Simulation of the fine structure of the 12 July 1996 Stratosphere-Troposphere Experiment: Radiation, Aerosols and Ozone (STERAO-A) storm accounting for effects of terrain and interaction with mesoscale flow

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[1] Vertical mixing of chemical tracers and optically active constituents by deep convection affects regional and global chemical balances in the troposphere and lower stratosphere. This important process is not explicitly resolved in global and regional models and has to be parameterized. However, mixing depends strongly on the spatial structure, strength, and temporal evolution of the particular storm, complicating parameterization of this important effect in the large-scale models. To better quantify dynamic fields and associated mixing processes, we simulate a thunderstorm observed on 12 July 1996 during the STERAO-A (Stratosphere-Troposphere Experiment: Radiation, Aerosols, and Ozone) Deep Convection field project using the Goddard Cloud Ensemble (GCE) model. The 12 July STERAO-A storm had very complex temporal and spatial structure. The meteorological environment and evolution of the storm were significantly different than those of the 10 July STERAO-A storm extensively discussed in previous studies. Our 2-D and 3-D GCE model runs with uniform one-sounding initialization were unable to reproduce the full life cycle of the 12 July storm observed by the CHILL radar system. To describe the storm evolution, we modified the 3-D GCE model to include the effects of terrain and the capability of using nonuniform initial fields. We conducted a series of numerical experiments and reproduced the observed life cycle and fine spatial structure of the storm. The main characteristics of the 3-D simulation of the 12 July storm were compared with observations, with 2-D simulations of the same storm, and with the evolution of the 10 July storm. The simulated 3-D convection appears to be stronger and more realistic than in our 2-D simulations. Having developed in a less unstable environment than the 10 July 1996 STERAO-A storm, our simulation of the 12 July storm produced weaker but sustainable convection that was significantly fed by wind shear instability in the lower troposphere. The time evolution, direction, and speed of propagation of the storm were determined by interaction with the nonuniform background mesoscale flow. For example, storm intensity decreased drastically when the storm left the region with large convective available potential energy. The model appears to be successful in reproducing the rectangular four-cell structure of the convection. The distributions of convergence, vertical vorticity, and position of the inflow level in the later single-cell regime compare favorably with the airborne Doppler radar observations. This analysis allowed us to better understand the role of terrain and mesoscale circulation in the development of a midlatitude deep convective system and associated convective mixing. Wind, temperature, hydrometeor, and turbulent diffusion coefficient data from the cloud model simulations were provided for off-line 3-D cloud-scale chemical transport simulations discussed in the companion paper by DeCaria et al. (2005).
1. Introduction

[2] It is well known that convective activity, which currently is not explicitly resolved in general circulation models (GCMs), plays an important role in atmospheric circulation contributing to upward transport of water vapor, momentum, and stratosphere-troposphere exchange. Strong convective storms generate gravity waves that perturb the tropopause and penetrate the stratosphere and mesosphere where they break and dissipate, depositing momentum and energy [Holton, 1982] that play an important role in the circulation of the middle atmosphere. Deep convection redistributes trace gases and aerosols from the boundary layer to the free troposphere [Chatfield and Crutzen, 1984; Dickerson et al., 1987; Stenchikov et al., 1996]. Chemical species detrained in the middle and the upper troposphere are advected for long distances, experiencing chemical transformation, and affecting regional and global chemical budgets [Pickering et al., 1990, 1992a, 1992b, 1996], eventually altering Earth’s radiative balance.

[3] Some of the important effects of convection are implemented in GCMs and chemical transport models (CTMs) in the form of parameterizations. However, the complexity of convective processes, the dependence of these processes on numerous factors, and nonlinear interaction with the mesoscale environment [Donner et al., 1999] limit the accuracy of these parameterizations.

[4] The Stratosphere-Troposphere Experiment: Radiation, Aerosols, and Ozone, Part A (STERAO-A) campaign was specifically designed to clarify the effects of midlatitude convection on tropospheric ozone, accounting for a comprehensive set of physical processes including lightning [Dye et al., 2000]. The most impressive thunderstorm in this campaign was observed on 10 July 1996 and has been discussed in detail by Dye et al. [2000], Skamarock et al. [2000, 2003], and Barth et al. [2001].

[5] To better understand the variability of the effects of convection and their dependence on the mesoscale environment we studied a convective storm observed over southeastern Wyoming, northern Colorado, and southwestern Nebraska on 12 July 1996, during STERAO-A. We discuss our results in this and a companion paper [DeCaria et al., 2005]. This paper deals with the reconstruction of dynamic fields that are used by DeCaria et al. [2005] for transport and chemistry experiments. In the companion paper we present results of tracer transport calculations for CO and other gases, which are reasonably well conserved over the lifetime of the storm. Accurate representation of convective transport in the model, along with observations of lightning flash rates and anvil NOx (NO + NO2), allowed DeCaria et al. to estimate the amount of NO production per flash. The dynamical fields were also used to drive a cloud-scale photochemical model to compute the effects of convective transport and lightning on tropospheric ozone, an important radiatively active trace gas in the upper troposphere.

[6] The 12 July STERAO storm is significantly different than the strongest STERAO storm, which occurred 2 days earlier on 10 July. The convection on 12 July developed in a significantly more stable environment than on 10 July. Therefore it was extremely difficult to produce the 12 July convection in the model simulations. It seems that both elevated terrain and a strongly nonuniform distribution of Convective Available Potential Energy (CAPE) played important roles in the 12 July storm transition from a multicellular line, to a rectangular four-cell structure, and then to a single intense cell that may have acquired supercell characteristics for a brief period. It is important to reproduce this fine structure of the storm in simulations because it significantly affects vertical convective mixing of tracers. We employed both 2-D and 3-D versions of the Goddard Cloud Ensemble (GCE) model [Tao and Simpson, 1989a, 1989b; Tao et al., 1991, 1993, 2003] to simulate different (but overlapping) phases of the storm. Our 2-D results have been discussed by DeCaria et al. [2000].

