#### Report on

# Development of a Lagrangian Particle Dispersion Model Compatible with the Weather Research and Forecasting (WRF) Model

Jerome D. Fast and Richard C. Easter Pacific Northwest National Laboratory

16 February 2006

## 1. Summary

The Weather and Research and Forecasting (WRF) model is a next-generation mesoscale meteorological forecast model that has been developed collaboratively among many government agencies and universities, including NCAR, NOAA, and the Air Force. WRF is expected to replace the MM5 model in the near future for many operational and research applications since MM5 development is no longer supported.

Lagrangian particle dispersion models (LPDMs) have been used for many years as tool to determine source-receptor relationships. Since WRF is a relatively new model, there are no LPDMs that are currently compatible with WRF as far as we know. We have adapted an existing LPDM called FLEXPART (Stohl et al., 2005) for use with WRF so that the multi-scale meteorological predictions made by WRF can be used in source-receptor analyses. The reasons FLEXPART was selected is because it has many capabilities including the calculation of forward dispersion, backward response functions, trajectory clusters, removal processes, concentrations, uncertainties, age spectra, and mass fluxes and the code is well-documented. However, FLEXPART is designed to perform particle dispersion computations based on wind fields derived from the ECMWF global forecast model.

We have therefore made extensive modifications of the FLEXPART code so that

- 1) the Net CDF output files produced by WRF are read directly,
- 2) the particle position computations correctly utilize the native WRF grid, and
- 3) the assumptions employed by the model are consistent with mesoscale models rather than global models.

In theory, one could develop software that would manipulate the WRF NetCDF output files to produce binary files compatible with FLEXPART; however, this would introduce an extra task that would create unnecessary I/O computational time and make running FLEXPART less efficient.

This report summarizes the changes made to FLEXPART, briefly describes how to use the new model that we call FLEXPART-WRF, and summarizes the capabilities of FLEXPART-WRF. The FLEXPART-WRF code should be considered a beta version. Although we have performed a number of tests, there may still be problems associated with certain configurations of the model that have not yet been checked. We also describe additional work needed to make FLEXPART-WRF more flexible and easier to use in an operational environment.

#### 2. Modification of FLEXPART

This section is a list of the changes made to the FLEXPART code.

#### 2.1 Modifications to the directory structure

The original top-level directory (which contained source code and was also used for running the code) was divided into a "src" directory containing the source code and makefile, and a "run" directory containing input and output files and subdirectories.

#### 2.2 Modifications to the makefile

- added new modules added to object list
- added links to netcdf library

## 2.2 Modules added to the source code

flexpart\_wrf.f: modified version of main program, replacing FLEXPART.f
map\_proj\_wrf.f: subroutines for map projection
map\_proj\_subaa.f: subroutines for map projection
read\_ncwrfout.f; reads WRF netcdf files

#### 2.3 Modifications to source code

Many modules had to be modified, that are listed below, to make FLEXPART compatible with WRF. Most of the changes arise because of the differences in the ECMWF and WRF coordinates systems, but other changes result from options we have added.

advance.f distance.f readoutgrid.f assignland.f getfields.f readoutgrid\_nest.f boundcond\_domainfill.f gridcheck.f readpartpositions.f readreceptors.f gridcheck\_nests.f calcmatrix.f init\_domainfill.f readreleases.f calcpar.f calcpar nests.f obukhov.f readwind.f calcpv.f readwind\_nests.f openouttraj.f calcpv\_nests.f openreceptors.f releaseparticles.f centerofmass.f outgrid\_init.f richardson.f outgrid init nest.f clustering.f timemanager.f conccalc.f partoutput.f verttransform.f partoutput\_short.f verttransform\_nests.f concoutput.f concoutput\_nest.f plumetraj.f writeheader.f convmix.f readavailable.f writeheader\_nest.f coordtrafo.f readcommand.f distance2.f readlanduse.f

#### 2.4 Additions to options file: /options/COMMAND

Four parameters have been added to the existing 22 parameters in the COMMAND file:

23. TURB\_OPTION. The default computation of turbulent wind components in FLEXPART, based on surface-layer scaling and local stability, is used when this

- parameter is set to 1. Setting this parameter to 0 turns off all turbulent wind components for trajectory computations. Setting this parameter to 2 permits turbulent wind components based on predicted turbulence kinetic energy (TKE). TURB\_OPTION = 2 is not functional yet and should not be used.
- 24. ADD\_SFC\_LEVEL. By default, FLEXPART uses meteorological quantities near the surface (10-m winds and 2-m temperature and humidity) in addition to those available on the meteorological model's vertical grid levels for determining turbulence quantities and particle transport/dispersion. The user can still choose this method by setting ADD\_SFC\_LEVEL = 1. The default methodology is useful for global model output that has coarse vertical grid spacing. For mesocale models, such as WRF, the vertical grid spacing near the surface is usually small and the lowest model level may be within 10 m of the ground. In this situation, the user may wish to set this parameter to 0, which would not add a 10-m computation level and the meteorology at the lowest model level would be used instead. ADD\_SFC\_LEVEL = 0 is not functional yet and should not be used.
- 25. SFC\_OPTION. By default, FLEXPART computes u\*, surface heat flux, and PBL height based on the mean meteorological input files. The user can still choose this method by setting the parameter to 0. Mesoscale models, such as WRF, usually compute these variables and it would be more consistent to use the values predicted by WRF. Setting this parameter to 1 makes the code read the variables directly from the WRF output files. For this case, the user must check the WRF registry so that u\*, surface heat flux, and PBL height are written to the NetCDF output files. If FLEXPART-WRF cannot find these variables, the code will then assume they are missing and compute u\*, surface heat flux, and PBL height by the default methodology. NOTE: if using SFC\_OPTION = 1 make sure that the first WRF output file is not used since u\*, surface heat flux, and PBL height are not defined in the wrfout\_\* files.
- 26. IOUTTYPE. The output files produced by FLEXPART are written in binary format by default. We found it useful to output the particle positions and concentrations in ASCII format that was easier to read by graphical software. The user can choose binary or ASCII output by setting this parameter to 0 or 1, respectively.

