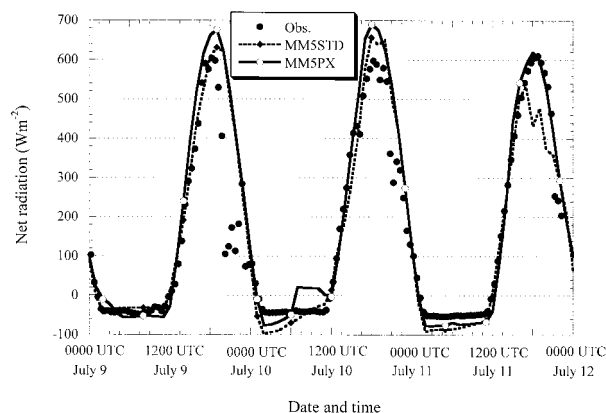


FIG. 5. Observed and modeled net radiation for the 3-day period from 0000 UTC 9 to 0000 UTC 12 Jul 1987.

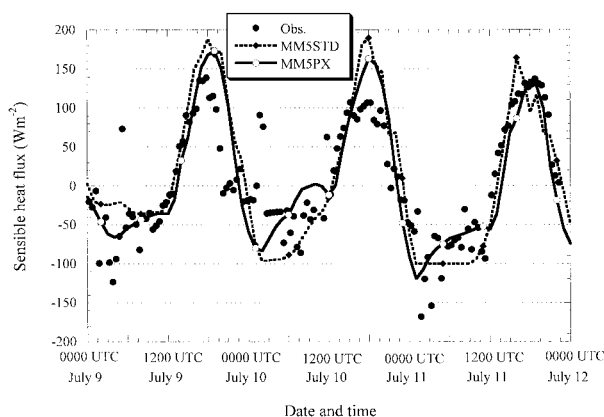


FIG. 6. As in Fig. 5 but for sensible heat flux.

aggregation of several vegetation categories using the values shown in Table 1. Note that the resultant gridcell value is very similar to the value specified for grassland (83 s m^{-1}) because this particular grid cell is dominated by grassland. Thus, the difference in $R_{\text{st min}}$ between the two models is mainly due to a revision of the value assigned to grass. The small differences of LAI, z_0 , and vegetation coverage of the 3D runs between the June and July cases reflect the vegetation growth in the two months.

b. Model and measurements comparison

1) THE JULY 1987 CASE

Figure 5 shows observed and modeled net radiation [R_n in Eq. (1) in PX95] at the FIFE site for the 3-day comparison period (0000 UTC 9–0000 UTC 12 July 1987). The modeled net radiation by both the MM5STD and MM5PX models was slightly overestimated for 9 and 10 July during the daytime. Note that both models used the same simple surface radiation scheme, so the modeled net radiation differs between them only because of differences in other model parameters such as ground temperature, precipitable water, and especially cloud cover. On 11 July 1987, MM5PX simulated net radiation at the surface very well as compared with observations. For the same day, MM5STD underestimated the net radiation because of clouds occurring around noon rather than in the late afternoon, as observations indicated. Consequently, MM5STD's simulations of sensible and latent heat fluxes were also underestimated for 11 July, as described below.

Figures 6 and 7 show comparisons between the measured sensible and latent heat fluxes and both model simulations for 9–11 July. Because the surface heat fluxes derived by Bowen ratio techniques and eddy correlation are similar (see PX95), here we plot only the fluxes measured by Bowen ratio techniques. Both models overestimated sensible heat flux (Fig. 6) for 9 and 10 July during midday and the afternoon, and simulated

it reasonably well at night and during the morning. This pattern is similar to the comparison of net radiation (Fig. 5) and is therefore probably related to both models' inability to simulate correctly the midday and afternoon partial cloudiness, which occurred on both days. Note that MM5STD simulated higher sensible heat flux than MM5PX even though its simulation of net radiation was generally lower. The sensible heat flux on 11 July was well simulated by MM5PX as compared with the observations; MM5STD tended to overestimate sensible heat flux in late morning before clouds occurred in the model and then to underestimate around noon.

