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INTERNATIONAL CENTRE FOR SCIENCE AND HIGH TECHNOLOGY
c/o INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS 34100 TRIESTE (ITALY) VIA GRIGNANO 9 (ADRIATICO PALACE) P.O. BOX 586 TELEPHONE 040-224572 TELEFAX 040-224575 TELEX 460449 APH I

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"Arco: a Particle Model for the Study of the Atmospheric Dispersion Under Complex Conditions"

F. DESIATO
Agenzia Nazionale per la Protezione dell'Ambiente
A.N.P.A. (EX-ENEA/DISP)
Rome, Italy

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ARCO
A PARTICLE MODEL FOR THE STUDY OF THE ATMOSPHERIC DISPERSION UNDER COMPLEX CONDITIONS

FRANCO DESIATO
ENEA - Direzione Centrale Sicurezza Nucleare
e Protezione Sanitaria, Roma

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Sommario

Il presente rapporto descrive il modello di dispersione atmosferica ARCO (Atmospheric Release in Complex Terrain) e il relativo codice di calcolo. ARCO è stato sviluppato dall'ENEA-DISP per lo studio su terreno complesso di rilasci accidentali o di routine da sorgenti puntiformi. Si tratta di un modello Lagrangiano, in cui la nube inquinante viene simulata mediante un elevato numero di pseudoparticelle la cui velocità è pari alla sòmma delle componenti di avvezione e di moto turbolento. Il campo di avvezione viene calcolato da un modello diagnostico di vento a cui ARCO è accoppiato, mentre la componente turbolenta viene calcolata con metodi statistici di tipo Monte Carlo e in base a diverse parametrizzazioni della struttura termica e dinamica dello strato limite atmosferico.

Abstract

The present report describes the atmospheric dispersion model ARCO (Atmospheric Release in COmplex terrain) and its related computer code. ARCO has been developed by ENEA-DISP for the study of accidental or routine emissions by point sources over complex terrain. It is a Lagrangian model, in which the pollutant plume is simulated by a large number of particles with a velocity which is the sum of the advection and turbulent components. The advection field is provided by a diagnostic wind field model coupled with ARCO, while the turbulent motion is computed using a Monte Carlo statistical technique and on the base of different parametrizations of the dynamic and thermal structure of the atmospheric boundary lay...

Index

Introduction

The short term dispersal of toxic pollutants into the atmosphere can be described by different types of models depending on the space and time scale, the complexity of topography and meterological conditions, and the purpose of the model evaluation, i.e. the output required in terms, for example, of averaging time of computed concentrations or accuracy in the localization of maximum concentration.

The most simple and widely used models are the Gaussian plume models, based on the statistical theory and empirical observations of the horizontal and vertical standard deviations σ_y and σ_z of the concentration distribution. To allow space and time variability of the meteorological conditions, including wind speed and direction, straight line plume models are often replaced by sequential puff models, with the option of puff splitting to take into account wind shear.

The dispersion in complex terrain or meteorological conditions requires the use of three-dimensional diffusion models coupled with objective or prognostic wind field models. With respect to Eulerian grid models, Lagrangian particle models have the advantage of being conceptually and computationally simpler and of avoiding numerical diffusion. Particle models can be purely deterministic or possess statistical characteristics. In the first case, particle motions are uniquely calculated based on some closure of the diffusion-advection equation; particle-in-cell models based on K-theory belong to this category. In the second case, Monte Carlo tecniques are used to produce semi-random perturbations and the dynamics of each particle represents just one realization of an infinite set of possible solutions.

The Environmental Modeling Division of ENEA-DISP has applied for several years the Atmospheric Diffusion Particle-in-Cell (ADPIC) model (Lange, 1978) in conjunction with the MATHEW mass consistent diagnostic wind field model (Sherman, 1978), originally developed at the Lawrence Livermore National Laboratory, for both the real time and the previsional assessment of the short term atmospheric dispersion in complex terrain. In ADPIC, Lagrangian "mass" particles are transported inside a fixed eulerian grid, and the diffusive velocity of the particles is derived based on K-theory.

