The Dispersion of Silver Iodide Particles from Ground-Based Generators Over Complex Terrain. Part II: WRF Large-Eddy Simulations Versus Observations

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The Dispersion of Silver Iodide Particles from Ground-Based Generators over Complex Terrain. Part II: WRF Large-Eddy Simulations versus Observations

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ABSTRACT

A numerical modeling study has been conducted to explore the ability of the Weather Research and Forecasting (WRF) model-based large-eddy simulation (LES) with 100-m grid spacing to reproduce silver iodide (AgI) particle dispersion by comparing the model results with measurements made on 16 February 2011 over the Medicine Bow Mountains in Wyoming. Xue et al.’s recently developed AgI cloud-seeding parameterization was applied in this study to simulate AgI release from ground-based generators. Qualitative and quantitative comparisons between the LES results and observed AgI concentrations were conducted. Analyses of turbulent kinetic energy (TKE) features within the planetary boundary layer (PBL) and comparisons between the 100-m LES and simulations with 500-m grid spacing were performed as well. The results showed the following: 1) Despite the moist bias close to the ground and above 4 km AGL, the LES with 100-m grid spacing captured the essential environmental conditions except for a slightly more stable PBL relative to the observed soundings. 2) Wind shear is the dominant TKE production mechanism in wintertime PBL over complex terrain and generates a PBL of about 1000-m depth. The terrain-induced turbulent eddies are primarily responsible for the vertical dispersion of AgI particles. 3) The LES-simulated AgI plumes were shallow and narrow, in agreement with observations. The LES overestimated AgI concentrations close to the ground, which is consistent with the higher static stability in the model than is observed. 4) Non-LES simulations using PBL schemes had difficulty in capturing the shear-dominant turbulent PBL structure over complex terrain in wintertime. Therefore, LES of wintertime orographic clouds with grid spacing close to 500 m or finer are recommended.

1. Introduction

Inadequate or uncertain targeting of seedable clouds from silver iodide (AgI) ground-based generators has been a complex and long-standing problem in winter orographic cloud-seeding programs. The efficacy of the ground-based seeding depends significantly on the effective dispersion of the seeding agent in orographic clouds over complex terrain. To address how AgI particles
released from ground-based generators disperse over complex terrain within the Wyoming Weather Modification Pilot Program (WWMPP), which is an outcome-focused randomized program (Breed et al. 2014), a focused field experiment was conducted between 9 February and 1 March 2011. Boe et al. (2014, hereinafter Part I) describes airborne measurements of AgI-based ice nuclei (IN) plumes from ground-based generators collected by Weather Modification, Inc. (WMI), Piper Cheyenne II research aircraft equipped with an updated National Center for Atmospheric Research (NCAR) acoustic IN counter (Langer et al. 1967, 1978; Langer 1973; Heimbach et al. 1977, 2008; Super et al. 2010). The airborne data were collected over the Wyoming Medicine Bow and Sierra Madre ranges on nine different days during the field experiment period.

Previous observational studies have documented the dispersion of ground-released AgI plumes over mountainous target regions. An airborne experiment conducted by Super (1974) studied the dispersion of an AgI plume on the Bridger Range in Montana using the original version of the NCAR acoustic IN counter. The plume width was \( \sim 28^\circ \) and was mostly confined to the lowest 500 m above the ridge line. A similar experiment conducted by Holroyd et al. (1988) over the Grand Mesa of Colorado showed that the median spread of AgI plumes was \( \sim 15^\circ \) and that the median plume height above the crest exceeded 500 m. They also pointed out that the dispersion efficiency was higher during cloudy days than clear days. Measurements of microphysical changes induced by seeding, such as high concentrations of small ice crystals, also indicated that AgI plumes have relatively narrow spreads and remain close to the ground (Super and Heimbach 1988; Super and Boe 1988; Huggins 2007). More recently, Geerts et al. (2010, 2011) showed, by means of reflectivity data from a profiling radar, that the impact of ground-based orographic cloud seeding was confined to the planetary boundary layer (PBL), about 1 km deep. Most of the aforementioned studies focused on AgI dispersion from a single ground-based generator while the field experiment within the WWMPP tried to assess the features of AgI plumes from both single and multiple ground-based generators, better representing the real WWMPP seeding experiments.

In addition to physical measurements of AgI plumes from ground-based generators by airborne and ground-based instruments, numerical models were used to investigate plume dispersion. In the air quality modeling community, Lagrangian particle trajectories and dispersion models are commonly used to simulate pollutant transport and the dispersion of hazardous materials. Commonly used models include the Hybrid Single Particle Lagrangian Integrated Trajectory (HYSPLIT) model (Draxler and Rolph 2014), the Second-Order Closure Integrated Puff (SCIPUFF) model (Sykes and Gabruk 1997), and the Flexible Trajectory (FLEXTRA) and Flexible Particle Dispersion (FLEXPART) models (Stohl et al. 1995, 2005). These models are usually run in an “offline” mode, which means that they are driven by meteorological reanalysis data or meteorological conditions generated by numerical forecast models. However, for certain types of applications such as aerosol–cloud–precipitation interactions and glaciogenic seeding effects on orographic clouds, “online” calculations of particle transport and dispersion are needed. The reason is that the transport and dispersion of such passive particles will impact the microphysics of clouds and precipitation, which also influences the flow dynamics through microphysics–dynamics feedbacks. These interactions are not represented in “offline” models.

Bruintjes et al. (1995) was probably the first study in the weather modification community that compared online-calculated gaseous tracer concentrations (SF\(_6\)), using a three-dimensional model, with the airborne in situ observations. This pioneering work demonstrated the capability of numerical models to qualitatively and quantitatively capture the dispersion of AgI over complex terrain. The interaction between the airflow and the topography was identified as the dominant factor in determining the dispersion and transport of tracer materials. Part of the discrepancy between the simulated and observed results can be explained by the relatively large grid spacing (2 km) used in Bruintjes et al. (1995). Schicker and Seibert (2009) found that a grid spacing of 2.4 km did not reasonably simulate flows over complex terrain while 0.8 km did reproduce characteristic flow features. Weigel et al. (2007) performed large-eddy simulations (LES) using a grid spacing of 350 m to investigate turbulent kinetic energy (TKE) evolution in a steep and narrow Alpine valley. They found that wind shear was the dominant production mechanism for TKE over such complex terrain. LES at 150m grid spacing showed that the stable stratification limited turbulent stress to the lowest few hundred meters near the surface of the mountain (Chow et al. 2006).