[7] The 3-D and 2-D GCE models are based on the same physics. The 2-D GCE model has been used extensively for storm-scale research and convective transport of trace gas studies in the tropics and midlatitudes [e.g., Tao et al., 1991, 1993, 1996; Pickering et al., 1991, 1992a, 1992b, 1993, 1998; Scala et al., 1990]. It has been tested in numerous environments and agreed well with both remote (such as radar and passive microwave) and in situ observations from aircraft penetrations. Stenchikov et al. [1996] have applied the 2-D GCE model for a case study of a strong convective storm over the Great Plains in North Dakota on 28–29 June 1989, which was observed in detail during the North Dakota Thunderstorm Project (NDTP) [Boe et al., 1992].

[8] The 3-D GCE model, which requires significantly more computer resources than the 2-D version, is actively used in studies of interactions of clouds with each other [Tao and Simpson, 1989a] and with their surroundings. It was successfully applied to better quantify heat, moisture, momentum, mass, and water budgets associated with deep convection [e.g., Tao and Simpson, 1989b, 1993, Tao et al., 1993] accounting for surface fluxes and their impact on precipitation, CAPE distribution, and boundary layer structure [Lynn et al., 2001; Baker et al., 2001; Lynn and Tao, 2001; Wang et al., 2003; Johnson et al., 2002]. Cloud-scale chemical tracer transport based on the 3-D GCE simulations is discussed by Pickering et al. [1996] and DeCaria et al. [2005]. A review of recent applications of the GCE model to the understanding of precipitation processes is given by Tao et al. [2003] and Tao [2003].

[9] We found that we had to modify both the 2-D and 3-D GCE models to use spatially nonuniform initial conditions and account for terrain effects in order to simulate the 12 July STERAO storm. The period of linear organization from about 2030 UTC to 2300 UTC was simulated by DeCaria et al. [2000] using the 2-D GCE model. The 2-D simulations of the 12 July storm were conducted along the 41°N cross section from 105°W to 100°W, accounting for terrain and nonuniform initial fields extracted from the National Centers for Environmental Prediction (NCEP) Eta forecast fields. Horizontal resolution was 1 km. The
vertical grid was nonuniform with 31 levels and finest resolution (220 m) was located near the surface. Our 2-D simulation of the 12 July thunderstorm produced a convective cell with characteristics similar to observed at the initial stage of the storm development, but it was difficult to expect that a chosen cross section would be suitable for an extended simulation period in such a region with strong nonhomogeneities in the initial and boundary conditions.

In the 2-D simulations the surface-based convection began as two isolated cells forced nearly simultaneously by the upslope flow. The storm intensity maximized in about 1.5 hours when the top of the convective cell reached 13 km. Further evolution is characterized by a developing single-cell structure and a rapid decay of the storm when it moved into a region with low CAPE along 41°N. The speed of the simulated 2-D storm was 2 times faster than observed.

On the basis of these findings, we concluded that using the 2-D approach we can simulate only the initial evolution of the 12 July thunderstorm (i.e., the development of a multicellular line along the Wyoming-Colorado border as simulated by DeCaria et al. [2000]). Here we use the 3-D GCE model in a 5-hour simulation to capture the further evolution of the storm, including the transition from linear multicell convection to a highly 3-D single cell system. The 3-D meteorological fields were provided for the offline transport experiments conducted in the companion paper.

The main objectives of this study are as follows: (1) reconstruct the complex fine structure of the July 12 STERAO storm; (2) account for interaction of convection with the terrain and mesoscale circulation; (3) produce 3-D dynamic fields for chemistry modeling; (4) compare 2-D and 3-D simulations to clarify limitations of the 2-D approach; and (5) compare simulations with observations and with the July 10 STERAO storm.

2. GCE Model

The GCE model hydrodynamics is based on a complete set of compressible, nonhydrostatic equations in a Cartesian coordinate system. A second-order finite differencing scheme with small nonoscillatory horizontal advection schemes with small implicit diffusion [Smolarkiewicz, 1983; Smolarkiewicz and Grabowski, 1990] are employed for spatial approximation.

Open boundary conditions of Klemp and Wilhelmson [1978b] are used at the lateral boundaries. Newtonian damping is applied to the potential temperature and components of horizontal velocity at the top of the domain at about 25 km. At the bottom the GCE model is coupled with the land surface/vegetation model of Boone and Wetzel [1999]. However, this scheme was not employed in the current simulation.

A parameterization of sub-grid turbulent mixing is based on the prognostic equation for turbulent kinetic energy [Deardorff, 1975; Klemp and Wilhelmson, 1978a; Soong and Ogura, 1980]. Turbulent mixing is handled in the cloud model using a turbulent diffusion approximation.

A Kessler-type scheme [Kessler, 1969; Houze, 1993] for liquid hydrometeors (cloud water and rain) and the three-category scheme of Lin et al. [1983] for solid hydrometeors (ice, snow, and hail) are employed to parameterize cloud microphysics. The hydrometeors are assumed to be spherical with exponential size distributions except for cloud water and cloud ice, which are monodisperse. The hydrometeors are advected with the air motion, mixed by turbulent processes, and affected by deposition and microphysical transformations. A noniterative saturation adjustment scheme accounting for water and ice was implemented by Tao et al. [1989].

