Implementation of a Random Displacement Method (RDM) in the ADPIC Model Framework

Donald L. Ermak
John S. Nasstrom
Allan G. Taylor

June 1995

This is an informal report intended primarily for internal or limited external distribution. The opinions and conclusions stated are those of the author and may or may not be those of the Laboratory.

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED *BS*

DISCLAIMER

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial products, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

This report has been reproduced
directly from the best available copy.

Available to DOE and DOE contractors from the
Office of Scientific and Technical Information
P.O. Box 62, Oak Ridge, TN 37831
Prices available from (615) 576-8401, FTS 626-8401

Available to the public from the
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Rd.,
Springfield, VA 22161

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

Contents

	Page
1. <i>Introduction</i>	1
2. <i>Eulerian and Lagrangian equations</i>	1
3. <i>Numerical solution</i>	2
3.1 Finite difference equations	2
3.2 Time step.....	3
4. <i>Validation of the RDM versus analytic solutions</i>	4
5. <i>Acknowledgments</i>	9
6. <i>References</i>	9
<i>Appendix I: RDM implementation</i>	10
<i>Appendix II: FORTRAN Namelist input parameters</i>	14

1. Introduction

The objective of this work was to implement a 3-D Lagrangian stochastic (also called random walk or Monte Carlo) diffusion method in the framework of the operational ADPIC (Atmospheric Diffusion Particle-In-Cell) code (Lange, 1989; Taylor et al., 1993). The Random Displacement Method, RDM, presented here and implemented in the ADPIC code, calculates atmospheric dispersion in a purely Lagrangian, grid-independent manner. Some of the benefits of this approach compared to the previously-used "particle-in-cell, gradient diffusion" method are (a) a sub-grid diffusion approximation is no longer needed, (b) numerical accuracy of the diffusion calculation is improved because particle displacement does not depend on the resolution of the Eulerian grid used to calculate species concentration, and (c) adaptation to other grid structures for the input wind field does not affect the diffusion calculation. In addition, the RDM incorporates a unique and accurate treatment of particle interaction with the surface.

2. Eulerian and Lagrangian equations

The Random Displacement Method (RDM) is based, as is the particle-in-cell, gradient diffusion method, upon the conservation of species principal expressed in the form of the 3-D, incompressible, Eulerian advection-diffusion equation:

$$\frac{\partial \bar{C}}{\partial t} = -\bar{u} \frac{\partial \bar{C}}{\partial x} - \bar{v} \frac{\partial \bar{C}}{\partial y} - \bar{w} \frac{\partial \bar{C}}{\partial z} + \frac{\partial}{\partial x} \left(K_x \frac{\partial \bar{C}}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial \bar{C}}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial \bar{C}}{\partial z} \right) \quad (1)$$

where $\bar{C}$ is the mean air concentration of the species; $\bar{u}$, $\bar{v}$, and $\bar{w}$ are the mean wind components in the x , y , and z directions, respectively; t is time; and K_x , K_y , and K_z are the eddy diffusivities for the three coordinate directions (the eddy diffusivity tensor is assumed to be diagonal).

The RDM uses stochastic differential equations that describe the same process as the advection-diffusion equation (1), but in a Lagrangian instead of an Eulerian framework (Boughton *et al.*, 1987; Ermak, 1992; Rodean *et al.*, 1992). The stochastic differential equations for the displacement of an idealized fluid element in the three coordinate directions are

$$dx = \bar{u} dt + (2K_x)^{1/2} dW_x, \quad (2a)$$

$$dy = \bar{v} dt + (2K_y)^{1/2} dW_y, \text{ and} \quad (2b)$$

$$dz = \bar{w} dt + \frac{\partial K_z}{\partial z} dt + (2K_z)^{1/2} dW_z, \quad (2c)$$

where $dW_{x,y,z}$ are three independent random variates with zero mean and variance dt , i.e.,

$$\begin{aligned}\overline{dW} &= 0, \\ \overline{dW^2} &= dt.\end{aligned}$$

In (2a-b) it has been assumed that turbulence is homogeneous in the horizontal, x and y , directions. Eqs. (2a-c) can be integrated in time to calculate independent trajectories representing the movement of individual fluid elements. In a numerical dispersion calculation, the released species is represented by a large number of marker particles (fluid elements), each with a specified species mass. The ensemble-mean concentration at any time t can then be calculated from the particle locations at time t and the species mass associated with each particle.