It is promising that high-resolution LES can reproduce flow features over complex terrain reasonably well. Moreover, high-resolution cloud-resolving LES capture the interactions between turbulent eddies and cloud microphysics over complex terrain. There is some observational evidence that PBL turbulence is important in snow growth in cold clouds hugging mountains (Geerts et al. 2011). This study does not examine cloud microphysical processes (the case study in question is a dry event), but it serves as a prerequisite study for follow-up observational and numerical work into the impact of glaciogenic seeding on microphysical processes in orographic clouds. Specifically, this
study examines the capability of LES at 100-m grid spacing using the Weather Research and Forecasting (WRF) model to capture AgI dispersion over mountainous topography for a case on 16 February 2011 described in Part I. The model results were evaluated using airborne and ground-based observations. Comparisons of model results between simulations with 500-m grid spacing and that of LES with 100-m grid spacing have also been conducted to provide guidance for future simulations. The observational experiment on 16 February and the numerical experiment are described in section 2 and section 3, respectively. The model–observation and model–model comparisons are presented in section 4 followed by discussions in section 5. The main conclusions are summarized in section 6.

2. Description of the observational experiment

Nine flights were conducted over the Medicine Bow and Sierra Madre mountains in Wyoming between 9 February and 1 March 2011. Operations required 1) that the region be devoid of low-level orographic clouds and snowfall to allow the aircraft to fly under visual meteorological conditions close to the terrain, and 2) that there be substantial flow over the mountain. The latter was ascertained by requiring that the Froude number be greater than one (Fr > 1). On one of the nine flights, between 2240 UTC 16 February and 0216 UTC 17 February 2011, the IN counter registered high IN concentrations on several flight legs, with some well above mountaintop level (Part I). Hereinafter, all times are in UTC. The IN counter at the surface site also recorded the passage of AgI plumes (Part I). Given the rich observational data, this case was chosen for an LES experiment.

The synoptic conditions during the observational period are illustrated in Fig. 1 using the North American Regional Reanalysis (NARR) data. These data have a spatial resolution of 32 km and are available every 3 h. The 700-hPa temperature (color shaded) was chosen because it roughly corresponds with the average mountain elevation above sea level. Moderately strong southwesterly flow persisted over a broad area ahead of a slowly progressing trough over California. Local cooling over the Medicine Bow Mountains (within the green circle) at about 2 K over 6 h was the result of cold-air advection and diurnal surface cooling. Wind speed and direction were fairly steady during this 6-h period. The Medicine Bow Mountains were devoid of low-level clouds, and there were altostratus overhead (Part I).

For this case, radiosondes were released from Saratoga, a town upwind of the Medicine Bow Mountains (Figs. 2a,b), at 2200 UTC 16 February and at 0100 UTC 17 February. The observed soundings along with those from model simulations are shown in Fig. 3. The sounding parameters averaged between the surface and the peak of the Medicine Bow Mountains are listed in the left column of Table 1. Based on the Saratoga soundings, the winds (speed and direction) did not change much and the atmospheric stability decreased slightly during a 3-h period. These sounding parameters are broadly consistent with the synoptic analyses.

![Fig. 1](image_url)
Five ground-based generators (red triangles in Fig. 2) were operated between 2148 UTC 16 February and 0115 UTC 17 February. The aircraft flew 8 legs transecting the plumes (see Fig. 2c and Fig. 6 for the flight pattern) and took measurements from 2319 UTC 16 February to 0035 UTC 17 February corresponding to local late afternoon.\(^2\) The flight legs were upwind of the steep mountain crest around Medicine Bow Peak to avoid boundary layer separation and vertical transport in the lee of this sharp crest, something commonly observed over this mountain range (J. R. French et al. 2013, personal communication). An IN counter, with a larger cloud chamber than the airborne version, was operated at the surface site (Mountain Meadow Cabin 9, as shown in Fig. 2) to detect AgI plumes in downwind regions. The generator operational times and flight times are listed in Table 2. More details about this case can be found in Part I.

3. Description of the numerical experiment

The WRF model (version 3.2.1; Skamarock et al. 2008) was run on two nested grids with grid spacings of 2500 and 500 m, respectively, driven by the NARR data in a non-LES mode initially. Hereinafter, these two domains are referred to “coarse resolution” or “non LES” domains. Since a practical technique that communicates information between the domain in a non-LES mode and the nested domain in an LES mode (two-way nesting) is generally unavailable in WRF (Moeng et al. 2007), a one-way nesting procedure was applied to drive the 100-m LES. The simulations on the two non-LES grids were spun up for 21 h from 0000 to 2100 UTC 16 February 2011. They were then run from 2100 UTC 16 February to 0300 UTC 17 February with an output interval of 20 min.

\(^2\) Local solar noon was at 1919 UTC, and sunset was at 0040 UTC on this day.
Subsequently, these outputs were processed to drive the LES over the same period with lateral boundary conditions being updated every 20 min. The topographies of the domains with different grid spacings are shown in Fig. 2. The 2500- and 500-m domains consist of 320 × 220 grid points, while there are 800 × 800 grid points for the LES domain. The vertically stretching coordinate as applied in Xue et al. (2010, 2012, 2013b,a) was adopted for all three domains. The vertical grid spacing is less than 200 m in the lowest 2000 m above ground level (AGL), which makes the grid aspect ratio of the LES domain less than two in regions experiencing the strongest AgI dispersion. For the LES domain, high-resolution elevation and land use type data from the U.S. Geological Survey (USGS) were applied. For the two coarse-resolution domains, regular USGS 30-s data were used.

In this study, the AgI cloud-seeding parameterization documented in Xue et al. (2013b,a) was applied to simulate the release of AgI particles from ground-based generators. The size distribution of AgI particles from the generators is assumed to follow a lognormal distribution with a mean diameter of 0.05 μm and a geometric standard deviation of two. The mean size of the AgI particle is slightly larger than was specified in Xue et al. (2013b,a) because of slightly different ingredients of the AgI solution. The vertical mixing or diffusion of AgI particles by the Mellor–Yamada–Janjić (MYJ; Janjić 2001) and the Yonsei University (YSU; Hong et al. 2006) PBL schemes was explicitly simulated in the non-LES domains. No PBL scheme was specified for the LES since we assumed that most of the terrain-induced eddies responsible for AgI vertical mixing would be appropriately resolved with a 100-m grid spacing. The same dynamic equations were applied for AgI mass mixing ratio and number concentration as other scalars (potential temperature and moisture, etc.) in the WRF model to account for resolved-scale advection and transportation. The details of the vertical diffusion of AgI in PBL schemes and the subgrid-scale (SGS) diffusion of AgI in LES can be found in the appendix. For the LES, a 1.5-order SGS TKE closure model was chosen (Deardorff 1980; Moeng 1984). A very short time step of 1/15 s was applied to ensure that the LES remained numerically stable. The detailed configurations of the WRF model for all domains are listed in Table 3.

