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ADPIC
A THREE-DIMENSIONAL COMPUTER CODE
FOR THE STUDY OF POLLUTANT DISPERSAL AND DEPOSITION
UNDER COMPLEX CONDITIONS

Rolf Lange

October 18, 1973

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ADPIC A THREE-DIMENSIONAL COMPUTER CODE FOR THE STUDY OF POLLUTANT DISPERSAL AND DEPOSITION UNDER COMPLEX CONDITIONS

Abstract

In line with the widening need and effort in the field of pollutant transport and diffusion studies from local to extended regional scales, it has become apparent that a fully three-dimensional approach must be taken, and in order to do computer studies, three-dimensional computer codes must be developed. ADPIC is such a code. It is a three-dimensional, Cartesian, particle-diffusion code, capable of calculating the time-dependent dispersion of inert or radioactive air pollutants under many conditions, including stratified shear flow, calms, topography, and wet and dry deposition, for individual or multiple

instantaneous or continuous sources and space- and time-variable diffusion parameters.

The code solves the three-dimensional diffusion-advection equation by the pseudo-velocity technique for a given mass-consistent advection field. The method is based on the particle-in-cell technique with the pollutant concentration represented by Lagrangian particles in an Eulerian grid mesh. ADPIC has been verified for a number of selected advection-diffusion problems for which analytic solutions are available, and has been found to give results to within $\pm 5\%$ of the analytic solutions.

Introduction

ADPIC (Atmospheric Diffusion Particle-in-Cell) is a numerical, three-dimensional, Cartesian, particle-diffusion code capable of calculating the time-dependent distribution of air pollutants under many conditions including strongly distorted advection wind fields, calm conditions, space variable surface roughness, wet and dry deposition, radioactive decay, and space- and time-variable diffusion parameters.

Basically, the code solves the three-dimensional advection-diffusion equation in its flux conservative form (pseudo-velocity technique) for a given mass-consistent advection field by finite difference approximations in Cartesian coordinates. The method is based on the particle-in-cell technique with the pollutant concentration represented statistically by imbedded Lagrangian marker particles in an Eulerian grid.¹⁻³

The code has two versions: A moving expanding grid version and a fixed grid version. The moving, expanding grid version is primarily designed to model single puff releases; the grid automatically expands and travels with the puff along its trajectory in the free atmosphere. This version is particularly

suitable for the study of free-air bursts, or the long-range study of a surface release. The fixed grid version is suitable for the study of instantaneous or continuous releases near or on the surface over a range of scales, loosely defined from close-in (5 to 10 km) to mid-range (10 to 200 km).

ADPIC Description

PSEUDO-VELOCITY METHOD

The pseudo-velocity method consists of the following: Given the nonlinear transport-diffusion equation

$$\frac{\partial \chi}{\partial t} + \bar{U}_A \cdot \bar{\nabla} \chi = \bar{\nabla} \cdot (K \bar{\nabla} \chi), \quad (1)$$

where χ is a scalar concentration, K the diffusion coefficient and $\bar{U}_A$ the (given) mass-consistent wind advection field, under the assumption of incompressibility we can replace the $\bar{U}_A \cdot \bar{\nabla} \chi$ term by $\bar{\nabla} \cdot (\chi \bar{U})$. Upon combining the two divergence terms, we can rewrite Eq. (1) in its flux conservative (pseudo velocity) form

$$\begin{aligned} \frac{\partial \chi}{\partial t} + \bar{\nabla} \cdot \left[\chi \left(\bar{U}_A - \frac{K}{\chi} \bar{\nabla} \chi \right) \right] \\ = \frac{\partial \chi}{\partial t} + \bar{\nabla} \cdot (\chi \bar{U}_P) = 0, \end{aligned} \quad (2)$$

where $\bar{U}_P = \bar{U}_A - \frac{K}{\chi} \bar{\nabla} \chi$ is the pseudo transport velocity.

The grid mesh of the code is represented by an Eulerian grid consisting of three-dimensional rectangular cells of uniform size. The concentrations χ are

defined at the centers of the cells and the velocities $\bar{U}_A$, $\bar{U}_P$ and $-\frac{K}{\chi} \bar{\nabla} \chi$ are defined at the cell corners. The locations of the particles, which represent the pollutant cloud statistically, are defined by their individual Lagrangian coordinates within the Eulerian fixed grid.

A time cycle of the code is divided into an Eulerian step and a Lagrangian step and proceeds as follows:

- Eulerian Step: The concentrations χ , given for each cell at the beginning of the cycle, are used to calculate the diffusivity velocities $U_D = -\frac{K}{\chi} \bar{\nabla} \chi$ which are then added to the given wind advection velocities $\bar{U}_A$ to yield a pseudo velocity $\bar{U}_P$ for each cell corner.
- Lagrangian Step: Each marker particle contained in a given cell is transported for one time step Δt with a velocity $\bar{U}_P$, which is computed from the pseudo-velocities $\bar{U}_P$ at the corners of the cell, and the particle coordinates $\bar{x}$ are determined by a volume weighting scheme

$$\bar{x}(\text{new}) = \bar{x}(\text{old}) + \bar{U}_P \Delta t. \quad (3)$$

Finally, a new concentration distribution χ is calculated from the new particle positions, thus ending the cycle.

The chief advantage of using such a hybrid Eulerian-Lagrangian scheme is that the fictitious diffusion inherent in a purely Eulerian scheme is eliminated. The truncation errors inherent in the finite difference algorithms remain, of course, and must be minimized by the choice of the time step.

BOUNDARY CONDITIONS

The boundary conditions are applied to a layer of boundary cells that surround or protrude into the grid.

Topography

Space-variable surface roughness in the form of topography protrudes into the basic grid block of the code. The code recognizes individual flagged grid cells as topography and uses the applicable boundary conditions. The proper modeling of particle deposition on the ground is greatly dependent on the way topography is treated. Dry deposition and deposition by gravity is treated by specifying a deposition velocity at the topographic surface.

Flux Boundary Conditions

Flux boundary conditions representing inflow or outflow of pollutant particles from the grid are cast in the form of conservation of total flux, $(\bar{U}_P \chi) = \text{constant}$ [see Eq. (2)]. An inversion layer capping the region of interest can be specified by a reflecting boundary condition, whence the total flux $(\bar{U}_P \chi) = 0$ at the inversion layer. In the case of the moving, expand-

ing grid version, the grid mesh will automatically expand when a pollutant particle from a growing puff enters a boundary cell.

OPTIONS IN ADPIC

Sources

Pollutant sources can be generated anywhere within the grid mesh or on an inflow boundary. When the pollutant distribution to be studied covers less than two grid cell lengths, the code diffuses the particles too slowly, so that for the case of sub-grid scale sources a special sub-grid treatment of the special source particles is employed.

Active Pollutants

The way in which ADPIC describes pollutants in terms of discrete mass (activity) particles makes the implementation of decay rate calculations very straightforward. Such processes as radioactive decay or prompt γ -ray dose (cloudshine) of pollutants in conjunction with atmospheric dispersion under complex conditions can be modeled.

Deposition

Surface deposition from gravity or turbulent impaction and washout of pollutants from rain clouds and the ensuing ground surface concentrations are modeled by cumulatively storing those particles that have reached the ground in a special two-dimensional deposition array.

COMPUTER COST

ADPIC requires large amounts of core storage space. Four three-dimensional

arrays arise from the Eulerian part of the time cycle: the concentration $\chi(I, J, K)$, and the three velocity components $\bar{U}(I, J, K)$, $\bar{V}(I, J, K)$, and $\bar{W}(I, J, K)$. The total size of the arrays is the number of grid cells ($I \times J \times K$). Four one-dimensional arrays arise from the Lagrangian part of the time cycle: the particle coordinates $X(N)$, $Y(N)$, and $Z(N)$ and the particle mass $M(N)$. Here N is the total number of ADPIC particles. In addition to these basic arrays, the boundary conditions and various options of the code require a good deal of computer memory storage. It is expected that most of the usable large core memory (about 340 000 decimal words) of a CDC 7600 computer will be needed to run ADPIC in its final form for a regional study. A rough upper limit size for such a problem would be 25 000 cells (50×50 in the horizontal $\times 10$ in the vertical) and 30 000 particles.

The estimation of computer time for such a problem is presently speculative. Most of the verification studies were run for a 3375-cell grid ($15 \times 15 \times 15$) with 4000 particles at roughly 0.01 min/cycle. The 25 000-cell, 30 000-particle regional grid is about seven times larger; hence, one might expect a computer time of 0.07 min/cycle. This is a computational speed about 100 times faster than the real-time value of 8 min/cycle that one would expect for a 5-km horizontal grid cell length and a 5-m/sec mean wind.

Scaling for ADPIC

Assuming that a 25 000-cell, 30 000-particle fixed grid size problem is a practical maximum size for ADPIC, based on the computer memory core

limitations discussed above, the resolution provided by the grid cells of such a problem can be discussed with regard to the distance scale of interest for a release study:

- Close-in (1 to 5 km). Each grid cell would correspond to from 20 to 100 m in the horizontal, roughly equivalent to the source size. Building wake effects, for example, may be studied on that scale.
- Mid-range (10 to 200 km). On this scale, the individual grid cell would correspond to from 200 m to 4 km in the horizontal. This would provide sufficient resolution to study the regional dispersion of pollutants away from the source. However, as has been pointed out, when the standard deviation of a pollutant distribution σ_x is equal to or less than ΔX , where ΔX is the grid cell length, ADPIC does not diffuse pollutants fast enough. Thus the lower bound on σ_x for a valid ADPIC calculation in this mid-range case lies between 400 m and 8 km.