Recently, the option for Monte Carlo statistical diffusion has been introduced into ADPIC (Lange, 1990). Afterwards, several reasons suggested the opportunity of developing a new code. At first, it was considered that it would be useful to drive the particles by three-dimensional wind fields computed in a terrain-following coordinate system instead of a Cartesian coordinate system. This may have some advantages in terms of simplicity and of better vertical resolution near the surface. Two wind field models with these characteristics (Ludwig, 1988; Moussiopoulos et al., 1988) are now available for this purpose at ENEA-DISP.

As a consequence of the Monte Carlo and of the terrain-following options, the convenience of eliminating the gridded structure of the model domain became evident. In addition, the possibility of using input data variable in space (roughness height) or in space and time (mixing height, Monin-Obukhov length, precipitation) was outlined. For these reasons, a new code (ARCO: Atmospheric Release in COmplex terrain) has been developed, which retains some modules fo the Monte Carlo version of ADPIC and includes the features mentioned above. The present report describes the physical assumptions adopted in ARCO, and some characteristics of the computer code.

ARCO is presently operational into the ENEA-DISP real time system for the assessment of the consequences of accidental releases into the atmosphere, ARIES-I (Atmospheric Release Impact Evaluation System - Improved) (Desiato and Maggi, 1991). ARIES-I has been develped on a cluster of VAX computers in VMS environment. Recently, a new version (ARIES-W) of the system has been developed on a RISC Workstation in UNIX environment, for the off-line assessment of the environmental impact of pollutant sources. In both ARIES-I and ARIES-W, ARCO is linked with other codes devoted to the preprocessing of meteorological and environmental data and the postprocessing of the computed concentration and deposition fields. It is also linked with two territorial data banks covering Italy, at high space resolution, and Europe, at lower space resolution, respectively.

1 - The model

1.1 Particle motion

ARCO solves the three-dimensional flux conservation equation,

$$\partial\chi/\partial t + \nabla\cdot(\chi U_p) = 0 \qquad (1)$$

where χ is the pollutant concentration and U_p is a pseudo transport velocity defined as the sum of the mean advection velocity U_a and a diffusive velocity U_d.

U_a is obtained from the space interpolation to the individual particle position, and the time interpolation to the current time step, of the three-dimensional gridded advection field computed by a diagnostic wind field model. The space interpolation of U_a is linear, with the exception of the vertical interpolation under the lowest layer, for which a power low with the exponent of a neutral surface layer (1/7) is used.

U_d is computed using the Langevin equation, whose solution in inhomogenous conditions presents several conceptual and numerical problems (Thomson, 1984; De Baas et al. 1986). In ARCO, the method suggested by Legg and Raupach (1982) is adopted, the vertical component equation being,

$$w(t+\Delta t) = aw(t) + b\sigma_w r + (1-a)T_L\, \partial\sigma_w^2/\partial z \qquad (2)$$

where w(t) is the vertical velocity at time t, r is a random number from a Gaussian distribution with zero mean and unit variance, T_L the Lagrangian integral time scale,

$$a=\exp(-\Delta t/T_L); \quad b=(1-a^2)^{1/2} \qquad (3)$$

The last term in (2) allows for inhomogeneous turbulence in which T_L and the standard deviation of the vertical wind component σ_w can vary with height. The two horizontal components of U_d are computed using analogous equations without the last term, because homogeneous turbulence is assumed in the horizontal in the absence of boundaries.

The time step Δt is computed for each particle as a fraction of the minimum among the three components of the Lagrangian time scale T_L.

