

MONTECARLO - A New, Fully-Integrated PC Software for the 3D Simulation and Visualization of Air Pollution Dispersion Using Monte Carlo Lagrangian Particle (MCLP) Techniques

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Abstract

This paper discusses the theoretical basis and the software implementation of a new version of the MONTECARLO computer package. This software provides a fully-integrated PC tool for: 1) processing meteorological data and calculating the parameters of the planetary boundary layer (PBL); 2) calculating the vertical profiles of the atmospheric turbulence parameters with a new, more rigorous and flexible parameterization; 3) running a Monte Carlo Lagrangian Particle (MCLP) model to simulate atmospheric dispersion of plumes under non-homogeneous, non-stationary conditions in flat or complex terrain; and 4) visualizing plume dynamics and air pollution concentrations using an integrated software, EWB-Air™ (<http://www.ssesco.com/files/ewb.html>), which produces three-dimensional (3D) views and animations superimposed over a digital map of the region.

1 Introduction and Overview

In the 1990s, MCLP models have become increasingly popular. The development of these techniques originates from the pioneering work of several researchers, including Smith (1968), Hall (1975), Watson and Barr (1976), Lamb (1978), and Zannetti (1981).

In MCLP applications, air pollution emissions of gases and particulate matter are simulated by a set of computational (or “fictitious”) particles that act like air pollution “tracers”. The trajectory of each particle is calculated by using pseudo-velocities that account for two main components: 1) the average transport, due to the mean wind velocity and 2) the unresolved turbulent fluctuations. The latter are simulated by generating pseudo-random velocity terms, with the aim of recreating – numerically – the randomness of atmospheric motion.

In comparison with other techniques (e.g., Gaussian plume models and gradient-theory grid models), MCLP models show a remarkable degree of spatial and temporal resolution. In particular, these models are capable of making full use of available meteorological measurements and information, since each particle moves according to the values of the meteorological parameters interpolated at the particle’s exact location. This feature allows MCLP models to provide realistic simulations of complex atmospheric dispersion phenomena, such as wind shear effects.

MCLP models have been well studied and improved in the last two decades. For example: Zannetti and Al-Madani (1983) suggested an approach to account for plume rise phenomena (see also Van Dop, 1992); Barentsen and Berkovicz (1984) introduced the use of two separate equations to simulate updrafts and downdrafts in convective conditions (see also DeBaas et al., 1986); Reid (1979) and Gifford (1982) identified the Langevin stochastic differential equation as the theoretical basis for MCLP models (see also Rodean, 1994); Zannetti (1986) defined a numerical scheme for the introduction of all cross-correlations among wind fluctuations; Lorimer (1986) introduced a kernel method for a cost-effective calculation of the concentration field; and Gopalakrishnan and Sharan (1997) introduced a simple approach to deal with heavy gas dispersion. In addition, MCLP models have been used in conjunction with meteorological models (HOTMAC[®] & RAPTAD[®] <http://chili.rt66.com/ysa/index.html>; RAMS & HYPACT <http://www.aster.com/>) to provide impressive plume simulations, especially in complex regions. These applications ranged from the regional/continental scale, e.g., Yamada’s (1992) simulation of the Chernobyl accident, to the local scale, e.g., the simulation of the Bhopal release, Boybeyi et al. (1995).

In spite of this theoretical development and testing, MCLP models present some difficulties in the correct use of the meteorological input. MCLP models require, as input, a complex set of meteorological variables that, in general, cannot be directly measured but can only be inferred from available measurements or the outputs of 3D meteorological models. These calculations are still based upon semi-empirical assumptions and clouded with uncertainty.

In this paper, we introduce a new version of our MCLP model, called MONTECARLO. This package presents several interesting features.

1. MONTECARLO allows the user to prepare a 3D meteorological input from a very limited set of meteorological measurements, using

the most advanced parameterization formulas for the planetary boundary layer (PBL).

2. The package includes a new routine that calculates theoretically-correct adjustment of the meteorological input when the meteorological averaging time is less than an hour.
3. The user is provided with advanced 3D visualization and animation capabilities, since MONTECARLO is fully integrated with the visualization program EWB-Air™ (EWB-Air is a trademark of SSESco <http://www.ssesco.com/files/ewb.html>).

For additional information on distribution and use of MONTECARLO, the reader is encouraged to contact the first author (zannetti@exponent.com).

2 Determination of Meteorological Parameters and Profiles in the PBL

MONTECARLO routines allow the user to calculate meteorological parameters and profiles in the entire PBL, based upon a limited set of meteorological measurements and information. The theories and numerical implementations are presented in Sozzi and Zannetti (in press) and will only be summarized here.