If the close-in shape of the distribution from a continuous source is known as a function of time, e.g., if $\sigma_x(t)$ is known for a Gaussian distribution, then sub-grid scale point sources can be treated directly in the mid-range scale problem. This may be the case for some ideal circumstances, but most probably, to be able to initially resolve a pollutant distribution that originates from a continuous 20-m large source with a mid-range grid scale, one must use a special method for providing an extended source that

is released into the mid-range problem. Similar scaling remarks hold, of course, in the vertical.

- Distant range (out to 1000 km). For this range, to retain the necessary resolution of the debris cloud, ADPIC should most likely be used in its moving-expanding grid version in a single or sequential puff approach to the study of an established plume. In this case, the ADPIC grid follows mean advection trajectory of the debris cloud and expands as the cloud expands.

OUTPUT

ADPIC's main output is pollutant concentration per grid-cell volume in terms of number of particles per cell and mass per particle as functions of time and grid cell location, from which either the cloud center or surface air concentration can be obtained in Ci/m^3 or g/m^3 .

Additionally, a special two-dimensional grid cell array keeps track of the cumulative deposition of pollutant on the surface in terms of pollutant radioactivity per grid cell area (Ci/m^2 or g/m^2).

Because the coordinates of each ADPIC particle are stored, sampling volumes other than grid cells can be used to obtain concentrations at the desired locations.

WASHOUT VERSUS RAINOUT

At present, the basic assumption for modeling removal of debris particles in ADPIC is that the base of the rain cloud is above the debris cloud and thus does

not protrude into the ADPIC grid mesh from above. For surface or near-surface pollutant releases, this seems to be a reasonable assumption, certainly for the close-in range and probably for most of the mid-range to about 100 km downwind. Thus, ADPIC will not treat in-cloud rainout, but has provisions for below-cloud washout.

Washout is treated in the following way in ADPIC. For a specified rain rate prevailing over a given surface area, a washout coefficient $\Lambda(r)$ is assumed as a function of debris particles of size r . Because of their limited number, each ADPIC particle is much larger than a debris particle. Therefore, an ADPIC mass particle is initially considered to represent an integrated debris particle size distribution over sizes such that

$$M(0) = \int_{r=0}^{\infty} m(r, 0) dr, \quad (4)$$

where $M(0)$ is the initial mass of an ADPIC particle and $m(r, 0)$ is the mass per unit radius of a debris particle of radius r at time 0. Constant density is assumed for the debris particles. $M(t)$, the mass of an ADPIC particle remaining after a time t in the rain for a given constant rain rate and raindrop size distribution, can then be written as⁴

$$\begin{aligned} M(t) &= \int_{r=0}^{\infty} m(r, t) dr \\ &= \int_{r=0}^{\infty} m(r, 0) e^{-\Lambda(r)t} dr. \end{aligned} \quad (5)$$

To account for the diffusion and transport of pollutant as calculated by ADPIC, this

function $M(t)$ is computed (or looked up from a table) at each ADPIC time step Δt . The fraction of mass $F(\Delta t)$ of an ADPIC particle washed out and deposited on the surface during one ADPIC time cycle then becomes

$$F(\Delta t) = \frac{M(t) - M(t+\Delta t)}{M(t)} = 1 - \frac{\int_{r=0}^{\infty} m(r, 0) e^{-\Lambda(r)(t+\Delta t)} dr}{\int_{r=0}^{\infty} m(r, 0) e^{-\Lambda(r)t} dr} \quad (6)$$

This fraction of mass loss per cycle for each ADPIC particle is stored cumulatively each cycle in a two-dimensional, surface deposition array.

DIFFUSION PARAMETERS

Because ADPIC is a three-dimensional Cartesian code and uses the turbulent flux diffusivity pseudo-velocity

$$\bar{u}_D = -\frac{\bar{K}}{\chi} \bar{\nabla} \chi, \quad (7)$$

to model diffusion, it can in principle accommodate the full Cartesian eddy diffusivity tensor $\bar{K} = K_{ij}$. In practice, isotropy of turbulence in the atmosphere is assumed, and only the diagonal terms K_{xx} , K_{yy} , and K_{zz} survive. In addition, it is generally assumed that the horizontal components of the diffusivity coefficients are the same, so that $K_{xx} = K_{yy}$. Even with these simplifications, the capability of ADPIC to model diffusion in three-dimensions with topography and inversions, under conditions of wind shear and with space- and time-variable diffusivity

coefficients, cannot presently be fully exploited largely because of the lack of a unified theory of diffusion in the atmosphere from which such diffusion coefficients can be obtained. Consequently, at least as a starting point, the various tested partial theories of diffusion in the atmosphere must be combined in a consistent way to provide diffusion coefficients for ADPIC.

For present purposes, diffusivity coefficients must be found that are valid for single puff or continuous plume releases which can grow from sources on the order of meters in size to debris clouds on the kilometer scale. When we consider time periods on the order of 12 h and geographical radii of interest on the order of 100 km, we are in a range where turbulent diffusivities are scale-dependent. Additionally, since the debris cloud may extend vertically through the entire turbulent mixing layer, the state of the thermal stability of the atmosphere must be taken into account. Constant K-theory will not be adequate for such requirements, and similarity theories will be chosen as the primary available framework upon which to base horizontal and vertical diffusivity coefficients for ADPIC.

Horizontal Diffusivity Coefficients

A large number of experimental studies have been summarized⁵ to show the validity of similarity theory in the inertial subrange of the atmosphere, as originally proposed by Kolmogoroff and discussed by Batchelor,⁶⁻⁸ for the horizontal spreading of clouds in the atmosphere from meter to kilometer sizes over times from minutes to several

days. The conclusion drawn is that for such scales the horizontal diffusivity coefficients take the form

$$K_{xx} = K_{yy} \propto \epsilon^{1/3} (\overline{\sigma_x^2})^{2/3}, \quad (8)$$

where ϵ is the rate of eddy-energy transfer in the inertial range and is a scaled function of height Z and average horizontal windspeed $\overline{U}(Z)$ above the surface,

$$\epsilon \propto \frac{(\overline{U}(Z))^3}{Z}, \quad (9)$$

and $\overline{\sigma_x^2}$ is the average horizontal dispersion of the cloud. For early times, when the initial cloud size in terms of its standard deviation σ_0 is important, the time rate of change of the dispersion is proportional to time t ,

$$\frac{d(\overline{\sigma_x^2})}{dt} \propto (\epsilon \sigma_0^2)^{2/3} t. \quad (10)$$

At late times, when $\sigma_0^2 \ll \overline{\sigma_x^2}$, the time rate of change of the dispersion becomes

$$\frac{d(\overline{\sigma_x^2})}{dt} \propto \epsilon t^2. \quad (11)$$

Vertical Diffusivity Coefficient

For the vertical diffusivity coefficient K_{zz} , the turbulent diffusion due to both the mechanical shear induced by the drag of the earth's surface on the atmosphere and the vertical thermal convection within the atmosphere must be taken into account. Within the first 50 to 100 m, the so-called surface layer of the atmosphere, the original similarity concepts of Obukhov,⁹ based on constant momentum and heat

flux, have been thoroughly analyzed and tested experimentally.¹⁰⁻¹⁹ The results can be considered as ample verification for choosing the Monin-Obukhov similarity parameter $\xi = Z/L$, where L is the Monin-Obukhov length and Z is the vertical height, as the primary independent variable representing the state of stability of the atmosphere in the surface layer to obtain the vertical diffusivity coefficient $K_{zz}(\xi)$. The functional relationship under this approach for K_{zz} is

$$K_{zz} = U_* k Z \frac{1}{\phi_m} = \left(\frac{kZ}{\phi_m} \right)^2 \frac{\partial \overline{U}}{\partial Z} \quad (12)$$

where U_* is the friction velocity, k is the von Karman constant,

$\phi_m = \frac{kZ}{U_*} \frac{\partial \overline{U}}{\partial Z}$ is a dimensionless wind shear, and $\overline{U}$ is the average horizontal windspeed. The function ϕ_m depends in the following way on the stability of the atmosphere:

$$\begin{aligned} \text{Stable: } \phi_m &= 1 + \gamma_1 \xi, \\ \xi &> 0, \quad L > 0 \end{aligned} \quad (13)$$

$$\begin{aligned} \text{Neutral: } \phi_m &= 1, \\ \xi &= 0, \quad L \rightarrow \infty \end{aligned} \quad (14)$$

$$\begin{aligned} \text{Unstable: } \phi_m &= (1 - \gamma_2 \xi)^{-1/4}, \\ \xi &< 0, \quad L < 0. \end{aligned} \quad (15)$$

Here γ_1 and γ_2 are empirical constants on the order of 4 to 5 and 14 to 16, respectively. For neutral conditions, $\phi_m = 1$, $\xi = 0$, and $L \rightarrow \infty$. The Obukhov length L has the form

$$L = - \frac{U_*^3 C_p \rho T}{kg H}, \quad (16)$$

where C_p is the specific heat of air at constant pressure, ρ the density of air, T the temperature, H the heat flux, and g the gravitational acceleration. Where L is not known, it can be found from its functional relationship to the Richardson number, R_i , for example.¹⁹