ARCO runs in a terrain following coordinate system with ground surface as zero vertical coordinate. The surface is seen as a perfect mirror for the partcle motion, so the sign of the vertical coordinate and of the vertical velocity of a particle are inverted if they become negative. The top of the mixing layer is also seen as a mirror in the unstable case, when the presence of an inversion lid is supposed to prevent the particle from diffusing above the unstable layer. The upper particle reflection is suppressed in the presence of plume rise, when the vertical coordinate of the particles is computed with a separate method (see 1.5)

1.2 Turbulence parameters

ARCO incorporates several subroutines for the estimate of σ_v and T_L profiles with different methods, also depending on the availability of turbulence measurements. The methods included at present are listed in tables 1 and 2. The stability condition of the boundary layer is defined on the base of the mixing height h and the Monin-Obukhov length L (Carruthers et al., 1991),

$h/L > 1$: stable; $-.3 < h/L < 1$: neutral; $h/L < -.3$: unstable. (4)

One approach is based on the parameterization summarized by Hanna (1982). For the wind fluctuation components:

stable: $\sigma_u = 2u_*(1-z/L)$; $\sigma_v = 1.3u_*(1-z/L)$; $\sigma_w = \sigma_v$ (5)

neutral: $\sigma_u = 2u_* \exp(-3fz/u_*)$; $\sigma_v = 1.3u_* \exp(-2fz/u_*)$; $\sigma_w = \sigma_v$ (6)

unstable: $\sigma_u = u_*(12-.5h/L)^{1/3}$; $\sigma_v = \sigma_u$;

$\sigma_w = .96w_*(3z/h-L/h)^{1/3}$ $z/h \leq .03$ (7)

$\sigma_w = \min[.96w_*(3z/h-L/h)^{1/3}, .763\sigma_w = .96w_*(z/h)^{.175}]$ $.03 < z/h \leq .4$

$\sigma_w = .722w_*(1-z/h)^{.207}$ $.4 < z/h \leq .96$

$\sigma_w = .37w_*$ $.96 < z/h < 1$

f is the Coriolis parameter and $w_* = u_*(-h/kL)^{1/3}$ is the convective velocity scale.

For the Lagrangian time scale components:

stable: $T_{Lx} = .15h/\sigma_u (z/h)^{.5}$; $T_{Ly} = .07h/\sigma_v (z/h)^{.5}$; $T_{Lz} = .1h/\sigma_w (z/h)^{.5}$ (8)

neutral: $T_{Lx} = .5z/\sigma_u (1+15fz/u_*)$; $T_{Ly} = T_{Lx}$; $T_{Lz} = T_{Lx}$ (9)

unstable: $T_{Lx} = .15h/\sigma_u$; $T_{Ly} = T_{Lx}$; $T_{Lz} = T_{Lx}$ (10)

When wind direction fluctuation measurements σ_θ and σ_φ are available, they can be used to derive σ_v vertical profiles. The sampling time of σ_θ should be of the same order or the time interval between two consecutive wind fields used for the advection term of the particle motion.

First, $\sigma_v(z_i) = \sigma_\theta(z_i)U(z_i)$ and $\sigma_w(z_i) = \sigma_\varphi(z_i)U(z_i)$ are computed from the available measurements at heights z_i; then, $\sigma_v(z)$ components at particle height z are obtained by linear interpolation between the closest lower and upper z_i and maintaining the relationships between σ_u and σ_v of (5,6,7). If only one measurement at z_n is available, or above the highest available measurements at z_n, the following equations are used:

stable:	$\sigma_u=2\sigma_v/1.3$;	$\sigma_v=\sigma_v(z_n)(1-z/h)/c$; $c=1-z_n/h$	$\sigma_w=\sigma_w(z_n)(1-z/h)/c$ $c=1-z_n/h$	(11)
neutral:	$\sigma_u=\sigma_v$;	$\sigma_v=\sigma_v(z_n)\exp(-.75z/h)/c$ $c=\exp(-.75z_n/h)$	$\sigma_w=\sigma_w(z_n)\exp(-.75z/h)/c$ $c=\exp(-.75z_n/h)$	(12)
unstable:	$\sigma_v=\sigma_u$	$\sigma_u=\sigma_v(z_n)$	$\sigma_w=.37w_*+c(1-z/h)$, $c=[\sigma_w(z_n)-.37w_*]/(1-z_n/h)$	(13)

Practically, the wind fluctuations profiles expressed through (11,12,13) are the same of (5,6,7), forcing the profiles to the observed values at the height of the available meaaurements z_n.