31 arc-s data (about 30-m resolution) over the area of interest were downloaded from the National Map Viewer and Download Platform for the LES domain.

4The abruptly changing topography introduces vigorous upward and downward motions close to the ground, which easily violate the vertical Courant–Friedrichs–Lewy criterion when a longer time step was applied.
In this study, the 100-m LES was driven by atmospheric conditions simulated by the 500-m non-LES simulation. Since the 500-m run contained no SGS TKE information, the initial and lateral boundary conditions of the 100-m LES domain interpolated from the 500-m non-LES results have zero SGS TKE value. However, these zero initial and boundary conditions do not impact the validity of the 100-m LES in this case. Most recently, Mirocha et al. (2014) investigated how TKE evolves using two nested LES domains within a mesoscale (non-LES) domain in an idealized setup. They found that the SGS TKE still develops in LES domains with zero SGS TKE initial and lateral boundary conditions (from the mesoscale simulation) when topography is present and when the wind/potential temperature are perturbed at the upwind boundaries. In this study, the real topography is much more complex than the idealized topography used in Mirocha et al. (2014). The complex terrain provides a broad range of scales that help spin up the SGS TKE in our simulation. Furthermore, the land surface types used in our LES represent the heterogeneity of the surface condition. Unlike the homogeneous surface conditions applied in Mirocha et al. (2014), such heterogeneity provides perturbations to the lower atmosphere, which works similar to wind/temperature perturbations in Mirocha et al. (2014) and accelerates the SGS TKE development in the LES domain. The relatively large LES domain (80 km × 80 km) used here allows the SGS TKE to build from the upwind boundaries well before reaching the area of interest (ground-based generators). Chow et al. (2006) and Weigel et al. (2007) also showed that the LES simulation of flow in a steep valley driven by European Centre for Medium-Range Weather Forecasts (ECMWF) data can reproduce observed wind, temperature, and TKE profiles reasonably well, which indicates that the complex terrain and real land surface types help the SGS TKE formation in the LES.

### 4. Results

#### a. Appropriateness of the LES

Before any LES results can be compared with the observations, the appropriateness of the LES must be assessed especially when the initial and later boundary conditions interpolated from the non-LES simulation

<table>
<thead>
<tr>
<th>Generators</th>
<th>Operational time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mullison Park (MP)</td>
<td>2148 UTC 16 Feb–0104 UTC 17 Feb</td>
</tr>
<tr>
<td>Barrett Ridge (BR)</td>
<td>2149 UTC 16 Feb–0106 UTC 17 Feb</td>
</tr>
<tr>
<td>French Creek Overlook (FCO)</td>
<td>2150 UTC 16 Feb–0111 UTC 17 Feb</td>
</tr>
<tr>
<td>Rob Roy 2 (RR2)</td>
<td>2151 UTC 16 Feb–0113 UTC 17 Feb</td>
</tr>
<tr>
<td>Beaver Creek Hills (BCH)</td>
<td>2152 UTC 16 Feb–0115 UTC 17 Feb</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Flight leg</th>
<th>Observational time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Leg 1</td>
<td>2319 UTC 16 Feb–2323 UTC 16 Feb</td>
</tr>
<tr>
<td>Leg 2</td>
<td>2326 UTC 16 Feb–2333 UTC 16 Feb</td>
</tr>
<tr>
<td>Leg 3</td>
<td>2335 UTC 16 Feb–2342 UTC 16 Feb</td>
</tr>
<tr>
<td>Leg 4</td>
<td>2345 UTC 16 Feb–2353 UTC 16 Feb</td>
</tr>
<tr>
<td>Leg 5</td>
<td>2355 UTC 16 Feb–0004 UTC 17 Feb</td>
</tr>
<tr>
<td>Leg 6</td>
<td>0007 UTC 17 Feb–0014 UTC 17 Feb</td>
</tr>
<tr>
<td>Leg 7</td>
<td>0017 UTC 17 Feb–0025 UTC 17 Feb</td>
</tr>
<tr>
<td>Leg 8</td>
<td>0027 UTC 17 Feb–0035 UTC 17 Feb</td>
</tr>
</tbody>
</table>

### Table 1. Summary of the sounding parameters. For the observations and the 500-m non-LES, the parameters were calculated over Saratoga (see Figs. 2a,b). For the 100-m LES, the parameters were calculated over the starred location shown in Fig. 2c.

<table>
<thead>
<tr>
<th>Parameters*</th>
<th>Obs</th>
<th>500-m non-LES</th>
<th>100-m LES</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \overline{U} ) (m s(^{-1}))</td>
<td>22</td>
<td>19</td>
<td>17</td>
</tr>
<tr>
<td>( \overline{U} ) dir (°)</td>
<td>227</td>
<td>225</td>
<td>221</td>
</tr>
<tr>
<td>( \delta ) (10(^{-2}) s(^{-1}))</td>
<td>1.25</td>
<td>0.70</td>
<td>1.21</td>
</tr>
<tr>
<td>( \delta ) dir (°)</td>
<td>250</td>
<td>265</td>
<td>272</td>
</tr>
<tr>
<td>( N ) (10(^{-2}) s(^{-1}))</td>
<td>0.77</td>
<td>1.01</td>
<td>1.10</td>
</tr>
<tr>
<td>Fr (–)</td>
<td>1.87</td>
<td>1.22</td>
<td>0.97</td>
</tr>
<tr>
<td>Ri (–)</td>
<td>0.38</td>
<td>2.07</td>
<td>0.83</td>
</tr>
<tr>
<td>( H_{LCL} ) (m AGL)</td>
<td>2280</td>
<td>1730</td>
<td>1327</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
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<th>Operational time</th>
</tr>
</thead>
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</tr>
<tr>
<td>Beaver Creek Hills (BCH)</td>
<td>2152 UTC 16 Feb–0115 UTC 17 Feb</td>
</tr>
</tbody>
</table>

* All parameters were calculated between 60 m AGL and the peak of the Medicine Bow Mountains. Here \( \overline{U} \) is the mean wind speed; \( \overline{U} \) dir is the direction of the mean wind; \( \delta \) is the bulk wind shear between 60 m AGL and the peak of the Medicine Bow Mountains; \( \delta \) dir is the direction of the wind shear; \( N \) is the Brunt–Väisälä frequency (average of the dry and the moist values); Fr = \( \overline{U}/(NH) \) is the local bulk Froude number, where H is the height of between 60 m AGL and the peak of the Medicine Bow Mountains; Ri = \( N^2/\delta^2 \) is the bulk Richardson number; and \( H_{LCL} \) is the height of the LCL above the ground.