A fundamental assumption in both the Eulerian formulation (1) and the Lagrangian formulation (2a-c) is that time and space scales of the turbulence are small relative to the time and space scales of the diffusion calculation to be performed. From an Eulerian view, the length scale ("eddy size") of the turbulence, L , is assumed to be small relative to the length scale of the spatial gradients of the concentration to be calculated, e.g., $L \ll \bar{c} / (\partial \bar{c} / \partial z)$. From a Lagrangian view, the time scale ("eddy lifetime") of the turbulence, τ , is assumed to be smaller than the time over which concentrations are to be calculated (i.e., $\tau \ll t$).

In the atmospheric boundary layer, turbulent time scales range from seconds to minutes. At the surface, they are typically assumed to be zero and to increase in a manner that is approximately linear with height. The rate of increase with height of the turbulent time scale near the surface is much higher under unstable, as opposed to stable, conditions. Therefore, for near-source diffusion from a point source the assumptions implicit in Eqs. (1) and (2a-c) become more valid, in general, for source heights closer to the surface and for more stable conditions. Conversely, for more elevated source heights and more unstable conditions (when the time and space scales of turbulence are greater) the assumptions are only valid for times and distances farther from the source, when the concentration distribution is more dispersed.*

3. Numerical solution

3.1 Finite difference equations

Assuming that K_x and K_y are constant in space, and that K_z varies linearly with height, i.e.,

* Models based on the Langevin equation are not limited by these assumptions, and can successfully model near-source dispersion under many conditions.

$$K_z(z) = K_z(z_i) + \left. \frac{\partial K}{\partial z} \right|_{z_i} (z - z_i) \quad (3)$$

a numerical solution of Eqs. (2a-c) can be constructed using the difference equations (Ermak, 1992):

$$\Delta x_i = \bar{u} \Delta t_i + [2K_{xi} \Delta t_i]^{1/2} \xi_{xi} \quad (4a)$$

$$\Delta y_i = \bar{v} \Delta t_i + [2K_{yi} \Delta t_i]^{1/2} \xi_{yi} \quad (4b)$$

$$\Delta z_i = \bar{w} \Delta t_i + \left(\frac{\partial K_z}{\partial z} \right)_i \Delta t_i + \left[2K_{zi} \Delta t_i + \left(\frac{\partial K_z}{\partial z} \right)_i^2 \Delta t_i^2 \right]^{1/2} \xi_{zi} \quad (4c)$$

where, for example, in the vertical direction,

$$\begin{aligned} \Delta z_i &= z(t_{i+1}) - z(t_i), \\ K_{zi} &= K_z(z_i, t_i), \\ \left(\frac{\partial K_z}{\partial z} \right)_i &= \left. \frac{\partial K}{\partial z} \right|_{\substack{t=t_i \\ z=z_i}}, \\ \Delta t_i &= t_{i+1} - t_i, \text{ and} \\ \xi_{zi} &= \text{a random number with zero mean } (\bar{\xi} = 0) \\ &\text{and variance of one } (\bar{\xi^2} = 1). \end{aligned}$$

The second-order term in (4c), $(\partial K / \partial z)^2 \Delta t^2$, is unique to our RDM. This term includes the effect of the linear variation of K during the finite time step, Δt , on the displacement variance, and is especially important close to the ground where K_z approaches zero in similarity theory parameterizations (Nasstrom (1995) described the K parameterization options available for the RDM). Particle trajectories can be numerically calculated by successively using (4a-c) and incrementing the particle position using, for example,

$$z(t_{i+1}) = z(t_i) + \Delta z_i. \quad (5)$$

Details on the implementation of (4-5) are given in Appendix A.

