Variational Assimilation of Precipitable Water Using a Nonhydrostatic Mesoscale Adjoint Model. Part I: Moisture Retrieval and Sensitivity Experiments

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ABSTRACT

Recently it has been proposed that the phase delay associated with the radio signals propagating from GPS satellites to a ground-based GPS receiving station can be used to infer the vertically integrated water vapor (precipitable water—PW) with a high degree of accuracy. Since a ground-based GPS receiving station is relatively inexpensive, a specially designed, dense GPS network can provide PW measurements with unprecedented coverage. Such a dataset can potentially have a significant impact on operational numerical weather prediction.

In this paper, a series of numerical experiments were conducted using a variational (4DVAR) data assimilation system based on The Pennsylvania State University—National Center for Atmospheric Research mesoscale model MM5 and its adjoint. The special soundings collected in SESAME (Severe Environmental Storms and Mesoscale Experiment) 1979 were used in two sets of experiments. In the first set, a 1-h assimilation window and an analysis of the observed PW data were used. All data were assumed to be available at the end of the assimilation window. The assimilation of PW data was found to effectively recover the vertical structure of water vapor and improve the quality of moisture analysis. The use of surface humidity data in addition to PW analysis resulted in further improvement in the quality of the retrieved moisture fields, particularly in the lower troposphere. The assimilation of PW and surface humidity data reduced the rms errors in the initial moisture analysis by as much as 40%. Such improvement cannot be achieved by assimilation of wind and temperature data, because they do not carry sufficient information on the moisture field. The authors also found that the assimilation of PW and surface humidity data can lead to significant improvement in short-range precipitation forecasts when used along with the wind and temperature data. The use of PW and surface humidity data in 4DVAR increased the threat score from 0.01 to 0.48 for 3-h forecasts and from 0.43 to 0.65 for 6-h forecasts.

SESAME 1979 is a case with intensive convective activity, and the forecast is strongly affected by moist diabatic processes. The intent here is to test the impact of including adjoints of moist physics (adjoints of the Kuo cumulus convective scheme and the grid-resolvable precipitation) in the 4DVAR system to PW assimilation results during the initial stage of the storm case. Thus, the assimilation window is extended from 1 to 3 h, and it is assumed that PW data were available at an interval of 3 h in the second set of experiments. The PW data assimilated are generated by the model simulation. It was found that the inclusion of moist physics in the 4DVAR system reduced the systematic biases of the model, allowed a better fit between the model and observed data, and resulted in an improved "optimal" initial condition and, consequently, a better short-range prediction. The threat score was increased from 0.30 to 0.50 in the 6-h forecasts following the assimilation cycle. These results suggest that the effects of physical parameterization should be included in a 4DVAR data assimilation system, especially for a situation with significant precipitation over a relatively long assimilation window (greater than 3 h). The sensitivity of the 4DVAR results to the initial guess field was also tested. The results of 4DVAR were found to be relatively insensitive to the quality of the initial condition (the guess field). Even with a very poor initial moisture field, 4DVAR was able to produce a high quality moisture analysis after the PW data were assimilated, although the number of iterations required had to be increased from 30 to 50.

1. Introduction

Atmospheric water vapor is an extremely important variable for short-range numerical weather prediction because moisture distribution is directly related to the formation of clouds and precipitation. Water vapor also plays a critical role in atmospheric processes that act over a wide range of temporal and spatial scales, from global climate to microphysics. Despite significant progress in remote sensing of wind and temperature, cost-effective profiling of atmospheric water vapor is still lacking. Recently, several techniques have been proposed for sampling vertically integrated water vapor. One such technique is the use of phase-delay information from a radio signal transmitted from a GPS satellite, which can be used to derive fairly accurate

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precipitable water (PW) measurements. Since a GPS ground station is relatively inexpensive, a large number of ground-based GPS stations can be deployed to provide unprecedented coverage of PW measurements at a temporal resolution of about 10 min (Bevis et al. 1992). Many other satellite instruments can also provide useful PW measurements, for example, the VISSR (Visible–Infrared Spin Scan Radiometer) Atmospheric Sounder (VAS) on the GOES-7 satellite. The PW observations can also be obtained from the Special Sensor Microwave/Imager (SSM/I) system. Rabin et al. (1991) discussed the quality of PW measurements retrieved from VAS and SSM/I. Illari (1989) showed that the satellite-derived PW data are of comparable quality to the radiosonde data. Although these systems can provide fairly accurate PW measurements, such data contain no information on the vertical structure of water vapor. Two questions can be asked. First, can the vertical structure of water vapor be retrieved through some retrieval algorithms? Second, would the PW measurements be useful for operational numerical weather prediction?

Kuo et al. (1993, hereafter referred to as KGW) used a simple iterative retrieval method to derive vertical profiles of specific humidity from PW observations, using the model humidity field as a first guess. The derived specific humidity profiles were then nudged into a model. It was found that the assimilation of PW was effective in recovering the vertical structure of water vapor with an accuracy much higher than that from statistical retrieval based on climatology. The improved analysis due to assimilation also led to improved short-range precipitation forecasts. Illari (1989) showed that the inclusion of satellite PW data in the ECMWF (European Centre for Medium-Range Weather Forecasts) humidity analysis had a small but positive impact on the rainfall forecast in the Tropics. Wu and Derber (1994) included the SSM/I PW observations in the NMC (National Meteorological Center) spectral statistical interpolation analysis system and found such data were effective in correcting a humidity bias over the western Pacific. They calculated the anomaly correlations of 5-day predictions and concluded that the inclusion of the PW observations improved the forecast, especially in the Southern Hemisphere where the conventional observations were sparse. Holt and Chang (1994) studied the impact of the SSM/I-measured PW data on the prediction of the ERICA (Experiment on Rapidly Intensifying Cyclones over the Atlantic) IOP 4 storm. They directly replaced the specific humidity with an “adjusted” moisture profile corresponding to the SSM/I PW measurements. The “adjusted” moisture profile was obtained from PW observations using the simple retrieval method proposed by KGW. Their results showed a moderately positive impact on explosive cyclone prediction with the incorporation of the PW measurements.

It is important to recognize that most retrieval methods need a priori information (or estimates) on the vertical structure of water vapor. For example, KGW made use of the model-predicted humidity fields as the first guess for their retrieval method. Other traditional methods obtain such information from climatology. Because the PW measurements contain no information on the vertical structure of water vapor, PW data can only be used to correct biases in the vertically integrated water vapor fields, not the detailed moisture structure in the vertical. As a result, the first-guess “background” moisture profiles can have a significant influence on the final results of the moisture retrieval.

Recently, we developed a 4DVAR system based on the Penn State–NCAR nonhydrostatic mesoscale model (MM5), including moist processes and planetary boundary layer physics. This paper makes use of this 4DVAR system for PW assimilation. The special soundings available from SESAME 1979 (Severe Environmental Storms and Mesoscale Experiment) were used to simulate a set of PW measurements, which were then assimilated into the 4DVAR system. The accuracy of the derived water vapor fields through variational assimilation of PW was assessed by direct comparison with the detailed specific humidity soundings. In some experiments mass and wind (and surface moisture data) were added, along with the PW observations, to the 4DVAR system to assess the relative importance of wind, temperature, and PW data in mesoscale data assimilation.

In a 4DVAR system, the vertical structure of water vapor is retrieved through an optimization procedure that minimizes the distance between model solution and PW observations. Theoretically, a priori information on the vertical structure of water vapor is not required if the number of observations is larger than the degrees of freedom of the control variable. The vertical structure of the moisture field is obtained as the “optimal” solution to the minimization problem under the dynamic constraints of the forecast model and its adjoint and the integrated constraint of the observed PW data. The initial guess should have little or no impact on the final results depending on the density of observations. Assessing the importance of the initial guess field in moisture retrieval using the 4DVAR approach is one of the objectives of this research.