## 2.5 Definition of release characteristics, receptor locations, and concentration grid

FLEXPART is designed for use with global model output defined on a latitude-longitude grid and particle positions are computed using that coordinate system. The coordinate system in WRF, however, is not defined in latitude and longitude but as either a Lambert conformal grid or polar stereographic grid. The u- and v-components of the wind in WRF are therefore not true east-west and north-south components. In FLEXPART-WRF, particle positions are computed using a grid coordinate system, defined in meters, based on the grid spacing of the outer nested domain. We have changed the code so that the release locations, particle positions, and concentration grid can be defined in meters for the extent of the outer nested domain of WRF where x=0 and y=0 at the southwest corner of the domain. However, the user is likely to still want to define release locations, particle positions, receptor locations, and concentration grid in terms of latitude and longitude. Both options are included in the code. When the latitude-longitude option is chosen, all horizontal positions are input and output as latitude and longitude (in degrees), but are converted to/from the grid meters

coordinates system (which is always used for internal computation) using map projection routines.

To choose the desired coordinate system, modify /src/includepar:

- Set  $iomode\_xycoord = iomode\_xycoord\_meters$  for input and output tin the meters coordinate system
- Set  $iomode\_xycoord = iomode\_xycoord\_latlon$  for input and output in the latitude-longitude coordinate system

The choice of coordinate system also affects the RELEASES, RECEPTORS, and OUTGRID input files so that the user needs to define parameters in the files in either meters or latitude/longitude:

#### /options/RELEASES

- Line 4: Lower left corner x coordinate of the release location
- Line 5: Lower left corner y coordinate of the release location
- Line 6: Upper right corner x coordinate of the release location
- Line 7: Upper right corner y coordinate of the release location /options/RECEPTORS
- Line 2: x coordinate of the receptor location
- Line 3: y coordinate of the receptor location

#### /options/OUTGRID

- Line 1: lower left grid cell x coordinate
- Line 2: lower left grid cell y coordinate
- Line 5: upper right grid cell x coordinate
- Line 6: upper right grid cell y coordinate

Note that the concentration output grid is defined by the outermost corners of the lower-left and upper-right grid cells. If one wants the concentration grid to essentially match the outermost WRF grid in terms of horizontal grid spacing and coverage, then set the outermost corners of the concentration-grid lower-left and upper-right cells to match the centers of the WRF-grid lower-left and upper-right cells, and set the output grid x and y dimensions to 1 less than the WRF grid x and y dimensions. With these settings, the centers of the concentration-grid cells will be shifted by  $\frac{1}{2} \Delta x$  and  $\Delta y$  from the centers of the WRF-grid cells.

#### 2.6. Other modifications

FLEXPART parameterized mesoscale wind velocity fluctuations because of the ECMWF global forecast model does not resolve mesoscale circulations. The mesoscale wind velocity components, usigold, vsigold, and wsigold in /src/advance.f are now set to zero because the parameterization is not appropriate when using mesoscale model wind fields.

#### 2.7 Vertical interpolation

By default, FLEXPART interpolates meteorological parameters from the ECMWF model's hybrid-pressure ("eta") levels to levels defined by a terrain-following Cartesian vertical coordinate. This simplifies the particle dispersion calculations, because the Cartesian level

spacing (Δz) does not vary horizontally. We choose to retain this feature in FLEXPART-WRF, although several modifications have been made to account for the differences between ECMWF and WRF. For example, vertical velocities in ECMWF output files are in "etadot" units whereas WRF vertical velocities are already in m s<sup>-1</sup>. The variables method\_z\_compute and method\_w\_terrain\_correction were added during code development and testing. The method\_z\_compute switches between computing heights with the hydrostatic approximation (which was done in the original FLEXPART) and using the WRF geopotential heights directly. The method\_w\_terrain\_correction was used to test several approaches for transforming and interpolating the WRF w (which is an absolute vertical velocity) to FLEXPART's terrain-following Cartesian vertical coordinate system. For both these variables, there should be no reason to change the values set in *verttransform.f*.

#### 3. Running FLEXPART-WRF

The user should read the paper by Stohl et al. (2005) that contains documentation on the code as well as the choice of parameters for the input files. We only describe the differences in how to run the code as a result of the modifications to make the code compatible with WRF.

Step 1: compile code (in the /src directory)

- Modify makefile to include the appropriate NetCDF paths and compiler flags for your system. Compiling the code with optimization turned on and bounds checking turned off greatly increases the model speed.
- Modify /src/includepar to change *iomode\_xycoord* to the desired input/output coordinate system.
- Type "make" to compile code. The executable name is *flexpart\_wrf*.