Above the surface layer and up to the turbulent mixing height, turbulence due to the surface stress eddies, thermal convection and wind shear decreases with height until it essentially disappears at the top of the mixing layer.²⁰ The similarity assumptions of constant momentum and heat flux are no longer valid in this region, and very little consensus exists among investigators at the present time as to the values of vertical diffusion parameters.²¹ This is largely due to the complex interactions of wind shear, lapse rate, Coriolis force, pressure gradients, eddy diffusivity, buoyant plumes, and topography in this region. It is generally assumed that the vertical diffusivity coefficient K_{zz} either remains constant up to the mixing or inversion height, where it sharply drops to a minimum value, or goes to a minimum there with some smooth functional dependence on height above the surface layer. In general, K_{zz} appears to be a strong function of the lapse rate.²²

Another reasonable starting point for obtaining a value for K_{zz} for ADPIC above the surface layer will be to rely on a statistically obtained power law profile for the vertical standard deviation σ_z of the form

$$\sigma_z = a \sigma_y x^b \quad (17)$$

where a and b are observationally

obtained stability category constants, σ_y is the horizontal wind fluctuation respectively, and x is the downwind distance from the source. From the relation between K-theory and statistical diffusion theory, the vertical diffusivity coefficient K_{zz} then becomes

$$\frac{d[\sigma(t)]^2}{dt} = 2K_{zz} \quad (18)$$

where t is the time of travel from the release point.²³⁻²⁵

In conclusion, with the flexibility available in ADPIC for assigning diffusion parameters, the basically accepted methods for their description, by empirical power law profiles coupled with stability categories and by Kolmogoroff's and Monin-Obukhov's L similarity theories, can be combined to give a starting point for a widened capability to model diffusion and transport of pollutants in the atmospheric boundary layer. Currently, a great deal of research effort is being expended on turbulent diffusion in the atmosphere, including the study of vertical gradients of wind and temperature profiles. Resulting descriptions of diffusion parameters can be quickly incorporated into ADPIC once they are consolidated and verified sufficiently to be considered operational.

ACCURACY OF ADPIC

Because the ADPIC time cycle is half Eulerian and half Lagrangian and because the original particle placement is determined by a random number generator, the discussion of the accuracy of ADPIC must remain largely empirical.

Five major factors contribute to the accuracy of the ADPIC method, and they will now be discussed in turn.

Basic Finite Difference Algorithms

As mentioned before, the cell concentrations are defined at the cell centers and the pseudo velocities $\bar{U}_p$ are defined at cell corners. The pseudo velocities contain both the advection velocities $\bar{U}_A$ and the diffusion velocities $\bar{U}_D$. Figure 1 shows this and the diffusion velocity algorithm resulting from this arrangement, displayed in a reduction to two dimensions for simplicity. The algorithm for the diffusivity velocity U_D has an upper limit $|U_D| \leq 2 \frac{K}{\Delta X}$ where K is the diffusion parameter and ΔX is the length of the cell. This feature prevents particles that are near the edge of a distribution, where there may be cells with just one particle interspersed with empty cells, from being moved too fast because of excessive diffusion velocities that occur under such conditions when the velocity and concentration grid is not staggered. For example, the algorithm for the diffusion velocity in a nonstaggered grid requires three cells,

$$\begin{array}{|c|c|c|} \hline x, U & x, U & x, U \\ \hline i-1 & i & i+1 \\ \hline \end{array}$$

$$U_i = -\frac{K}{2\Delta X} \frac{(x_{i+1} - x_{i-1})}{x_i} \quad (19)$$

It can easily be seen that if $x_i = 0$, $U_i \rightarrow \infty$.

The truncation errors contained in the ADPIC diffusion velocity algorithm can be investigated by expanding it in a Taylor series. Consider the one-dimensional case,

$$U_{i+1/2} = -\frac{K_{i+1/2}}{\Delta X} \frac{(x_{i+1} - x_i)}{x_{i+1/2}} \quad (20)$$

Let the subscript be dropped for $i+1/2$ and expand x_{i+1} and x_i in Taylor series about $i+1/2$ to the first contributing error term:

$$U = -\frac{K}{\Delta X} \cdot x \left[x + x' \frac{\Delta X}{2} + \frac{1}{2} x'' \left(\frac{\Delta X}{2} \right)^2 + \frac{1}{6} x''' \left(\frac{\Delta X}{2} \right)^3 - \left\{ x - x' \frac{\Delta X}{2} + \frac{1}{2} x' \left(\frac{\Delta X}{2} \right)^2 - \frac{1}{6} x''' \left(\frac{\Delta X}{2} \right)^3 \right\} \right] \quad (21)$$

$$U = -\frac{K}{\Delta X} \cdot x \left[x' \Delta X + \frac{1}{24} x''' \Delta X^3 \right] = -\frac{Kx'}{x} - \frac{K}{24} \frac{x'''}{x} \Delta X^2 \quad (22)$$

Fig. 1. Velocity algorithm. (a) grid mesh; (b) diffusivity.

The first term on the righthand side is the exact differential expression for the diffusivity velocity; the second term is the first contributing error term. Forming the ratio of the ADPIC diffusion velocity, Eq. (20), to the exact differential diffusion velocity, we obtain a measure of the importance of the error term

$$\frac{U_{ADPIC}}{U_{EXACT}} = 1 - \frac{\chi'''}{\chi'} \frac{(\Delta X)^2}{24}. \quad (23)$$

For most problems, the third derivative χ''' is sufficiently smaller than the first derivative χ' so as to make the error term small.

The Number of Eulerian Cells per Problem

It is important to have enough grid cells to resolve a given particle distribution well enough to make the concentration gradients calculated from the cell concentrations representative of the actual gradients. While the particle positions per cell may indicate some sub-grid resolution, it is important to point out that the numerical solutions of the diffusion equation are defined on the Eulerian grid. To get a feeling for how well a distribution must be resolved to give reasonable answers, consider Eq. (23) above for the case of a one-dimensional Gaussian distribution:

$$\chi = \frac{Q}{\sigma} e^{-X^2/2\sigma^2}. \quad (24)$$

Let us find the derivatives χ' and χ'''

$$\chi' = -\frac{QX}{\sigma^3} e^{-X^2/2\sigma^2}. \quad (25)$$

$$\chi''' = \frac{QX}{\sigma^5} \left[3 - \frac{X^2}{\sigma^2} \right] e^{-X^2/2\sigma^2}. \quad (26)$$

Substituting Eqs. (25) and (26) into (23), we obtain

$$\frac{U_{ADPIC}}{U_{EXACT}} = 1 - \frac{1}{24} \left(\frac{X^2}{\sigma^2} - 3 \right) \frac{\Delta X^2}{\sigma^2}. \quad (27)$$

Using the fact that 99% of all particles in a one-dimensional Gaussian distribution lie within $x = 3\sigma$, we can substitute $x = 3\sigma$ in Eq. (27) and obtain

$$\frac{U_{ADPIC}}{U_{EXACT}} = 1 - \frac{\Delta X^2}{4\sigma^2}. \quad (28)$$

This indicates that when the cell size ΔX is large compared to the standard deviation of a particle distribution, ADPIC diffuses too slowly.

It appears that Eq. (27) indicates that for $X^2 = 3\sigma^2$ the error term vanishes regardless of the grid spacing. In this case, $\chi''' = 0$ and higher-order derivatives in the Taylor expansion of χ must be retained to get a meaningful expression.

The Number of Particles per Cell

Inasmuch as the ADPIC particles represent a quantized density, it is desirable to have as many particles per cell as possible. The upper limit of this number is obviously dictated by computer storage. ADPIC assigns a fictitious cell volume to each particle of the same size and shape as the basic grid cell. Thereby, in calculating the concentration field from the particles, each particle will contribute some fractional part of its mass to eight nearest-neighbor cells in

proportion to the overlap of its "volume" with the cell volumes of the neighbor cells. This procedure smoothes out the concentration field and in return the diffusion velocity field which is computed from it, and is consistent with the fact that the Eulerian part of the cycle cannot resolve sub-grid-scale phenomena. As the result of many problems run it can be said that, empirically, due to this smoothing technique as few as one particle per cell on the average will yield meaningful results. With fewer particles per cell than that, i.e., when particles have no neighbors within one cell length around them, the ADPIC diffusivity velocity algorithm (see Fig. 1) moves the particle to a grid point and "freezes" it there.

Particle Generation

ADPIC uses a random number generator to generate input particle distributions, either of constant density or Gaussian. It has been found that generating a Gaussian puff of standard deviation σ with several thousand particles represents a fairly good sample population, and the generated particle distribution is close to Gaussian. However, in the case of continuous sources where particle economy dictates that no more than a few hundred particles can be generated per cycle, each batch appears somewhat "lumpy." To some extent, because of many such batches these lumps average out when the batches start overlapping and diffusing. But since a particle is moved with a weighted average velocity of the velocities at the eight corners of the cell it is in, lumps of particles that were generated very close together in space tend to hold

together. As the most extreme example, two particles generated with exactly the same coordinates will never move apart. Individual placement of thousands of source particles is extremely impractical even if a good way could be found to do it in the case of a Gaussian distribution. For the case of a particle distribution that is well resolved by ADPIC grid cells, a method has been found to "smooth" the random number generator distribution without disturbing the shape of the Gaussian distribution. This method will be discussed later under ADPIC Verification.

Boundary Conditions

Due to the part-Eulerian, part-Lagrangian makeup of ADPIC, the boundary conditions break up into one set of conditions imposed on the Eulerian velocity field and one set imposed on the Lagrangian particles. Both sets must be consistent with each other.