Short-wave and long-wave radiative transport is implemented following Chou and Kouvaris [1991], Chou and Suarez [1999], Chou et al. [1995, 1999], and Kratz et al. [1998]. The spectral approximation is conducted on 16 spectral intervals in the solar and thermal infrared (IR). The solar radiation scheme includes absorption due to water vapor, CO2, O3, and O2, aerosols and cloud hydrometeors, as well as Rayleigh scattering and scattering by clouds and aerosols. The long-wave scheme accounts for the effects of both gaseous (CO2, H2O, O3, N2O, CH4, CFCs) and hydrometeor absorption.

The GCE model uses a Cartesian grid with the altitude over a flat surface as the vertical coordinate. It originally did not account for terrain and assumes uniform initialization from a single sounding. To apply the 3-D GCE model for a case-study in a region with strong spatial inhomogeneities, we have modified it to use nonuniform initial distributions of the meteorological fields and account for terrain effects, as we did previously with the 2-D GCE model [DeCaria et al., 2000]. We account for the dynamical effect of terrain by keeping all components of the velocity equal to zero on and under terrain during the course of the calculations. This effectively obeys a "no slip" boundary condition at the surface and prevents any hydrodynamic fluxes of energy, momentum, or mass through the terrain. This approach is similar to the immersed boundary method first proposed by Peskin [1981] that is now widely used for calculating hydrodynamic flows with complex boundaries using finite difference methods in Cartesian coordinates [Iaccarino and Verzicco, 2003; Mittal et al., 2004].

In this study we integrated the model in a domain of 360 km by 328 km in the x and y directions, respectively. Positive x direction is from west to east, and positive y direction is from south to north. The horizontal grid spacing was 2 km in both horizontal directions, and 0.5 km in the vertical. The grid dimensions were 180 × 164 × 50 in the x, y, and z directions, respectively. For this spatial resolution, the time step that allowed numerically stable calculations was 3 s. We also applied additional damping at the lateral boundaries to prevent growth of the convective disturbances near the boundaries especially at the southern border of the domain.

3. Observed Storm Development

DeCaria et al. [2000] give a detailed description of synoptic conditions for 12 July. Continuous radar coverage was provided by the Colorado State University CHILL radar at Greeley, Colorado (40.45°N; 104.64°W). The National Oceanic and Atmospheric Administration (NOAA) WP-3D aircraft gathered Doppler radar data, flying legs parallel to the line of convection. The airborne Doppler radar was scanned 20° forward and aft of the
flight track, which allowed the reconstruction of the 3-D airflow field [Jorgensen et al., 1996]. The University of North Dakota Cessna Citation II measured CO, NO, O₃, hydrocarbons, cloud physics, and meteorological data. The WP-3D measured these variables plus a variety of additional chemical species. Visible satellite imagery is available during the entire period of storm development. Figure 4 of DeCaria et al. [2000] shows a satellite photograph with the anvil produced by the storm just north of the Colorado-Wyoming border oriented in a west-to-east direction at 2215 UTC. Strong convective activity is also seen to the south from a separate storm in east-central Colorado.

Figure 1. Colorado State University CHILL radar 4.50-km constant altitude plan position indicator (CAPPI) radar reflectivity factor (dBZ) obtained for the period (a) 2127 UTC, (b) 2207 UTC, (c) 2258 UTC, and (d) 0113 UTC. The ordinate and abscissa refer to distance in kilometers from the radar facility located at Greeley, Colorado (40.45°N, 104.64°W). The maximum reflectivity occurred at the position of the plus symbol. Figures 1c and 1d have the WP-3D aircraft track superimposed.

[21] The Colorado State University CHILL radar imagery (Figure 1) shows that during the early stages of growth from 2046 UTC to 2141 UTC, multiple, relatively weak, separated convective cells were located in southeastern Wyoming (Figure 1a). Between 2141 UTC and 2212 UTC, convective cells strengthened and organized in a linear structure with the highest reflectivity gradients generally located along the southern flank (Figure 1b). By 2258 UTC the storm developed a four-cell spatial structure with the strongest convection at the eastern flank (Figure 1c). The storm moved to the east-southeast with the leading edge reaching the Wyoming-Colorado border by 2304 UTC. The convection evolved further from an elongate structure into a
more oblate form containing a strong reflectivity signature at the western periphery of the cloud complex between 2258 UTC and 2330 UTC. By 2330 UTC, the convection acquired more of a southeast propagation with a speed of about 8 m/s. In addition to this somewhat deviant motion, the radar reflectivity pattern developed a V-signature in the midtroposphere clearly indicating a 3-D storm-scale circulation characteristic of severe convection. Strong reflectivity gradients remained at the southwestern edge of the storm with an extensive anvil blowing off to the northeast. The northeastern-most convective cell dominated and by 0113 UTC on 13 July only this single intense convective cell remained (Figure 1d). The separate convective activity to the south is also clearly seen on the radar image for 0113 UTC (Figure 1d).

4. Initialization of Convection

[22] The thermodynamic diagram of temperature, dew point, and wind composited from the soundings at Fort Morgan, Colorado, at 1956 UTC and aircraft data taken by the NOAA WP-3D at 2200 UTC ahead of the storm shows instability in the lower troposphere [see DeCaria et al., 2000, Figure 3]. However, the CAPE was as low as 700 m$^2$s$^{-2}$, which is almost a factor of 2.5 less than on 10 July when it reached 1850 m$^2$s$^{-2}$. The significant portion of instability on 12 July could be attributed to the strong wind shear that reached ~35 m s$^{-1}$ in the 6-km layer above the terrain in the region where the storm initially developed. The bulk Richardson number of approximately 7 supports development of supercell convection (if CAPE is sufficient).