Step 2: modify the input files (in and below the /run directory)

- Edit the pathname file to include the path of the run directory and location of WRF output files.
- Edit the AVAILABLE file to include a list of WRF output files to be used and the corresponding times of the files.
- Edit the /options/COMMAND, /options/RELEASES, /options/RECEPTORS, and options/OUTGRID files for the desired application. Note that values for many of the parameters will depend on the type of coordinate system desired. The value in the /src/includepar and the input files must have the same coordinate system. See Section 2.5 for the affected parameters.

The user has the option of using WRF input from one domain or from multiple nested domains if available. All or some of the domains can be used. When multiple nested domains are used, particle positions are determined using the winds from the highest resolution domain that overlaps the particle's current position. Particles are free to be transported into and out of nested domains. If the user employs nested domains, then multiple entries are needed in the pathnames file for the locations of the WRF output files. Separate AVAILABLE files are also needed for nested domains. For example, AVAILABLE.grid2 is the naming convection for the WRF output from domain 2. The user

can run FLEXPART with only one of the WRF nested domains if desired. In that situation the third nested domain would become "grid 1" in FLEXPART.

The COMMAND file contains a parameter called NESTED\_OUTPUT that implies that concentration fields can be produced for multiple output grids. This option does not work and only one output grid for concentration fields can be used per run.

The OUTGRID file also contains the vertical spacing of the 3-D output concentration fields. The resulting concentration field grid has a terrain-following Cartesian vertical coordinate. For simulations that use multiple nested WRF domains, the topography on the outer grid is used to compute the terrain-following coordinate. In areas of complex terrain where a high-resolution concentration field grid is desired, one should run FLEXPART with only one domain using the innermost nested domain from WRF as input with a concentration field grid that does not exceed the dimensions of the WRF domain.

## Step 3: run flexpart\_wrf

- If there are problems in the set up of the run, FLEXPART usually prints out information as to what is wrong.
- FLEXPART output is written to files in the /run/output directory. Separate output files are written for each output date/time. The naming convention is:

grid\_conc\_yyyymmddhhssss: 3-D concentration fields

grid\_pptv\_yyyymmddhhssss: 3-D mixing ratio fields in ppt

receptor\_conc; concentrations determined at receptor sites

receptor\_pptv: mixing ratios, in pptv, at receptor sites

partposit\_yyyymmddhhssss: x, y, and z locations and auxiliary information for each particle

#### Step 4: use model output

• There is no GUI for FLEXPART. It is currently up to the user to have software that can produce graphical output or analyze the output.

#### 4. FLEXPART-WRF tests

We have used WRF simulations of circulations over central Mexico to perform several tests the trajectory, particle dispersion, and concentration field computations produced by FLEXPART-WRF. This region was chosen because of the complex terrain. The outer grid encompassed Mexico with a grid spacing of 22.5 km while inner nested grids were centered over Mexico City with grid spacings of 7.5 and 2.5 km.

# 4.1 Forward Dispersion

We next describe a series of FLEXPART-WRF runs that simulates the multi-day transport and mixing of pollutants emitted from Mexico City between 26 February and 4 March 1997. The first run continuously releases 10,000 particles from a 1225 km² box in the Mexico City valley between 06 and 18 LST 26 February. The next run is identical to the first, except that the particles are released during the following 12-h period between 18 LST 26 February and

06 LST 27 February. The rest of the runs release particles during subsequent 12-h intervals until 06 LST 2 March. In this way, the multi-day particle plume can be segregated by release time that corresponds to daytime and nighttime release periods. For these runs, TURB\_OPTION was set to 1, ADD\_SFC\_LEVEL was set to 1, SFC\_OPTION was set to 0 and IOUTTYPE was set to 1 in the COMMAND file.

Examples of the particle plume location at various times are shown in Figs. 1 - 9. The synoptic winds were primarily southwesterly during the period so that the particle plume was transported to the northeast. During the daytime, particles were mixed within the convective boundary layer up to 2 to 3 km AGL over Mexico City. As the ambient mid-troposphere winds transport the particles to the northeast, the plume became decoupled from the surface over the Gulf of Mexico. The decoupling produced layers in the mid-troposphere that were often relatively thin. While particles were transported relatively quickly out of the central plateau, a wide distribution of particles from daytime and nighttime periods mixed together over the Gulf of Mexico. Note that the center of mass computations are based on only those particles within the computational domain; therefore, some caution should is warranted when a large fraction of the particles have been transported out of the domain.

Figure 10 is a plot of the concentrations resulting from the particle positions at 06 LST 28 February that correspond to Fig. 4a. A uniform kernel is used to compute concentrations that smooth out some of the spatial variations in the particle plume.

Time series of concentrations at two surface receptor sites downwind of Mexico City are shown in Fig. 11. Lower concentrations were produced during the daytime releases as a result of mixing with the convective boundary layer. Higher concentrations were produced at night because the particles released tend to be confined to a shallow layer near the surface. Lower concentrations were also produced at the second receptor site (dashed line) since it is located further away from Mexico City. A small portion of the particles released between 06 and 18 LST 26 February and between 18 LST 28 February and 18 LST 1 March remain over the central plateau. Particles released at other times are transported beyond the plateau and are not circulated back over the receptor locations.

# 4.2 Coordinate System Comparison

In another test, FLEXPART-WRF was run in trajectory mode to produce trajectories based on the meter and latitude-longitude coordinate system input/output options. In both runs, the trajectory was released from Mexico City and tracked for 72 hours. As seen in Fig. 12, the trajectories are nearly identical.