Except for the cloudy afternoon of 9 July, the latent heat flux (Fig. 7) simulated by MM5PX compared very well with the measurements for the 3-day period, which suggests that the model is well able to simulate evapotranspiration accurately in such vegetated areas (see Table 2). The latent heat flux simulated by MM5STD, however, was underestimated for most of the three days, particularly during cloud-free periods. This result, combined with MM5STD's tendency to overestimate sensible heat flux even when clouds are not an issue, such as the late morning of 11 July, suggest a bias toward dry surface conditions. Of course, this bias is specific

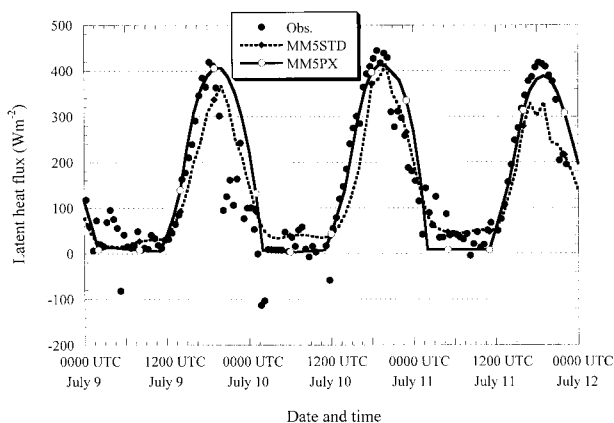


FIG. 7. As in Fig. 5 but for latent heat flux.

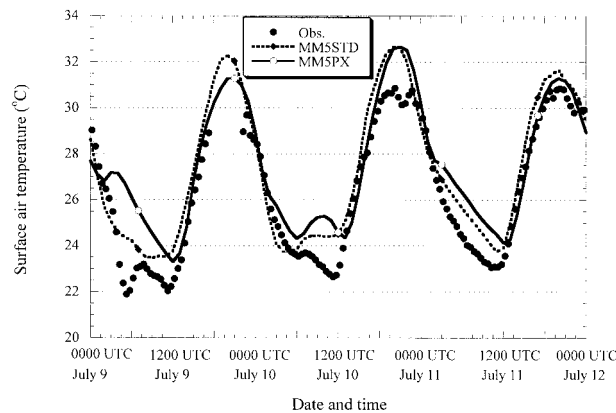


FIG. 8. As in Fig. 5 but for surface air temperature.

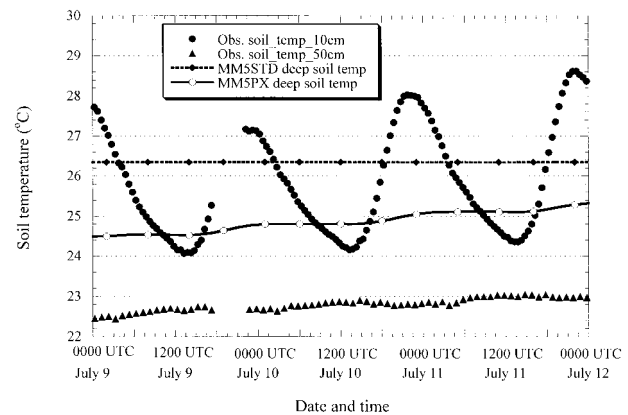


FIG. 9. As in Fig. 5 but for soil temperature.

to this case, because MM5STD cannot dynamically adjust moisture in response to variations in soil moisture, soil type, or vegetation characteristics.

Figure 8 shows the modeled and observed surface air temperature at measurement height (1.5 m) for the three-day period. We used sensible heat flux and temperature at the lowest model layer (~ 18 m) to estimate the temperature at the 1.5-m height. The simulations by each model are similar except for the peak temperature on 9 July, when the MM5STD temperature was about 1°C higher than the MM5PX temperature. Unfortunately, the observations were missing for the middle of the day on 9 July, so the peak temperature cannot be evaluated. On 10 July, both models overestimated the surface air temperature by about 1.5°C at the peak. This result is consistent with the similar oversimulation of net radiation and sensible heat flux by both models (Figs. 5 and 6) on 10 July, which again is linked to the failure of either model to simulate accurately the midday cloudiness. On 11 July 1987, the surface air temperature results by both models compared very well with observations, with MM5PX slightly closer to the measurements. Note that surface winds were strong ($10\text{--}15\text{ m s}^{-1}$) during this day, which suggests that horizontal advection may be more important than local surface fluxes in determining the local surface air temperature. Therefore, the good comparison to measurements at this site reflects a realistic regional simulation by the land surface model.

To illustrate the soil temperature and its evolution during the 3-day period, we plotted the observed soil temperatures at 10 and 50 cm, the substrate temperature from MM5STD, and T_2 (the 1-m average soil temperature) from MM5PX in Fig. 9. In MM5STD the deep soil temperature is a constant value equal to the diurnal mean of surface air temperature in the previous day of simulation, but in MM5PX T_2 can vary according to Eq. (2) in PX95. This ability to vary allows MM5PX to simulate the multiday trends such as the gradual warming evident in the measurements at both soil depths (10 and 50 cm). The ability of T_2 to track long-term

trends has been tested more extensively in a seasonal (3.5 month) simulation that will be described in Part II.