The advection velocity field is adopted entirely by ADPIC from MACAW, a computer code that calculates a Mass Consistent Advection Wind field similar to the method used by Dickerson,²⁶ and will not be discussed further here other than to point out that it is compatible with the assumption in ADPIC of incompressibility and conservation of mass.

The two basic boundary conditions imposed on the pseudo-velocity field in ADPIC $\bar{U}_p = \bar{U}_A + \bar{U}_D$ are constant mass flux, $(\chi\bar{U}) = \text{constant}$, corresponding to inflow and outflow of particles, and zero mass flux $(\chi\bar{U}) = 0$, corresponding to reflection of particles from the boundary. There are intermediate cases as, for example, deposition of particles at the

topography, in which case a deposition velocity is specified. The chief cause of error incurred by velocity boundary conditions that has stubbornly plagued numerical simulations of all kinds is the lack of ability to specify the outflow boundary conditions. In the kind of studies that ADPIC has so far been used for, the concentration field is smooth enough by the time it reaches the outflow boundary that the boundary velocities can be specified by postulating a constant flux of particles through the boundary grid cell layer.

The particle boundary conditions are very simple. If a particle has been found to have left the grid during a cycle, it is either annihilated or counted as deposited or is reflected, according to the type of boundary specified.

TIME-STEP CALCULATION

ADPIC stability is rather insensitive to the length of the time step per cycle; however, since the i th particle transport

is done by a forward differencing scheme

$$\bar{x}_i^{n+1} = \bar{x}_i^n + U_p^n \cdot \Delta T, \quad (29)$$

diffusion occurs too fast when ΔT becomes too large. It has been found satisfactory to limit the transport of the fastest particle in the problem to not allow it to move further than one cell octant per time step. (In one dimension this is equivalent to half a cell length.) ADPIC finds the largest total velocity $U_p = U_A + U_D$ that any particle sees and computes the time step according to the following equation:

$$\Delta T = F \cdot \left[\text{Minimum of} \left(\frac{\Delta X}{|U_{PM}|}, \frac{\Delta Y}{|V_{PM}|}, \frac{\Delta Z}{|W_{PM}|} \right) \right] \quad (30)$$

where F is an input number between 0 and 1/2 and ΔX , ΔY , ΔZ are the cell lengths and $|U_{PM}|$, $|V_{PM}|$, $|W_{PM}|$ are the absolute values of the maximum pseudo velocities at any cycle.

Finally, the time step ΔT is allowed to drop rapidly if required, but is limited to an increase of only a factor 1.3 from cycle to cycle to avoid instabilities.

ADPIC Verification

INSTANTANEOUS SOURCES (PUFFS)

General Discussion

All instantaneous source verification problems were run on the expanding grid version of ADPIC. In this version the grid automatically expands by a given ratio independently in any of the three coordinate directions as soon as a particle is entering a boundary cell. In this manner boundary velocities need not be known and are set equal to zero,

and no particles ever leave the grid. No matter how small the source, it can be resolved by the ADPIC grid from the beginning, and remains well resolved provided the puff does not get too distorted.

The initial Gaussian distribution of the particles is generated by calling a random-number generator. To generate a particle, the particle generator picks a random coordinate X and then computes the Gaussian probability $P_X = \exp(-X^2/$

$2\sigma_0^2$) that the particle would be found at that coordinate. It then picks another random number between zero and one. If this number is less than the probability P_X , the particle is "allowed." If the number is greater than P_X , the particle is "disallowed" and a new random coordinate X is picked and so on, until all particles are generated. To guard against too many disallowed particles at the edge of the distribution where $P_X \rightarrow 0$, there is a cutoff on the coordinate X which is input into the code.

It was found that even for large samples of several thousand particles thus generated from the random generator, there were gaps and lumps of particles in the coordinate distribution. Further smoothing of the initial distribution was obtained in the following way: Since the total number of particles, the cell size of ADPIC, and the standard deviation of the Gaussian distribution to be generated are known, one can first compute the number of particles that should be contained in a given cell. After that, the random particle placement routine described above is employed for that cell by picking random coordinates within the cell until all particles for that cell are generated subject to the constraint of the Gaussian distribution. This method results in a considerably less lumpy distribution.

The following verification problems for puff diffusion were all compared against the analytic Gaussian solutions to the diffusion-advection equation as

described for each problem. These are the solid lines in the following plots. The error bars shown for the ADPIC solutions were obtained by plotting the highest and the lowest particle concentration per cell as obtained by scanning four planes of symmetry for each problem in which the concentrations of corresponding cells should be the same. Because of the random nature in which the particles are generated, this corresponds essentially to running the same problem four times and sampling the same cell each time. The error bars thus are a good indication of the errors introduced by the quantization of density into particles and the above mentioned lumpiness of the random number generator. When the generator smoothing technique is not used, the error bars become roughly twice as large as the ones shown in the accompanying verification plots.

The following verification problems were run on ADPIC to study instantaneous sources: Number 3-2-15, puff diffusion with constant diffusion parameter K , $K_{xx} = K_{yy} = K_{zz}$; Number 3-3-24B, puff diffusion with scale-dependent K ; Number 3-3-26, puff diffusion with constant K in simple shear flow. These problems will now be discussed in turn.

Instantaneous Source Diffusion with Constant K

Problem 3-2-15 was run to compare ADPIC for the case of puff diffusion in three dimensions with constant K with the Gaussian solution to the diffusion advection equation of the form

$$\chi(x, y, z, t) = \frac{Q}{(2\pi)^{3/2} (\sigma_{x0}^2 + 2K_{xx}t)^{1/2} (\sigma_{y0}^2 + 2K_{yy}t)^{1/2} (\sigma_{z0}^2 + 2K_{zz}t)^{1/2}} \times \exp \left[-\frac{1}{2} \left(\frac{x^2}{\sigma_{x0}^2 + 2K_{xx}t} + \frac{y^2}{\sigma_{y0}^2 + 2K_{yy}t} + \frac{z^2}{\sigma_{z0}^2 + 2K_{zz}t} \right) \right]. \quad (31)$$

A spherically symmetric Gaussian puff distribution of 3896 particles with a standard deviation of $\sigma_{0x} = \sigma_{0y} = \sigma_{0z} = 2\Delta X$ was generated at the center of a $14 \times 14 \times 14$ originally cubical ADPIC grid of cell size $\Delta X = \Delta Y = \Delta Z = 10$ m, and was allowed to diffuse. The diffusion parameters were $K_{xx} = K_{yy} = 1 \times 10^4$ cm²/sec, $K_{zz} = 10$ cm²/sec. The problem ran 60 cycles and 286 300 sec during which time the grid expanded automatically many times, with the final cell size being $\Delta X = \Delta Y = 394$ m, $\Delta Z = 16.9$ m.

Figures 2 and 3 show the initial particle distribution at $T = 0$. Figure 4 shows the particle distribution at Cycle 60, $T = 286$ 300 sec in the X-Z plane. Figure 5 shows the same in the X-Y plane. Figures 6 and 7 show the particle concentrations per original cell volume at Cycle 60 in the X-Z plane along the X-axis and Z-axis respectively.

Instantaneous Source with Scale-Dependent $K(t)$

Problem 3-3-24B was run to compare ADPIC against an analytic solution for the case of scale-dependent diffusion.

It is shown in reference²⁷ that the variance σ^2 of a Gaussian distribution can be expressed in the following closed form for scale-dependent diffusion in the atmosphere:

$$\sigma^2(t) = \left(\sigma_0^2 + \frac{2}{3} C \epsilon^{1/3} t \right)^3 \quad (32)$$

where σ_0 is the original standard deviation of the distribution, C a constant of order unity, ϵ is the energy dissipation rate in the atmosphere, and t is time. When this expression is substituted into the expression for the similarity theory diffusivity parameter

$$K(t) = C \epsilon^{1/3} \sigma^4/3(t) \quad (33)$$

we obtain K as a function of ϵ and time:

$$K(t) = C \epsilon^{1/3} \left(\sigma_0^2 + \frac{2}{3} C \epsilon^{1/3} t \right)^2. \quad (34)$$

To match the observation that at very late times at the upper end of the turbulence scale K becomes a maximum constant K_{MAX} , Walton²⁷ uses as a form for $K(t)$

$$K(t) = \left[\frac{1}{K_{MAX}} + \frac{1}{K(t)_{Eq. (34)}} \right]^{-1}. \quad (35)$$

This $K(t)$ was put into ADPIC in the same form for $K_{yy}(t)$ and $K_{zz}(t)$, but with different constants. For $K_{yy}(t)$:

$$K_{yyMAX} = 5 \cdot 10^9 \text{ cm}^2/\text{sec}, \quad \sigma_{y0} = 204 \text{ m};$$

and for $K_{zz}(t)$:

$$K_{zzMAX} = 1 \cdot 10^4 \text{ cm}^2/\text{sec}, \quad \sigma_{z0} = 33.4 \text{ m}.$$

For both the y and z directions, $\epsilon = 2.0$ and $C = 1$. The results of ADPIC were

Fig. 2. Initial particle distribution at $T = 0$, X-Y plane, problem 3-2-15.