Two more methods for the evaluation of the wind fluctuation components are included in ARCO. The first is based on the equations summarized by Gryning et al. (1987):

if L>0: $\sigma_u=u_*[2(1-z/h)]^{1/2}$; $\sigma_v=\sigma_u$ $\sigma_w=1.4u_*(1-z/h)^{3/4}$ (14)

if L<0: $\sigma_u=u_*[.35(-h/kL)^{2/3}+(2-z/h)]^{1/2}$ $\sigma_v=\sigma_u$

$\sigma_w=u_*\{1.5[z/(-kL)]^{2/3}\exp(-2z/h)+(1.7-z/h)\}^{1/2}$ (15)

The second is based on Carruthers et al. (1991)

stable: $\sigma_u=2.5u_*(1-.5z/h)^{3/4}$; $\sigma_v=.8\sigma_u$; $\sigma_w=.52\sigma_u$ (16)

neutral: $\sigma_u=.5u_*(i-.8z/h)$; $\sigma_v=.8\sigma_u$; $\sigma_w=.52\sigma_u$ (17)

unstable: $\sigma_u=(w_*^2+6.25T_{wn}^2u_*^2)^{1/2}$; $\sigma_v=(.3w_*^2+4T_{wn}^2u_*^2)^{1/2}$;

$\sigma_w=[.4T_{wc}^2+(1.3T_{wn}u_*/w_*)^2]w_*^2$, (18)

with $T_{wc}=2.1(z/h)^{1/3}(1-.8z/h)$, and $T_{wn}=1-.8z/h$.

As far as the Lagrangian time scales are concerned, in alternative to (5,6,7) values of $T_{Lx}=T_{Ly}=T_{Lz}$ independent on height and functions of the stability category as in Neumann (1978) can be selected (table 3). The stability category is evaluated based on roughness height, Monin-Obukhov length and friction velocity (Sutherland and Hansen, 1986).

Both wind fluctuations and Lagrangian time scale components ar not allowed to be lower than threshold values, tipically .1 m/s for σ_u and σ_v, .01 m/s for σ_w and 3 s for T_L.

TABLE 1

σ_u, σ_v	σ_w	ITURB
σ_θ measurement (11,12,13)	Hanna (5,6,7)	1
σ_θ measurement (11,12,13)	σ_ϕ measurement(11,12,13)	2
Hanna (5,6,7)	Hanna (5,6,7)	3
Gryning et al. (14,15)	Gryning et al. (14,15)	4
Carruthers et al. (16,17,18)	Carruthers et al. (16,17,18)	5

TABLE 2

T_L	ITLAG
Hanna (8,9,10)	1
Stability (table 3)	2

Methods included in ARCO for the evaluation of wind fluctuation components and Lagrangian time scale; in parenthesis are the equations in the text. ITURB and ITLAG are flags for selecting the methods in the SITE input file (see 2.2).

TABLE 3

Stability cat.	T_L (s)
A	2400
B	1700
C	700
D	750
E	1000
F	2250

Values of the Lagrangian time scale as a function of the stability category.

1.3 Meteorological parameters

Roughness height, mixing height, Monin-Obukhov length and precipitation data are given as input to ARCO either as two-dimensional fields or as uniform values over the whole domain.

The friction velocity field is computed at each time step,

$$u_*(x,y)=kU(z_1)/[\ln(z_1/z_0)-\psi(z_1/L)+\psi(z_0/L)] \tag{19}$$

where $U(z_1)$ and z_0 are the first level wind speed and the roughness height interpolated at (x,y), respectively. The stability functions ψ are (van Ulden and Holtslag, 1985):

stable: $\psi=-17[1-\exp(-.29z/L)]$ (20)

unstable: $\psi=2\ln[(1+X)/2]+\ln[(1+X^2)/2]-2\tan^{-1}(X)+\pi/2,\ \ X=(1-16z/L)^{1/4}$ (21)

1.4 Particle generation

The size and shape of the source can be modeled through the definition of the three standard deviations of a Gaussian distribution and the six coordinates of the "cut-off" of the Gaussian distribution, representing the physical boundaries of the source.

A random number generator is used to compute the initial particle coordinates compatible with the source definition. The duration of the first time step for the calculation of the motion after the generation is also assigned randomly to each particle, to allow the simulation of a continous release.