One of the most important parameters provided by meteorological models to air quality models is PBL height, which determines the vertical extent of rapid mixing of air pollutants. Many physical processes and parameters can affect the PBL height, such as heat fluxes, ground and near-surface temperature, and vertical temperature and moisture profiles. Figure 10 shows the PBL height for 11 July 1987 estimated from observations and simulated by MM5STD and MM5PX. The “observed” PBL height is derived from radiosonde measurements using the bulk Richardson number method suggested by Holtslag et al. (1990), as is used in MM5PX. As mentioned before, in MM5STD when the Blackadar PBL scheme is used, PBL height is calculated only under convective conditions, when the Blackadar convective PBL scheme defines the top of the PBL as the limit of free convection plus a 20% buoyancy over-

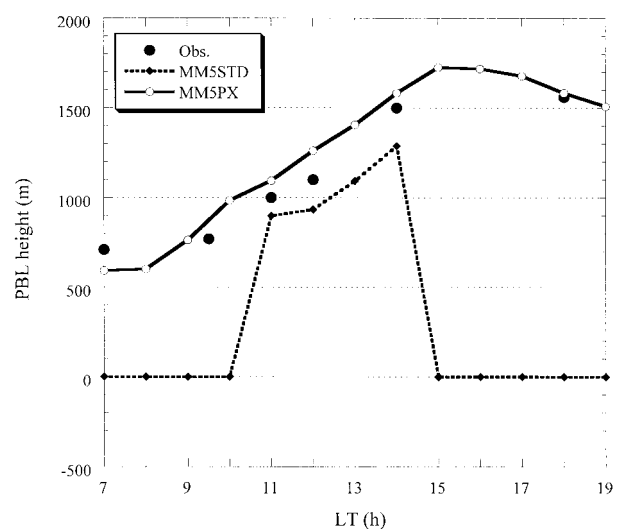


FIG. 10. Observed and modeled PBL height for 11 Jul 1987 at local time (LT).