[23] We were unsuccessful at simulating a sustainable storm using uniform initial conditions based on the composite soundings from DeCaria et al. [2000] with either the 2-D or 3-D GCE model. In this study we have developed 3-D nonuniform initial fields and accounted for the effects of terrain to simulate a storm similar to the observed one using a modified version of the 3-D GCE model.

[24] To construct nonhomogeneous initial conditions for our simulations we utilized routine forecast and analysis fields from the NCEP Eta Model [Mesingher et al., 1988; Rogers et al., 1996]. The Eta Model data were provided by NCEP in gridded binary (GRIB) format on an irregular Eta-model horizontal grid with resolution about 32 km. The Eta Model data included surface pressure, surface elevation, and 3-D fields of pressure, temperature, water vapor mixing ratio, and horizontal wind components on 26 pressure levels for the entire United States. These data were first interpolated to a regular horizontal grid with 0.5° grid spacing and vertical grid identical to that used in the cloud model. After choosing a 3-D domain for the cloud model simulations, the fields are then projected onto the cloud model’s horizontal grid.

[25] Although a finer terrain profile could have been used, the Eta Model terrain profile was chosen in order to keep the initial meteorological fields, which are also derived from the Eta Model, dynamically consistent at the lower boundary. The pressure field is adjusted to make it consistent with the GCE model formulation. This helps to decrease the generation of gravity and sound waves during an approximately 15-min spin-up period. Applying nonuniform initial conditions and corresponding boundary conditions allows us to account for interaction of the storm with the mesoscale features, (e.g., upslope flow, nonuniform spatial distribution of CAPE, and wind shear) which developed in the region because of larger-scale circulation processes not accounted for in our calculations. Interactions with mesoscale features appear to play an important role in thunderstorm life cycle, as does the mesoscale response to the deep convection that modifies CAPE and wind shear background distributions in the calculation domain [e.g., Donner et al., 1999].

[26] For our relatively short-term simulations we have chosen initial fields from the middle of the period of storm development to better characterize the entire period. The Eta analysis fields were not available for this particular time. Therefore we constructed the initial conditions using most suitable Eta forecast fields. The most recent available data were forecast fields from the 1200 UTC 12 July Eta Model run. Eta Model data were extracted from the 6-hour forecast (valid 1800 UTC 12 July) and the 12-hour forecast (valid 0000 UTC 13 July.) The 12-hour forecast valid at 0000 UTC 13 July was chosen for initial conditions over the 6-hour forecast valid at 1800 UTC because the Eta Model was slow in developing the post-frontal upslope flow, a critical component for convection along the mountains of the Front Range. Observations from Laramie, Wyoming, (located near 105.6°W) at 1800 UTC showed a 4 m s$^{-1}$ easterly wind component, while an easterly wind component was absent in the Eta 6-hour forecast valid at that time at Laramie’s longitude. In contrast, the 12-hour Eta forecast fields did contain an easterly component at Laramie’s longitude, and were in much closer agreement with the observations at 1800 UTC. The 12-hour forecast fields also verified better than the 6-hour fields for the zonal wind speed above 400 hPa. Temperature and surface pressure from the 12-hour Eta forecast are also in a good agreement with observations. However, water vapor mixing ratio is slightly underestimated [DeCaria et al., 2000].

[27] Figure 2 shows the Eta fields used for initial and boundary conditions. The fields are shown in the domain used for our 3-D GCE simulations. Figure 2a depicts the land elevation (shown by isolines with contour interval of 100 m) and vectors of surface wind. The easterly upwind flow tends to force convection at the initial phase of the storm evolution. The maximum value of CAPE (Figure 2b) in the storm region is about 700 m$^2$s$^{-2}$, which is consistent with the composite soundings from DeCaria et al. [2000]. CAPE reaches its maximum value in the relatively narrow region elongated along the mountain ridge.

[28] In the 3-D simulations convection (in accordance with observations) has been initiated at the border of the region with relatively high CAPE at about (41.1°N, 104.5°W) near the northwest corner of the model domain (Figure 2b). CAPE in this region was only 600 m$^2$s$^{-2}$ which is barely enough to support initial storm development. This explains why the simulation was sensitive to the position where the storm is initialized. If the position of initial disturbances is shifted to the region where CAPE is 500 m$^2$s$^{-2}$, the storm would not develop. The CAPE distribution also plays an important role in the long-term storm development. The southeastward propagation of the storm follows the higher values of CAPE. As soon as
DeCaria et al. activity seen on the satellite and radar images (see corresponding to the location of separate strong convective highest values of CAPE farther south in the domain collapsed much earlier than was observed. The regions of rapidly out of the area with high CAPE very quickly and 2-D simulation conducted along 41°

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5.1. Model Configuration

5.3-D GCE Calculations

Figure 2. Eta Model fields used for initialization of the GCE model simulations. (a) Land elevation (m) and surface wind vectors. (b) CAPE (J kg⁻¹ m⁻²). The domain corresponds to the domain used in our 3-D calculations.
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the storm propagates away from the region with CAPE above 600 m s⁻², it dissipates quickly. For example, in the 2-D simulation conducted along 41°N the storm moved rapidly out of the area with high CAPE very quickly and collapsed much earlier than was observed. The regions of highest values of CAPE farther south in the domain correspond to the location of separate strong convective activity seen on the satellite and radar images (see DeCaria et al. [2000, Figure 4] and Figure 1).