3.2 Time step

In the ADPIC code, a gridded wind field is used for the mean wind components, $\bar{u}$, $\bar{v}$, and $\bar{w}$ in (4a-c). Consequently, the time step used in the numerical solution is

restricted to prevent a particle from moving more than a single mean wind grid cell in any time step due to mean wind advection plus diffusion. Furthermore, for accurate time integration of concentration in the concentration grid, the time step is also restricted to prevent any particle from moving through more than a single concentration grid cell in any time step (this results in conservatively small time steps when the concentration distributions span many sampling grid cells).

In the RDM, the time step is determined separately for each particle. The eddy diffusivity and the spatial derivative of the vertical eddy diffusivity are evaluated analytically at the particle position at each time step. The particle time steps for all particles are forced to synchronize at necessary times, such as when meteorological parameters change, source parameters change, wind input data changes, particle concentrations are to be saved, status messages are to be written, or graphics output is to be written.

4. Validation of RDM versus analytic solutions

To validate the implementation of the RDM, calculations were performed and compared to three types of exact analytic solutions of the advection-diffusion equation (1). First, a successful no-diffusion, advection-only comparison was made to confirm that a Gaussian concentration distribution is accurately advected through the concentration sampling grid and that the time-integrated concentration is accurately calculated. Second, a series of point source releases at various elevations under uniform mean wind speed and constant K_x , K_y , and K_z conditions were simulated. Again, the RDM results were in excellent agreement with the analytic solutions which are time-dependent Gaussian concentration distributions with standard deviations $\sigma_{x,y,z} = (2K_{x,y,z}t)^{1/2}$. Finally, a more complex case of inhomogeneous turbulence was simulated and compared with the analytic solution. Details of this latter comparison and its results follow.

This case study was chosen to test the RDM under inhomogeneous turbulence conditions that included significant interaction of the dispersing plume with the lower boundary. The release scenario involved a continuous source at the ground surface,

$$z_s = 0, \quad (6a)$$

with a unit source rate,

$$Q_c = 1 \text{ g/s}. \quad (6b)$$

The eddy diffusivities and mean wind speed were chosen to be representative of a neutral surface layer, as follows:

$$K_z(z) = 0.1z \text{ m}^2/\text{s}, \quad (6c)$$

$$\bar{u} = 5 \text{ m/s}, \quad (6d)$$

$$\sigma_y(x) = 0.15 x^{0.92} \text{ m, and} \quad (6e)$$

$$K_x = 0. \quad (6f)$$

K_y was calculated using the relationship

$$K_y = \frac{1}{2} \frac{d}{dt} \sigma_y^2.$$

The grid used for calculating the concentration from the particle positions was nested in the horizontal with a resolution of 3.125 m in the innermost (fourth) nested grid near the source and 50 m in the outermost grid. The vertical resolution was 5 m. The domain was 2 km in the horizontal and 210 m in the vertical.

The RDM-calculated mean concentrations were compared to concentrations obtained by using the following analytic solution to the advection-diffusion equation taken from Brown *et al.* (1993):

$$\bar{C}(x, y, z) = \frac{Q_c}{(2\pi)^{1/2} K_1 x \sigma_y(x)} \exp\left(\frac{-y^2}{2\sigma_y^2(x)}\right) \exp\left(\frac{-\bar{u}z}{K_1 x}\right). \quad (7)$$

This solution for the mean concentration (e.g., g/m³) assumes (a) a continuous point source with source strength Q_c (e.g., in g/s); (b) the vertical eddy diffusivity is a linear function of height, $K_z(z) = K_1 z$; (c) a Gaussian horizontal concentration distribution with standard deviation, $\sigma_y(x)$; (d) no alongwind diffusion, i.e., $K_x = 0$; (e) the mean wind speed, $\bar{u}$, is constant with height; (f) zero vertical mass flux at the ground surface; and (g) the source location is at coordinates $x=0$, $y=0$, and $z=0$.