The user is required to specify the roughness length in the study area or, alternatively, the land-use type (e.g., cultivated land, urban, etc.). Then, the program calculates the turbulent vertical flux of sensitive heat (H_0) from the global solar radiation (R_g), where R_g is calculated from cloudiness, latitude, longitude, and time of the day. If $H_0 \leq 0$, this parameter is recalculated later.

The program calculates, at each meteorological station for each hour of the day, the friction velocity (u_*), the stability parameter ($1/L$), where L is the Monin-Obukhov length, the scale temperature (T_*), the convective velocity scale (w_*), the mixing height (h_{mix}), and if $H_0 < 0$ (stable conditions), the thickness of the night time, ground-based, inversion layer (h_{inv}).

The above parameters are used to calculate the meteorological profiles above every meteorological station. The wind is interpolated from two values provided by the user, the first value represents the surface wind (e.g., 10 meters above the ground) and the second value is an estimate of the wind at the top of the PBL. Similarly, the potential temperature, if needed, is also interpolated/extrapolated throughout the PBL.

MONTECARLO calculates the vertical profiles of the variables actually required as a meteorological input by the MCLP model, i.e.,

- The standard deviation of the streamwise wind component σ_u
- The standard deviation of the crosswind wind component σ_v
- The standard deviation of the vertical wind component σ_w
- The Lagrangian time scale in the streamwise direction T_{Lu}
- The Lagrangian time scale in the crosswind direction T_{Lv}
- The Lagrangian time scale in the vertical direction T_{Lw}

All these calculations are based on well-known parameterizations of the atmospheric surface layer (ASL) and the PBL, where these parameterizations are implicitly based upon an averaging time of an hour. However, when MCLP models are run, it is often possible to use shorter averaging times for wind data. It is not uncommon, for example, to have wind data (speed and direction) provided as 5-minute averages. Under these conditions, the "hourly" formulas introduced above may lead to an overestimation of atmospheric dispersion rates. Under these circumstances, the new version of our MONTECARLO model introduces corrective terms, based upon a rigorous spectral theory of atmospheric diffusion (see Sozzi and Zannetti, in press).

We believe that this is an important new feature of MONTECARLO and that applications of MCLP models that do not include our corrective terms can overestimate atmospheric diffusion, especially horizontal diffusion.

3 Example Simulation Results

Plume simulation results are readily displayed using the EWB-Air program. Sets of particle location information generated and stored during a plume simulation may be viewed from any angle in conjunction with regional map data, as shown in Figures 1 and 2. In addition, concentration data may be visualized as color-filled contours overlaid on the map, as shown in Figure 3.

Particle plume data and concentration grid data can be written to disk at user-specified frequencies (e.g., every 2 minutes of simulation time). This allows for animation of both the plume and concentration fields using EWB-Air. Such animations can be critical in evaluating plume dispersion over time and the effects of changing meteorological conditions and emission rates.

4 The MONTECARLO Package

The MONTECARLO software ensemble consists of the MONTECARLO plume simulation program (written in FORTRAN), the EWB-Air visualization system, and a pair of data conversion routines for translating MONTECARLO results into EWB-Air format. The MONTECARLO program and the data conversion utilities are DOS applications that can be run from within the Microsoft Windows™ operating system. The EWB-Air program provides a Windows-based graphical user interface for visualization of MONTECARLO results.

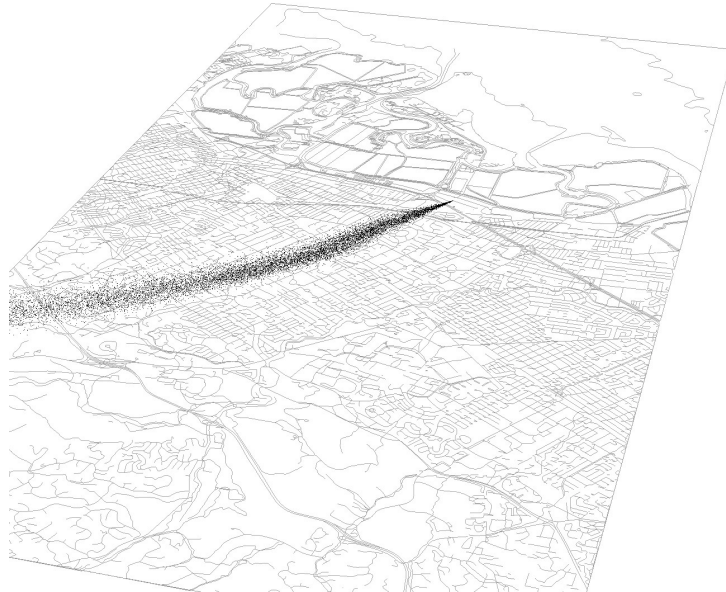


Figure 1. Three-dimensional aerial view of simulated plume superimposed on a regional map.