Fig. 3. Plot of initial particle distribution at $T = 0$. Problem 3-2-15.

compared with the analytic Gaussian solution to the diffusion-advection equation

$$\chi(y, z, t) = \frac{Q}{2\pi(\sigma_{y0}^2 + 2K_{yy}T)^{1/2}(\sigma_{z0}^2 + 2K_{zz}T)^{1/2}} \times \exp\left[-\frac{1}{2}\left(\frac{y^2}{(\sigma_{y0}^2 + 2K_{yy}T)} + \frac{z^2}{(\sigma_{z0}^2 + 2K_{zz}T)}\right)\right] \quad (36)$$

in which K_{yy} and K_{zz} are of the time-dependent form of Eq. (35).

ADPIC was run in a two-dimensional mode in the y - z plane for this problem with the X dimension degenerate. This was achieved by allowing only four cells in the X direction and setting σ_{x0} in the particle generator equal to a very large number so that the probability that a particle can be found along the x -axis $P_x = \exp(-X^2/2\sigma_{x0}^2)$ goes to one everywhere. As a result, the particle density

in the x -direction is constant. In addition, K_{xx} was set equal to zero everywhere and the particle flux set equal to zero at the $X_{\max}$ and $X_{\min}$ boundaries.

The number of particles initially generated in a two-dimensional Gaussian distribution was $3168/\Delta X$ where ΔX is the cell width in the degenerate X -direction. σ_{0y} was 204 m and σ_{z0} was 33.4 m. The number of cells was $4 \times 14 \times 14$ in the x, y, z direction respectively. The problem was run to 100 cycles, $T = 37\,720$ sec. Figures 8 and 9 show the particle distribution at cycle 0 in the y and z dimensions. Figures 10 and 11 show the same at cycle 100, $T = 88\,720$. Figure 12 is a plot of relative particle concentration per cell at cloud center versus time.

Instantaneous Source Diffusion in Simple Shear Flow

Problem 3-3-26 was run to compare ADPIC with the analytic solution of Quesada²⁸ for puff diffusion in shear flow. The analytic solution advanced by Quesada²⁸ is of the form

$$\frac{\chi(x, y, z, t)}{\chi_0} = \frac{\exp[-y^2/(1+4\tau)] \exp(-F/G)}{[(1+4\tau)G]^{1/2}} \quad (37)$$

where

$$\begin{aligned} F &= (x' - \mu z'\tau)^2 (1+4\tau) \\ &\quad + 4\mu z'\tau^2 (x' - \mu z'\tau) + z'^2 \\ &\quad \times (1+4\tau + \frac{4}{3}\mu^2\tau^3) \\ G &= (1+4\tau)^2 + \frac{4}{3}\mu^2\tau^3 (1+\tau), \end{aligned}$$

all expressed in the dimensionless quantities

Fig. 4. Particle distribution at Cycle 60, $T = 286\,300 \text{ s}$, X-Z plane, problem 3-2-15.

Fig. 5. Particle distribution at Cycle 60, $T = 236\,300$ s, X-Y plane, problem 3-2-15. Inner circle: concentration = $1/e$ central concentration.

Fig. 6. Plot of particle concentration per original cell volume at cycle 60, X-Z plane, along the X-axis. Problem 3-2-15.

Fig. 7. Plot of particle concentration per original cell volume at cycle 60, X-Z plane, along the Z-axis. Problem 3-2-15.

Fig. 8. Initial particle distribution Y-Z plane, problem 3-3-24B.

Fig. 9. Initial particle distribution, Y-Z plane, along the Y- and Z-axes, problem 3-3-24B.

Fig. 10. Particle distribution at Cycle 100, $T = 88\,720 \text{ s}$, Y-Z plane, Problem 3-3-24B.

Fig. 11. Plot of particle distribution, Y-Z plane, along the Y- and Z-axes at Cycle 100, $T = 88\,720$ s, problem 3-3-24B.

$$\mu = Sa/D, \tau = tD/a^2, x' = x/a,$$

$$y' = y/a, z' = z/a$$

with $a = \sqrt{2\sigma_0}$ the initial cloud radius in terms of the initial standard deviation of the particle distribution. $D = K_{xx} = K_{yy} = K_{zz}$ are the constant diffusion parameters. $S = (\partial U / \partial z)$ is the shear factor which is introduced into the ADPIC problem via the advection wind field in the x-z plane in the following way:

$$U_A = U_{A0} + SZ. \quad (38)$$

Letting $U_{A0} = 0$, we obtain a constant shear in the x-z plane with the mean advection defined as zero at the cloud center. To calculate the ADPIC cell concentration $\chi(x, y, z, t)$, we multiply

Fig. 12. Plot of relative particle concentration per cell at cloud center versus time. Problem 3-3-24B.

the analytic solution Eq. (37) through by $x_0 = Q \cdot \Delta V / [\sigma_0^3 (2\pi)^{3/2}]$, where Q is the number of particles in the puff and ΔV is the cell volume.

ADPIC models shear by superimposing the advective velocity field $\bar{U}_A$ which contains the shear on the diffusion velocity field $\bar{U}_D$. In this problem, a spherically symmetric Gaussian particle distribution with an initial standard deviation $\sigma_0 = 20$ m was generated at the center of an ADPIC

grid mesh of $20 \times 20 \times 20$ cubical cells of cell size $\Delta X = \Delta Y = \Delta Z = 7$ m. The expanding grid version of ADPIC was used. The simple shear in the x-z plane was introduced with the advection velocity field in the form of Eq. (38) with $S = 0.125 \text{ sec}^{-1}$. The problem ran to 120 cycles, $T = 6328$ sec and the diffusion parameters were $K_{xx} = K_{yy} = K_{zz} = 10^6 \text{ cm}^2/\text{sec}$. The grid expanded many times, each time by a factor of 1.3 in

Fig. 13. Particle distribution at cycle 20, $T = 5.3$ s, X-Z plane, problem 3-3-26.

the respective coordinate direction until at the last cycle 120, the cell size was $\Delta X = 194\,500\text{ m}$, $\Delta Y = \Delta Z = 466\text{ m}$.

Figures 13, 14, 15, 16 and 17 show the ADPIC particle distribution in the x-z plane at various times. Figures 18 and 19 show the particle cell concentrations of ADPIC versus distance in the $\pm x$ and $\pm z$ directions respectively at $T = 62.54\text{ sec}$, cycle 50. The fact that

the distributions on the plots are not symmetric with respect to $x = 0$ is due to the location of the cell centers nearest the x-axis being $1/2 \Delta X$ away from the axis. Figures 20 and 21 similarly display the cell concentrations at $T = 6328\text{ sec}$, cycle 120. Due to the influence of the shear, the resolution of the particle distribution by the grid becomes poorer at late times and ADPIC begins to diffuse

Fig. 14. Particle distribution at cycle 50, $T = 62.5\text{ s}$, X-Z plane, problem 3-3-26.

Fig. 15. Particle distribution at cycle 80, $T = 464 \text{ s}$, X-Z plane, problem 3-3-26.

Fig. 16. Particle distribution at cycle 120, $T = 6328$ s, X-Z plane, problem 3-3-26.

Fig. 17. Particle distribution at cycle 120, $T = 6328 \text{ s}$, Y-Z plane, problem 3-3-26.

Fig. 18. Plot of particle cell concentration versus distance at cycle 50, $T = 62.54$ s, X-Z plane, along the X-axis, problem 3-3-26.

Fig. 19. Plot of particle cell concentration versus distance, cycle 50, $T = 62.54$ s, X-Z plane, along the Z-axis, problem 3-3-26.

Fig. 20. Plot of particle cell concentration versus distance, cycle 120, $T = 6328$ s, X-Z plane, along the X-axis, problem 3-3-26.

Fig. 21. Plot of particle cell concentration versus distance, cycle 120, $T = 6328$ s, X-Z plane, along the Z-axis, problem 3-3-26.

too slowly. The beginning of this effect can be seen in Figs. 20 and 21. Figure 17 shows an end view looking along the x-axis into the y-z plane at late time. No shear is active in this plane and the distribution is circular, as one would expect for a pure diffusion problem. Figure 22 shows the relative puff center concentration as a function of time for both the analytic solution and ADPIC.

CONTINUOUS SOURCES (PLUMES)

General Discussion

Continuous sources are generated in ADPIC by releasing sequential puffs. The individual puffs are created each time cycle by a special source subroutine that works on the same basis as the one discussed in the section on Particle Generation under Accuracy of ADPIC. The number of particles generated for each puff is governed by the equation:

$$M^n = \frac{\dot{Q} \cdot \Delta T}{PM} \quad (39)$$

where M^n is the number of particles created at cycle n , $\dot{Q}$ is a constant release

Fig. 22. Relative cloud center concentrations, puff diffusion in simple shear flow, problem 3-3-26.

rate in grams per second (curies per second) and PM is the mass in grams (or activity in curies) per particle, and ΔT is the ADPIC time step.

The fixed grid mode of ADPIC is appropriate to treat continuous sources because the entire plume length of interest together with topography and meteorology must be covered by the grid mesh. As pointed out in the sections on Accuracy of ADPIC and Scaling for ADPIC, the standard deviation of a source size must be on the order of a grid cell size for the shape of the source distribution to be resolved by the grid mesh, and this

represents the major difficulty when near point sources as from stacks are involved. The problem must be solved by first obtaining an extended source from a near point source which then is well resolved for ADPIC. Such an extended source can be obtained in three ways of increasing complexity:

1. An extended source is calculated simply by Gaussian puff diffusion of the source puffs until the puffs have reached a size that is resolved by the grid mesh and then input into ADPIC.