Section 2 describes the variational method for PW assimilation. Section 3 presents results from a set of 1-h data assimilation experiments. We assume that PW data are available only at one time level, and we assess the ability of 4DVAR in retrieving the vertical structure of water vapor through a 1-h PW assimilation. In section 4, we presents results from another set of 3-h data assimilation experiments designed to evaluate the impact of initial guess and moist physics on the results of the assimilation and the subsequent short-range prediction. The summary and discussions are presented in section 5, along with a plan for future work.
2. Methodology

a. Variational formulation

In this study, we use the adjoint technique for data assimilation. A detailed description of this technique can be found in Le Dimet and Talagrand (1986) and Navon et al. (1992). A cost function that measures the distance between the model solution and direct (model forecast variables, such as wind, temperature, and water vapor, etc.) and indirect (such as radiances, PW, etc., fields not used as model predictive variables) observations is defined as a function of the model initial condition:

\[ J(x_0) = \sum_{r_1} W_r [f(t_{r_1}) - f^{\text{obs}}(t_{r_1})]^2 + \sum_{r_2} \gamma [PW(t_{r_2}) - PW^{\text{obs}}(t_{r_2})]^2, \]  \hspace{1cm} \text{(2.1)}

where the first term measures the distance between model variable \( f \) and direct observations \( f^{\text{obs}} \), where \( f \) can be wind, temperature, or specific humidity, and the second term includes the impact of PW observations. Here \( W_r \) and \( \gamma \) are weighting coefficients, \( t_r \) and \( t_\gamma \) are times when observations are available, and \( t_0 \) represent the beginning and ending time of the assimilation window. Here \( W_r \) are diagonal matrices obtained by taking the inverse of the square of the maximum difference of model variables between the observations at the beginning and the ending time of the assimilation window (see Navon et al. 1992). A value of \( \gamma = 30 \) is used to make the second term having the same orders of magnitude as the first term in (2.1).

The model used in this study is the Penn State–NCAR mesoscale model version 5 (MM5) described by Grell et al. (1994) and Dudhia (1993). MM5 is a nonhydrostatic model that evolved from the hydrostatic version (MM4) described by Anthes et al. (1987). The version of MM5 used in this study includes a Kuo-type cumulus parameterization scheme, a grid-resolvable scale nonconvective precipitation parameterization, and a bulk aerodynamic parameterization of the planetary boundary layer (PBL) processes. The adjoint of an adiabatic version of MM5 was recently developed by Zou et al. (1995). In this study, we have added the adjoint of the aforementioned physical parameterization schemes. The adjoint version of moist parameterization was constructed by linearizing the original nonlinear scheme around the basic state at every time step while keeping the “on–off” switches the same as in the nonlinear model and then transposing the tangent linear model (TLM). Numerical experiences of Zou et al. (1993), Zupanski (1993), Verline and Cotton (1993), and Bao and Warner (1993) showed that it is feasible to apply the adjoint of moist processes to 4DVAR using models ranging from a simple one-dimensional cloud model to complicated primitive equation models. The minimization procedure used the limited-memory quasi-Newton method of Liu and Nocedal (1989), which is the most efficient and robust unconstrained minimization method, as shown in Zou et al. (1993).

b. Assimilation of PW data

In this study, we used the specific humidity analysis that was produced by KGW based on the special 3-h soundings collected during SESAME 1979. The observed PW is obtained from the vertical integration of the specific humidity analysis

\[ PW^{\text{obs}} = \frac{p^*}{g} \sum_{k=1}^{KX} q_{\text{obs}}(k) \Delta \sigma(k), \]  \hspace{1cm} \text{(2.2)}

where \( q_{\text{obs}}(k) \) is the specific humidity analysis at the \( k \)th layer, \( \Delta \sigma(k) \) is the layer thickness of the model at the \( k \)th layer, \( KX \) is the total number of layers, and \( p^* \) is defined as \( p_s - p_l \), where \( p_s \) is the surface pressure, and \( p_l \) is the pressure at the top of the model (100 hPa).

In a nudging data assimilation procedure, only the direct observations (observations of model predictive variables) can be assimilated into the model. Therefore, in order to assimilate the observed PW measurements, KGW first developed an iterative retrieval method to derive an “interim” specific humidity field from PW obs, and this interim specific humidity field was then nudged into the model. In 4DVAR, PW obs can be directly assimilated into the model. The 4DVAR minimizes a cost function, such as (2.1), which measures the distance between the model and the observed PW fields by controlling the initial conditions, and the resulting optimal initial condition and its subsequent forecast represent a best fit to the observations within the assimilation window.

Since PW is not a model predictive variable, it is necessary to include an operation on model variable \( q \), which results in model PW

\[ PW = Q q, \]  \hspace{1cm} \text{(2.3)}

where \( Q \) is a constant matrix defined as
Here $\mathbf{PW}$ and $\mathbf{p}^*$ are vectors of dimension $IX \times JX$, and $\mathbf{q}$ is a vector of dimension $IX \times JX \times KK$:

$$
\mathbf{PW} = \begin{pmatrix}
    \vdots \\
    \mathbf{pw}_l \\
    \vdots \\
\end{pmatrix}, \quad 
\mathbf{p}^* = \begin{pmatrix}
    \vdots \\
    \mathbf{p}_l^* \\
    \vdots \\
\end{pmatrix}, \quad 
\mathbf{q} = \begin{pmatrix}
    \vdots \\
    \mathbf{q}_l \\
    \vdots \\
\end{pmatrix},
$$

where $l = J + (J - 1) \times JX, l' = k + (J - 1) \times KK + (J - 1) \times JX \times KK, I, J, \text{ and } K$ represent indices of meridional, zonal, and vertical grid points, and $IX, JX, \text{ and } KK$ are the total number of grid points in the three directions.

Before assessing the impact of PW observations on the optimal solution of the minimization problem, we need to calculate the gradient of the second term of $J$. The derivation is similar to the one presented by Zou et al. (1995), who directly assimilated the refractivity observations into the model. Following Zou et al. (1995), $\nabla J$ can be obtained by integrating the adjoint model from the final time $t_f$ to the initial time $t_0$ with the following forcing terms:

$$
2W_f[\mathbf{f}(t_f) - \mathbf{f}^{\text{obs}}(t_f)],
$$

$$
2\gamma \mathbf{Q}^T[\mathbf{PW}(t_f) - \mathbf{PW}^{\text{obs}}(t_f)],
$$

which are added at times $t_o$ and $t_o$, respectively, during the backward integration of the adjoint model. Therefore, the gradient of the cost function augmented by the information of PW (2.1) can still be obtained by a single integration of the adjoint model from time $t_0$ to $t_f$.

Having the values of the cost function and the gradient, any large-scale unconstrained minimization (see Zou et al. 1993) can be employed to iteratively find the minimum of the cost function, which produces the best fit to the PW observations (or possibly other data) available between time $t_0$ to $t_f$ in a least squares sense. If the descent algorithm produces negative specific humidity in the retrieved IC at some points, they will be replaced by a very small positive value $10^{-12}$ at the beginning of the forward model integration. The corresponding adjoint calculation is implemented also at the end of the adjoint model integration. Having obtained the optimal initial conditions at $t_0$, we integrate the nonlinear model forward to obtain the model state at $t_f$, which is saved and compared with the detailed specific humidity soundings.

3. Numerical experiments using 4DVAR as a retrieval method

a. Experiment design

In SESAME 1979, 3-h soundings were available during the 24-h period of 1200 UTC 10 April to 1200 UTC 11 April at approximately 35 stations over the central United States with an average station separation of approximately 250 km. KGW conducted a careful objective analysis of these 3-h soundings. This study made use of their analyses. Readers are referred to KGW for the detailed analysis procedure.