5. 3-D GCE Calculations

5.1. Model Configuration

[29] We found that the 2-D GCE model failed to describe the extended evolution of the storm when it obtained a 3-D structure after about 2300 UTC [DeCaria et al., 2000]. The 2-D model also produced a storm that moved much faster than the observed one. This is mainly because the 3-D interactions of the storm with the terrain and mesoscale circulation define direction and speed of the storm propagation, and led to the development of the observed fine spatial structure of the convection. Therefore we modified the GCE model to include the effects of terrain and the capability to use nonuniform initial fields as discussed above. For the 3-D simulations, we have to choose a smaller domain than in our 2-D calculations. However, it covers an area of 380 km × 328 km which is large enough to follow the storm evolution for about 5 hours until it dissipates. The simulations start from the initial conditions constructed from the Eta fields for 0000 UTC (Figure 2). Horizontal resolution was 2 km in both the east-west and north-south directions. Vertical spacing was 500 m with 50 vertical levels. As in the work by Skamarock et al. [2000], we did not include in this simulation the effects of radiation and of latent and turbulent surface heat fluxes, as they are of secondary importance for short-term convective processes developing in an unstable meteorological environment, such as that considered here.

[30] Because the simulated 12 July storm moved to the southeast (consistent with observations), the domain was shifted in this direction and convection was initialized in the northwestern corner of the domain to allow convection sufficient space to proceed to the southeast as in the observations. A three-cell east-west-oriented linear convective structure was initialized with the potential temperature perturbation Δθ,

\[
\Delta \theta = 8 \theta \sum_{i=1}^{3} \exp \left[ -\frac{(x-x_i)^2}{\sigma_x^2} - \frac{(y-y_i)^2}{\sigma_y^2} - \frac{(z-z_i)^2}{\sigma_z^2} \right],
\]

where \(x_i, y_i, z_i\) are coordinates of the center of perturbations measured from the south-west corner of the domain and from sea level

\[
x_1 = 104.75° W, y_1 = 41.1° N, z_1 = 3500 m,
\]

\[
x_2 = 104.50° W, y_2 = 41.1° N, z_2 = 3500 m,
\]

\[
x_3 = 104.25° W, y_3 = 41.1° N, z_3 = 3500 m.
\]

The widths and amplitude of perturbations are \(\sigma_x = 5\) km, \(\sigma_y = 5\) km, \(\sigma_z = 1.5\) km, and \(8\theta = 4\) K.

[31] The position and the structure of the initial perturbation in the model corresponds to the position of the multicellular line which evolved between 2046 and 2120 UTC (Figure 1a). In the following 5 hours the observed storm proceeded to northeastern Colorado and developed into a 3-D rectangular four-cell structure that evolved into a single intense cell, and then dissipated. In our 3-D simulations we focused on the period of storm evolution that followed the initial stage studied by DeCaria et al. [2000] onward to its dissipation at about 0130 UTC on 13 July 1996 (see Figure 1).

[32] Some numerical complications caused by using non-uniform initial fields were associated with the large CAPE at the southern part of the model domain (Figure 2b). This region is not of primary interest but was included to allow our simulated storm sufficient space to develop and move southeastward. As a result, a very strong convective system developed at the southern boundary consistent with observations (see Figure 1d). That system interfered with the boundary conditions causing numerical instability.
We extended the domain as far south as available computer RAM allowed, but a very large domain would be necessary to move the southern boundary to a convectively stable region. Therefore we applied nudging type boundary conditions in a five-point belt along the lateral boundaries \cite{Davies, 1976; Robert and Yakimiw, 1986; Yakimiw and Robert, 1990}. In this boundary belt the three velocity components were relaxed to their initial values. That helped to stabilize the numerical solution for the entire period of the simulation. We believe it is important to keep this region of convective instability in the southern part of the domain because it allows us to more realistically calculate the time evolution of the mesoscale flow that interacts with the 12 July STERAO storm.

5.2. Results

To evaluate the simulated storm structure, we conducted comparisons of calculated radar reflectivity distributions in the middle and upper troposphere with the CHILL radar reflectivities and in situ aircraft observations. The atmospheric flow in the single intense cell regime has been evaluated using Doppler radar from WP-3D measurements that are available only at the final stage of the storm evolution.

Figure 3 shows the simulated radar reflectivity in the middle troposphere at the 4.5-km level (for visualization purposes only the part of the simulation domain where the storm is developing is shown) for comparison with the CHILL radar observations in Figure 1. On the basis of the CHILL radar observations discussed above and lightning observations presented by DeCaria et al. \cite{2005}, we assume that the beginning of the run corresponds to 2030 UTC. The very early stages of storm development proceeded more rapidly in the model than was observed. Therefore we have advanced the times of our comparisons with observations by 50 min. At 40 min after the beginning of the simulation (roughly corresponds to 2200 UTC), we see in Figure 3a a linear convective structure similar to the radar image at 2207 UTC in Figure 1b. The middle cell shows two closely located reflectivity maxima exhibiting a minor tendency for splitting. However, at 90 min (corresponds to 2250 UTC) this linear structure has fully evolved into the four-cell rectangular structure as in observations at 2258 UTC (Figure 1c). Consistent with observations the rectangle has
dimensions of about $40 \times 20$ km with the longer sides slightly rotated to the southeast. At the southern border of the domain we see disturbances that propagate from the region of instability. The four-cell structure continues to move southeastward (Figure 3c and 3d). The southeasternmost cell is gradually becoming the most intense. The other cells are decaying because the southeasternmost cell first processed the CAPE and left a more stable environment for the other cells. In the observations, there is clear competition between the two easternmost cells with the northeasternmost cell being slightly stronger (Figure 1c).