In this study, the 100-m LES was driven by atmospheric conditions simulated by the 500-m non-LES simulation. Since the 500-m run contained no SGS TKE information, the initial and lateral boundary conditions of the 100-m LES domain interpolated from the 500-m non-LES results have zero SGS TKE value. However, these zero initial and boundary conditions do not impact the
contain no SGS properties. The first general and important question about such a simulation is how much spinup time is needed. In this study, the coarse-resolution domains were spun up for 21 h before the generators were turned on. However, limited computational resources prevented us from performing a long LES spinup simulation. Here, we investigate the spinup time issue by analyzing the kinetic energy power spectrum as described in Errico (1985) and Skamarock (2004).

The instantaneous 1D kinetic energy spectra at 15-min intervals averaged over the entire horizontal domain (excluding 10 grid points near boundary in each direction) between the surface and 2000 m AGL are plotted from 0 to 120 min in Fig. 4. The height of 2000 m AGL was chosen because most of the terrain-induced turbulent eddies are only active below this level and the vertical resolution of the model is also appropriate for an LES below this altitude, as shown later in this study. The blue line in each panel represents the $k^{-5/3}$ ($k$ is the wavenumber) slope, which indicates the inertial subrange of the kinetic energy spectrum (Kolmogorov 1991). The LES domain covers 80 km $\times$ 80 km, which means that the largest scale in the energy spectrum is still within the mesoscale range; therefore the spectrum follows the inertial slope at most scales. The deviation of the spectrum from the inertial subrange at scales less than 1 km ($\sim 10^{-3}$ m$^{-1}$ in per wavelength space) is due to the numerical diffusion of the integration scheme in the model (Bryan et al. 2003; Skamarock 2004) and to the vertical averaging.

Apparently, the initial wind field that was interpolated from the 500-m results did not produce the correct spectrum (0-min spectrum in Fig. 4). The wind field was adjusting to the underlying complex terrain 15 min into the LES. The turbulence at small scales injected energy into the wind field at large scales, causing an "overshoot" of the spectrum with respect to the inertial slope. Such adjustments and overshooting still existed after 30 min into the simulation. At 45 min, the wind field reached a balanced state and produced a spectrum following the inertial subrange at scales greater than 1 km. The spectrum remained basically unchanged after 45 min. Such a steady-state spectrum will not be achieved if the synoptic conditions change significantly during this period. Based on the evolution of the model kinetic energy power spectrum, we conclude that the LES needs about 45 min to spin up in this specific case. Since the AgI particles were released from the generators after 48 min in the LES, the dispersion of these particles should be properly simulated by the balanced flow field.

Another important verification of LES is that the SGS TKE should be small compared to the total or resolved-scale TKE. LES by definition requires the model to resolve eddies at the most energetic scales. The energy at unresolved scales must be modeled or parameterized. The profiles of total TKE, SGS TKE, and half of the vertical velocity variance (vertical momentum flux) are illustrated in Fig. 5 for both the upwind and downwind regions. The upwind region is defined as the 360 $\times$ 360 grid points in the southwest corner of the domain while the downwind region is the 440 $\times$ 440 grid points in the northeast corner. The profiles from 0 to 2000 m AGL represent values of these terms temporally averaged between 2145 UTC 16 February and 0115 UTC 17 February (operational time of the generators) and spatially averaged within the upwind and downwind regions.

For both the upwind and downwind regions, the SGS TKE is a small portion of the total TKE at each level. The SGS TKE to total TKE ratio is around 10%–20% in the lowest 200 m and becomes less than 10% above 200 m. The higher ratio close to ground agrees with previous LES studies of a buoyancy-driven PBL (Deardorff 1980; Moeng 1984). Since the atmosphere was stable and windy, the flow in the downwind region was approximately between a resonance state and a boundary layer separation regime ($1 < Fr < 1.7$; Table 1) (Stull 1988). Because no terrain-induced gravity waves or mountain wave breaking existed in this case and the interactions between the flow and terrain were weaker in the downwind region, a weaker TKE profile

<table>
<thead>
<tr>
<th>Table 3. Model configurations.</th>
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<tbody>
<tr>
<td>Configurations/domains</td>
</tr>
<tr>
<td>Simulation time</td>
</tr>
<tr>
<td>Time step</td>
</tr>
<tr>
<td>Output frequency</td>
</tr>
<tr>
<td>Radiation</td>
</tr>
<tr>
<td>PBL</td>
</tr>
<tr>
<td>Surface</td>
</tr>
<tr>
<td>Microphysics</td>
</tr>
<tr>
<td>Turbulence</td>
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<td></td>
</tr>
</tbody>
</table>

1 The peak of the Medicine Bow Mountains is roughly at grid point (360, 360).
exists in the downwind region than in the upwind region. The profiles of vertical velocity variances (Fig. 5) highlighted the fact that the majority of the TKE resided in the horizontal dimension because the wind shear was the dominant TKE production mechanism in this case (see detailed discussions in section 5). These profiles also indicated a PBL height of about 1000 m AGL in this case, which agrees with the observations of Geerts et al. (2010, 2011). Such a PBL height suggests that the vertical grid spacing used in the LES was appropriate.

b. Sounding comparisons

After the appropriateness of the LES is justified, model-simulated and observed meteorological conditions are compared in this section. Since the NARR data were used to drive the simulations, comparisons of synoptic fields between the model and the NARR data are inappropriate. We then compare the sounding information at Saratoga in this section.

The observed and simulated soundings at 2200 UTC 16 February and 0100 UTC 17 February are plotted in

![Kinetic energy power spectrum](image-url)
low-level wind directions than the 100-m LES. However, such differences are mainly due to the different sounding location used in the 100-m LES. Comparisons of low-level winds between 500-m non-LES and 100-m LES at the sounding location in the 100-m domain showed better agreement than Fig. 3, although a slight wind direction discrepancy still existed (not shown). The easterly component of the wind field in 100-m LES is attributed to the numerical boundary effect and the drainage flow caused by the strong low-level inversion and local topography gradient.