2. If the local scale length of diffusion at the position of the particle can be obtained, a diffusivity velocity for that particle can be calculated from this length independent of the ADPIC method. In essence, this implies that the local sub grid scale particle distribution is known for the source particles for which it cannot be obtained by the regular ADPIC method.
3. Finally, the extended source can be obtained by separately computing the close-in problem with ADPIC in which the source is resolved by the grid from the beginning, and the extended source particle distribution thus obtained is used as input to drive the larger scale ADPIC problem.

In all but the simplest cases, Method 1 above will not result in a representative extended source because by the time the source particle distribution has reached the size required, it would have interacted with the topography and have been subjected to time- and space-varying winds.

Method 3 is the most accurate of the three, but also the most cumbersome. Because of time-varying meteorology and due to the statistical nature of the particle generation, it requires that a close-in problem can run for extended source input for every time step of the large-scale ADPIC problem.

Method 2 represents essentially a compromise between 1 and 3 in that it assumes knowledge of the local sub-grid diffusion scales in terms of the diffusion parameters K and a Gaussian distribution, but allows the meteorology and topography

to interact with the source particles.

This method was adopted to treat sub-grid scale sources in ADPIC, and is discussed in detail in the next section, together with its verification in problems 3-3-25 and 3-3-25a.

After that follows the discussion of three problems comparing the results of continuous sources in ADPIC with numerically integrated analytic solutions: Problem 2-3-27 with a continuous source and no advection, essentially the "calm" problem, from a well-resolved source; Problem 2-3-29G continuous source with diffusion and a 2-m/s advection field and sub-grid scale source; and Problem 2-3-29I which is like 2-3-29G but with a 10-m/s advection field.

The continuous source problems just mentioned were compared to a numerical time integration of the Gaussian solution of the diffusion-advection equation for the concentration field of successive puffs. Consider a single, spherically symmetric, Gaussian puff of initial size σ_0 and constant diffusivity K , released via a constant source rate $\dot{Q}$ over an infinitesimal time period dt into a constant advection field in the $+x$ direction of magnitude U (m/s). The equation for the time rate of change of the concentration field can be written (Ref. 29, p. 267):

$$\frac{d\chi(x, y, z, t)}{dt} = \frac{\dot{Q} dt}{(2\pi)^{3/2} (\sigma_0^2 + 2 K t)^{3/2}} \times \exp \left\{ -\frac{1}{2} \left[\frac{(x - Ut)^2 + y^2 + z^2}{\sigma_0^2 + 2 K t} \right] \right\}. \quad (40)$$

When this equation is integrated over infinitely many such puffs in time from

$t = 0$ to some time $t = T$, we obtain the continuous source concentration field $\chi(x, y, z, t)$ in space and time:

$$\chi(x, y, z, t) = \frac{\dot{Q}\Delta V}{2\pi^{3/2}} \int_0^T \frac{dt}{(\sigma_0^2 + 2Kt)^{3/2}} \times \exp \left\{ -\frac{1}{2} \left[\frac{(x - Ut)^2 + y^2 + z^2}{\sigma_0^2 + 2Kt} \right] \right\} \quad (41)$$

where the equation has been multiplied through by the ADPIC cell volume ΔV to obtain χ in units of particles per cell. This integral, Eq. (41), was programmed and numerically integrated on the computer to an accuracy of 0.0001 particles/cell and the solution was used to compare with cell concentrations computed by ADPIC at selected points in space and time.

Sub-grid Scale Source Particle Treatment

As shown in the section Accuracy of ADPIC, when the particle distribution in ADPIC cannot be resolved by the grid mesh, errors in diffusion rates occur. This situation is found when one tries to model continuous sources that are considerably smaller than a cell volume. (The difficulty does not arise in the case of instantaneous sources, as these can be run on the expanding grid version and be well resolved from the beginning.) For such continuous sources in the presence of advection the problem is compounded because the larger the advection, the further the errors of the initially poor resolution of the source particle distribution are carried downwind.

If an assumption can be made about the shape of the source particle distribution at early times until the distribution

has spread out enough to represent an extended source, resolved by the grid mesh, the source particles can be diffused in accordance with such a distribution until such time. It should be kept in mind that the only purpose of this source particle treatment is to provide ADPIC with reasonably representative extended source for the study of larger-scale three-dimensional phenomena like varying meteorology, diffusion parameters and topography over distances of hundreds of kilometers, the effect of which are not very sensitive to the exact shape of the source. If effects near the source are to be investigated, the close-in ADPIC problem will have to be run separately. With this in mind, let us assume the sub-grid scale source is Gaussian in character and that it remains locally Gaussian until its standard deviation σ is approximately equal to the size of a grid cell and represents an extended source. At this point, the locally Gaussian assumption is discarded and ADPIC calculates diffusion by its concentration gradient method. It will now be shown how this assumption leads to a sub-grid scale diffusivity velocity and how this velocity is integrated to diffuse source particles. This approach treats horizontal and vertical diffusion of the particles independently. For simplicity, the case for the one-dimensional Y direction is illustrated.

For a Gaussian distribution, the concentration field for a puff is described by

$$\chi = \frac{Q}{(2\pi)^{1/2} \sigma_y} \exp \left(-\frac{1}{2} \frac{y_D^2}{\sigma_y^2} \right) \quad (42)$$

where χ is the particle concentration, Q

the source, σ_y the standard deviation and y_D the distance of the particle from the center of the distribution. From the definition of the diffusion flux

$$xV_D = -K_y \frac{\partial x}{\partial y} \quad (43)$$

we can, by dividing through by x , obtain the definition of diffusion velocity

$$V_D = -\frac{K_y}{x} \frac{\partial x}{\partial y} = -K_y \frac{\partial(\ln x)}{\partial y} \quad (44)$$

where V_D is an average diffusion velocity and K_y the diffusion parameter. Calculating $\ln x$ from Eq. (42) and substituting in (44), we obtain for the diffusivity velocity

$$V_D = -K_y \frac{\partial}{\partial y} \left[\ln \frac{Q}{(2\pi)^{1/2}} - \ln \sigma_y - \frac{1}{2} \frac{y_D^2}{\sigma_y^2} \right] \\ = \frac{K_y y_D}{\sigma_y^2} \quad (45)$$

From the earlier discussion on scale-dependent diffusion, we have the two equations

$$K_y = \epsilon^{1/3} \sigma_y^{4/3} \quad (33)$$

$$\sigma^2 = \left(\sigma_0^2 + \frac{2}{3} \epsilon^{1/3} t \right)^3 \quad (32)$$

where C has been set equal to 1.

Substituting these into the equation for V_D , Eq. (45), we obtain after some algebra

$$V_D = \frac{y_D}{\left(\frac{\sigma_0^2}{\epsilon} \right)^{1/3} + \frac{2}{3} t} \quad (46)$$

This diffusivity velocity is independent of the ADPIC grid mesh and is the desired one defined at the coordinate (y_D, t) of a given source particle. It is important to point out that y_D here is the absolute value of the distance from the particle to the diffusion center as can be seen from its definition in Eq. (42). This "diffusion distance" y_D coincides with the actual y -coordinate of the particle position in ADPIC only when the origin in ADPIC is the same as the diffusion center and in the absence of advection or buoyancy terms. Similarly, t represents here the "age" of the particle since its creation and t coincides with the actual ADPIC problem time only in the case of a single puff source.

Study of Eq. (46) shows that in the case of a true point source, when $\sigma_0 \rightarrow 0$, or at late time when $(\sigma_0^2)^{1/3} \ll \frac{2}{3} t$ for any size source,

$$V_D = \frac{y_D}{\frac{2}{3} t} \quad (47)$$

Hence it is a property of a Gaussian distribution that all those particles for which the diffusion distance y_D divided by the diffusion time t is a constant ratio will have the same diffusion velocity V_D . Also, Eq. (46) shows that if a particle gets generated as part of a Gaussian source distribution of size σ_0 at a distance y_{0D} at $t = 0$, its initial diffusion velocity is

$$V_D = \frac{y_0}{\left(\sigma_0^2 / \epsilon \right)^{1/3}} \quad (48)$$

For the case of constant K , Eqs. (33) and (32) become respectively

$$K = K_{\text{constant}} \quad (49)$$

$$\sigma^2 = \sigma_0^2 + 2 K t. \quad (50)$$

In parallel development as for the scale-dependent case, we obtain then an expression for the diffusivity velocity

$$V_D = \frac{y_D}{\frac{\sigma_0^2}{K} + 2t}. \quad (51)$$

The validity of Eq. (51) above, under the assumptions made, is shown by two ADPIC calculations at the end of this chapter.

Since also

$$V_D = \frac{\partial y_D}{\partial t}, \quad (52)$$

Eq. (51) can be integrated in time since neither ϵ , σ_0 nor K are here functions of y or t . This integration is carried out each ADPIC cycle over the applicable time step Δt . From Eqs. (51) and (52) for the constant K case, the integral equation is

$$\int_{y_D}^{y_D + \Delta y} \frac{dy_D}{y_D} = \int_t^{t + \Delta t} \frac{dt}{\frac{\sigma_0^2}{K} + 2t}. \quad (53)$$

Integrating (53) and solving for Δy_D

$$\Delta y_D = y_D \left\{ \left[1 + \frac{\Delta t}{\left(\frac{\sigma_0^2}{2K} \right) + t} \right]^{1/2} - 1 \right\} \quad (54)$$

where Δy_D is the distance diffused by the source particle during time step Δt , y_D is the diffusion distance at the begin-

ning of the cycle, Δt is the ADPIC time step and t is the "age" of the source particle at the beginning of the cycle.