An objective of this study is to assess the ability of 4DVAR assimilation to recover the detailed moisture structure with the assimilation of one-time-level PW data. For this purpose, we conducted a very short time period (1 h) data assimilation between 1700 and 1800 UTC 10 April. This simulates the situation in which only one-time-level PW data are available at 1800 UTC 10 April. Such 4DVAR experiments are similar to retrieval experiments with the MM5 and its adjoint acting as a strong dynamic constraint. Due to the short assimilation window, the computational expense of 4DVAR is reduced.

Specifically, we began the 4DVAR at 1700 UTC 10 April. The initial guess fields were interpolated from the analyses at 1200 UTC 10 April and 0000 UTC 11 April. During the 1-h period, we assimilated the PW observations at 1800 UTC 10 April. We then compared the derived specific humidity fields with the detailed SESAME humidity soundings at 1800 UTC 10 April to assess the ability of 4DVAR in retrieving the water vapor field from the PW observations. Note that when only the PW observations were assimilated (experiment 4 in Table 1), the first term on the right-hand side of (2.1) was omitted in such an experiment.

Another objective of this study is to determine the relative importance of PW data and other meteorological fields (such as wind, temperature, or both), as well as the added value of PW data, on the results of wind and temperature assimilation and precipitation forecast. In view of the fact that high resolution (in time) wind and temperature observations are available from a potential network of wind profilers and radio acoustic sounding systems, we need to assess the impact of PW assimilation in an environment in which wind and temperature observations are available.

A set of seven numerical experiments were conducted (see Table 1) to assess the value of one-time-level PW data on moisture retrieval and precipitation forecasts. The first three experiments (experiments 1–3) are forecast experiments without a data assimilation cycle. These experiments use a diabatic version of MM5, including Kuo-type cumulus parameterization, grid-resolvable nonconvective precipitation parameterization, and bulk PBL parameterization with surface energy fluxes and friction. The remaining four experiments (experiments 4–7) are data assimilation experiments using the 4DVAR technique. The data assimilation was conducted during the 1-h period between 1700 and 1800 UTC 10 April 1979 using an adiabatic version of the MM5 and its adjoint. After the data assimilation procedure, the diabatic version of MM5 was used to carry out the forecast steps as described above. We have conducted additional 4DVAR experiments, making use of the diabatic version of MM5 and its adjoint during the 1-h assimilation period, and found that the results are not significantly different from those
Table 1. Summary of numerical experiments.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Guess IC</th>
<th>Period (UTC)</th>
<th>Observation</th>
<th>Model</th>
<th>IC</th>
<th>Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td>1700–1800</td>
<td>PW</td>
<td>adiabatic</td>
<td>analysis</td>
<td>diabatic</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>4</td>
<td>intp.</td>
<td>1700–1800</td>
<td>PW</td>
<td>adiabatic</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>intp.</td>
<td>1700–1800</td>
<td>PW, $q_e$</td>
<td>adiabatic</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>intp.</td>
<td>1700–1800</td>
<td>$u$, $v$, $T$</td>
<td>adiabatic</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>intp.</td>
<td>1700–1800</td>
<td>PW, $q_e$, $u$, $v$, $T$</td>
<td>adiabatic</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

A set of one-time-level retrieval experiments

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Guess IC</th>
<th>Period (UTC)</th>
<th>Observation</th>
<th>Model</th>
<th>IC</th>
<th>Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>$q$ intp.</td>
<td>1800–2100</td>
<td>PW</td>
<td>diabatic</td>
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<tr>
<td>9</td>
<td>$q$ avg.</td>
<td>1800–2100</td>
<td>PW</td>
<td>diabatic</td>
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<td></td>
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<tr>
<td>10</td>
<td>$q$ avg.</td>
<td>1800–2100</td>
<td>PW</td>
<td>diabatic</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

A set of two-time-level OSSE experiments

* Analysis at 1200 UTC 10 April.

using the adiabatic models. Two reasons might explain this fact. First, there is little precipitation during the assimilation period of 1700 and 1800 UTC 10 April. Second, the effects of physical parameterization are minimized for a 1-h assimilation. In section 4, we will reevaluate the effects of moist physics on data assimilation during a 3-h period when significant precipitation was occurring.

The control experiment (experiment 1) was initialized at 1800 UTC 10 April 1979 (defined as $t = 0$ h) and integrated for 12 h. The model domain covered the central United States, with an area of 2200 km × 1960 km. The initial condition was obtained from an objective analysis of rawinsonde and surface observations at 1800 UTC 10 April (see KGW for details), which included the detailed three-dimensional structure of wind, temperature, and moisture. This experiment serves as a reasonable measure of the lower bound of rms errors for the other experiments. The lateral boundary conditions were obtained by linear interpolation of objective analyses at 12-h intervals.

Experiment 2 is similar to experiment 1, except it was initialized at 1200 UTC 10 April using all the available observations at that time. The predicted humidity fields at 1800 UTC 10 April represent a typical 6-h forecast. Experiment 3 was initialized at 1800 UTC 10 April, similar to the control. However, its initial condition was obtained by linear interpolation of analyses at 1200 UTC 10 April and 0000 UTC 11 April. The interpolated analysis would certainly have a lower quality than the original analysis at 1800 UTC 10 April. Experiment 3 serves as the benchmark (upper bound of rms errors) for all the other data-assimilation experiments (experiments 4–7).

All the 4DVAR experiments (experiments 4–7) begin at 1700 UTC 10 April and use the time-interpolated analyses at that time as their initial guess. This initial guess is iteratively modified by assimilating different combinations of observations taken at 1800 UTC 10 April. Experiment 4 assimilates PW data only; experiment 5, PW and surface humidity data; experiment 6, wind and temperature; and experiment 7, PW, surface humidity, wind, and temperature data. The optimal initial conditions obtained from these data assimilation experiments are valid at 1700 UTC 10 April. The model is then integrated forward for 1 h to 1800 UTC 10 April, and at that time, the model solutions are compared with observed soundings to assess the accuracy of the derived three-dimensional specific humidity fields. The model state at 1800 UTC 10 April is then used as the initial condition for the subsequent 12-h forecasts to examine the impact of 4DVAR assimilation of various data (particularly, the PW observations) on rainfall prediction.

The computational domain has a mesh size of 49 × 55, with a grid spacing of 40 km. There are 10 levels in the vertical, and these are evenly spaced. Integrations of both the MM5 and its adjoint are performed with a 3-min time step. It should be noted that there are some important differences between the MM5 model used here and the MM4 model used in KGW, aside from the fact that the MM4 used in KGW had 23 σ levels in the vertical. First, MM4 was a hydrostatic model, and second, the Blackadar (1979) PBL formulation was used in KGW. The MM5 used here is a nonhydrostatic mesoscale model with a bulk PBL scheme.

b. Results from the 4DVAR retrieval experiments

Figure 1 shows the variation of the cost function (Fig. 1a) and the norm of the gradient (Fig. 1b), $\nabla J$, with the number of iterations during the minimization procedure for experiment 4. There is a significant reduction in $J$ during the first few iterations. It basically
reaches its minimum within five iterations. The norm of $\nabla J$ decreases by two orders of magnitude in 10 iterations. This shows that the minimization procedure converges rather fast, and the 4DVAR can effectively assimilate the PW data into the model.

Figure 2 shows the PW fields at 1800 UTC 10 April derived from the KGW analysis (PW$_{AN}$), the time-interpolated analysis (PW$_{IN}$), the 6-h forecast from experiment 2 (PW$_{6h}$), and the 1-h forecast of experiment 4 following the 4DVAR assimilation of PW observations (PW$_{VA}$). A comparison between PW$_{AN}$ and PW$_{IN}$ and a comparison between PW$_{AN}$ and PW$_{6h}$ show that both the time-interpolated analysis and the 6-h forecast have significant errors. For example, a band of high PW over northern Texas and southern Arkansas and another band of low PW immediately to its south are evident in the 6-h forecast (PW$_{6h}$) but not in the analysis (PW$_{AN}$). There are also significant differences between PW$_{IN}$ and PW$_{AN}$ over central and southern Texas. The time-interpolated PW analysis appears to underestimate the integrated water vapor over these regions. In sharp contrast, PW$_{AN}$ and PW$_{VA}$ are almost identical to each other.