Sounding parameters were calculated between 60 m AGL and the peak of the Medicine Bow Mountains (Table 1). Observations below 60 m were not included because of artifacts introduced during the sounding launch. The model data below 60 m were removed as well because of the unrealistic values caused by the erroneous soil moisture initialization. Similar to what was found in Fig. 3, both simulations generated realistic wind direction between the surface and the mountain peak. The 500-m run simulated slightly better wind speed than the 100-m LES. But the 100-m LES captured wind shear and shear direction changing trend better than the 500-m simulation. Both runs simulated a more stable atmosphere than the soundings with the 100-m LES being slightly more stable than the 500-m simulation. As a result, both simulations underpredicted Fr and overpredicted the Richardson number Ri. The possible reasons for the more stable low-level atmosphere simulated by the model will be discussed in next section. Nevertheless, both simulations showed the same downward trend in stability as in the observations. Because of the moist nature of the NARR-driven simulations, the simulated lifted condensation level (LCL) heights were lower than observed. The LCL height was especially low in the 100-m LES at 0100 UTC 17 February. Despite the moist bias aloft and close to the ground simulated by the model, both the 500-m non-LES and the 100-m LES captured the general features of the flow in the PBL where the dispersion of AgI particles occurred.

c. AgI concentration comparisons

As discussed in Part I, the IN counter has a time-distributed delay averaging 80 s from the ingestion of atmospheric IN to their detection. Thus, the measurements in the form of IN count rate (s⁻¹), accounting for the 80-s delay, are plotted along the flight tracks in Fig. 6. Figure 6a reveals that the horizontal spread of the AgI plumes was not significant, with the majority of the plumes evident

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6 Saratoga, as a small urban area that is not resolved by the NARR data, has higher surface temperature and lower soil water content than its surroundings.

7 Wind shear turned counterclockwise in both observations and the 100-m LES, whereas it turned clockwise in the 500-m simulation.
in the immediate downwind vicinity of the generators. However, since the flight legs were vertically orientated, the horizontal spread of the plumes at low levels may have been wider. The temporal smoothing of IN measurements (and thus spatial dispersion because of the aircraft movements) was not accounted for in Fig. 6. Thus, in reality, the IN plumes may be narrower than suggested in Fig. 6a (see Part I for details). Figure 6b illustrates the vertical structure of the observed AgI plumes. The vertical coordinate is referenced to mean sea level (MSL). The highest count rates (>10 s\(^{-1}\)) were observed in the lowest leg and the count rates generally decreased with increasing altitude. The features of observed AgI plumes in this case agreed with many previous observational studies (Super 1974; Holroyd et al. 1988, 1995; Super and Heimbach 1988; Super and Boe 1988).

Figure 7 shows 3D depictions of LES-simulated AgI plumes and wind fields at 2230 UTC 16 February, 0000 UTC 17 February, and 0130 UTC 17 February. The wind field showed little change during the 3-h period, which is consistent with the analyses presented in previous sections. Spatially, the high-level wind showed constant wind speed and almost uniform wind direction while the low-level wind was forced by the complex topography and presented higher variability than the wind field aloft. The midlevel wind was more variable than the high-level wind but was less variable than the low-level wind.

In Fig. 7, the visible blue plumes indicate AgI particles with number concentration greater than 100 L\(^{-1}\), which roughly corresponds to one IN count per second in the airborne observations—the lowest concentration measurable with the IN counter in its configuration used in this experiment (see Part I for details). The AgI plumes remained narrow during this period. The plumes from generators Mullison Park (MP), Barrett Ridge (BR), and Beaver Creek Hills (BCH; see Fig. 2 for locations) merged into one large plume at 0000 UTC 17 February, but the plumes from generators French Creek Overlook (FCO) and Rob Roy 2 (RR2) stayed separate throughout the simulation. The general morphology of these plumes in the horizontal compared qualitatively well with the observations (Fig. 6a). The vertical extent of the simulated plumes are also illustrated in Figs. 7b(1)–(3). Most of the time, the plumes were draped over the mountain with high concentrations of AgI particles close to the ground. Note that the plume from RR2 (the southeastern generator) had more vertical dispersion than the others including FCO whose plume experienced more variable terrain during this period. Such results indicate that terrain changes alone are not responsible for lofting AgI particles and local stability and TKE are also important.

To better compare the vertical structure of the AgI plumes, the AgI concentrations are plotted along two cross sections (as indicated by two black dashed lines in Fig. 2c) in Fig. 8 for the same times as shown in Fig. 7. The two cross sections, orientated northwest to southeast and about 6 km apart, were chosen to cover the flight legs 3–8. Also plotted are the TKE isoline of 1 m\(^2\) s\(^{-2}\) (red
lines) and cloud water mixing ratio (black lines). Similar to Fig. 7b1, the plume from RR2 (the southernmost plume) reached a higher altitude than the others at 2230 UTC 16 February (Figs. 8a1,b1). The plumes from FCO (the center plume) and RR2 had AgI concentrations greater than 10^5 m^-3 or 100 L^-1 (colors warmer than yellow) above the maximum observation altitude of 3800 m MSL at this time (Figs. 8a1,b1). The envelope of the plumes' upper edges is collocated with the active turbulence region (red outlines), which implies that turbulent mixing is the primary mechanism for AgI vertical dispersion. Since the instantaneous plume morphology is an integrated reflection of the turbulent eddy history, occasional mismatches between the plumes' upper edges and the instantaneous TKE isoline are reasonable.

Figures 8a2 and 8b2 show that at 0000 UTC 17 February, the turbulence was not as active in the plume locations as 1.5h earlier. Correspondingly, the plumes stayed close to the ground. Only a small portion of the plume from the FCO generator reached 3800 m MSL with a AgI concentration greater than 10 L^-1 (see yellow areas in Fig. 8b2). This match between low turbulent activity and weak AgI vertical extent confirms that
turbulent eddies are primarily responsible for the vertical dispersion of AgI particles. Also at this time, clouds started to form above 4000 m MSL, consistent with the sounding analyses in section 4b. At the later time (0130 UTC 17 February), the turbulence became strong again over the plume regions. As a result, the AgI plumes reached higher than 1.5 h earlier. The clouds grew into a deck, located just above the plumes. Visual observations showed that there was a cloud deck close to this altitude when the airborne observations were taken (see Fig. 5 in Part I).

Figure 8 shows that the turbulence was more active over the southern part of the domain. Indeed, the southern portions of these cross sections are part of the upwind region and the northern parts are associated with the downwind region because of the southerly component of the prevailing low-level wind. Based on the analyses shown in section 4a, the TKE is stronger in the upwind region than in the downwind region. The isoline of $TKE = 1 \text{ m}^2 \text{s}^{-2}$ is almost exactly the cutoff for the downwind TKE (see Fig. 5). Thus, not many TKE structures showed up in the northern part of the cross sections in Fig. 8. The TKE budget terms in this case will be analyzed in detail in section 5.