# 4.3 Effect of SFC\_OPTION and PBL Parameterization

An example of the differences in particle dispersion between simulations that employed the default computation of u\*, heat flux, and PBL depth (SFC\_OPTION = 0) and u\*, heat flux, and PBL depth directly from WRF (SFC\_OPTION = 1) is shown in Fig. 13. The YSU PBL parameterization was used in WRF for both simulations. The predicted particle plume and

concentration fields at 15 LST, 9 h after the particles began to be released at 06 LST, were qualitatively similar.

When the MYJ PBL parameterization is used in WRF, changing SFC\_OPTION has a larger impact on the predicted particle plume as seen in Fig. 14. More of the particle plume remains within the Mexico City valley when SFC\_OPTION = 0. It is not clear at present why FLEXPART-WRF is more sensitive to SFC\_OPTION for the MYJ PBL parameterization, but the user needs to be aware of such differences.

The PBL parameterization in WRF itself leads to differences in the dispersion computations and the user needs to be aware which PBL parameterization is more suited to a particulate application. As shown in Fig. 15, the predicted particles plumes at 00 LST 2 March 1997 for simulations that employ either the YSU or MYJ PBL parameterization are both transported to the northeast. However, more of the particles from the MYJ simulation remained within the Mexico City valley because the stronger thermally-driven circulations produced in WRF that used the MYJ PBL parameterization. The higher convective boundary layer heights from the YSU simulation also transported particles farther aloft where they could be influenced by the ambient flow.

## 5. Capabilities of FLEXPART-WRF

We have tested the primary capabilities of the code including:

- Forward / backward dispersion
- Forward / backward trajectories
- Receptor concentrations
- Clustered trajectories

Forward simulations have been more thoroughly tested than backward simulations. We have not had time to thoroughly test other capabilities of the code including emission variation files, removal processes, uncertainties, age spectra, mass fluxes, and the simulation of atmospheric trace gases such as stratospheric ozone.

#### **6.** Future Developments

The beta version of FLEXPART-WRF should work for most forward/backward trajectory and dispersion applications. Nevertheless, our experience with the code has identified several issues that should be addressed for long-term use of FLEXPART-WRF including:

Graphical Output: There is currently no graphical user interface (GUI) for FLEXPART. Since modifying the input files and running FLEXPART is relatively simple, a GUI may not be needed for the input. However, it would be very useful to have some sort of graphical product. All of the output is produced by binary or ascii files and it is up to the user to plot the results. Another useful graphing approach would utilize a Graphical Information System (GIS) so that model results could be displayed on many different types of layers and/or maps.

PNNL has several staff with experience in GUI and GIS programming that could be brought in on a project to develop a FLEXPART-WRF interface.

<u>Turbulence</u>: It would be useful to have the turbulent components consistent with WRF TKE. A placeholder has been set in the COMMAND file using the TURB\_OPTION=2 option, but this option should not be used. Some time was spent deriving u'<sup>2</sup>, v'<sup>2</sup>, and w'<sup>2</sup> from the predicted TKE, but the task was not completed to ensure that the code was stable for a variety of meteorological conditions. Another possible approach is to set the turbulent components in the Langevin equation to be proportional to the TKE vertical profiles and not dependent on boundary layer scaling and PBL height.

<u>Testing of Input Options:</u> We have not had test all possible combinations of input options in the COMMAND file. Some of our tests have shown that some combination of options do not work as advertised. For example, we had problems using a time averaging period of less than one hour. Additional tests are needed to identify combinations of input options that do not work and possibly providing fixes for them.

<u>Client-specific needs:</u> We have chosen to retain much of the functionality of running the code using the default input files: COMMAND, RELEASES, RECEPTORS, etc. For certain applications, the user may have to run the code multiple times to produce output that addresses a specific question. To reduce the time needed to modify input files and run multiple simulations, the code would need to be modified.

<u>Near-surface meteorological quantities:</u> FLEXPART computes 10-m winds and 2-m temperature based on the coarse output from the ECMWF model. For a mesoscale model such as WRF, the vertical grid spacing may be small so that meteorological quantities are already computed near the ground. We have set a placeholder in the COMMAND file by setting ADD\_SFC\_LEVEL = 0 to deactivate the interpolation of surface quantities and rely on WRF predicted variables, but this option is not function and it should not be used.

Computational Efficiency: Our experience is that the trajectory and particle dispersion in FLEXPART-WRF predictions take longer than one would expect. We have not fully tested where the computational time is being used and have run the code on only one Linux computer cluster. For example, 11-h dispersion simulations with releases of 10000, 100000, and 1000000 using NetCDF input files and ascii output files takes about 1, 2, and 6 minutes to complete, respectively. A simple trajectory run takes about 1 minute as well so the computational time for one and ten thousand particles is not very different. It is likely that most of the computational time is simply I/O required to read the WRF NetCDF files and write the output files. WRF has options for different types of output formats that have not been tested for speed. If I/O is not the problem, then it would be useful to determine which part of the code takes up the majority of the computational time. It is likely that some efficiency can be gained by re-organizing parts of the code. FLEXPART is highly modular with many modules, making it relatively easy to understand and change the code. However, for our aerosol model development we have found that having fewer subroutine calls greatly reduces the overall computational time.

<u>Map factors:</u> Particle positions and motions are calculated using the WRF map projection grid. Map factors should be (but are not yet) included in these calculations. For simulation domains covering a few thousand km, the map factors are close to unity (especially for the Lambert conformal projection), and neglecting the map factors should have little effect. Bigger errors could occur with larger simulation domains.