Figs. 1-3 show results comparing concentrations calculated using the RDM to those calculated by the analytic solution (7). Figs. 1 and 2 show excellent agreement between the contours of concentration from the analytical solution and the RDM, respectively, at a height of 10 m for a horizontal domain extending 1.8 km downwind of the source. The RDM contours in Fig. 2 are not as smooth as those in Fig. 1 due to the different concentration grid resolutions within different nested grids in the RDM computational domain. Fig. 3 also shows excellent agreement in a plot of concentration calculated by the analytic solution (solid line) and by the RDM (individual points) versus height at a downwind distance of 1.5 km along the centerline of the plume. Note the highly non-Gaussian shape of the vertical concentration profile. This exponential behavior of the concentration profile is primarily due to the linear variation with height of the vertical eddy diffusivity near the ground.

Figure 1. Contours of mean concentration (g/m^3) calculated by the **analytic solution** given in Eq. (7) with assumptions (6a-f) at a height of 10 m in a horizontal domain of 1.8×1.8 km. Contour levels are 3×10^{-5} (innermost), 1.5×10^{-5} , 3×10^{-6} , and 1×10^{-6} g/m^3 (outermost), as in Fig. 2. The units of the x and y axes are kilometers from the source location. Contours were drawn using a uniform 320 by 320 dimension horizontal array of concentration values.

Figure 2. Contours of mean concentration (g/m^3) calculated by the RDM with assumptions (6a-f) at a height of 10 m. Contour levels are 3×10^{-5} (innermost), 1.5×10^{-5} , 3×10^{-6} , and $1 \times 10^{-6} \text{ g/m}^3$ (outermost), as in Fig. 1. The units of the x and y axes are kilometers from the source location. Contours were drawn using concentration values from four nested grids with a resolution of 3.125 m in the innermost grid near the source and 50 m in the outermost grid. Note the domain used to plot these contours is slightly larger than in Fig. 1, but the scale is the same.

Figure 3. Mean concentration (g/m^3) versus height (m) calculated by the RDM (points) and the analytic solution (solid line) given by Eq. (7) with assumptions (6a-f) at a downwind distance, x , of 1.5 km at the centerline ($y = 0$) of the plume. RDM concentrations represent grid-cell volume averages and analytic concentration values were volume-averaged in a similar manner for comparison.

5. Acknowledgments

We would like to thank H.C. Rodean, E. Näslund, R. Lange, and L.A. Lawson for their help with earlier versions of the random displacement method. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract number W-7405-Eng-48.

6. References

- Boughton, B.A., J.M. Delaurentis, and W.E. Dunn (1987) A stochastic model of particle dispersion in the atmosphere, *Boundary-Layer Meteorol.*, **40**, 147-163.
- Brown, M.J., S.P. Arya, and W.H. Snyder (1993) Vertical dispersion from surface and elevated releases: an investigation of a non-Gaussian plume model, *J. Appl. Meteorol.*, **32**, 490-505.
- Ermak, D.L. (1992) Dense-Gas Dispersion Advection-Diffusion Model. *Proceedings JANNAF Safety and Environmental Protection Subcommittee meeting*, Aug. 10-14, 1992, Chemical Propulsion Information Agency, CPIA Pub. 588, pp. 215-224. Also, Lawrence Livermore National Laboratory, Livermore, CA, publication UCRL-JC-109697.
- Lange, R. (1989) Transferability of a Three-Dimensional Air Quality Model between Two Different Sites in Complex Terrain, *J. Appl. Meteorol.*, **28**, 7, pp. 665-679
- Nasstrom, J.S. (1995) *Turbulence parameterizations for the RDM version of ADPIC*, UCRL-ID-120965, Lawrence Livermore National Lab., Livermore, California.
- Rodean, H.C., R. Lange, J.S. Nasstrom, and V.P. Gavrilov (1992) Comparison of two stochastic models of scalar diffusion in turbulent flow. Preprint, Tenth Symposium on Turbulence and Diffusion, 29 Sept.-2 Oct. 1992, Portland, OR. Published by the American Meteorological Society, Boston, MA.
- Taylor et al. (eds.), (1993) *User's Guide to the MATHEW/ADPIC Models*, UCRL-MA-103581 Rev. 2.0, LLNL, Livermore, CA, .