The qualitative comparisons between the observations and LES-simulated AgI dispersion presented so far indicate that the horizontal spread of the simulated AgI plumes was similar to what was observed and the simulated plumes extended to the highest observational altitude with comparable AgI concentrations. Quantitative comparisons are needed to further assess the usefulness of the LES results. Therefore, we plotted the contour frequency by altitude diagrams (CFAD) of airborne measurements (all of the data from flight legs 1 to 8) and LES results in Fig. 9. In each panel, the $x$ axis represents the IN count rate per second (the AgI count rate converted from the concentration for model results), the $y$ axis is the altitude (m AGL), and the frequency (ratio of AgI-altitude data points over total number of samples) is color shaded. The observations numbered 2918 along the flight legs, and they are plotted in the CFAD format in Fig. 9a. To make the comparisons as
consistent as possible, we identified the 2918 grid points corresponding to the locations of all the measurements in space. Since the LES results were output every 5 min (see Table 3), it is impossible to match the exact timing of each measurement. Therefore, the average value of each grid point between 2315 UTC 16 February and 0035 UTC 17 February (the observational period as listed in Table 2) was plotted in Fig. 9b. The observed AgI concentrations as a whole are a subset of the entire AgI concentration space (a continuous temporal–spatial manifold), such that the observations should be bounded by the maximum possible values in the entire concentration space. Thus, we also plotted the maximum AgI count rate from each of the 2918 grid points between 2315 UTC 16 February and 0035 UTC 17 February in Fig. 9c.

Figure 9 shows that low values of both observed and simulated AgI count rate (<2 s⁻¹) dominated the appearance frequency at all altitudes (blue to green or even red colors). The CFAD of the average simulated AgI count rate resembled the observed CFAD below about 400 m AGL, but it deviated in the AgI count rate comparison between 400 and 1000 m AGL. In this layer, the LES-averaged CFAD overestimated the frequency of small values (low AgI concentration) and underestimated the large values (high AgI concentration). As discussed previously, the vertical dispersion of AgI particles was largely determined by the turbulent eddies, which are highly intermittent in space and time. The LES-averaged CFAD (over 1 h and 20 min) significantly smoothed out the intermittency and underestimated
AgI concentration in comparison with the observed CFAD. In contrast, the maximum LES-simulated AgI concentrations resulting from the strongest turbulent eddy during the measurement period should encompass the observed values. Figure 9c shows that the maximum LES-simulated CFAD overestimated the frequencies of large values at almost all altitudes. Quantitatively, the observations lie between the two LES-simulated CFADs, which means that it is possible to choose model AgI concentrations in flight tracks' corresponding grids to reproduce almost exactly the same CFAD as observed within the flight window. Considering the uncertainties associated with the observations and the LES, the CFAD comparisons show reasonable agreement between the observed and LES-simulated AgI concentrations.

Measurements of IN concentrations at the surface site (Mountain Meadow Cabin 9) were also collected in the downwind region of the airborne measurements in this case (see Fig. 2c for the location of this site). Because of the larger chamber and fixed location, the detection threshold of this ground-based IN counter (about 5 L$^{-1}$) is lower than the airborne version (higher sensitivity). Figure 10 shows histograms of 15-min averaged AgI concentration between 2200 UTC 16 February and 0300 UTC 17 February for observations at the surface site (Fig. 10a), results of the LES at the closest grid point to the site (Fig. 10b), and results of the LES averaged over the 9 x 9 closest grid points to the site (Fig. 10c). The model values were taken from the first layer, which is about 7 m AGL at the surface site. The LES generally overpredicted AgI concentrations at the surface site but remained within one order of magnitude. The overpredicted AgI concentrations maybe caused by 1) the uncertainty of AgI source strength from ground-based generators, 2) errors in the simulated wind direction, and 3) the inefficient vertical dispersion by the turbulent eddies.

Relative to point 1, the actual size distribution of AgI particles from the pyrotechnic generator varies from generator to generator at different times. A slight change of the mean mass diameter and spread of the distribution will easily result in an order of magnitude difference in AgI concentration. For example, doubling the mean mass diameter will decrease the AgI concentration by 8 times. As for point 2, the LES-simulated wind direction was more southerly than the observed wind in the first half of the simulation. Thus, more AgI particles were advected from the RR2 generator to the surface site in the model. The arrival of the AgI plume on the surface site is an integrated result of advection, transportation, and dispersion of AgI particles along the path from RR2 to the site. Any errors in wind direction, TKE strength, and local stability within the path will impact the arriving time and concentration magnitude of the AgI plume at the site. Although the model overestimated the AgI concentrations at the surface site, it captured the trends quite well. In regard to point 3, a recent study by Zhang et al. (2013) revealed that low-level wind and temperature are not well simulated by the WRF model in complex terrain. The underestimate of wind speed by the 500-m non-LES simulation is apparent in this study (see Table 1). The weaker low-level wind might be the result of inaccurate conditions in NARR data and WRF's deficiency in simulating correct wind fields at low level. A direct result of such an underestimate in wind speed is the lower Fr and the higher Ri, and subsequently a more stable low-level atmosphere simulated by the non-LES run. Mirocha et al. (2014) showed that the LES driven by a mesoscale model generally underpredict the wind simulated by the mesoscale model because of not-fully developed turbulence. Such a result is also valid in our study, as Table 1 also showed that inherited from 500-m non-LES results, the LES simulated even weaker low-level winds and a more stable lower atmosphere. Accordingly, the more stable atmosphere simulated by the LES generated less active TKE than reality, which resulted in weaker vertical mixing and a higher concentration of AgI particles close to the ground.
d. LES and non-LES comparisons

Based on the 100-m LES comparisons using the airborne and ground-based measurements of AgI number concentration, the LES was shown to reasonably capture the AgI dispersion characteristics over the Medicine Bow Mountains in the 16 February 2011 case. If we assume the LES reasonably represents reality even though discrepancies between LES and observations still exist, we can use the high-resolution LES results to validate other simulations with lower resolutions. The practical purpose of such validations is to find out, given affordable computational resources, what model setup can provide a reasonable estimate of AgI dispersion over complex terrain that finally impacts the orographic cloud and leads to precipitation enhancement on the ground. Here, we provide an example of such validations using CFADs of simulated AgI concentration and profiles of total AgI number.

To conduct the validations, three additional simulations over the domain with 500-m grid spacing were performed. Each run was a one-way nesting simulation driven by the outputs of the 2500-m simulation. The output frequency was set to 5 min to match that of the 100-m LES. One of the runs was the LES, one a non-LES using the MYJ PBL scheme, and one a non-LES using the YSU PBL scheme. All these 500-m simulations were spun up for 45 min as in the 100-m LES case. Though the 500-m domain is larger than 100-m domain, the kinetic energy spectrum tends to reach steady state within 45 min too (not shown). This is partially because the orographic cloud and leads to precipitation enhancement on the ground. Here, we provide an example of such validations using CFADs of simulated AgI concentration and profiles of total AgI number.