After the very initial stage of development, the overall time evolution of the storm and the speed of propagation are very similar to observations. For 150 min of evolution (from 40 to 190 min of simulation) shown in Figure 3 and 4, the southeasternmost cell that developed into a marginal supercell moved by about 35 km to the south and 60 km to the east, covering a distance of 70 km with average speed of 7.8 m/s. This is in a very good agreement with the observed storm propagation speed derived from CHILL radar observations (Figure 1). The 3-D model captures the directionality and the speed of propagation of the storm much better than in the 2-D simulation where the storm moved 2 times faster than in observations.

Figure 4 shows the evolution of the simulated reflectivity in the upper troposphere at 10 km (approximately the middle of the detrainment layer) starting from 120 min of storm simulation onward to the supercell formation. At 120 min all four cells are seen at 10 km, but the cells at the southern flank of the system have larger CAPE than the cells at the northern flank of the system. The southeasternmost cell gradually became the strongest one. This cell dominates, producing the largest anvil with total hydrometeor mixing ratios of more than 5 g/kg and simulated reflectivity about 50–55 dBZ. At 190 min into the simulation (corresponding to 0030 UTC on 13 July) the storm developed into a single intense cell (or marginal supercell) consistent with the radar observations at 0113 UTC (Figure 1d). As in Figure 1d the simulation also shows clear interaction with the convection at the southern border of the domain. The simulated single intense cell moves southeastward to the area with low CAPE and transforms slightly faster than in observations. The convective cell is still relatively strong at 210 min (roughly corresponding to 0050 UTC) as seen in Figure 4d.
with the anvil blowing to the northeast as in the observations (Figure 1d). The simulated convection dies in about 30 min (at 0120 UTC on 13 July) slightly earlier than observed. However, the last stage of the storm simulation (after 210 min) is less realistic. The convective cell leaves the region with high CAPE at about 220 min and begins to decay and to strongly accelerate to the east, presumably because of interaction with the mesoscale flow modified by other convective processes developing in the domain. This analysis shows that the initial nonuniform distribution of CAPE and the mesoscale transformation of the flow in the entire domain, as affected by the STERAO storm and the strong convection in the southern part of the domain (that modify CAPE and wind shear), are the most important factors that define the long-term evolution and the fine structure of the storm.

[37] This analysis shows that 3-D dynamics produce a storm structure significantly different compared with the storm structure that DeCaria et al. [2000] obtained in the 2-D simulations. The 3-D flow has more degrees of freedom and allows for more complex storm development. For example, the flow in the upper troposphere in 2-D simulations tends to move above and below the anvil enhancing vertical mass exchange. In the 3-D simulations, upper-troposphere flow tends to move around the anvil in a horizontal plane without production of a significant vertical wind component. The storm has more flexibility to develop in the 3-D nonuniform background and appears to be stronger than the 2-D storm. The mesoscale structure introduced by initial conditions is vitally important to storm evolution because we were even unable to produce sustainable convection using uniform initialization from soundings. In this case the dynamic instability in the lower troposphere adds energy to sustain strong convection. The more flexible 3-D dynamics allowed the storm to take advantage of more of the available instability than in the 2-D simulations. The wind shear in the upper troposphere defines the evolution of the anvil, the horizontal transport of pollutants, and their dilution rate. However, the processes in the anvil are also very sensitive to the microphysical parameterization.

[38] The stronger 3-D convection translates into a more intensive vertical transport of pollutant tracers from the boundary layer into the upper troposphere. Tables 1 and 2 show, respectively, maximum vertical flux and mixing ratio of CO in the 2-D and 3-D simulations for three subsequent times at various altitudes. The 3-D convection consistently produced larger fluxes and higher concentrations of CO at all altitudes above the boundary layer.

Table 1. Maximum Upward Flux (g m$^{-2}$ s$^{-1}$) Calculated by DeCaria et al. [2000] Using 2-D GCE Model Compared With That Obtained in This Study Using 3-D GCE Model

<table>
<thead>
<tr>
<th>Altitude</th>
<th>2100 UTC</th>
<th>2200 UTC</th>
<th>2300 UTC</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>2D</td>
<td>3D</td>
<td>2D</td>
</tr>
<tr>
<td>3 km</td>
<td>2.33 × 10$^{-4}$</td>
<td>2.85 × 10$^{-4}$</td>
<td>3.65 × 10$^{-4}$</td>
</tr>
<tr>
<td>5 km</td>
<td>4.72 × 10$^{-4}$</td>
<td>6.79 × 10$^{-4}$</td>
<td>6.06 × 10$^{-4}$</td>
</tr>
<tr>
<td>7 km</td>
<td>4.55 × 10$^{-4}$</td>
<td>8.24 × 10$^{-4}$</td>
<td>1.13 × 10$^{-3}$</td>
</tr>
<tr>
<td>9 km</td>
<td>9.42 × 10$^{-5}$</td>
<td>6.86 × 10$^{-4}$</td>
<td>1.16 × 10$^{-3}$</td>
</tr>
<tr>
<td>11 km</td>
<td>no convective influence</td>
<td>3.00 × 10$^{-4}$</td>
<td>7.37 × 10$^{-4}$</td>
</tr>
<tr>
<td>13 km</td>
<td>no convective influence</td>
<td>no convective influence</td>
<td>1.62 × 10$^{-4}$</td>
</tr>
</tbody>
</table>

[39] To analyze the fine spatial and dynamic structure of the convection in the single cell stage of the 12 July storm, we consider the vertical cross section (Figure 5) that goes through the core of the cell at y = 160 km at 190 min into the calculations (Figure 4c). We evaluate the simulation by comparing the results with the airborne Doppler radar observations. Because of the slightly faster development of the simulated storm at this stage we have chosen for comparison the airborne Doppler radar observations at 0105 UTC on 13 July 1996 that are approximately 30 min later than the simulated time.