Appendix I: RDM implementation

For brevity, only the vertical direction will be discussed in the following. The equations for the horizontal directions are of the same form as the vertical equations except there are no terms with spatial derivatives of the eddy diffusivities.

In describing the vertical displacement, it is convenient to represent the new particle height, z_{i+1} , after a time step Δt_i ($\equiv t_{i+1} - t_i$) as the sum of four terms: the initial particle height z_i , the mean wind displacement $\bar{w}\Delta t_i$, the mean diffusive displacement Δz_i^* , and random diffusive displacement $\Delta z_i'$, i.e.,

$$z_{i+1} = z_i + \bar{w}\Delta t_i + \Delta z_i^* + \Delta z_i'. \quad (\text{A1})$$

Recalling (4c), the mean diffusive displacement is seen to be

$$\Delta z_i^* = \left(\frac{\partial K_z}{\partial z} \right)_i \Delta t_i, \quad (\text{A2a})$$

and the random diffusive displacement is described by the following mean and variance:

$$\overline{\Delta z_i'} = 0, \quad (\text{A2b})$$

and

$$\overline{\Delta z_i'^2} = 2K_z \Delta t_i + \left(\frac{\partial K_z}{\partial z} \right)_i^2 \Delta t_i^2 \equiv \sigma_{zi}^2 \quad (\text{A2c})$$

The random diffusive displacement, $\Delta z_i'$, is obtained from a uniform probability distribution function

$$P(\Delta z_i') = \begin{cases} \frac{1}{2\sqrt{3}\sigma_{zi}}, & \text{if } -\sqrt{3}\sigma_{zi} < \Delta z_i' < \sqrt{3}\sigma_{zi}, \\ 0, & \text{elsewhere,} \end{cases} \quad (\text{A3})$$

where σ_{zi} is defined in (A2c). This distribution function has the correct mean and variance as specified in (A2b) and (A2c), respectively. A value of $\Delta z_i'$ can then be calculated using

$$\Delta z_i' = 2\sqrt{3}\sigma_{zi}(r - 0.5), \quad (\text{A4})$$

where r is a uniform random number on (0,1).

Equations (A1), (A2a), and (A4) provide a method for calculating the new particle height z_{i+1} that is consistent with (4c) and is used when there is no possibility that the new

calculated particle height will be below the ground surface. However, when the initial particle height, z_i , is sufficiently close to the ground, or more specifically when

$$z_i < \sqrt{3}\sigma_{zi} - \bar{w}\Delta t_i - \Delta z_i^*, \quad (\text{A5})$$

this procedure must be modified to ensure that the final particle height is above ground. One of two procedures is used to treat the particle interaction with the ground depending upon whether the diffusivity K_z is or is not a function of height.

When K_z is *not* a function of height, the new particle height, z_{i+1} , is simply reflected above ground level whenever z_{i+1} is less than zero. Thus, (A1) becomes

$$z_{i+1} = |z_i + \bar{w}\Delta t_i + \Delta z_i^* + \Delta z_i'|. \quad (\text{A6})$$

where $|\dots|$ indicates the absolute value. This is the reflective boundary condition that is commonly used when K is constant. Here we have approximated the Gaussian probability distribution with a uniform probability distribution that has the identical first two moments as the Gaussian distribution. The error introduced by this approximation is essentially zero for practical purposes after only a few time steps, and, in general, is much less than the error associated with using a finite number of particles to describe the species spatial distribution.