Figure 3 plots vertical profiles of rms errors of specific humidity at 1800 UTC 10 April, as verified against the specific humidity soundings at 36 sounding stations for four separate fields: 1) the time-interpolated analysis ($q_{IN}$), 2) the 6-h forecast, using analysis at 1200 UTC 10 April as the initial condition ($q_{6h}$), 3) the retrieved specific humidity analysis as a result of PW assimilation ($q_{VA}$), and 4) the KGW analysis ($q_{AN}$). The results show that $q_{IN}$ has an rms error exceeding 2 g kg$^{-1}$ at $\sigma = 0.75$ and 0.85. The vertically integrated rms error in specific humidity (VQRMS) is 1.153 g kg$^{-1}$. The $q_{6h}$ has less error at these two levels but it has a larger error at the lowest model level. The VQRMS (1.084 g kg$^{-1}$) is slightly smaller than that of $q_{IN}$. The assimilation of PW observations resulted in a more accurate water vapor field as compared with $q_{IN}$ throughout the troposphere. It should be noted that the initial guess for 4DVAR (based on the interpolated analysis) at 1700 UTC 10 April has a quality similar to $q_{IN}$. The VQRMS for $q_{VA}$ is 0.915 g kg$^{-1}$. At some levels, the difference between $q_{VA}$ and $q_{IN}$ is larger than 0.5 g kg$^{-1}$. This is truly encouraging because there is no information on the vertical structure of moisture in the PW field. Yet the 4DVAR is capable of retrieving that information by assimilating the PW data directly into the model.

To have a better understanding of the effectiveness of PW assimilation, we show in Fig. 4 the specific humidity field at $\sigma = 0.85$ for $q_{AN}$, $q_{IN}$, and $q_{VA}$ at 1800 UTC 10 April. A comparison between $q_{IN}$ and $q_{AN}$ shows that the time-interpolated analysis has significant errors in several places. For example, it misses the high humidity over southern Texas and the tight moisture gradient over northern Mississippi and Alabama. The specific humidity over the southern tip of Texas has a maximum of 14.6 g kg$^{-1}$ in $q_{AN}$, while that in $q_{IN}$ is only 7 g kg$^{-1}$. The moisture gradient over northern Mississippi and Alabama is considerably diffused in $q_{IN}$. The assimilation of PW results in a significant improvement in both of these areas. The specific humidity in $q_{VA}$ is brought up to 13 g kg$^{-1}$ over southern Texas, and the moisture gradient is restored in northern Mississippi and Alabama.

As a way to evaluate the quality of the derived humidity fields, we calculate the correlation coefficient of the derived humidity fields (experiment 4) at 1800 UTC 10 April with the final moisture analysis prepared by KGW and present the results in Fig. 5 as a dashed line. The correlation coefficient between the interpolated moisture field and the KGW analysis is shown in Fig. 5 as a thick solid line. The results indicate that the 4DVAR assimilation of PW observations has significantly increased the accuracy of the moisture fields throughout the lower half of the troposphere. This assessment is supported by the significant improvement.
in the correlation coefficients after assimilation. For example, the correlation coefficient for the interpolated field is about 0.62 at $\sigma = 0.65$. It is increased to 0.85 after PW assimilation.

Next, we will assess the added value of the surface moisture observations since such data are available routinely at a fairly high temporal and spatial resolution. We show in Fig. 6 the rms errors of specific humidity at 1800 UTC 10 April for the time interpolated analysis ($q_{IN}$, thick solid line) and the retrieved specific humidity fields with PW assimilation (experiment 4; dashed line) and with PW and surface humidity assimilation (experiment 5, dotted line). The results indicate that the inclusion of surface humidity data not only improves the retrieved humidity field at the lowest model level, it also improves the moisture fields at $\sigma = 0.85$ level.

Significant progress has been made over the past decade in the development of remote sensing instruments to profile wind and temperature. Therefore, it would be desirable to assess the value of PW data in an environment in which measurements of wind and temperature are available. Experiments 6 and 7 assimilate a combination of wind, temperature, PW, and surface moisture observations. Figure 6 shows the rms errors of specific humidity at 1800 UTC 10 April for experiment 6 (assimilation of wind and temperature; dot–dashed line). The assimilation of wind and temperature improves the moisture field only slightly by reducing the VQRMS from 1.153 g kg$^{-1}$ ($q_{IN}$; no as-
FIG. 3. The rms errors of the time-interpolated specific humidity field $q_{AN}$ (thick solid line), the 6-h model-predicted specific humidity field $q_{AN}$ (dash-dotted line), the retrieved specific humidity field after assimilating the precipitable water $q_{VA}$ (dashed line), and the KGW analysis $q_{AN}$ (thin solid line), all valid at 1800 UTC 10 April 1979. The numbers in the figure are VQRMS.

(c) Analysis of bias and nonbias errors

The important questions to ask are the following: 1) How detailed vertical structure of specific humidity? 2) How much does the PW and $q$ assimilation reduce the bias and, more importantly, nonbias errors? Bias error ($E_b$) simulation) to 1.093 g kg$^{-1}$. This shows that the wind and temperature fields contain little or no information on the water vapor field. The assimilation of wind and temperature does not lead to significant improvement in the water vapor field. Nevertheless, some slight improvements are noted in the mid troposphere, possibly because of better advection of the water vapor field as a result of wind assimilation. Figure 5 shows the vertical profiles of the correlation coefficient of the specific humidity for experiment 5 (dotted line) and experiment 6 (dotted-dashed line), in addition to experiment 3 (thick solid line) and experiment 4 (dashed line). The correlation coefficients of the specific humidity field are increased by the wind and temperature data assimilation (experiment 6, dot-dashed line in Fig. 5). However, the maximum improvement is obtained by assimilating the PW and surface moisture data. It should be noted that even though the assimilation of wind and temperature only leads to slight improvements in the moisture field, as will be shown later, it has a significant impact on precipitation forecasts. With the assimilation of wind and temperature data, the dynamical fields (convergence, divergence, trough, and ridge) are better defined, which has a direct influence on the precipitation prediction.

FIG. 4. The specific humidity $q$ at $\sigma = 0.85$ of the analysis ($q_{AN}$ in experiment 1), the time interpolated $q$ ($q_{AN}$ in experiment 3), and the retrieved $q$ assimilating only the precipitable water observations ($q_{VA}$ in experiment 4). The contour interval is 1 g kg$^{-1}$. 
Fig. 5. The correlation coefficient of the specific humidity field at 1800 UTC 10 April between the control and experiment 3 (no data assimilation, thick solid line), experiment 4 (assimilation of PW, dashed line), experiment 5 (assimilation of PW and surface moisture, dotted line), and experiment 6 (assimilation of wind and temperature, dot–dashed line). The numbers in the figure are the vertically integrated correlation coefficients.

represents error in the vertically integrated specific humidity (PW) and nonbias error \( E_{nb} \) is the error excluding bias error, which are defined as

\[
E_b(n) = |\bar{q}(n) - \bar{q}^{\text{obs}}(n)|
\]

\[
E_{nb}(n) = \left( \frac{\Delta \sigma}{(KX - k_{\text{obs}} + 1)} \right) \sum_{k = k_{\text{obs}}}^{KX} \{ [q(k, n) - \bar{q}(n)] - [q^{\text{obs}}(k, n) - \bar{q}^{\text{obs}}(n)] \}^{1/2},
\]

where

\[
\bar{q}(n) = \frac{\Delta \sigma}{(KX - k_{\text{obs}} + 1)} \sum_{k = k_{\text{obs}}}^{KX} q(k, n),
\]

\[
\bar{q}^{\text{obs}}(n) = \frac{\Delta \sigma}{(KX - k_{\text{obs}} + 1)} \sum_{k = k_{\text{obs}}}^{KX} q^{\text{obs}}(k, n).
\]

Here \( q(k, n) \) and \( q^{\text{obs}}(k, n) \) are the model and observed specific humidity at the \( n \)th station on the \( k \)th level (see Fig. 7a), \( k_{\text{obs}} \) is the highest level where observations are available, and \( \Delta \sigma \) is the thickness of model layers.