[40] In Figure 5a we see that the simulated radar reflectivity reaches a maximum value of 50–55 dBZ at 4–5 km which corresponds to the altitude of the approximately 60–70 dBZ observed maximum. However, the simulated reflectivity (~55 dBZ) at 9–10 km is greater than in observations. The top of the convection is between 12 and 13 km, and the axis of the convective cell is at about 60° to the horizon. The simulated vertical velocity in the updraft (Figure 5b) exceeds 14 m s$^{-1}$ and reaches a maximum at 9 km. The air in the downdrafts in the middle and upper troposphere descends with the speed of ~2 to ~4 m s$^{-1}$. The relatively intense downward motion in the lower troposphere is produced by an inflow in the convective cell. We will discuss it in more detail below.

[41] The width of the updrafts in the convection is about 10 km. The cloud top altitude at the period of maximum intensity reaches 13 km as in the observations. The maximum vertical velocity in the course of the simulated 12 July storm evolution was about 20 m s$^{-1}$, which is consistent with the WP-3B radar observations. All these characteristics are weaker than for the 10 July storm (which produced vertical velocities of more than 30 m s$^{-1}$). This result is consistent with the less unstable meteorological environment on 12 July.

Table 2. Maximum CO Mixing Ratio (ppbv) Calculated by DeCaria et al. [2000] Using 2-D GCE Model Compared With That Obtained in This Study Using 3-D GCE Model

<table>
<thead>
<tr>
<th>Altitude</th>
<th>2100 UTC</th>
<th>2200 UTC</th>
<th>2300 UTC</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2D</td>
<td>3D</td>
<td>2D</td>
</tr>
<tr>
<td>3 km</td>
<td>128.67</td>
<td>130.46</td>
<td>126.52</td>
</tr>
<tr>
<td>5 km</td>
<td>124.87</td>
<td>130.46</td>
<td>122.86</td>
</tr>
<tr>
<td>7 km</td>
<td>119.06</td>
<td>130.46</td>
<td>121.49</td>
</tr>
<tr>
<td>9 km</td>
<td>104.42</td>
<td>130.04</td>
<td>123.26</td>
</tr>
<tr>
<td>11 km</td>
<td>no convective influence</td>
<td>122.65</td>
<td>128.03</td>
</tr>
<tr>
<td>13 km</td>
<td>no convective influence</td>
<td>no convective influence</td>
<td>107.60</td>
</tr>
</tbody>
</table>
Figures 5c and 5d show observed reflectivity and vertical velocity from the WP-3D radar. In the observations the updraft is offset with respect to the maximum of reflectivity. The core of the convection is located ~10 km east of the location of maximum rainwater, which is in the subsiding air in the lower troposphere. The intensity of the updraft oscillates in time reaching a maximum value about 20 m s\(^{-1}\), but at this moment it is weaker than in the simulation. However, the maximum altitude of the reflectivity distribution moves toward the updraft current position and reaches about 13 km ASL.

The simulated horizontal wind convergence is shown in Figure 6a. A region of large positive convergence indicating the most intensive inflow is located in the 4–6 km layer. Above this level the air is moving upward (see Figure 5b) while below it the air is moving downward and hits the ground, producing the diverging flow along the Earth’s surface seen in the lowest kilometer. Convergence at 5 km is fairly large reaching 4 \(\times\) 10\(^3\) s\(^{-1}\). Integrating convergence over a 10 × 10 km horizontal region and 1-km depth layer we computed that inflow is about 1.5 \(\times\) 10\(^8\) kg s\(^{-1}\). The negative convergence in the upper troposphere (UT) shows that anvil exhaust from the convective cell maximizes at ~10 km. The secondary convergence regions seen at 11 and 14 km probably correspond to generation of gravity waves by the convection.

Strong wind convergence generates cyclonic rotation. This positive angular momentum is advected upward with the airflow and stabilizes the convective updraft. The vertical component of vorticity is especially strong in the middle and upper part of the convective cell at altitudes of 5–12 km. The vertical vorticity component (Figure 6b) reaches 8 \(\times\) 10\(^3\) s\(^{-1}\), which is equivalent to an angular velocity of about 4 \(\times\) 10\(^{-3}\) s\(^{-1}\) and a revolution time around the center of the cell of about half an hour. In the region of the downward flow below the level of inflow negative vorticity is generated.

Figures 6c and 6d show convergence and the vertical component of vorticity, respectively, calculated using WP-3D Doppler radar wind fields. Because of the lack of observations, the entire picture cannot be seen. The observed convergence and vorticity are weaker than calculated in the same proportion as observed vertical velocity is weaker than calculated, but the spatial structure is practically identical. In Figure 6c we see positive convergence at 4–5 km level and negative convergence at 7–11 km.
Positive vorticity is seen above the inflow level at 6 km and negative vorticity below.

In Figures 7a and 7b we show horizontal cross sections at the levels of maximum inflow (5 km) and maximum outflow (10 km). Figure 7a shows convergence and horizontal velocity vectors. We see that most intensive inflow is from the north and northwest. Below the convergence region the wind is blowing to the southeast. This structure is similar to the observed shown in Figure 7c that also shows a strong rear-inflow jet.