The CFADs of AgI concentration over the 100-m LES domain (for 500-m simulations, it is a subset of the domain as indicated by the black box in Fig. 2b) during the AgI release period (2145 UTC 16 February to 0115 UTC 17 February) are plotted in Fig. 11 for the 100-m LES and the other three 500-m simulations. The x axis is model-simulated AgI concentration from $10^{-3}$ to $10^{3} \text{m}^{-3}$ in a logarithmic scale. The y axis and color shaded areas are the same as described in Fig. 9. The data sample included all the model data below 1800 m AGL over the indicated domain and from all output records. The large data population resulted in much smoother CFADs compared to those in Fig. 9.

The CFAD of the 500-m LES looks very similar to that of the 100-m LES. Both CFADs showed high frequencies of data that are confined in concentration between $10^{2}$ and $10^{7} \text{m}^{-3}$ and in altitude between 0 and 3000 m AGL. For the lower concentration range, the 500-m LES also predicted a similar pattern to the 100-m LES (blue belt from $10^{-3}$ to $10^{3} \text{m}^{-3}$ and from 300 to 1000 m AGL). Such features were also captured by the 500-m MYJ simulation, but it did not simulate the high concentration features evident in both LES results. Basically, the 500-m MYJ simulation predicted a much shallower mixed layer than in the LES runs. Similarly, the 500-m YSU simulation also simulated a very shallow mixed layer in which very high concentrations of AgI stayed close to the ground. Some local maxima close to $10^{3} \text{m}^{-3}$ at about 200 m AGL were also predicted by the 500-m YSU simulation.

The different properties of AgI vertical dispersion simulated by these modeling approaches can be found in the profiles of total AgI number as well. As shown in Fig. 12, the 500-m LES predicted a similar profile to the 100-m LES when the generators were turned off. The AgI number is greatest in the 100-m LES between 150 and 1700 m AGL. The 500-m MYJ simulation reproduced the trend of the LES results but underpredicted the number by more than an order of magnitude between 200 and 1500 m AGL. The 500-m YSU simulation completely missed the main features produced by the LES runs and simulated a very inactive PBL with minimum vertical dispersion. Both LES profiles show fewer AgI number close to ground compared to non-LES runs, which indicates that the low-level vertical dispersion is stronger in LES mode.

Based on the CFAD and AgI number profile comparisons, the LES with 500-m grid spacing mostly reproduced the 100-m LES AgI dispersion characteristics. Non-LES runs using PBL schemes had difficulty in capturing the shear-dominant turbulent PBL structure over complex terrain in wintertime. The grid spacing of 500 m applied here is within the “terra incognita” identified by Wyngaard (2004). Traditional mesoscale models using PBL schemes and finescale LES were not designed to operate at this resolution. Gibbs et al. (2011) provided an example showing that the employment of a PBL scheme on the range of 1 km or less could lead to degrading results. The comparisons performed here indicated that both the SGS model for LES and PBL schemes for non-LES simulations need to be revised or even new PBL scheme needs to be developed in complex terrain at 500-m grid spacing. For practical purposes, we tentatively suggest that LES with a grid spacing close to 500 m or finer may adequately simulate AgI dispersion over complex terrain and wintertime orographic clouds when the new SGS model and new PBL schemes are absent for time being. On a coarse grid, the MYJ PBL scheme appears to best simulate the glaciogenic seeding of wintertime orographic clouds.

5. Discussion

The wintertime PBL over complex terrain is not consistent with the traditional buoyancy-driven mixed-layer
concept. This statement can be confirmed by analyzing the profiles of TKE budget terms in the TKE tendency equation.\(^8\) A symbolic form of the TKE tendency equation can be written as

\[
\frac{dTKE}{dt} = \text{BUOY} + \text{SHEA} + \text{ADVT} + \text{TUTR} + \text{PRAD} + \text{DISS},
\]

where \(\frac{dTKE}{dt}\) is the TKE tendency or storage term (Stull 1988), BUOY is the buoyant production term, SHEA is the shear or mechanical production term, ADVT is the TKE advection term, TUTR is the turbulent transport term, PRAD is the pressure adjustment of correlation term, and DISS is the dissipation term. Figure 13 illustrates the profiles from 0 to 2000 m AGL of the BUOY, SHEA, ADVT, TUTR, and PRAD terms over the upwind region (same as in Fig. 5) during the AgI release time (2145 UTC 16 February to 0115 UTC 17 February). The storage term and dissipation term are ignored to make the plot more readable.

Since this experiment was carried out in late afternoon local time on an overcast winter day, the buoyancy played an insignificant role in TKE production. Actually, it worked as a destruction term since the atmosphere

\(^8\) The complete equation can be found in Stull (1988).
was stably stratified. Wind shear, on the other hand, dominated the TKE production between 100 and 600 m AGL. Such a deep shear layer consistently generating turbulent eddies does not exist in a traditional convective PBL over flat terrain. The breakdown of the shear term indicates that the negative values below 100 m AGL are associated with the persistent positive vertical kinematic eddy fluxes ($u'w' > 0$ and $v'w' > 0$) even if the shears are positive ($du/dz > 0$ and $dv/dz > 0$). Such features are suspected to relate to the interactions between the fine-scale terrain properties and the low-level wind field, or they might be just the result of mismatch between the lowest mass point height and the first-level coordinate height (Moeng et al. 2007). Further work should be done to decode this phenomenon. Both buoyancy-driven and shear-driven turbulent eddies are anisotropic. Buoyant turbulence is more vertically oriented while shear-induced turbulence is strongest in the horizontal. The shear-dominant TKE production shown in Fig. 13 explains the small fraction of the vertical component to the total TKE in the PBL as shown in Fig. 5.

The turbulent advection, transport, and pressure adjustment terms showed similar vertical patterns with the destruction of turbulence at low levels and the production at high levels. However, the interception of the curve and the zero line increases from 400 m AGL for advection to about 600 m AGL for transport and to about 900 m AGL for the pressure adjustment term.

Each of these terms might work as production or destruction terms locally, but integrated over the horizontal and the vertical they effectively become zero. These terms only adjust or redistribute turbulent energy generated by buoyancy and shear. Figure 13 shows that these mechanisms moved the turbulent energy generated in the wind shear layer to higher levels. The pressure adjustment term was responsible for the nonnegligible TKE above 1000 m AGL as shown in Fig. 5.

The discussion on the TKE budgets indicates that the wintertime PBL over complex terrain is very different from the summertime convective PBL over flat terrain. In this case, the wind shear induced by the rough terrain existing in a relatively deep layer dominates the TKE production that is horizontally orientated. Such a shear-driven turbulent layer is not only responsible for AgI dispersion but is also believed to enhance orographic precipitation by increasing riming efficiency as proposed in Houze and Medina (2005). In this case, the shear-driven turbulent layer is entirely within the PBL, as evident from the TKE profile, in contrast to the elevated shear zone in Houze and Medina (2005). Clearly, PBL turbulence is ubiquitous over complex terrain (where winter storms are usually accompanied by strong winds), thus orographic precipitation may rather generally be enhanced by PBL turbulence, as suggested by Geerts et al. (2011). Furthermore, the longwave radiation cooling of the cloud deck could invigorate the underlying turbulence, which would enhance the scalar dispersion and snow growth.