The number of particles ng to be generated at each time step Δt, is given as input; up to five species of pollutants with their own deposition velocities and half life can be considered at a time. If Q_n is the release rate of the nth species, the initial amount of a particle m is given by $q_{m,n}=Q_n\ \Delta t/ng$.

Release rates and source height, as well as the exit temperature and vertical velocity for plume rise calculation, can vary with time with a stepwise shape.

1.5 Plume rise

Plume rise due to buoyancy or momentum of the released pollutant is included in ARCO in a relatively simple way. First, the effective height $z_s+\Delta h$ of the source is computed, using formulas derived by Briggs for the different stabilities and following a scheme similar to that suggested by Turner (1985), including the partial penetration of the plume into the stable layer above the mixing height (fig. 1). Then, a vertical displacement Δz is added to the vertical coordinate of a particle at each time step, with $\Delta z \alpha t^{2/3}$ for buoyancy plume rise and $\Delta z \alpha t^{1/3}$ for momentum plume rise; the rise is suppressed when the age of a particle exceeds the time of maximum rise t_m.

Following the scheme in fig. 1, the Froude number Fr, the stack tip downwash correction factor f, and the buoyancy flux F_b, and the neutral-unstable momentum plume rise are first calculated:

$Fr=v_s^2/[gd(T_s-T_a)/T_a];$ (22)
$f=3(v_s-u_s)/v_s;$ (23)
$F_b=gv_sd^2(T_s-T_a)/4T_s;$ (24)
$\Delta h_{um}=3dv_s/u_s;$ (25)

v_s is the vertical exit velocity; d is the source diameter; T_s and T_a are source and ambient air temperatures, respectively; u_s is the wind speed at the release point.

In the stable case (L>0) the left side of the flow chart is valid, the equations for momentum and buoyancy plume rise being:

$\Delta h_{sm}=.646[v_s^2d^2/(T_su_s)]^{1/3}T_a^{1/2}/(\delta\theta/\delta z)^{1/6};$ (26)
$\Delta h_{sbv}=2.6(F_b/u_ss)^{1/3};$ $\Delta h_{sbc}=5F_b^{1/4}/s^{3/8};$ $\Delta h_{sb}=\min(\Delta h_{sbv},\Delta h_{sbc})$ (27)

$s=(g/\theta)\delta\theta/\delta z$ is the Brunt-Vaisala frequency; the potential temperature gradient $\delta\theta/\delta z$ is set to .01 C/m. Δh_{sbv} and Δh_{sbc} are plume centerline rises predicted by Briggs in wind and calm conditions, respectively (Weil and Brower, 1984).

In the neutral and unstable cases (L≤0) the right side of the flow chart is valid, the equations for buoyancy plume rise being:

$\Delta h_{ubv}=24(F_b/u_s^3)^{.6}(z_s+200F_b/u_s^3)^{.4};$ $\Delta h_{ubc}=24(F/u_s^3)^{.6};$ (28)
$\Delta h_{ub}=\min(\Delta h_{ubv},\Delta h_{ubc})$

Δh_{ubv} gives the lowest values for high wind speeds; Δh_{ubc} gives the lowest values for low wind speeds. If the estimated effective height $z_s+\Delta h_u$ is higher then mixing height, the