Figure 2. Top view of simulated plume showing effects of variations in local meteorology.

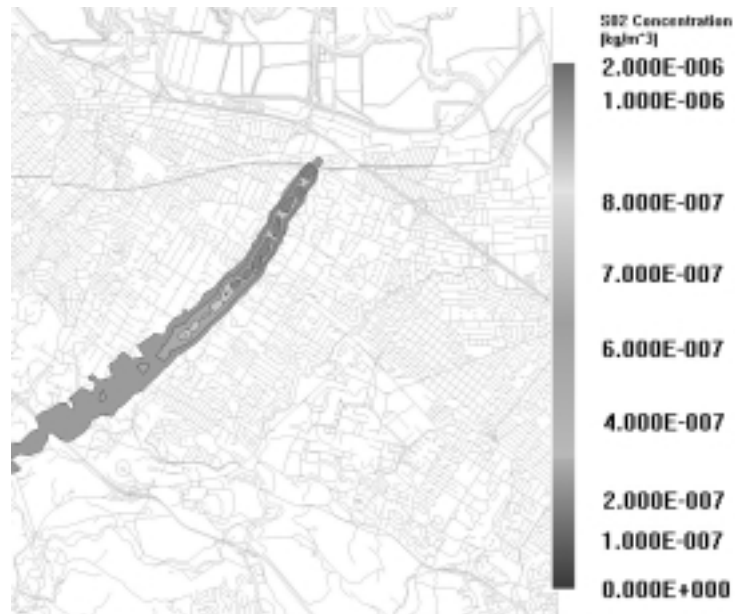


Figure 3. Instantaneous ground level concentration contours corresponding to plume shown in Figures 1 and 2.

A typical plume simulation begins with preparation of a set of input data files for the MONTECARLO program. These files include 1) a run parameter file, 2) a meteorology data file, 3) a meteorological station coordinates data file, 4) an emission data file, and 5) a local topography data file. All files are ASCII text files, which can be assembled easily using a text editor or spreadsheet program.

The run parameter file defines the simulation domain, source locations, and data input and output frequencies. The meteorology data file contains periodic readings of such parameters as wind speed, wind direction, temperature, pressure, and cloud cover. The meteorological station coordinates file contains the UTM coordinates of at least three meteorological stations within the simulation domain corresponding to the meteorological data input through the meteorology data file. The emission file contains periodic readings of source stack emission rates used to compute the mass of each plume simulation particle. The topography data file defines the local ground surface elevation (relative to sea level) over the simulation domain on a regular rectangular grid in UTM X- and Y-coordinates.

After the five input data files are prepared, the MONTECARLO program is started and runs in a DOS window. Progress messages are written to the display periodically as the simulation proceeds. The program also generates a run summary file that lists input parameters and tracks the numbers of active and inactive particles during the simulation. A particle becomes inactive when it

passes outside of the simulation domain. During a plume simulation run, the program sequentially writes particle location information and concentration grid information to output files for later post-processing with EWB-Air.

Upon completion of a MONTECARLO simulation, the user runs two data conversion utilities to prepare the particle location and concentration data for input to EWB-Air. These utilities run interactively in DOS windows, prompting the user for inputs related to several post-processing options.

In order to display MONTECARLO plume and concentration data over a regional map in EWB-Air, the user must prepare an optional map data file. A readily available source for map data in the United States is the US Geological Survey web site (<http://edcwww.cr.usgs.gov/doc/edchome/ndcdb/ndcdb.html>). Digital line graph (DLG) maps can be downloaded and converted into EWB-Air map format using a set of simple utility programs provided with EWB-Air. In addition, the user can convert the simulation domain topography data into EWB-Air format and drape the map over the topography in the EWB-Air display.

The EWB-Air program is invoked from an icon on the Windows Start menu. The user, using a built-in file browser, loads the data files containing particle location information, concentration information, and map and topography data. The EWB-Air software provides a wide variety of data display options for visualizing and animating plume simulation results viewed from any angle. Option configurations can be saved to files for rapid redisplay in a later EWB-Air session.

5 Conclusions

We believe that the current version of the MONTECARLO program represents a substantial improvement in using MCLP models. The code provides an enhanced level of user-friendliness and provides unique visualization/animation capabilities. More importantly, the code now incorporates important correction terms for the treatment of time intervals less than an hour.

We are currently expanding this package to include meteorological models, both diagnostic and prognostic.

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