<u>Vertical Interpolation:</u> As stated previously, FLEXPART interpolates the meteorological parameters to a terrain-following Cartesian vertical coordinate. Because of the finer vertical grid spacing typically used by mesoscale models, it is more conceptually pleasing not to vertically interpolate the meteorological quantities. However, we think the vertical interpolation is not a significant problem.

We will be performing some of these tasks during the summer and fall of 2006 and expect to release an update later this year.

**Acknowledgements:** This work was supported by the U.S. Air Force.

#### References

Stohl, A., C. Forster, A. Frank, P. Seibert, and G. Wotawa, 2005: Technical Note: The Lagrangian particle dispersion model FLEXPART version 6.2. *Atmos. Chem. Phys. Disc.*, 5. 4739-4799.

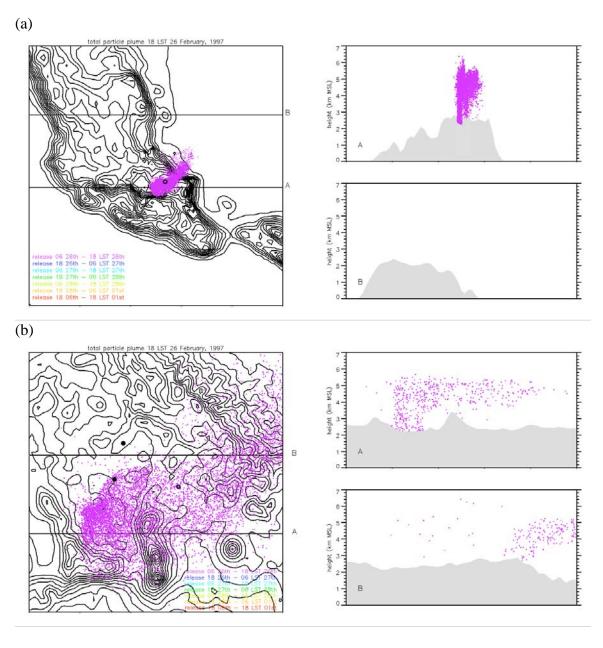


Figure 1. Simulated particle plume at 18 LST 26 February from a (a) regional and a (b) local perspective. The spatial extent of the plots corresponds to domains 1 and 3 for the regional and local perspectives, respectively. Black contours denote topography and the color of small particles denote the release period. The large filled colored circles denote center of mass of the particle plume. Two black circles in (b) denote receptor sites north of the Mexico City valley. Particles within 22.5 km and 2.5 km of lines A and B are shown in the vertical cross sections.

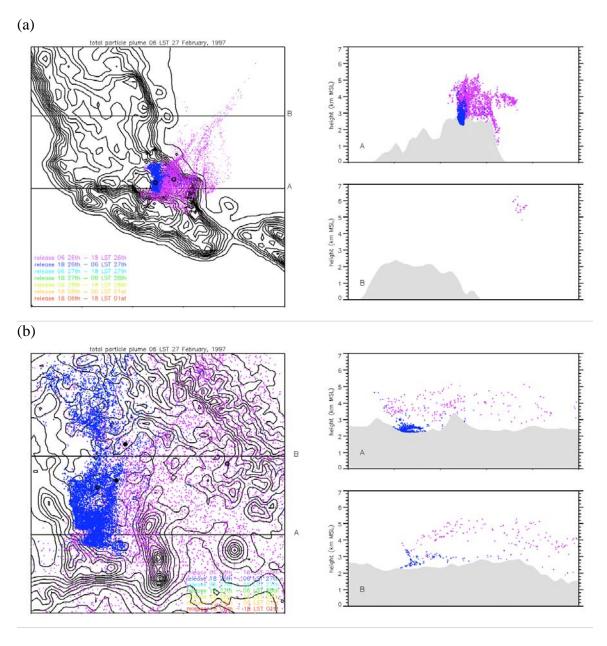


Figure 2. Same as Fig. 1, except at 06 LST 27 February.

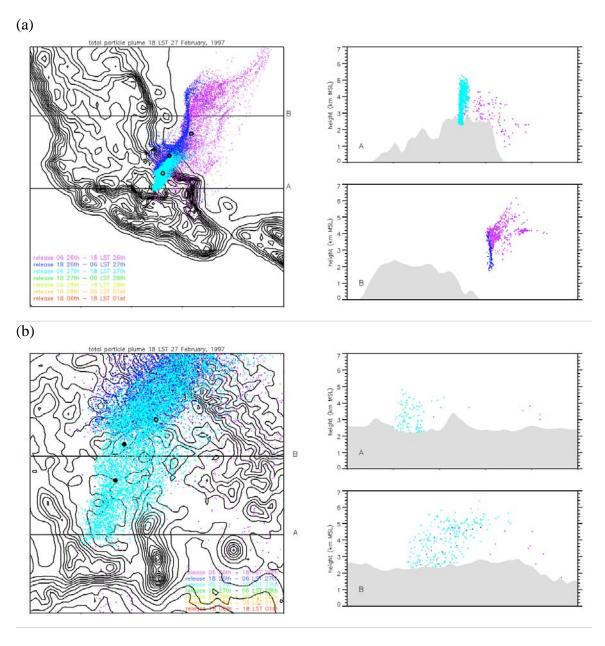


Figure 3. Same as Fig. 1, except at 18 LST 27 February.