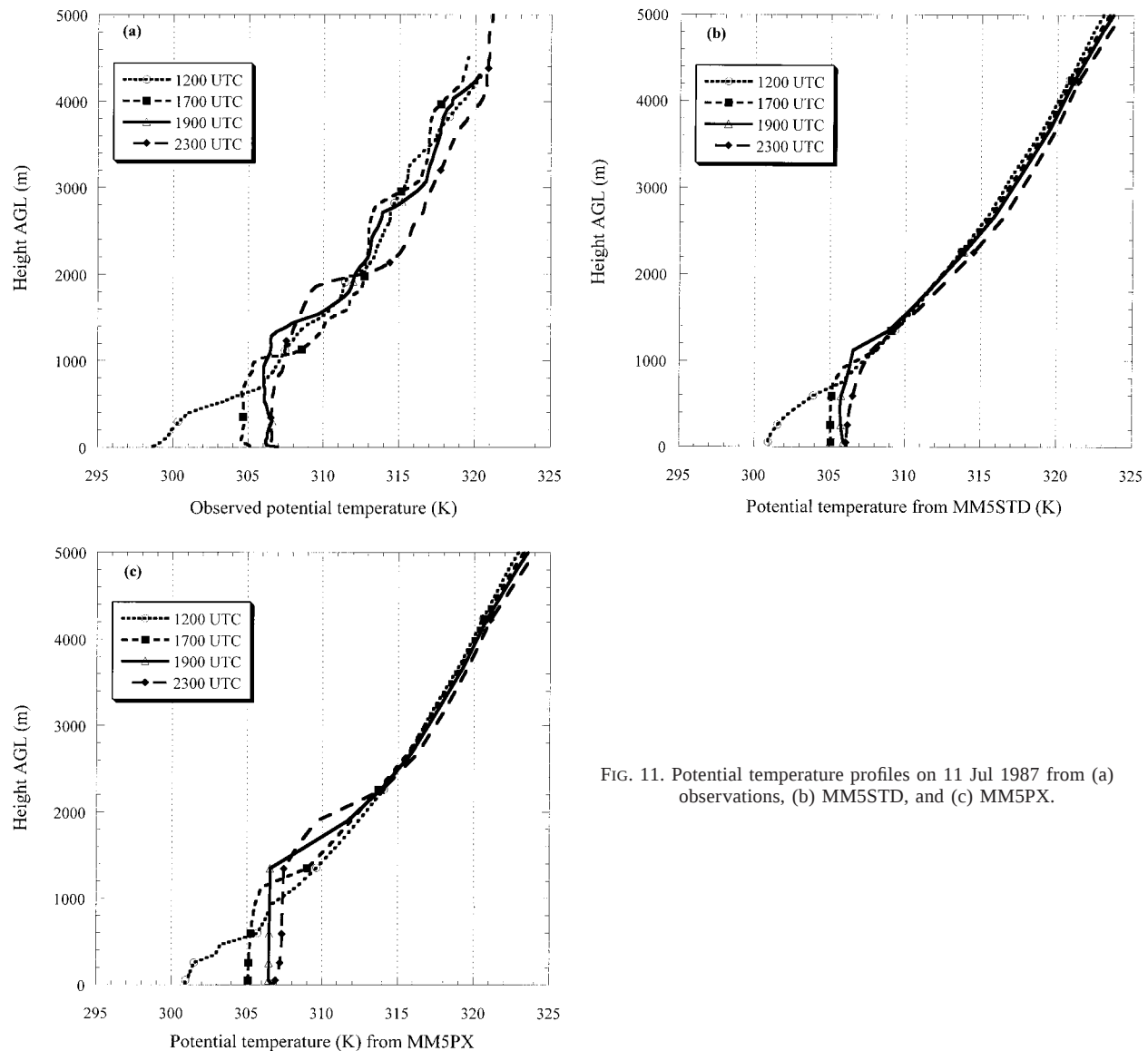


FIG. 11. Potential temperature profiles on 11 Jul 1987 from (a) observations, (b) MM5STD, and (c) MM5PX.

shoot. The MM5STD scheme not only underestimated the PBL height for the hours that were classified as convective (1100–1400 LT), but also ceased to give a convectively driven PBL by 1500 LT. During nonconvective conditions, the Blackadar PBL scheme in MM5STD reverts to a local eddy diffusion algorithm (Blackadar 1976), which makes no distinction of the PBL. The consequence of this early cessation of PBL parameterization is a less well mixed and more shallow layer in the later afternoon, which can be seen in the soundings discussed below (Fig. 11). MM5PX, on the other hand, modeled the entire diurnal evolution of the PBL and late afternoon peak PBL height very well in comparison with observations.

The effects of the new land surface scheme and PBL model applied in MM5PX can be examined in more

detail by comparing modeled vertical potential temperature profiles to measurements at several times of the day. Figure 11 shows potential temperature profiles derived from (a) radiosonde soundings and modeled profiles from (b) MM5STD and (c) MM5PX for four times during the day of 11 July 1987, from morning to late afternoon. In the morning (0700 LT or 1200 UTC), both models similarly overestimate the potential temperature in the lowest 400 m, and the near surface potential temperature by about 2 K. The overestimation near the surface can be partially attributed to the limited vertical resolution of the model, because Fig. 8 shows about a 1-K overprediction at the 1.5-m measurement height during the morning of 11 July. The remaining overestimation throughout the 400-m layer may be related to the underestimation of the very large negative (down-

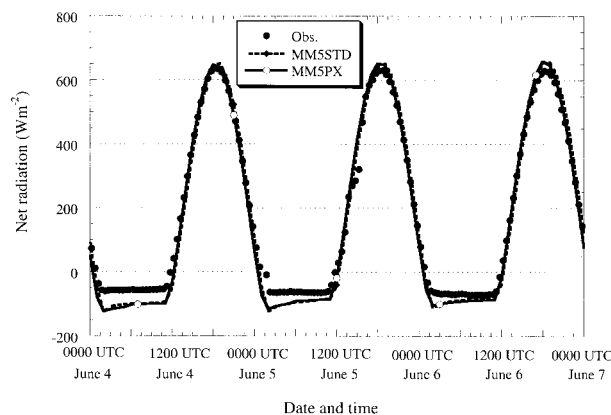


FIG. 12. Observed and modeled net radiation for the 3-day period from 0000 UTC 4 to 0000 UTC 7 Jun 1987.

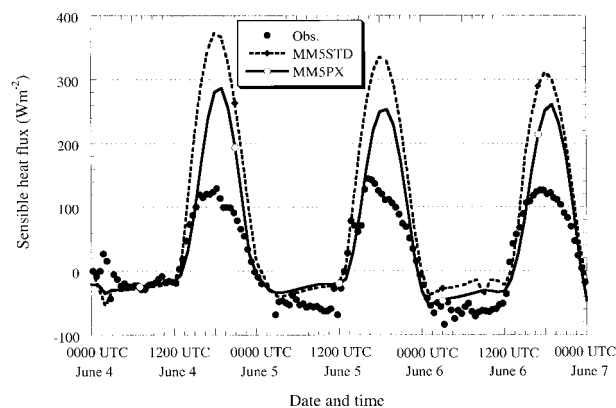


FIG. 13. As in Fig. 12 but for sensible heat flux.