A similar integration of Eq. (46) for the scale-dependent diffusion case results in

$$\Delta y_D = y_D \left\{ \left[1 + \frac{\Delta t}{\left[\frac{3}{2} \left(\frac{\sigma_0^2}{\epsilon} \right) + t \right]^{1/3}} \right]^{3/2} - 1 \right\}. \quad (55)$$

The actual distance traveled by a source particle during one cycle in the ADPIC grid can now be computed by adding the distance Δy_A from advection to the distance Δy_D diffused during a time step:

$$\Delta y = \Delta y_D + \Delta y_A = \Delta y_D + V_A \cdot \Delta t$$

where V_A is the weighted advection velocity obtained in the same way as for regular non-source ADPIC particles.

The various updated values at cycle $n+1$, the actual source particle coordinate in ADPIC y , the diffusion distance y_D and the particle age t are then calculated and stored for each individual source particle for the next cycle, i. e.,

$$y^{n+1} = y^n + \Delta y \quad (56)$$

$$y_D^{n+1} = y_D^n + \Delta y_d \quad (57)$$

$$t^{n+1} = t^n + \Delta t. \quad (58)$$

For continuous sources, sets of Gaussian distributions of size σ_0 of source particles are generated as discussed earlier. All those particles generated during the same

cycle will have a variety of initial diffusion distances y_D according to the Gaussian distribution, but all will have the same initial age, namely $t = 0$. After one cycle of diffusion in the manner discussed above, their age will be $t = \Delta t_1$ where Δt_1 is the ADPIC time step, and after two cycles $t = \Delta t_1 + \Delta t_2$ and so on. So at any one time there will exist several sets of source particles, each set of different age. When a given set of source particles that started out with a standard deviation σ_0 representative of the source size has diffused to a distribution size with a standard deviation $\sigma \approx \Delta Y$ where ΔY is the ADPIC cell length, the whole set is considered a suitable extended source and is released from its source particle status and is considered to consist of regular ADPIC particles. The test for release is made against t , the particle-set age at every time step. In the meantime, source particles are subject to the same boundary conditions as regular particles, with deposition on the topography being one of the most important, to provide a reasonable extended source. While the source particles are treated independent of regular ADPIC particles as a sub-grid scale distribution, they are counted

together with the regular particles in determining the particle concentration field in ADPIC which is used to calculate the diffusion velocities for the regular particles.

The special source diffusivity velocity for the constant K case, Eq. (51), was tested on ADPIC for its validity with two problems. This was accomplished by replacing in the code the expression for calculating the diffusion velocity in the y -direction,

$$V_D = -\frac{K}{\bar{x}} \frac{\Delta x}{\Delta Y} \quad (59)$$

by the special prescription, Eq. (51),

$$V_D = \frac{y_D}{\frac{\sigma_0^2}{K} + 2t} \quad (51)$$

and similarly for the other two velocity components U_D and W_D in the x - and z -directions, thereby making ADPIC particles special source particles for the duration of the entire problem.*

A 4000-particle single release with a spherically symmetric Gaussian distribution of $\sigma_0 = 2\Delta Y$ was generated in a

* It can be shown analytically that (59) and (51) are equivalent in the limit of

$$\left[\frac{1}{2} \frac{y_D \Delta Y}{(\sigma_0^2 + 2Kt)} \right]^3 \text{ and } \frac{\Delta Y^2}{2(\sigma_0^2 + 2Kt)} \text{ both being } \ll 1, \text{ by substituting}$$

$$\Delta x = \frac{Q}{(2\pi)^{1/2}} \frac{1}{(\sigma_0^2 + 2Kt)^{1/2}} \left\{ \exp \left[-\frac{(y_D + \Delta Y)^2}{2(\sigma_0^2 + 2Kt)} \right] - \exp \left[-\frac{1}{2} \frac{y_D^2}{(\sigma_0^2 + 2Kt)} \right] \right\}$$

$$\text{and } \bar{x} = \frac{Q}{(2\pi)^{1/2}} \frac{1}{(\sigma_0^2 + 2Kt)^{1/2}} \exp \left[-\frac{(y_D + \frac{1}{2}\Delta Y)^2}{2(\sigma_0^2 + 2Kt)} \right] \text{ into Eq. (59) above.}$$

Fig. 23. Relative puff center concentration for a source particle puff, problem 3-3-25 and 3-3-25A.

cubical $14 \times 14 \times 14$ cell ADPIC grid and left to diffuse according to Eq. (51). The initial cell size was $\Delta X = \Delta Y = \Delta Z = 10$ m. The diffusion parameter was $K = 10^4 \text{ cm}^2/\text{s}$.

Problem 3-3-25 used a time-step coefficient $F = 0.4$ in the time-step calculation,

$$\Delta t = F \cdot \frac{\Delta Y}{|V_D|_{\text{MAX}}}, \quad (60)$$

while problem 3-3-25A used an $F = 0.1$. Figure 23 shows the relative puff center concentrations as a function of time for both problems and for the analytic solution. The problem with the larger time-step coefficient diffuses a little too fast which is to be expected in the light of the

time-step discussion in the section, Time-Step Calculation.

When $\sigma_0^2 \ll 2Kt$, at late times,

$$\frac{X}{X_0} \propto t^{-3/2}. \quad (61)$$

This corresponds to a slope of $-3/2$ on log-log paper, and is plotted for comparison with the late-time ADPIC solutions in Fig. 23.

Continuous Source: Diffusion Only (Calm Condition)

Problem 2-3-27 was run to compare ADPIC results with the numerically integrated analytic expression, Eq. (41), discussed previously, for the case of a continuous succession of spherically

symmetric Gaussian source puffs of size σ_0 released each cycle into a fixed ADPIC grid of $28 \times 28 \times 14$ cubical cells and left to diffuse. The ADPIC cell size is 1000 m in the x, y, and z directions, $\sigma_0 = 2\Delta X = 2000$ m, i.e., the size of the source is well resolved by the grid mesh and special source particles are not used. Advection $U_A = V_A = W_A = 0$. The diffusion parameters $K_x = K_y = K_z = 10^7 \text{ cm}^2/\text{s}$.

The problem ran for 100 cycles to 42 450 s. The total number of particles generated was 21 222, giving an average number of 212.22 particles generated per cycle. A total of 5772 particles left the grid through the boundary, leaving 15 550 particles in the problem at the end. Figures 24, 25, 26 and 27 show the cathode-ray-tube display of the particle distribution at various times. Figure 28 compares

Fig. 24. Initial particle distribution, X-Y plane, continuous source, diffusion only, problem 2-3-27. Source bars indicate two standard deviations of source size.

Fig. 25. Particle distribution at cycle 20, $T = 8234 \text{ s}$, X-Y plane, problem 2-3-27.

Fig. 26. Particle distribution at cycle 60, $T = 24\,830 \text{ s}$, X-Y plane, problem 2-3-27.

Fig. 27. Particle distribution at cycle 100, $T = 42\,450 \text{ s}$, X-Y plane, problem 2-3-27.

Fig. 28. Plot cell center concentrations along section A, Fig. 26. Continuous source: Diffusion only, problem 2-3-27.

Fig. 29. Plot of cell concentrations along section B, Fig. 27. Continuous source: Diffusion only.

the analytic solution and the ADPIC solution in terms of number of particles per cell (defined at cell centers in ADPIC) versus distance along section A as located in Fig. 26. Similarly, Fig. 29 shows the ADPIC versus analytical solution comparison for a section indicated in Fig. 27.

Continuous Source: Diffusion and Advection

Problems 2-3-29G was run to compare the results of ADPIC with the numerically integrated expression, Eq. (41), for the case of a continuous succession of spherically symmetric Gaussian source puffs of size σ_0 released each cycle into the fixed ADPIC grid of $28 \times 28 \times 14$ cubical cells and subjected to diffusion and a constant advection velocity in the +X direction of $U_A = 2$ m/s. Each cell was 1000 m in the x, y, and z directions. The size of the source is $\sigma_0 = 20$ m, hence is not resolved by the ADPIC grid, and the special source particle treatment

discussed in the section on Instantaneous Source Diffusion with Constant K, is employed. The diffusion parameters are $K_x = K_y = K_z = 10^7$ cm²/s. The problem ran for 167 cycles and 23 470 s and the total number of particles generated was 23 472, giving an average of 140.5 particles generated per cycle. A total of 12 371 particles left the grid due to advection and diffusion, leaving 11 413 particles still in the problem at the end. The number of particles lost per cycle and particles generated at the source per cycle became equal at cycle 126, $T = 17\,330$ s, indicating that the plume had reached a steady state. Figures 30, 31, 32 and 33 show the CRT display of the particle distribution in the x-y plane at various times. Figures 34 and 35 show comparisons between ADPIC concentrations and the analytic solution along sections A and B whose locations are indicated in Fig. 31. Figures 36 and 37 show the same comparisons at late times along sections C and D, as located in Fig. 33.

Fig. 30. Particle distribution at cycle 17, $T = 1852 \text{ s}$, X-Y plane, problem 2-3-29G.

Fig. 31. Particle distribution at cycle 46, $T = 5526$ s, X-Y plane, problem 2-3-29G. Sections refer to planes along which cell center concentrations are sampled for comparison with analytic solution.

Fig. 32. Particle distribution at cycle 72, $T = 9073 \text{ s}$, X-Y plane, problem 2-3-29G.

Fig. 33. Particle distribution at cycle 167, $T = 9073 \text{ s}$, X-Y plane, problem 2-3-29G. Sections refer to planes at which all center concentrations are sampled for comparison with analytic solution.