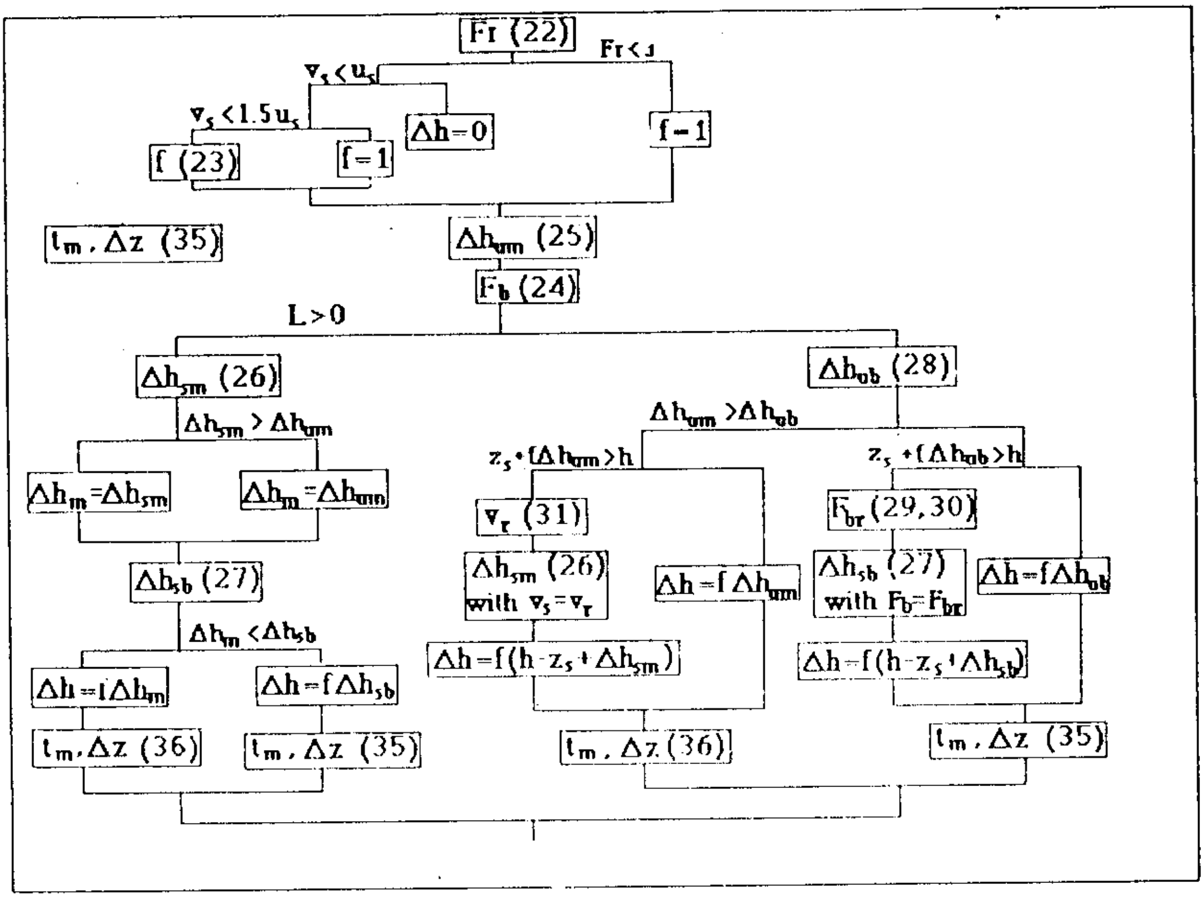

Fig. 1 - Flow chart of plume rise calculation in ARCO. In parenthesis are the equations as numbered in the text. Meaning of symbols:
Δh: plume rise; subscripts: s=stable; u=unstable; m=momentum; b=buoyancy; Fr: Froude number; f: stack tip downwash factor; u_s=wind speed at release height; v_s=release vertical velocity; v_r=residual vertical velocity; F_b=buoyancy flux; F_{br}=residual buoyancy flux; L=Monin-Obukhov length; h=mixing height; z_s=release height; t_m=time of maximum rise; Δz=particle vertical displacement in a time step.

residual buoyancy F_{br} or momentum v_r of the plume at the top of the mixing layer are calculated and used to calculate the rise in the upper stable layer with (27) or (26) respectively, in which u_s is replaced by wind speed at the top of mixing layer:

$$F_{br}=.0055[\Delta h-(h-z_s)]u_s^3/\{1+z_s/[\Delta h-(h-z_s)]\}^{2/3} \quad \text{if } \Delta h_{ub}=\Delta h_{ubv} \qquad (29)$$

$$F_{br}=u_s\{[\Delta h-(h-z_s)]/30\}^{5/3} \quad \text{if } \Delta h_{ub}=\Delta h_{ubc} \qquad (30)$$