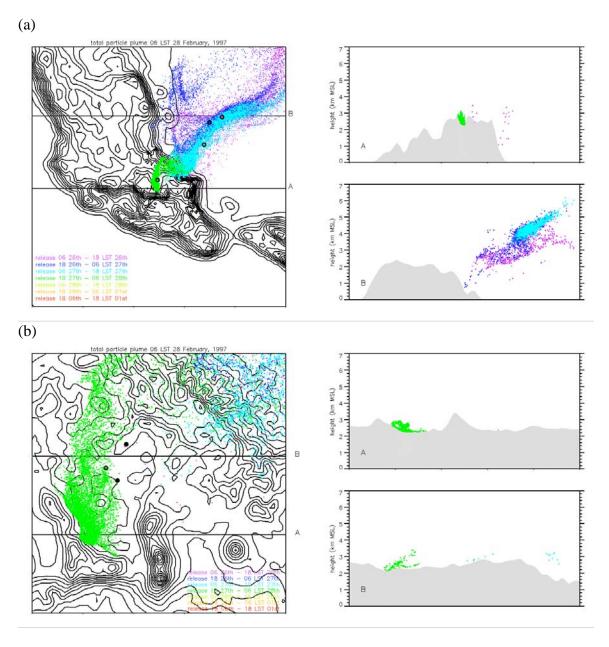


Figure 4. Same as Fig. 1, except at 06 LST 28 February.

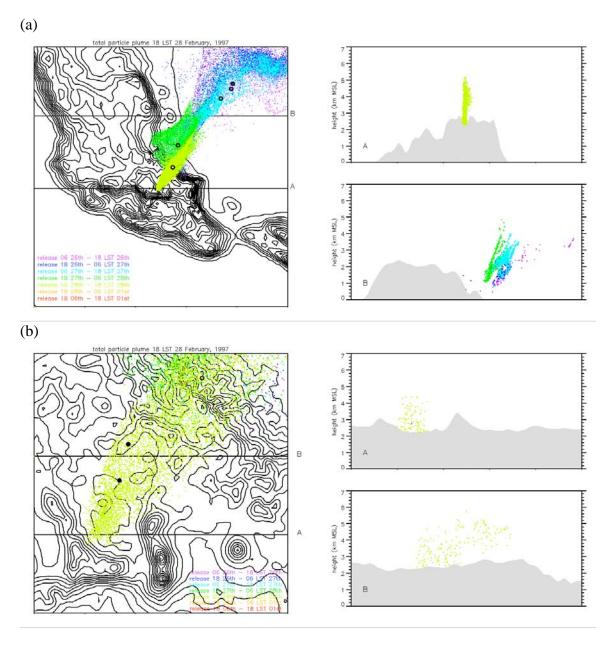


Figure 5. Same as Fig. 1, except at 18 LST 28 February.

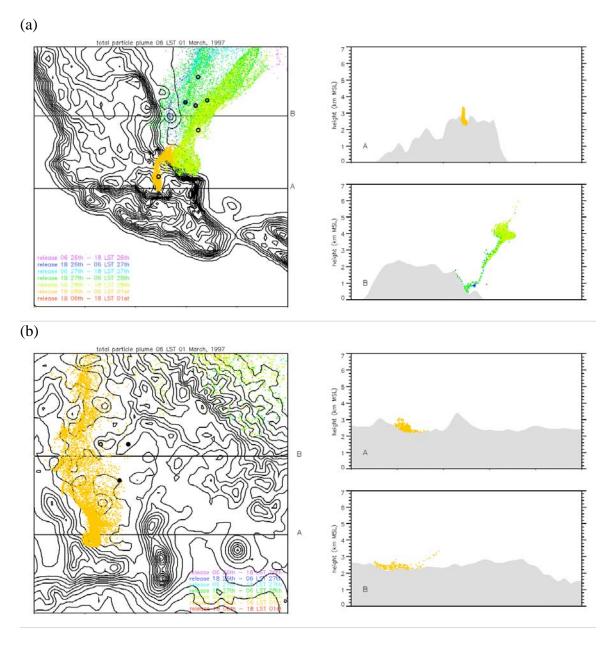


Figure 6. Same as Fig. 1, except at 06 LST 1 March.

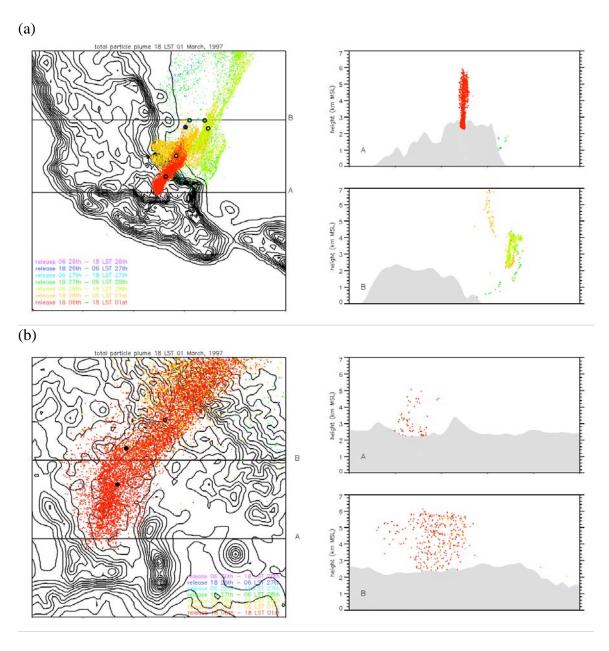


Figure 7. Same as Fig. 1, except at 18 LST 1 March.