Figure 7 shows loci of rawinsonde stations, the total rms error, the bias error \( E_b \), and the nonbias error \( E_{nb} \) for the guess field \( q(n) \). We observe that for most stations (for example, stations 260, 353, and 13) the nonbias error is about 70% of the total rms error, which means that the PW assimilation can reduce the total rms error at least by about 30%. However, we notice that there are a few stations (such as stations 1 and 19) that have large rms errors (3.73 g kg\(^{-1}\) at station 1 and 2.14 g kg\(^{-1}\) at station 19) and small bias errors (0.48 g kg\(^{-1}\) at station 1 and 0.50 g kg\(^{-1}\) at station 19). Since the assimilation of PW observations should contribute mainly to the removal of the bias error, it would be interesting to examine the reduction of nonbias error in experiments 4 and 5.

Since the PW observations at 1800 UTC are directly assimilated in experiments 4 and 5, the bias error obviously becomes very small and the rms errors left in the "optimal" IC contain mostly the nonbias error. Therefore, we show in Fig. 8 the nonbias error distribution for experiments 4 and 5 at 1800 UTC 10 April. Nonbias error is significantly reduced, for instance, for station 260 (2.51 g kg\(^{-1}\) in experiment 3; 1.53 g kg\(^{-1}\) in experiment 4; and 1.41 g kg\(^{-1}\) in experiment 5) and station 353 (1.47 g kg\(^{-1}\) in experiment 3; 1.36 g kg\(^{-1}\) in experiment 4; and 1.14 g kg\(^{-1}\) in experiment 5). Of particular interest are the results of stations 1 and 19, where the bias errors in the guess fields are small. Assimilation of PW observations (Fig. 8a) does not significantly reduce the rms errors of these stations. However, adding the surface moisture data to the PW assimilation (experiment 5) results in a large reduction of nonbias error at station 1 but not at station 19 (Fig. 8b). It would be interesting to examine the vertical profiles of the specific humidity at stations 353, 1, and 19, which represent three different types of soundings.

Fig. 6. The rms errors of the specific humidity field at 1800 UTC 10 April with no data assimilation (thick solid line), experiment 4 (assimilation of PW only, dashed line), experiment 5 (assimilation of PW and the surface moisture, dotted line), and experiment 6 (assimilation of the wind and temperature, dot–dashed line). The numbers in the figure are VQRMS.
Station 353 represents a sounding having large moisture bias error in the guess field; station 1 represents a sounding having small bias error, where adding the surface moisture to the PW assimilation is quite effective in reducing the nonbias error; and finally station 19 represents a sounding with small bias error where the assimilation of both the surface moisture and PW data could not reduce the nonbias error.

At station 353 (Fig. 9a), the specific humidity profiles of experiments 4 (dashed line) and 5 (dotted line) are brought closer to actual sounding (thin solid line) without significantly changing the vertical structure of moisture. The soundings at station 1 (Fig. 9b) has a sharp maximum at $\sigma = 0.85$ and a minimum at the lowest model level. However, the time-interpolated sounding (thick solid line) has a gradual decrease of specific humidity with height, which results in a positive error at the lowest level and a negative error at $\sigma = 0.85$. Errors at these two levels cancel each other and result in a very small bias error (0.48 g kg$^{-1}$) at this station. Therefore, assimilation of PW observation (dashed line) alone does not bring much improvement to the vertical structure of moisture at this station (thick solid line). However, when the surface moisture is added to the PW assimilation, the resulted moisture profile (dotted line) resembles the actual sounding (thin solid line) quite well. This is a result of the combined effects of PW and surface moisture assimilation.
It is interesting to note that 4DVAR can make use of PW and surface moisture information to create a dramatic change in the vertical structure of moisture, making it consistent with the observations. This is a very good example showing that both the PW and surface moisture observations are important for the moisture retrieval. A more complicated situation occurs at station 19 (Fig. 9c), where the actual moisture sounding (thin solid line) has one local minimum at \( \sigma = 0.85 \) and two maxima at \( \sigma = 0.95 \) and \( \sigma = 0.75 \). The PW assimilation (dashed line) is effective in reducing the systematic bias error, but it does not change the vertical structure of moisture significantly. The addition of surface moisture data (dotted line) does not bring further improvement because the specific humidity at the surface after the PW assimilation is already very close to the observations. Notice that this is also the station that has the largest nonbias error within the whole domain (see Fig. 8b). Obviously, more information is required

**Fig. 8.** Nonbias errors of (a) experiment 4 and (b) experiment 5 at 1800 UTC 10 April. Contour interval is 0.5 g kg\(^{-1}\).

**Fig. 9.** The specific humidity profiles at stations (a) 353, (b) 1, and (c) 19 in experiment 3 (thick solid line), experiment 4 (dashed line), experiment 5 (dotted line), and the actual soundings (thin solid line), all valid at 1800 UTC 10 April.
to recover the actual moisture structure for such sounding. The GPS occultation data (Zou et al. 1995), which provides additional information on the vertical structure of moisture, may be quite useful for this purpose.

d. Precipitation forecast

In this section, we examine the impact of PW assimilation on precipitation forecasts. This was assessed by conducting forward model integration using a full-physics version of MM5 (as described earlier) following the 1-h data assimilation window.

Figure 10 shows the 3-h accumulated precipitation during the 12-h period ending at 0600 UTC 11 April. This figure was originally shown in KGW but is reproduced here for the sake of convenience. As discussed in KGW, heavy precipitation did not start until 1800 UTC 10 April. Intense convection first occurred over southwestern Oklahoma, corresponding to the Wichita Falls tornado outbreak. The precipitation quickly expanded into a line pattern, and by 0000 UTC 11 April it covered nearly all of Oklahoma and southern Kansas (Fig. 10b). A well-defined northeast–southwest line had developed by 0300 UTC 11 April and produced heavy precipitation at its leading edge over eastern Kansas and central Oklahoma. Precipitation of lesser amounts was found over western Kansas to the rear of the squall line. This convective system continued to expand and move eastward. By 0600 UTC 11 April, an elongated line of precipitation (approximately 750 km in length) was found over Missouri, Oklahoma, and Texas, with three distinct centers in each of these states. During the next 6 h, this squall line continued to move eastward and maintained its intensity (not shown).

As a benchmark for the subsequent data assimilation experiments, we first show the precipitation forecast for the control experiment (experiment 1: Fig. 11). This experiment was initialized with the analysis of KGW using all the available surface and upper-air data collected at 1800 UTC 10 April. Figure 11a shows that by 2100 UTC 10 April precipitation took place over the border of Oklahoma and Texas at a location to the southeast of the observed 3-h rainfall (Fig. 10a). The intensities are quite comparable between the observed and predicted precipitation. We note that the model precipitation has a considerable larger areal coverage (see the 1-mm contour). This is possibly caused by the Kuo-type convective parameterization and the relatively coarse horizontal resolution (40 km). In the next 3 h, the model precipitation expanded in the northeast direction in a manner similar to the observed precipitation. Aside from the eastward shift and broad areal extent, the model precipitation associated with this convective system looks remarkably similar to the observation. One model error is the precipitation over the Texas panhandle, which was not observed. In the ensuing 6 h, the model precipitation continued to move eastward and expand in areal coverage in a way similar to the observations. For the 3-h accumulated precipitation ending at 0600 UTC, the control experiment also produced three distinct rainfall maxima over southwestern Missouri, southern Oklahoma, and central Texas. Although the loci of these precipitation maxima are not perfect, the shape of the model precipitation compares favorably with the observations. Overall, the precipitation forecast from this control experiment is reasonably good, except for the southward shift throughout the forecast. Given the relatively coarse horizontal (40 km) and vertical (10 level) resolution, as well as the simple precipitation parameterization used here, this is fairly encouraging.