Figures 7b and 7c show the vertical component of vorticity and horizontal wind vectors at 10 km. We see that the main anvil exhaust from the convective cell is to the east both in simulations (Figure 7b) and in observations (Figure 7c). However, the simulation also produced a moderate northerly component that is absent in observations. The structure of the observed and simulated vorticity fields is similar. It shows a south-north-oriented dipole with positive vorticity at the core of the convective updraft and negative vorticity to the north. Negative vorticity is stronger in the observations.

The simulated turbulent diffusion coefficient was relatively large (reaching 600 m²/s) at the level of inflow at 6 km (Figure 8). The turbulent mixing was assumed to be isotropic. The region of strong turbulence has dimensions of 25 × 20 km, which was much larger than the cross section of the updraft. At this level, turbulent kinetic energy (TKE) was generated both by thermal instabilities and wind shear. It is important to note that in the anvil at 12 km (Figure 8b) the turbulent diffusion coefficient was still relatively large, reaching 320 m²/s, which corresponds to a mixing length of more than 100 m. Intense turbulence in the anvil was maintained by vertical advection of TKE and dynamic instabilities enhanced by oscillations of the convective cell. The large values of the coefficient in the anvil indicate that turbulence could significantly contribute to redistribution of chemically active compounds transported by convection to the upper troposphere. This process must be accounted for in the transport calculations. Turbulence at the top of the convective cell even could affect stratosphere-troposphere exchange. However, in the 12 July storm the strength and altitude of the convective cell is not enough (tropopause was at ~15 km) to cause a sizable stratosphere-troposphere mass exchange (contrary to the 10 July storm). Consistently, ozone measurements from the UND Citation aircraft did not show any intrusions.
of stratospheric air with high ozone mixing ratios in the upper troposphere.

In the above discussion we characterized the terminal phase of the 12 July storm as a single intense cell or marginal supercell regime. This is consistent with the relatively weak CAPE observed on 12 July. However, we have shown that the convective cell possessed a rotating updraft and developed in a strong wind shear environment (\(35 \text{ m s}^{-1}\) in the 6-km layer above terrain). CHILL radar images also show that between 0058 and 0214 on 13 July there are occasions when V-shaped indentations ("notches") developed in the reflectivity field. These may be indicative of the weak echo region that is a characteristic feature of a supercell convection. Therefore we can characterize the 12 July single cell convection as a single intense cell marginally reaching supercell status.

6. Summary

Upward convective transport occurs in narrow updrafts on very fine spatial scales of atmospheric flow. The dynamical fields required for a posteriori simulation of this transport cannot be obtained from observations and have to be reproduced in model simulations. The fine structure of the convective flow and turbulent diffusion are crucially important for correct simulation of transport of chemical species from the boundary layer and LT into the UT/LS.

Here we used the 3-D version of the GCE model to simulate the 12 July STERAO storm. To correctly describe the spatial structure of this storm, we implemented terrain and nonuniform initial conditions in the 3-D version of the GCE model. We showed that with these modifications the 3-D GCE model is capable of simulating the transition from the linear multicell convection to a highly 3-D single severe cell. The archived meteorological fields from the cloud model simulation were evaluated using available observations and used as input to the Cloud-Scale Chemical Transport Model (CSCTM) [DeCaria et al., 2005].

Mesoscale models like RAMS, MM5, ARPS, and WRF provide capabilities for accounting for terrain and nonuniform initial fields that allow them to better reproduce...
mesoscale development interactively with the storm evolution. Here we showed that accounting for these effects improves a GCE model simulation. We found that dynamic fields from the GCE model output every 10 min provide a well-balanced input into our cloud-scale chemical transport model, not producing any spurious sources or sinks of mass. No “mass-fixing” routine, that we have found necessary when using output from mesoscale models, was needed in this case.

[53] The major results of this study can be formulated as follows.

[54] 1. The GCE model with terrain and nonuniform initialization was able to reproduce the correct observed development of the 12 July 1996 STERAO storm. The simulation produced storm spatial structure and temporal evolution that compare favorably with observations. Direction and speed of storm propagation are in good agreement with those derived from radar observations.

[55] 2. The 3-D simulation allowed reproduction of the entire life cycle of the storm from linear multicell structure to highly 3-D intense single cell (or marginal supercell convection). However, it seems in our simulation that the southeastern (rather than the northeastern as observed) convective cell became the most intense. This may have resulted because interaction between the cells is highly unstable and small sporadic perturbations can cause intensification of one cell at the expense of another. It suggests that some assimilation of observed information could be beneficial.

[56] 3. The 2-D approach does not allow us to describe the entire evolution of the storm, but does provide useful estimates of the storm development during the quasi-linear development phase of the storm for about the first 2 hours. The 3-D convection, consistently with observations, appears to be stronger than 2-D convection and initiated more intensive vertical transport of tracers from the boundary layer into the upper troposphere.

[57] 4. The 12 July STERAO storm is significantly different than the one on 10 July since it developed in an environment with much lower CAPE. The structure of simulated convection for this case appears to be much more sensitive to the detailed spatial distribution of initial meteorological fields, terrain effects, and boundary conditions. However, the 12 July storm produced relatively strong convection significantly affecting the chemical structure of the upper troposphere [see DeCaria et al., 2005], although it did not cause significant stratosphere-troposphere exchange. This study shows that parameterization of convection in the marginally unstable environment might need special attention.

References