ward) sensible heat flux (see Fig. 6) on the night of 10 July. At 1700 UTC (local noon), both models produce a fairly well mixed boundary layer with a mixed-layer potential temperature very close to the observations. As noted above, MM5PX produced a deeper mixed layer than MM5STD at this time, with the observations falling in between. In the afternoon at 1400 LT (1900 UTC), MM5PX modeled the vertical profile of potential temperature very well in comparison with observations, and MM5STD underestimated the height of the well-mixed layer as well as the potential temperature in the mixed layer. By the early evening (1800 LT or 2300 UTC) the two models had diverged even more, particularly with respect to the much cooler layer above the residual mixed layer, which may indicate a more extensive entrainment zone produced by MM5PX. It is striking that MM5STD produces little variation in potential temperature above 1400 m while MM5PX shows considerable changes in potential temperature up to 2000 m in a manner quite similar to the observations. These differences between the models are probably related more to the different PBL models than to the different land surface schemes. In particular, by using the bulk Richardson number to define the depth of the PBL and by continuing boundary layer scaling to define vertical mixing beyond the free convective period, MM5PX can better represent vertical mixing in the entrainment zone caused by vertical wind shear in this layer.

2) THE JUNE 1987 CASE

The modeled net radiation by both MM5STD and MM5PX compared well with the observations for the 3-day comparison period (0000 UTC 4–0000 UTC 7 June 1987) in Fig. 12. This demonstrates that the models' radiation scheme was able to simulate radiation fluxes under clear sky very accurately. However, for the same period, both models significantly overestimated the peak sensible heat flux (Fig. 13) and undersimulated the peak latent heat flux (Fig. 14) in comparison with

observations, with MM5PX's simulations closer to the observed values. MM5STD has the tendency to overestimate sensible heat flux and underestimate latent heat flux when the moisture availability is too small in comparison with the actual soil moisture. For the MM5PX model, the bias in the partitioning of the net radiation into sensible and latent heat fluxes was mostly due to the dry air humidity in the PBL, which is shown in Fig. 15 for 1800 UTC (1300 LT) 6 June 1987. The modeled mixing ratio profiles in the PBL were so dry (profiles at other times not shown here) that the stress function of air humidity F_3 in Eq. (7) was about 0.3 near midday, indicating partial closure of the stomata. To study the sensitivity of the stress function and the latent heat flux to the air humidity level in MM5PX, we did an experiment with a modified F_3 using the observed mixing ratio through the MM5 objective analysis routine rather than the model-simulated mixing ratio. The value of the stomatal resistance [R_{st} in Eq. (7)] was reduced from 226 to 167 $s\ m^{-1}$, and the latent heat flux was increased from 260 to 310 $W\ m^{-2}$ at the peak time. This result indicated how much the air humidity near the surface could affect the latent heat flux even though the transpiration process is nonlinear. The land surface model

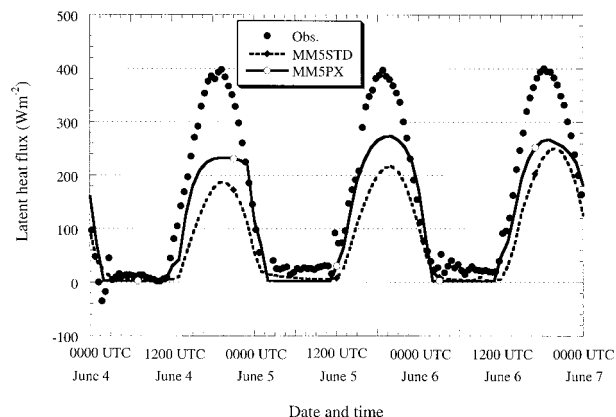


FIG. 14. As in Fig. 12 but for latent heat flux.

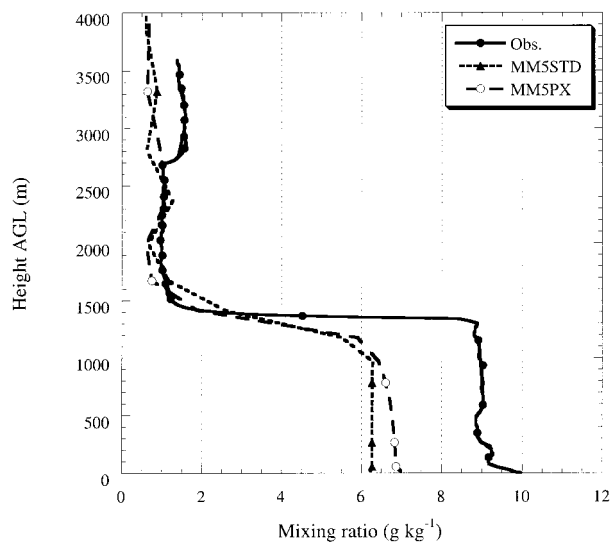


FIG. 15. Vertical profile of observed and modeled mixing ratio at 1800 UTC (1300 LT) 6 Jun 1987.

indeed helped but could not fully eliminate the underestimation of air humidity in the PBL (see Fig. 15), which was probably caused by other processes in MM5 and is out of the scope of this paper.