Initialized with interpolated analyses, the precipitation for experiment 3 is notably weaker (Fig. 12a) than in the control (Fig. 11a). For example, the maximum 3-h accumulated rainfall ending at 2100 UTC was 7.9 mm over the Oklahoma–Kansas border for experiment 3 at a location far north of the observations with an amount far short of the control (13.7 mm). There is a significant difference in the rainfall distribution between these two experiments in the next 3 h. Experiment 3 produced a northwest–southeast zone of precipitation extending from Nebraska to Arkansas (Fig. 12b), distinctly different from the control, which produced a northeast–southwest band of precipitation. During the following 3 h, experiment 3 produced significant precipitation over northern Texas, while the control concentrated its precipitation over eastern Oklahoma. Even by the end of the 12-h forecast, visible differences in rainfall distribution are quite evident. In summary, we see that when the model was initialized with an interpolated analysis, the precipitation forecast was degraded considerably compared with both the observations and the control experiment. It produced considerably weaker precipitation initially. Later, the rainfall distribution became quite different from the control.

The assimilation of wind and temperature fields (experiment 6) resulted in significant improvement in the model flow fields (not shown). Also, there was some improvement in the model precipitation during the first 3-h forecast (Fig. 13a). The rainfall maximum is now located over northern Texas instead of the Kansas–Oklahoma border. Later in the period, improvements over the experiment with no assimilation (experiment 3) become more evident, as the rainfall distribution began to more closely resemble that of the control. Particularly, during the 6-h period ending at 0600 UTC 10 April, the line pattern of precipitation associated with the squall line was well captured (see Figs. 13c and 13d).

The assimilation of PW and surface humidity observations led to improvement in the precipitation forecast early in the period. For example, the maximum 3-h accumulated rainfall ending at 2100 UTC was 7.9 mm at a location almost identical to that of the control (Fig. 14a). Later in the periods, the pre-
precipitation distribution continues to show improvement over the experiment without data assimilation. However, the assimilation of PW and surface humidity data (experiment 5) does not perform better than the experiment that assimilates wind and temperature (experiment 6). This is particularly evident during the later periods. For example, the 3-h precipitation ending at 0300 UTC 11 April (Fig. 14c) in experiment 5 shows a precipitation maximum over south-central Oklahoma, while both the control and experiment 6 place the maximum precipitation farther to the north and east. The linear precipitation pattern associated with the squall line over eastern Oklahoma and northern Texas found in the control and experiment 6 was not as evident in experiment 5. The final 3-h rainfall of experiment 5 was even worse as compared with the control. These results suggest that the assimilation of one-time-level PW and surface humidity data without the supporting wind and temperature information cannot improve precipitation forecasts over a sustained period.

The best precipitation forecasts are obtained when PW and surface humidity data were assimilated along with the wind and temperature information (experiment 7; Fig. 15). The precipitation forecasts during the first 3 h between experiment 7 and the control are almost identical. Later in the periods, aside from some minor differences, the rainfall distribution and intensity are remarkably similar between these two experiments. Comparison of results from experiments 6 and 7 indicates that the assimilation of PW and surface humidity data adds significant value to
wind and temperature assimilation in improving precipitation forecasts.

To provide an objective measure on the impact of data assimilation on precipitation forecasts, we calculate the threat score for all the experiments as verified against the precipitation forecast of the control. Since we conducted one-time-level data assimilation in experiments 4–7, we have chosen to present the verification results against the control. In this way, we can more clearly see the effects of 4DVAR assimilation of various variables. Notice that a three-dimensional analysis of specific humidity is used in experiment 1 but not in experiments 4–7. The results for the precipitation threshold of 5 mm are presented in Fig. 16. Initialized with interpolated analysis, experiment 3 (thick solid line) has a threat score close to zero during the first 6 h. By the end of the 12-h forecast, it gradually increases to about 0.30. The assimilation of PW data alone (dashed line) increases the threat score by 0.05–0.1 during most of the 12-h forecast period. The inclusion of surface humidity data (dotted line) provides an additional improvement of 0.1–0.15 in threat score during the first 6-h period. Its impact later in the forecast is very small. The assimilation of wind and temperature (dot–dashed line) has little impact during the first 3-h forecast. However, later in the period, its impact is considerably larger than that of PW and surface humidity assimilation. The best results are obtained when PW and surface humidity data are assimilated along with the wind and temperature data (long-dashed line). The threat scores during the entire 12-h forecast for experiment 7 are generally greater than 0.55. This
is truly remarkable because no detailed information on the vertical structure of atmospheric water vapor is available in the PW data. Yet the assimilation of PW and surface humidity adds considerable value to the wind and temperature assimilation. The impact on the precipitation forecast as a result of PW and surface humidity data assimilation during the first 6 h is particularly impressive. For example, the threat score was increased from 0.01 to 0.48 for 3-h forecast (ending at 2100 UTC 10 April) and from 0.43 to 0.65 for 6-h forecast (ending at 0600 UTC 10 April) as a result of adding PW and surface humidity data to wind and temperature assimilation (experiment 7 versus experiment 6).

In our analysis of the model precipitation forecasts from various 4DVAR experiments, we found that most of the precipitation was produced by the Kuo-type convective parameterization. As described in Kuo (1974) and Kuo and Anthes (1984), the precipitation produced by the Kuo-type scheme is directly related to moisture convergence. To gain further insight into the effects of 4DVAR on precipitation forecasts, we show in Fig. 17 the vertically integrated moisture convergence (IMC) at 1800 UTC 10 April for several experiments, which is defined as

$$M_c = \frac{1}{g} \int_0^\sigma \nabla \cdot (p^* \nu g) \, d\sigma,$$  \hspace{1cm} (3.5)

where $g$ is gravity and $\nu$ is specific humidity. The KGW analysis shows an area of moisture convergence over northern Texas (Fig. 17a), with a maximum of 16.1 MCU (moisture convergence unit, defined as 1 MCU = $10^{-5}$ g s$^{-1}$ cm$^{-2}$), corresponding to the region of
precipitation in the control run (Fig. 17a). With the assimilation of PW and surface humidity data (Fig. 17b), the maximum IMC in experiment 5 is 20 MCU. The area covered by the 10-MCU contour is larger than that in the control. The assimilation of wind and temperature (experiment 6; Fig. 17c) has a maximum of 9.9 MCU over northern Texas, considerably weaker than that in the control. Again, the best results are obtained with PW, surface humidity, wind, and temperature assimilation (experiment 7, Fig. 17d). The pattern and intensity of moisture convergence are almost identical to those of the control. Three hours later, the IMC in the control has grown to nearly 29.5 MCU (Fig. 18a), while that in experiment 5 has been reduced to 11.6 MCU (Fig. 18b). Here we again see that the assimilation of PW and surface moisture data without the wind and temperature observations is not sufficient to simulate the evolution of the moisture convergence. The assimilation of wind and temperature (experiment 6) did better than the assimilation of PW and surface humidity data (experiment 5). The maximum IMC in experiment 6 grew to 22.1 MCU, closer to that of the control as compared with experiment 5. The best forecast is again obtained in experiment 7, when PW and surface moisture data were assimilated along with the wind and temperature data. These results show that the assimilation of PW and surface humidity data by themselves has a positive but limited impact on the short-range precipitation forecast. However, when these data are used in combination with the wind and temperature data, they are quite effective in improving the short-range precipitation forecasts.
4. Sensitivity to initial guess and model physics