When K_z is a function of height and is linear near the ground with a value of zero at the ground surface (i.e., $K_z = K_z(z) = vz$, near the ground and v is a constant), the reflective boundary condition is not valid and introduces excessive error. In this case, the probability distribution function for the random diffusive displacement, $\Delta z_i'$, is approximated by the sum of two uniform distributions, rather than the single uniform distribution defined by (A3). The "double-block" probability distribution function for $\Delta z_i'$ used in this case is

$$P(\Delta z_i') = \begin{cases} p_1, & \text{if } -\bar{z}_{i+1} < \Delta z_i' < 0, \\ p_2, & \text{if } 0 < \Delta z_i' < \Delta z_{i\text{MAX}}', \\ 0, & \text{elsewhere,} \end{cases} \quad (\text{A7})$$

where

$$\bar{z}_{i+1} = z_i + \Delta z_i^*,$$

$$\Delta z_{i\text{MAX}}' = \frac{3\sigma_{zi}^2}{\bar{z}_{i+1}},$$

$$p_1 = \frac{\Delta z'_{iMAX}}{\bar{z}_{i+1}(\bar{z}_{i+1} + \Delta z'_{iMAX})}, \text{ and}$$

$$p_2 = \frac{\bar{z}_{i+1}^2 p_1}{(\Delta z'_{iMAX})^2}.$$

The random diffusive displacement, $\Delta z'_i$, can then be calculated as follows:

$$\Delta z'_i = \begin{cases} \frac{r_i}{p_1} - \bar{z}_{i+1}, & \text{if } r_i < p_1 \bar{z}_{i+1}, \\ \frac{(r_i - p_1 \bar{z}_{i+1})}{(1 - p_1 \bar{z}_{i+1})} \Delta z'_{iMAX}, & \text{if } r_i \geq p_1 \bar{z}_{i+1}, \end{cases} \quad (A8)$$

where r_i is a uniform random number on (0,1).

This approach to calculating the total diffusive displacement ($\Delta z_i^* + \Delta z'_i$) when the diffusivity is a function of height and linear near the ground has two unique features. First, it yields the exact values for the first and second moments of the total diffusive displacement and, second, it provides a value for the new particle position, z_{i+1} , in the absence of the mean wind $\bar{w}$, that is always greater than zero. Consequently, reflection at the ground surface is not needed to correct an unacceptable total diffusive displacement that puts the particle below the ground surface.

Finally, the new particle position, z_{i+1} , is then calculated by adding in the old particle position, z_i , and the mean wind displacement, $\bar{w}\Delta t_i$, using an equation of the same form as (A6), namely

$$z_{i+1} = |z_i + \bar{w}\Delta t_i + \Delta z_i^* + \Delta z'_i|, \quad (A9)$$

where the mean diffusive displacement, Δz_i^* , is calculated from (A2a), as before, and the random diffusive displacement, $\Delta z'_i$, is calculated from (A8) rather than (A4). The reflection condition implied by the absolute value sign in (A9) is applied to correct minor error, if any, in the mean wind displacement, $\bar{w}\Delta t_i$, that places the particle below the ground surface.

The above discussion of the RDM calculation of the vertical displacement and its treatment of the interaction with the ground surface basically applies when the terrain is flat. In general, a particle can end up below the ground surface as the result of minor errors in both the vertical and horizontal displacements as the code attempts to advect and diffuse the particle over and/or around the "step" representation of terrain in ADPIC.

The general procedure within ADPIC to ensure that particles remain above the ground surface is as follows: (1) If the terrain elevation of the new particle (x,y) location is less than or equal to the terrain elevation before the displacement, then the particle is simply reflected vertically. Otherwise, the particle height is shifted up one grid level at a time (up to a specified maximum number of shifts) in an attempt to place the particle above terrain; (2) If step (1) fails to place the particle above terrain, then the code returns the particle to its initial displacement height below the terrain and attempts to move the particle horizontally around the terrain; and (3) If step (2) fails to place the particle above terrain, then the particle is returned to its original location and no displacement of the particle occurs.

Appendix II: FORTRAN Namelist input parameters

(NOTE: Namelist parameters controlling the turbulence/K parameterizations for the RDM are not listed below. See UCRL-ID-120965, "Turbulence parameterizations for the RDM Version of ADPIC", Appendix B, for descriptions of these namelist input parameters.)