Because the sensible heat flux simulated by both models was overestimated, the modeled midday surface air temperature at measurement height (1.5 m) for the 3-day period (Fig. 16) was also higher than the observed, with smaller oversimulations by MM5PX. However, both models captured the warming trend over the three days. The increase of the peak surface air temperature during the three days from MM5PX (2°C) is more realistic than that from MM5STD (1.7°C) when compared with the measured increase (2.3°C). The observed soil temperatures at 10 and 50 cm, the substrate temperature from MM5STD, and T_2 (the 1-m average soil temperature) from MM5PX are plotted in Fig. 17. As mentioned before, in MM5STD the deep soil temperature does not

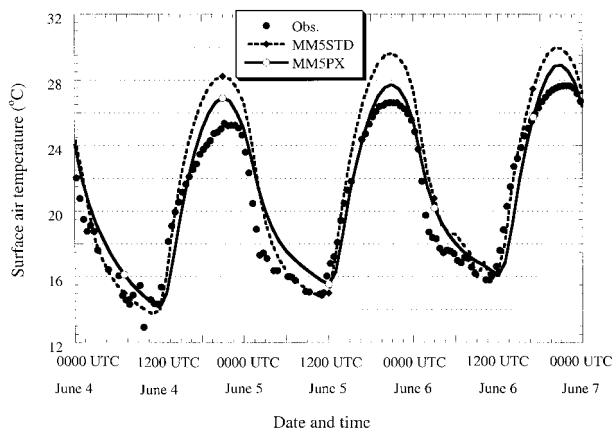


FIG. 16. As in Fig. 12 but for surface air temperature.

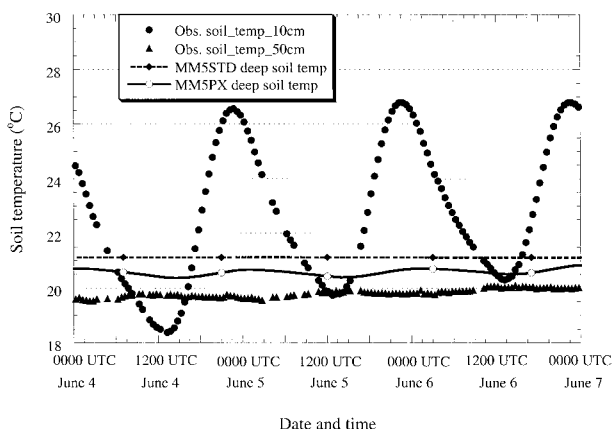


FIG. 17. As in Fig. 12 but for soil temperature.

vary with time in one simulation run, but it does in MM5PX. The obvious warming trend in the surface air temperature was much less evident in the observed soil temperatures and was essentially absent from the MM5PX deep soil temperatures.

Figure 18 shows the PBL height for 6 June 1987 estimated from observations and simulated by MM5STD and MM5PX. Both models underestimated the PBL height in the early morning but later on modeled the PBL height very well in comparison with observations. Note that the PBL from MM5STD was not defined after 1800 LT, because this model computes PBL height only for convective conditions, but the PBL from MM5PX was still over 1000 m. Further details of the PBL can be seen from vertical potential temperature profiles. Figure 19 shows potential temperature profiles derived from (a) radiosonde soundings, and simulated profiles from (b) MM5STD and (c) MM5PX models for

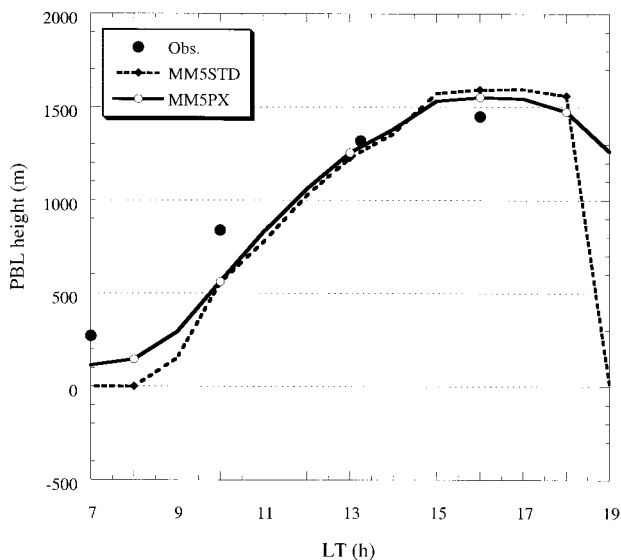


FIG. 18. Observed and modeled PBL height for 6 Jun 1987 at local time (LT).