The results presented in section 3 focused on 4DVAR assimilation of one-time-level PW and surface humidity data. An adiabatic version of MM5 and its adjoint was used in the 4DVAR assimilation system, and the initial guess was provided by linear interpolation of analyses at 1200 UTC 10 April and 0000 UTC 11 April. Two issues can be raised, one concerning the initial guess, and the other related to model physics. We should not expect that the solution to the variational problem of one-time-level PW data assimilation be unique since the atmospheric water vapor is a three-dimensional quantity, with significant horizontal and vertical variation at any given time. The PW analysis is an integrated quantity, only with horizontal variations. The specification of three-dimensional water vapor structure using a one-time-level two-dimensional PW analysis is, by definition, an incomplete observation problem. The 4DVAR assimilation using one-time-level PW data can improve upon the quality of the initial guess moisture field. However, when PW data are available at several time levels during the assimilation period, the solution to the variational problem may become unique. Concerning the impact of physical processes on the results of 4DVAR retrieval experiments, we have repeated a number of 4DVAR experiments presented in section 3 using a full-physics version of MM5 and its adjoint. We found that the results of moisture retrieval and precipitation forecasts are not very sensitive to physics. Two reasons might be given to explain this lack of sensitivity to model physics. One is that 1 h is a relatively short assimilation period. Model physics has a limited influence on the results.
The other reason is that there was little precipitation between 1700 and 1800 UTC 10 April. Therefore, precipitation physics should not have played an important role. In this section, we present results from additional experiments designed to address these two issues.

In this second set of experiments, we performed 4DVAR assimilation of PW data during the 3-h period of 1800 UTC to 2100 UTC 10 April. The PW analysis at 1800 UTC and the 3-h forecast of PW from the control (valid at 2100 UTC) were used as the "observed" PW data. We have chosen to use the observing system simulation experiment (OSSE) framework instead of a real-data framework in this study, with the intention of gaining some "theoretical guidance" on this problem. This is necessary because the simplified version of the MM5 model was used in this study, and the detailed structure of the convective systems observed in this case is difficult to simulate using a 40-km model. In addition, the limit in computing resources does not permit the use of the adjoint of a high-resolution version of MM5 with sophisticated physics. The cost of finishing 30 iterations for experiments 8 and 9 is about 3 CPU hours on a single processor of CRAY-YMP and requires 14.1-MW memory.

Experiments 8–10 assimilated PW data at both 1800 UTC and 2100 UTC 10 April during the 3-h assimilation period. The PW data at 2100 UTC 10 April was generated by the control experiment. In all these three experiments, the initial guess of the wind, temperature, pressure, and vertical velocity were obtained from the KGW analysis at 1800 UTC 10 April (identical to the control). The only differences between the experiments are the initial guess for the humidity fields and the physics used in the 4DVAR system. In experiment
high (with values greater than 1.5 g kg$^{-1}$) during the first 6-h forecast. It gradually decreases to 1.35 g kg$^{-1}$ by the end of the 12-h forecast. Using the "optimized" initial moisture fields (experiment 9, solid line), the VQRMS is drastically reduced from 1.54 to 1.15 g kg$^{-1}$ at 1800 UTC 10 April. The differences between these two forecasts using the original guess humidity field (experiment 9g) versus the optimal humidity field (experiment 9) remains fairly large during the first 6 h of the forecasts. The differences in VQRMS between the time-interpolated guess humidity field (experiment 8g; long-dashed line) and its corresponding optimal humidity field (experiment 8; dot–dashed line) are considerably smaller. The differences in VQRMS between experiments 8 and 9, both with optimal moisture fields, are in the range of 0.05–0.1 g kg$^{-1}$ during the 12-h forecast period. Figure 20b shows the threat score of the 3-h rainfall precipitation at the threshold of 5 mm for experiments 8 (dot–dashed line), 8g (long-dashed line), 9 (solid line), and 9g (dotted line). Again we see dramatic improvement in precipitation forecasts as a result of 4DVAR assimilation of PW data. Regardless of how the initial guess moisture field is obtained, the assimilation of PW data improved the threat score by more than 0.30 during the first 6 h of the forecast. The differences between experiments 8 and 9 are very small for a 3-h forecast. They become larger later in the forecast, with differences in threat scores close to 0.1. It is interesting to note that the threat score for experiment 9 is better than experiment 8g. This shows that the assimilation of two-time-level PW data can correct a very poor moisture field and produce better precipitation forecasts than the one that uses time-interpolated analysis. We conclude that the quality of the initial guess moisture field has a small impact on the retrieved water vapor fields when PW data were provided at both the beginning and the end of the assimilation period. The 4DVAR was effective in correcting a very poor initial guess field with PW assimilation. The sensitivity of precipitation forecast to initial guess is very small initially (comparing experiments 8g and 9g) but becomes moderately large later in the forecasts. Given the dramatic differences between the two initial guess moisture fields, our results suggest that the 4DVAR is relatively insensitive to the quality of the guess fields.

We next examine the effects of moist physics on a 4DVAR system. Figure 21 shows the vertical profiles of rms errors in wind, temperature, and specific humidity for experiments 9 (solid line) and 10 (dashed line) after 30 iterations. We note that with the inclusion of moist physics, the rms errors in the "optimal" initial state are reduced by more than 50% for the wind fields in the upper and lower troposphere. The improvement in the upper-level temperature field is equally impressive. At $\sigma = 0.25$, the rms temperature error in experiment 10 (adiabatic) is close to 1°C, while that in experiment 9 (diabatic 4DVAR) is about 0.4°C. The reduction of temperature errors is smaller in the lower
troposphere. However, an important result is that the inclusion of moist physics shows definitive improvements in the optimal initial states in wind and temperature fields. Positive impact is also found in the moisture field throughout the troposphere, except for a shallow layer at $\sigma = 0.85$. The improvements in the moisture field are smaller because PW data were assimilated in both experiments.

To gain insight into the differences between adiabatic and diabatic 4DVAR, we showed in Fig. 22 the differences in wind fields between experiments 9 and 10 at $\sigma = 0.25$ (Fig. 22a) and $\sigma = 0.85$ (Fig. 22b) at 1800 UTC 10 April after an optimal initial state is obtained (after 30 iterations). We found that the effect of the moist physics is not random. Rather, it produced organized change in the flow fields. In the upper level, it produced an organized divergent flow, with wind speed exceeding 4 m s$^{-1}$ over many places. The center of the upper-level divergence was located over the Oklahoma-Kansas region, where heavy precipitation took place. In the lower troposphere, convergence is noted in the difference flow fields. The difference wind also shows that the moist physics induced persistent southeasterly flow at the lower levels, which enhanced moisture fluxes from the Gulf of Mexico into the Central United States. The broad-scale low-level convergence and upper-level divergence, and the enhanced moisture transport, are factors that can contribute to enhanced precipitation over the central United States and support the continued evolution of the convective system.
Figures 22c and 22e show the errors of the retrieved temperature fields (differences between the optimal state and the temperature analysis of KGW) at $\sigma = 0.25$ for experiments 10 (adiabatic, Fig. 22c) and 9 (diabatic, Fig. 22e). It is interesting to note that the errors are considerably larger for diabatic 4DVAR. Over a number of places, the errors in the optimal initial state after diabatic 4DVAR are as large as 2.5°C. Over regions where convective systems are taking place between 1800 and 2100 UTC, the temperature errors are generally greater than 2.0°C. In contrast, the temperature errors associated with the diabatic 4DVAR are considerably smaller, they are less than 0.25°C over regions of precipitation. There are some isolated areas where diabatic 4DVAR temperature errors exceed 1.5°C. These all occurred over regions away from the convective system and are possibly related to errors in the original temperature analysis (for example, measurement errors or inconsistency between wind and temperature analyses). Similar results are found at $\sigma = 0.85$ (Figs. 22d,f). Again, the temperature errors of adiabatic 4DVAR (Fig. 22d) are considerably larger than that of the diabatic 4DVAR (Fig. 22f). This is very interesting because a high quality temperature field at 1800 UTC 10 April was used as the initial guess field (same as control) prior to 4DVAR. With moist physics, the 4DVAR produces a solution much closer to the KGW final analysis (thus, lower errors). However, when moist physics is absent, the adiabatic 4DVAR still has to modify the initial guess in order to minimize the cost function. That modification can actually cause errors in the “optimal” initial temperature field when moist physics is missing. In summary, we found that including moist physics in 4DVAR pro-
duced organized changes in wind and temperature fields and minimized their errors. These changes appear to favor enhanced precipitation. The question then becomes: Would these changes lead to improved precipitation forecasts?