ADPIC_CONTROL namelist

DIFF_METHOD

New option:

DIFF_METHOD = 'RDM'

Diffusion is calculated with the Random Displacement Method (RDM). For this method, the types of horizontal and vertical turbulence parameterizations to be used for K_z and K_H respectively, by the RDM must be specified using the parameters TURB_PARAM_VERT and TURB_PARAM_HORZ.

ADPIC_METPARAMS namelist

DIFF_ON_X

Flag which allows user to turn diffusion off in x (east-west) direction. (Note: x is not downwind distance in this case)

(Default: DIFF_ON_X = 'Y')

DIFF_ON_Y

Flag which allows user to turn diffusion off in y (north-south) direction.

(Default: DIFF_ON_Y = 'Y'). (Note: y is not crosswind distance in this case)

DIFF_ON_Z

Flag which allows user to turn diffusion off in z (vertical) direction.

(Default: DIFF_ON_Z = 'Y')

INTERP_WINDS_STEP_MEAN

A character variable ('y'/'n') which allows a more accurate interpolation of winds at the mean position during the random vertical displacement. If 'y', a more accurate calculation is possible in instances where winds change rapidly in the vertical. The default ('n') provides reasonably accurate results for most instances.

TIMESTEP_GLOBAL_FRACT

A parameter which can be used to decrease the global timestep. Values represent a decimal fraction multiplier of the timestep determined internally based on global input/output events. Allowed values are 0. to 1., (default is 1.)

MAX_GLOBAL_DELTA_T

A parameter which can be used to limit the global timestep to a specific value. A positive number representing a timestep (secs) is input if this feature is to be active. (No default)

TIMESTEP_LOCAL_MAX

A parameter (secs) which can be used to provide an upper limit for the local (particle-specific) timestep used to calculate particle movement. This parameter is likely used only in sensitivity studies of the RDM calculation scheme. (Default: 'infinity')

TIMESTEP_LOCAL_MIN

A parameter (secs) which can be used to provide a lower limit for the local (particle-specific) timestep. This parameter is likely used only in sensitivity studies of the RDM calculation scheme. (Default: 0.0)

TIMESTEP_LOCAL_FRACT

A parameter (decimal fraction) which multiplies the internally calculated local (particle-specific) timestep, scaling it either upward or downward. If timestep_local_min and/or timestep_local_max are set, those limits have precedence over a timestep determined by scaling from this variable (timestep_local_fract). (Default: 1.0)

NESTS_DELTA_T_CALC

The RDM calculation scheme allows the local timestep to be determined by the local sampling cell size. If a particle lies inside the innermost nest, nest level 4, the particle's local timestep is restricted so that the mean movement will be less than the smallest (most constricting) nested cell dimension. Maintaining this limit is most important for the integrated air concentration sampling option. If representative integrated air concentrations are not required, the nest level can be decreased, allowing longer local timesteps (and a faster calculation). Possible values are 0, 1, 2, 3, and 4, where 0 represents the case where the largest (main) grid cell dimension alone is used to determine the local timestep. (Default value: 4, meaning the innermost nest level)

A note on time steps: Global versus local

There are two types of time steps used in RDM diffusion method in ADPIC. The *global time step* is the time interval between consecutive input/output events which may affect all particles, e.g., times at which a MATVEL file needs to be read, a CONC*.BIF file

needs to be written, a time at which a time-varying met or source parameter becomes valid, times for particle plots to be generated, or times for status messages to be written. The *local time step* is set independently for each particle based on the eddy diffusivity and mean wind at its location, and is used to calculate the mean wind advection and diffusion for each particle. The local time step is less than or equal to the global time step. To provide accurate and stable mean wind advection calculation using the gridded mean wind field, as well as accurate time-integrated concentration calculations in the concentration grid, this local time step is restricted so particles move no more than one mean wind or concentration grid cell (whichever is smaller) per time step. Successive local time steps are used for a particle until its age matches the time at the end of the current global time step. After all particles have advanced to the time corresponding to the global time step, the appropriate input/output operations are done.