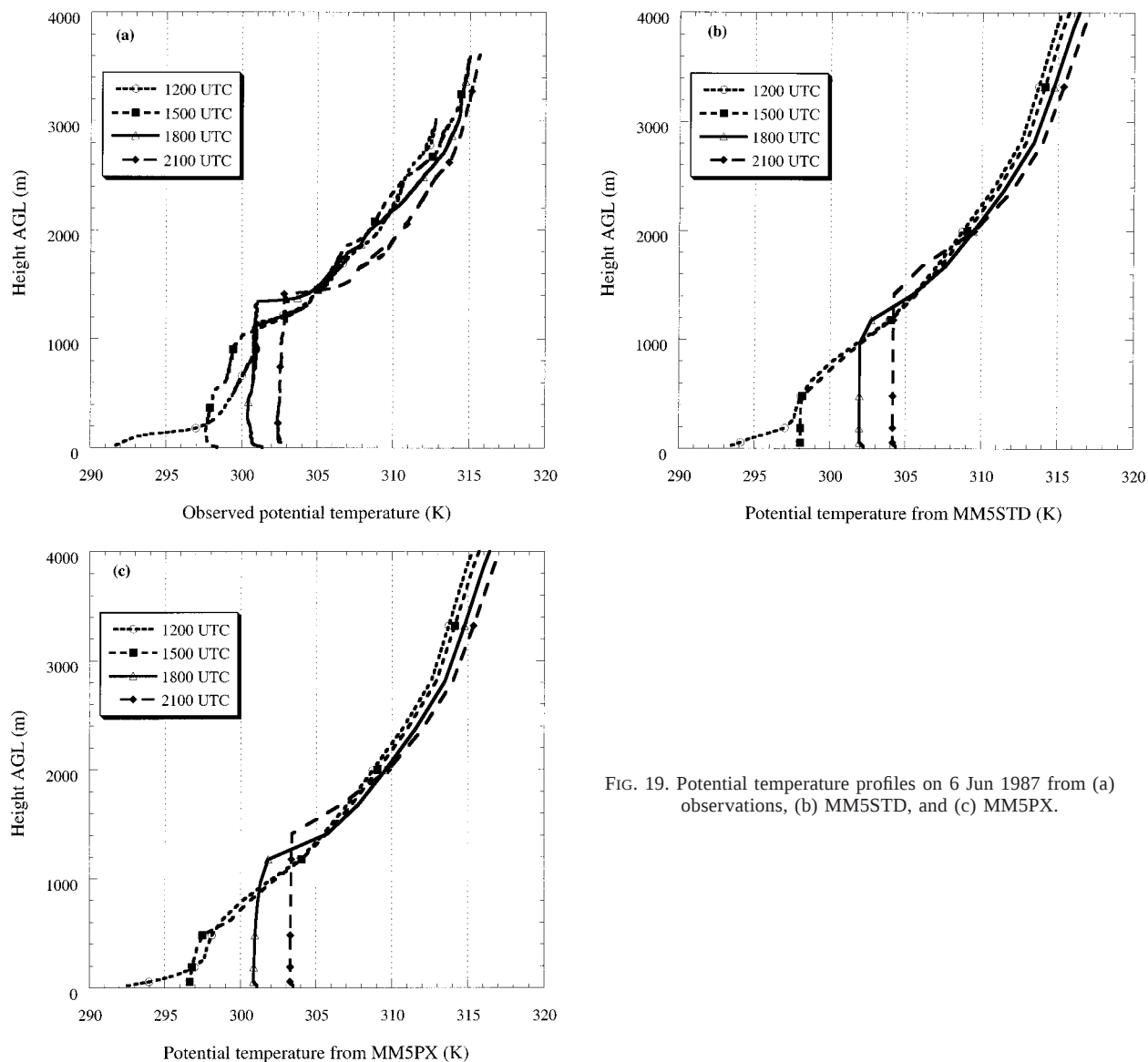


FIG. 19. Potential temperature profiles on 6 Jun 1987 from (a) observations, (b) MM5STD, and (c) MM5PX.

four times during the day of 6 June 1987, from morning to afternoon. In the morning (0700 LT or 1200 UTC), both models slightly underestimated the potential temperature near the surface but shifted to the overestimation as the day progressed. In the afternoon (1300 LT or 1800 UTC and 1600 LT or 2100 UTC) the observations and the models showed very well mixed boundary layers. However, at both sounding times the positive bias of the potential temperature from MM5STD was about 2 K throughout the mixed layer while the bias from MM5PX was only around 0.5 K.