The answer to this question is positive and is illustrated in Fig. 23. With the inclusion of moist physics in 4DVAR (experiment 9, solid line), the threat score at the 5-mm threshold has increased from 0.30 (experiment 10; dashed line) to 0.50 at the 3-h forecast and 0.25 to 0.5 at the 6-h forecast. This is truly remarkable. Using the same PW data during the 3-h assimilation window, the inclusion of moist physics produced a significant impact on short-range precipitation forecasts. The differences between experiment 9 and experiment 9g (no assimilation; dotted line) are even more dramatic. Obviously, inclusion of moist physics produces a better fit between the model solution and the data. Consequently, a better initial state is obtained, which leads to improved subsequent forecasts.

5. Summary and conclusions

Although cost-effective profiling of atmospheric water vapor is not yet available, several remote sensing systems are capable of providing highly accurate precipitable water measurements. Such data are potentially useful for operational numerical weather prediction. However, in order to make use of such data for operational forecasting, an effective data assimilation method should be developed. In this paper, we conducted a series of experiments using a variational data assimilation system based on the Penn State–NCAR mesoscale model MM5 and its adjoint. These experiments were conducted using the special sounding data collected during the SESAME 1979 experiment.

In the first set of experiments, we assumed that only one-time-level PW data were available. The data assimilation was limited to a 1-h window between 1700 and 1800 UTC 10 April. We found that the assimilation of PW data can recover useful information on the vertical structure of water vapor and improve the quality of the initial guess moisture field. The vertically integrated rms errors in the initial guess moisture field were reduced by 20% as a result of PW assimilation. The addition of surface humidity data in the 4DVAR was found to be quite effective in further improving the quality of moisture analysis in the lower troposphere. Compared to the original guess field, the assimilation of PW and surface humidity data reduced the rms errors in the moisture field by as much as 40%. The assimilation of wind and temperature reduced the moisture errors only by about 5%. This shows that the wind and temperature data do not contain sufficient information on the moisture fields. Assimilation of moisture data (such as PW measurements or surface humidity observations) is necessary to improve the quality of moisture analysis.

The improved moisture analysis as a result of PW assimilation led to improvements in short-range precipitation forecasts. The threat score at the 5-mm threshold was increased by nearly 0.1 due to PW assimilation. The inclusion of surface humidity data was found to be quite effective in further improvement in precipitation forecast, particularly during the first 6 h. However, we found that the assimilation of wind and temperature (without PW or moisture data) had a stronger impact on short-range precipitation forecasts than the assimilation of PW and surface moisture data later in the forecast. This shows that having an accurate description of the dynamic fields (through wind and temperature assimilation) is more important than improving the moisture analysis. The best results were obtained when PW and surface humidity data were assimilated in combination with the wind and temperature data. Our results indicate that when wind and temperature observations are available, the addition of PW and surface humidity data in the 4DVAR system drastically improves the precipitation forecast. For example, the threat score for the 3-h accumulated rainfall during the first 3-h forecast
carried out in an OSSE framework, in which the initial condition and 3-h forecasts from a control experiment were used to provide the "observed" PW data. We

was raised from 0.01 to 0.48 due to the addition of PW and surface moisture data in the 4DVAR system. With the continued deployment of wind profiler systems and other remote sensing systems, wind and temperature data can potentially be available over the continental United States at a fairly high temporal and spatial resolution. Our results suggest that the assimilation of PW and surface moisture data can lead to significant improvement in short-range quantitative precipitation forecasts when used along with the wind and temperature data.

In the second set of experiments, we carried out 3-h assimilation of PW data to test the sensitivity of 4DVAR to the initial guess field (prior to data assimilation) and moist physics. This set of experiments was
Fig. 22. The differences in wind fields at $\sigma = 0.25$ (a) and $\sigma = 0.85$ (b) at 1800 UTC 10 April for the optimal initial states between experiments 9 and 10, and the errors of the retrieved temperature fields at $\sigma = 0.25$ (c) and $\sigma = 0.85$ (d) for experiments 10 and 9 ($\sigma = 0.25$; $\sigma = 0.85$). The contour intervals are 2 m s$^{-1}$ for (a) and (b), 0.5°C for (c) and (e), and 0.25°C for (d) and (f). The maximum vector in (a) and (b) represents a wind of 7.3 and 2.4 m s$^{-1}$, respectively.
found that even when a very poor initial moisture analysis was used as the guess field (at zero iteration), 4DVAR was quite effective in producing a high quality moisture field after PW assimilation. The “optimal” initial state assimilating two-time-level PW data in a 3-h window is only slightly sensitive to the quality of the initial guess field. However, the number of iterations required depends on the quality of the guess field. In our experiments, the number of iteration was increased from 30 to 50 when a poor guess field was used. The “optimal” state using a poor guess field has a slightly higher error in the moisture fields and a lower score in precipitation forecasts. It is particularly encouraging to find that even with a horizontally homogeneous guess moisture field, 4DVAR was able to produce a good quality moisture field with PW assimilation. The weak sensitivity to the guess field is a very important property of 4DVAR, which differentiates itself from the simple nudging technique.

Our results also show that the inclusion of moist physics in the MM5 and its adjoint during the 3-h assimilation process leads to significant improvements in the derived “optimal” initial state and the subsequent short-range precipitation forecasts. The inclusion of moist physics in the 4DVAR process produced marked, organized differences in the resulting wind, temperature, and moisture fields. Generally, we found enhanced upper-level divergence, low-level convergence, and increased moisture fluxes in the vicinity of the precipitating area. These differences supported the continued evolution of the given precipitating system and provided a better fit to the observed data. Consequently, the skill score in the subsequent precipitation forecast increased dramatically as a result of including moist physics in the assimilation system. These results are significant and encouraging. They clearly show that the development and inclusion of the adjoint of various model physical processes in the 4DVAR system can reduce the model systematic biases and produce a better fit between the model and the data and, consequently, a better data assimilation and an improved forecast. One should expect the effects of physics to become even more important as the duration of the assimilation window is lengthened.

Currently, PW can be measured remotely in several satellite-based and ground-based remote sensing instruments (see appendix A in KGW). The horizontal and temporal resolution of these PW measurements are much higher than what we could derive from the special 3-h soundings of the SESAME case, which has a horizontal resolution of approximately 250 km. Therefore, several questions remain to be addressed. (i) How does the horizontal and temporal resolution impact the quality of the retrieved three-dimensional specific humidity field and the rainfall prediction? (ii) How does the accuracy of the 4DVAR results change as the resolution of the PW measurements increases? (iii) What would be the expected optimal resolution of PW measurements for short-term rainfall prediction? It is also important to properly define an error covariance matrix and a background term in the cost function for the assimilations of PW measurements. Future work will also show whether or not there is a significant positive impact on forecast quality from the direct use of both the PW measurements and 3-h rainfall observations over a 3- or 6-h assimilation window using a model with a higher vertical resolution. All of these problems need to be addressed before we can draw a general conclusion on the impact of PW assimilation to numerical weather prediction.

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