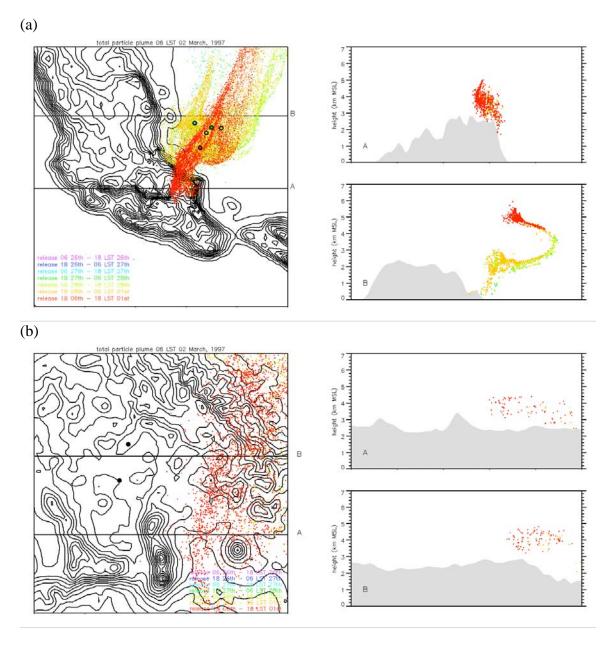


Figure 8. Same as Fig. 1, except at 06 LST 2 March.

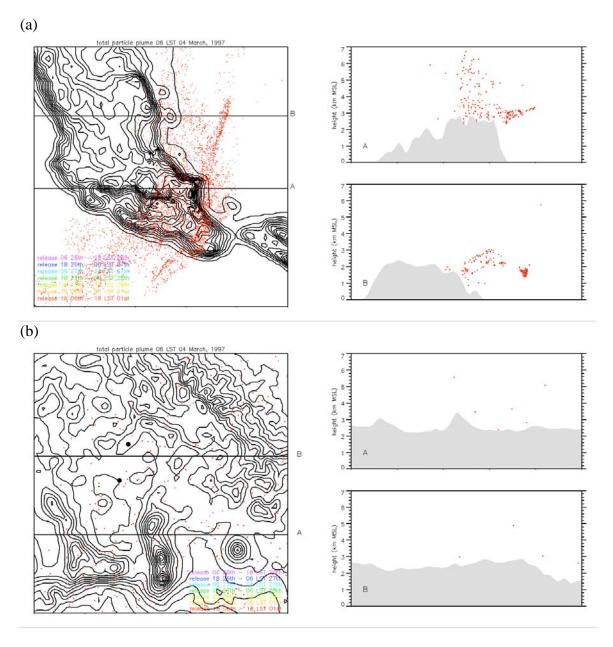


Figure 9. Same as Fig. 1, except at 06 LST 4 March.

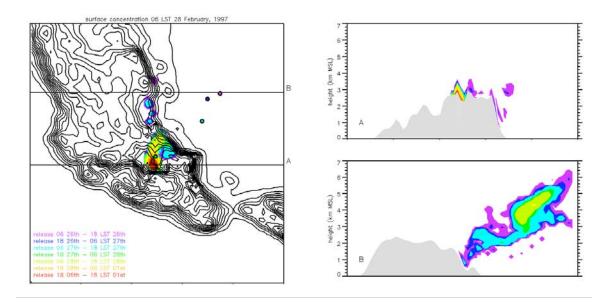


Figure 10. Same as Fig. 4a, except concentrations derived from the particle plume is shown.

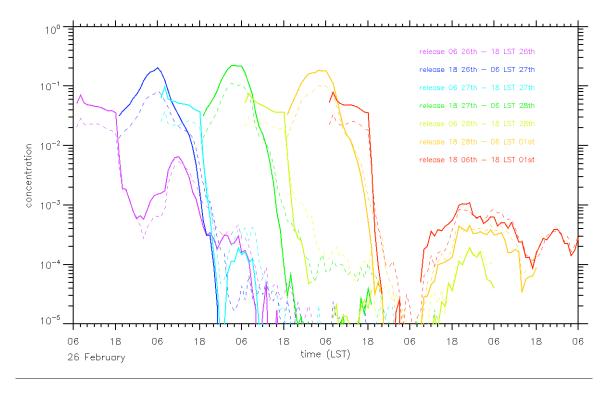


Figure 11. Time series of concentrations at two receptor sites denoted as black dots north of Mexico City in Fig. 1b. Solid and dashed lines denote concentrations at the receptors closest to and furthest from the Mexico City release area, respectively.

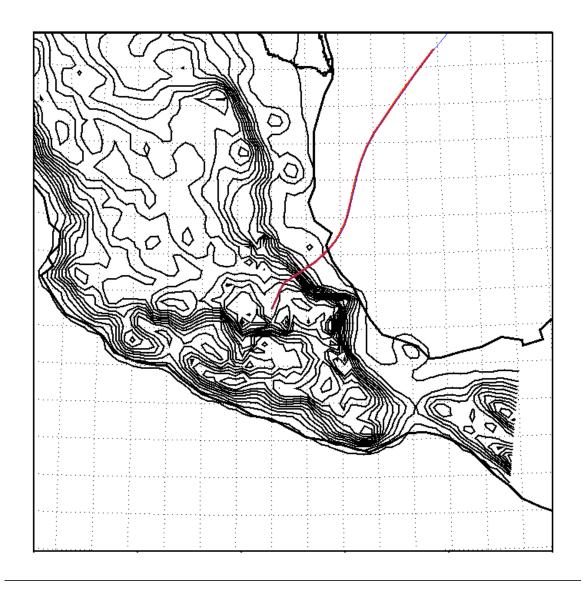


Figure 12. Comparison of forward trajectories computed using the meter (red) and latitude-longitude (blue) coordinate systems in FLEXPART-WRF.