AgI contamination over target areas from the previous seeding operations is a practical problem for many

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9 Under such stable conditions, an air parcel displaced vertically by turbulent eddies will experience a buoyancy force pushing it back to its original place (Stull 1988).
randomized wintertime orographic cloud-seeding programs. Usually, the mean wind speed and the target scale are used to calculate the average AgI dissipation time. However, the interactions between the topography and the low-level wind have been shown to be very complex in this study. The actual AgI dissipation time is believed to be different than the simple calculated value. This problem is difficult to address by the physical experiments performed by WMI but it is relatively easy to answer using the LES results. Based on this LES, it took about 1.5 h for AgI plumes to transport and dissipate away the target region after seeding ceased. This time is significantly longer than the simple calculated dissipation time of 50 min.

6. Conclusions

A numerical modeling study has been conducted to explore the ability of the WRF-based LES model to reproduce AgI particle dispersion by comparing the model results with measurements made on 16 February 2011 over the Medicine Bow Mountains in Wyoming. The recently developed AgI cloud-seeding parameterization (Xue et al. 2013b,a) was applied in this study to simulate AgI release from ground-based generators. Qualitative and quantitative comparisons between LES results and observations from soundings, aircraft, and ground-based instruments were conducted. Analyses on TKE features within the PBL and comparisons between a 100-m LES and simulations with 500-m grid spacing have been performed as well. The main conclusions of this study are as follows:

1) Despite the moist bias close to the ground and above 4 km AGL, the LES with 100-m grid spacing captured the essential environmental conditions and simulated a slightly more stable PBL relative to the observed soundings at Saratoga.

2) Wind shear is the dominant TKE production mechanism in wintertime PBL over complex terrain, and it generates a PBL of about 1000-m depth. The terrain-induced turbulent eddies are responsible for the vertical dispersion of AgI particles.

3) The LES-simulated AgI plumes were shallow and narrow, in agreement with inherently limited observations. The LES overestimated AgI concentrations close to the ground mainly because of a more stable simulated condition than the real atmosphere.

4) Non-LES simulations using PBL schemes had difficulty in capturing the shear-dominant turbulent PBL structure over complex terrain in wintertime. A LES approach should be applied for wintertime orographic clouds with a grid spacing close to 500 m or finer.

The LES was shown to reasonably simulate the AgI dispersion over the complex terrain in this study. Using the AgI cloud-seeding parameterization, more LES runs are being performed to investigate the glaciogenic cloud-seeding effect of the wintertime orographic clouds.

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APPENDIX

Vertical Diffusion of AgI in Non-LES Simulations and SGS Diffusion of AgI in LES

The vertical mixing or diffusion of any passive scalars by the MYJ and YSU PBL schemes and the SGS diffusion of any passive scalars in LES mode in the WRF model are described in the following sections. In this study, the AgI mass mixing ratio and number concentration were treated as two passive scalars in the WRF model that are mixed and diffused by the same equations below.

a. Vertical diffusion in MYJ PBL scheme

The MYJ scheme implements a nonsingular version of the Mellor and Yamada (1982) level-2.5 turbulence closure model through the full range of atmospheric turbulent regimes. The prognostic TKE equation in the MYJ scheme is parameterized as

$$\frac{d(l/q)}{dt} = \frac{\alpha(l/q)^4 + \beta(l/q)^2}{\gamma(l/q)^4 + \delta(l/q)^2 + 1} - \frac{1}{B_1} \tag{A1}$$

where $l$ is the master length scale, $q$ is the square root of twice the TKE, and $B_1$ is a constant. The coefficients denoted by Greek letters depend on buoyancy and shear of driving flow. The master length scale is first determined from diagnostic equations and is then adjusted to satisfy a nonsingularity criterion as described in Janjić (2001). The diffusion coefficients...
\(K_m\) and \(K_h\) are computed from \(q\) and \(l\) as described in Janjić (2001). The vertical fluxes of a passive scalar \(s\) are then calculated as

\[
\langle w's \rangle = -K_h \frac{\partial s}{\partial z}, \tag{A2}
\]

b. Vertical diffusion in YSU PBL scheme

The YSU scheme uses the countergradient terms to represent fluxes due to nonlocal gradients in the mixed layer. The mixing in the free atmosphere is dependent on local diffusion. For the mixed layer \((z \leq h)\), where \(h\) is the boundary layer depth, the turbulent diffusion equations for any prognostic variable including passive scalars \(s\) can be expressed by

\[
\frac{\partial s}{\partial t} = \frac{\partial}{\partial z} \left[ K_s \left( \frac{\partial s}{\partial z} - \gamma_s \right) - \left( \langle w's \rangle \right)_h \left( \frac{z}{h} \right)^3 \right], \tag{A3}
\]

where \(K_s\) is the corresponding eddy diffusivity depending on the momentum diffusivity \((K_m)\) and the Prandtl number \(Pr\), \(\gamma_s\) is the countergradient correction term, and \(\left( \langle w's \rangle \right)_h\) is the flux at the inversion layer. The YSU scheme explicitly treats the entrainment process through the asymptotic flux term at the inversion layer, the total diffusivity is found by taking the geometric mean of the entrainment diffusivity and the local diffusivity. In the free atmosphere, the YSU scheme uses a local diffusion scheme, or the so-called local-\(K\) approach.

c. SGS diffusion in LES mode

The 1.5-order SGS TKE model calculates the momentum diffusivity \((K_m)\) as

\[
K_m = C_k l \sqrt{\varepsilon}, \tag{A4}
\]

where \(C_k = 0.1\) is a constant; \(\varepsilon\) is the SGS TKE, for which a separate equation is solved; \(l\) is the isotropic length scale, which can be obtained from

\[
l = \min[(\Delta x \Delta y \Delta z)^{1/3}, 0.76e^{1/2}N^{-1}]. \tag{A5}
\]

The eddy viscosity coefficient for scalar \(s\) \((K_s)\) is given by \(K_s = Pr^{-1}K_m\), with \(Pr^{-1} = 3\) for the horizontal and \(Pr^{-1} = 1 + 2/\Delta z\) for the vertical. The SGS diffusion of scalar \(s\) in three dimensions is given by

\[
\langle u_i s \rangle = -2K_s \frac{\partial s}{\partial x_i}, \tag{A6}
\]

where \(i = 1, 2, 3\) for the \(x, y, \) and \(z\) dimensions.

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