5. Summary

A new advanced land surface/PBL model has been developed and implemented into the MM5 modeling

system to improve its PBL simulation, which is extremely important for air quality applications. The goal of this effort was to develop a land surface model that includes the essential surface and vegetation processes and is computationally efficient enough to run in mesoscale models. The new land surface model was originally based on the ISBA model (NP89) but has since undergone many modifications. In particular, three of the four empirical environmental functions that control stomatal resistance have been replaced as a result of newer literature and sensitivity experiments. Also, to overcome uncertainties in initialization of soil moisture, a data assimilation scheme is used to nudge soil moisture indirectly using surface observations of air temperature and relative humidity. Rather than assigning soil and vegetation parameters on the basis of the dominant land

use and soil type category in each grid cell we developed new gridcell aggregation procedures for soil and vegetation parameters such as soil texture, leaf area index, minimum stomatal resistance, roughness length, and vegetation coverage.

This land surface model has many similarities with and some important differences from the NCEP land surface model (Chen et al. 1996), which is implemented in the MM5. Both models have a similar level of complexity and both use empirical stomatal resistance parameterizations based on NP89, although our empirical functions have been more extensively revised. An important difference between these models is our soil moisture nudging scheme. This feature is particularly useful for air quality applications, which is our primary concern, because we mostly perform retrospective simulations where 4DDA can be used for the entire period. We look forward to comparison studies between these two schemes within the MM5 system.

The modified MM5 with the land surface/PBL model (MM5PX) was tested for two cases based on FIFE measurements. The results from MM5PX were compared with observations as well as with results from standard MM5 (MM5STD) simulations for the same period. No special site-specific treatments for the FIFE measurements were applied to soil and vegetation parameters other than the general methodologies described in section 3. Overall, for the case study of 9–11 July 1987, MM5PX demonstrated its capabilities of responding realistically to soil moisture and evapotranspiration, as shown by the simulation of surface fluxes and PBL height. MM5PX also simulated the PBL evolution and potential temperature profiles better than MM5STD, as compared with observations. Furthermore, MM5PX captured the warming trend evident in soil temperature observations over the multiday period.

The MM5PX simulations for the 4–6 June 1987 FIFE case study showed lesser improvements over the MM5STD as compared with measurements. Although the dry bias in the MM5PX simulations, indicated by the surface sensible and latent heat fluxes, was less than in the MM5STD results, they were still substantial. Clearly the large undersimulation of surface and boundary layer humidity (Fig. 15) contributed to the models' underestimation of stomatal conductance and, consequently, surface moisture flux. In spite of this dry bias in the surface heat fluxes, MM5PX simulations of surface level and mixed-layer temperatures compared well with measurements and were substantially better than the MM5STD simulations.

This paper (Part I) presents the land surface model description and some very limited evaluation against field data and the standard MM5. Part II of this paper will extend the evaluation of MM5PX to much longer simulation periods that include seasonal changes in vegetation. Therefore, Part II will describe, in detail, vegetation growth algorithms and evaluation against NDVI data. The soil moisture nudging scheme will also be

described in more detail along with sensitivity testing. Last, a chemical dry deposition model that utilizes the bulk stomatal resistance along with the surface and boundary layer meteorological output from the MM5PX to estimate dry deposition velocities of many chemical species relevant to air quality issues will be described. Part II will feature the evaluation of modeled surface fluxes of heat, moisture, and chemical dry deposition through comparison to two multimonth field experiments in the eastern United States.

Acknowledgments. The 1-km soil texture datasets for the conterminous United States are developed at the Earth System Science Center in the College of Earth and Mineral Sciences at The Pennsylvania State University under the support of NASA's Earth Observing System Program and NOAA's Global Energy and Water Cycle Experiment Continental-Scale International Project. The authors thank Ms. Tanya Otte and Ms. Donna Schwede of EPA for their technical review and valuable suggestions. We also thank Ms. Jeanne Eichinger of MCNC for her careful editing of this paper. The U.S. Environmental Protection Agency through its Office of Research and Development funded the research described here under cooperative agreement CR-823628 to the MCNC-Environmental Programs. It has been subjected to agency review and approved for publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

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