Fig. 34. Plot of cell center concentrations along section A, Fig. 31. Continuous source: Diffusion and advection, $U = 2$ m/s, $K = 1.0 \times 10^7$ cm²/s. Source size: STD $\sigma_0 = 20$ m, problem 2-3-29G.

Fig. 35. Plot of cell center concentrations along section B, Fig. 31. Continuous source: Diffusion and advection, $U = 2$ m/s, $K = 1.0 \times 10^7$ cm²/s, problem 2-3-29G.

The poor agreement on Figs. 34 and 36 near the source point between ADPIC and analytic cell concentrations is due to the fact that the source is not well resolved. However, it is important to keep in mind that while the cell concentration averages of ADPIC in this region are not repre-

Fig. 36. Plot of cell center concentrations along section C, Fig. 33. Continuous source: Diffusion and advection, $U = 2$ m/s, $K = 1.0 \times 10^7$ cm²/s, problem 2-3-29G.

Fig. 37. Plot of cell center concentrations along section D, Fig. 33. Continuous source: Diffusion and advection, $U = 2$ m/s, $K = 1.0$, problem 2-3-29G.

sentative because of the grid coarseness, they are not used to compute the diffusion of the source particles; rather, the special sub-grid scale source particle diffusion scheme is employed and the actual source particle coordinates as depicted

in the CRT Figs. 30, 31, 32, 33 are correct. Thus a proper extended source distribution is eventually provided and the false close-in cell concentrations do not introduce errors into the rest of the grid, as can be seen by the good agreement between ADPIC and the analytic solution at larger distances away from the source.

Problem 2-3-29I is the same problem as 2-3-29G initially. It is run, however, with a larger advection velocity $U_A = 10$ m/s in the positive x-direction, resulting in a narrower plume and somewhat different particle budget and total running time. The problem ran 101 cycles and $T \approx 32$ s. There was no need to run it any longer since after about 77 cycles $T = 2712$ s, the plume reached

a steady state with a constant number of particles of about 7900. The total number of particles generated was 12 092 at an average generation rate of 119.7 particles/cycle. A total of 4185 particles left the grid at the end of the problem, leaving 7909 particles in the problem.

Figures 38, 39, 40, 41 and 42 show the particle positions at various times. Figures 43 and 44 compare ADPIC with the analytic solution along sections A and B as located in Fig. 40 at an earlier time when the plume has not yet reached a steady state. Figures 45 and 46 compare ADPIC with the analytic solution along sections C and D as located on Fig. 42 at a time when the plume has reached the steady state.

Fig. 38. Particle distribution at cycle 9, $T = 306 \text{ s}$, X-Y plane, problem 2-3-29I.

Fig. 39. Particle distribution at cycle 27, $T = 924.5 \text{ s}$, X-Y plane, problem 2-3-29I.

Fig. 40. Particle distribution at cycle 35, $T = 1203 \text{ s}$, X-Y plane, problem 2-3-29I. Sections refer to cross-sectional planes at which cell concentrations are compared to analytic solution.

Fig. 41. Particle distribution at cycle 53, $T = 1832 \text{ s}$, X-Y plane, problem 2-3-39I.

Fig. 42. Particle distribution at cycle 101, $T = 3632 \text{ s}$, X-Y plane, problem 2-3-391. Sections refer to cross-sectional planes at which all concentrations are compared to analytical solution.

Fig. 43. Plot of cell center concentrations along section A, Fig. 40. Continuous source: Diffusion and advection. $U = 10$ m/s, $K = 1.0 \times 10^7$ cm²/s. Source size: STD $\sigma_0 = 20$ m, problem 2-3-29I.

Fig. 45. Plot of cell center concentrations along section C, Fig. 42. Continuous source: Diffusion and advection. $U = 10$ m/s, $K = 1.0 \times 10^7$ cm²/s. Source size: STD $\sigma_0 = 20$ m. Problem 2-3-29I.

Fig. 44. Plot of cell center concentrations along section B, Fig. 40. Continuous source: Diffusion and advection. $U = 10$ m/s, $K = 1.0 \times 10^7$ cm²/s, problem 2-3-29I.

Fig. 46. Plot of cell center concentrations along section D, Fig. 42. Continuous source: Diffusion and advection. $U = 10$ m/s, $K = 1.0 \times 10^7$ cm²/s, problem 2-3-29I.

VERIFICATION SUMMARY

Table 1 summarizes the ADPIC validation problems for a comparison of their agreement with the analytic solutions. The percentage errors listed refer to the deviation of ADPIC from the analytic solutions in terms of standard deviations σ of the various concentration distribution cross sections shown in the indicated figures.

Even though the number of cells and particles in the verification problems was moderate, the results indicate that ADPIC diffuses and advects particle

distributions over long periods of time, over many orders of magnitude in size, and for varied specifications of advection and diffusion parameters in three dimensions, to within a $\pm 5\%$ error of the analytically calculated standard deviation for such distributions. If more cells and more particles are used, correspondingly smaller errors can be expected.

Two points should be raised. First, the errors introduced by the lumpiness in the random number generator discussed in the section on Particle Generation under Accuracy of ADPIC adversely affect the accuracy of ADPIC. No detailed

Table 1. Comparison of ADPIC verification problems with the analytic solutions.

(1) Problem No.	(2) Coordinated direction	(3) Time (s)	(4) σ analytic (m)	(5) σ ADPIC (m)	(6) ADPIC errors (%)	(7) Figure No.
3-2-15	x	286 300	757	770	+2	6
	z	286 300	31.2	32.0	+3	7
3-3-24B	y	0	204	200	-2	9
	z	0	33.4	34.5	+3	9
	y	87 720	1.37×10^5	1.40×10^5	+2	11
	z	87 720	4100	4200	+2	11
3-3-26	x	62.54	282	280	-1	18
	z	62.54	58.5	58.0	-1	19
	x	6 328	2.58×10^5	2.65×10^5	+3	20
	z	6 328	560	580	+4	21
2-3-27	x	24 830	3150	3300	+5	28
	x	42 450	3300	3400	+3	29
2-3-29G	y	5 526	2620	2750	+5	35
	y	23 470	4700	4550	-3	37
2-3-29I	y	1 203	1200	1250	+4	44
	y	3 288	1750	1800	+3	46

Column (1) contains the problem number. Column (2) lists the direction of sampling as indicated on the corresponding figure. Column (3) is ADPIC problem time. Columns (4) and (5) are the standard deviations of the particle concentration distributions for the analytic solutions and the corresponding ADPIC results respectively. Column (6) shows the percentage error of ADPIC, Column (5), with respects to the analytic solution, Column (4). Column (7) refers to the figure in the report which shows the concentration distribution cross sections to which the standard deviations, Columns (4) and (5), pertain.

study has yet been made of the extent of this effect but as an example, the standard deviation of a puff of particles right after they were generated in ADPIC at $T = 0$ was computed and is shown in Table 1, problem 3-3-24B. Despite the fact that the random number generator was "instructed" to generate a particle distribution with a standard deviation of 204

and 33.4 respectively, the actually obtained particle placement corresponded to a standard deviation of 200 and 34.5, producing an initial error of -2% and +3% respectively. Second, the dimensions and diffusion parameters for the various problems are chosen for verification purposes against closed analytic solutions and in some cases do not represent physically meaningful scenarios.

Conclusions

ADPIC was created with the realization that the study and prediction of the transport, diffusion and deposition of atmospheric pollutants from various sources from local to extended regional scales requires a three-dimensional approach to computer modeling. Most air pollution scenarios involve time- and space-varying advection fields (shear) and diffusion parameters, topography, precipitation and gravitational effects for a variety of active or inert sources and are inherently three-dimensional in nature.

ADPIC was developed with capabilities to treat all these aspects of pollutant dispersal over short or long times with good accuracy for any specified source term, with the exception, for the present, of photochemistry. The pseudo-velocity and particle-in-cell method was chosen for ADPIC chiefly because of its advantage of eliminating the fictitious diffusion inherent in purely Eulerian codes. The other big advantage of this method is, that with the coordinates, mass, activity and "age" of each particle known at all times, the treatment of dry deposition,

washout from rain, radioactive decay, radioactive cloud-dose calculations and multiple instantaneous or continuous sources of various sizes and duration, becomes very convenient.

With the development of the three-dimensional, mass-consistent wind-field model MACAW,²⁶ which is used to provide the full three-dimensional space and time-varying advection field to ADPIC, pollutant dispersion studies of any desired complexity including stratified shear flow and calm conditions can be undertaken. By the same token, ADPIC can accommodate the full time- and space-varying diffusivity tensor K_{ij} , but currently only the usual three diagonal terms are used to describe scale-dependent atmospheric diffusion.

ADPIC has undergone an extensive verification effort, the most important cases of which are described in this report, and it has been shown to compare with the corresponding analytic solutions to within a few percent. Since meteorological and pollution data frequently considerably exceed a few percent error, ADPIC can be considered a sensitive

tool for the full-scale numerical study of pollutant dispersal in the atmosphere.*

* Since the writing of this report ADPIC has been applied extensively on the regional scale in the USAEC Reactor Safety Study (Prof. Rassmussen Panel) and it will be further verified against regional tracer release experiments during the coming fiscal year.

Although ADPIC has so far not been applied to water pollution problems, there is no reason why it could not be used, together with the appropriate advection flow field and diffusion parameters, to study the dispersion parameters, to study the dispersion of pollutants in water.

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