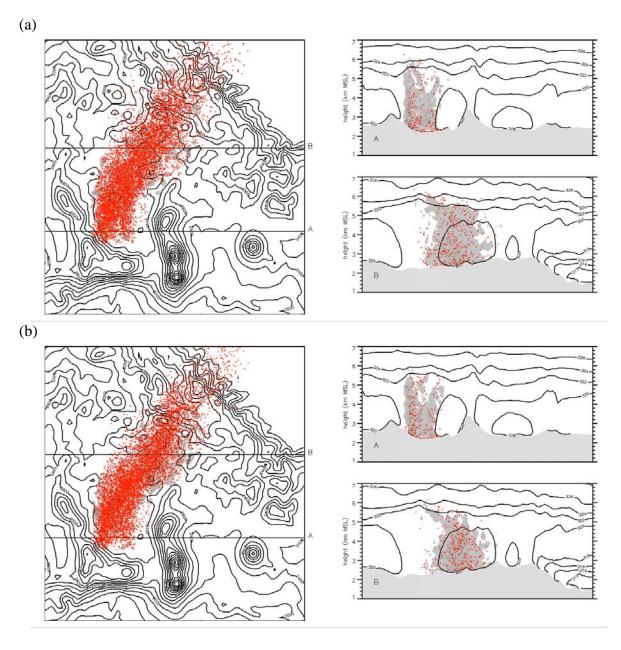


Figure 13. Comparison of forward dispersion over central Mexico at 15 LST 1 March 1997 using the YSU PBL parameterization in WRF and (a) SFC\_OPTION = 0 and (b) SFC\_OPTION = 1 in FLEXPART-WRF. Gray shading denote particle concentration at the surface (left) and along the vertical cross sections (right). Black contours denote topography (left) and potential temperature (right).

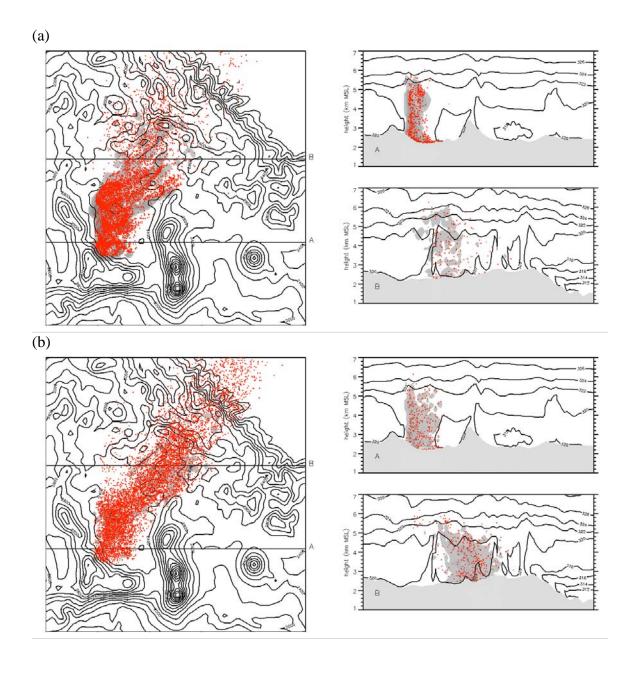


Figure 14. Same as Fig. 13, except that the WRF simulation employs the MRF PBL parameterization.

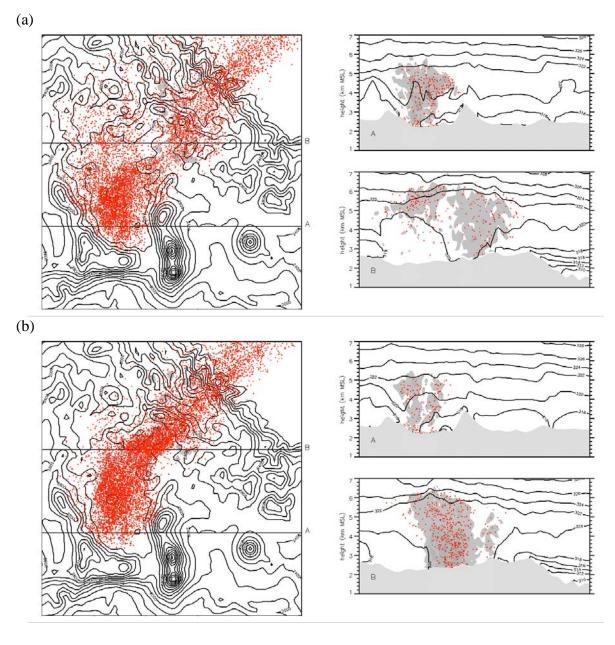


Figure 15. Comparison of forward dispersion over central Mexico at 18 LST 1 March 1997 using the (a) YSU and (b) MYJ PBL parameterizations in WRF and SFC\_OPTION = 1 in FLEXPART-WRF. Gray shading denote particle concentration at the surface (left) and along the vertical cross sections (right). Black contours denote topography (left) and potential temperature (right).