$$v_r=[\Delta h-(h-z_s)]/(3du_s) \qquad (31)$$

The plume penetration in the upper stable layer Δh_s is then added to mixing height, the total rise being:

$$\Delta h=(h-z_s)+\Delta h_s \qquad (32)$$

In all cases, once calculated the total rise Δh, the following transitional rises $\Delta h(t)$ are assumed (Briggs, 1975):

$$\Delta h(t)=1.6(F_b/u_s)^{1/3}t^{2/3} \qquad \text{for buoyancy plume rise} \qquad (33)$$

$$\Delta h(t)=8.3(F_m/u_s)t^{1/3} \qquad \text{for momentum plume rise} \qquad (34)$$

where $F_m=(T_a/T_s)(.5v_sd)^2$ is the momentum flux. Then, a vertical displacement Δz is added at each time step Δt to particles with age t less then t_m.

$$\Delta z=1.07(F_b/u_s)^{1/3}t^{-1/3}\Delta t; \qquad t_m=.5\Delta h^{3/2}(F_b/u_s)^{-1/2} \qquad \text{for buoyancy plume rise} \qquad (35)$$

$$\Delta z=.66(F_m/u_s)^{1/3}t^{-2/3}\Delta t; \qquad t_m=.12\Delta h^3(u_s/F_m) \qquad \text{for momentum plume rise} \qquad (36)$$

1.6 Concentration and deposition

For the calculation of ground level air concentrations, a kernel density distribution is assigned to each particle. The shape of the distribution should be optimized to balance the needs of limiting the number of particles and smoothing the concentration field on one hand, and of maintaining a good resolution and avoiding extra diffusion on the other.

In ARCO, a Gaussian density distribution is considered. The horizontal standard deviations σ_x and σ_y are expressed as fractions of the linear dimensions of the model domain; the vertical standard deviation σ_z is expressed directly in metres. The concentrations are computed on a rectangular grid whose spacing is specified as input.

If the release height is low and there is no plume rise, so that maximum concentrations are expected in the vicinity of the source, the concentrations are computed on four rectangular nested grids centered at the release point. Each grid has a double spacing with respect to the inner. This prescription allows to obtain concentration contour lines more realistic near the source. In this case σ_x and σ_y depend also on the grid spacing underlying the particle position.

The ground level air concentration at point (i,j) is given by:

$$C(i,j)=\Sigma_m 2q_m[\sigma_x\sigma_y\sigma_z(2\pi)^{3/2}]^{-1}\exp[-(x_m-x_i)^2/2\sigma_x^2]\exp[-(y_m-y_j)^2/2\sigma_y^2]\exp[-(z_m)^2/2\sigma_z^2] \quad (37)$$

where q_m, x_m, y_m and z_m are the pollutant amount and the coordinates of the particle m.

Dry deposition is calculated over the same grid of air concentration, and accumulated over each time step, as well as time integrated air concentrations. A deposition velocity is required for each pollutant. In principle, it depends on turbulence and surface resistance, however ARCO only considers an average value which is representative of the average terrain and turbulence conditions during the transport of the pollutant.

At each time step, the increment in deposited amount of a pollutant with average deposition velocity v_d at grid point (i,j) is given by:

$$D(i,j)=C(i,j)v_d\Delta t \quad (38)$$

Wet deposition is included in ARCO with a scheme analogous to puff models. The contribution of a particle to wet deposition at point (i,j) in a time step Δt is given by:

$$w(i,j) = \Lambda q(2\pi\sigma_y^2)^{-1}\exp[-(x-x_i)^2/2\sigma_y^2]\exp[-(y-y_j)^2/2\sigma_y^2]\Delta t \quad (39)$$
$$\Lambda=Wr^{.8}(i,j),$$

where W is the washout coefficient, r is the rain intensity in mm/h in the time interval Δt at point (i,j), q is the pollutant amount of the particle and (x,y) are the particle coordinates.

The eventual scavenging by dry and wet deposition and first order chemical reaction is taken into account through the depletion of the particles by exponential reductions of the pollutant amount of the particles:

$$q(t+\Delta t)=q(t)\exp[-v_d\Delta t(.5\pi)^{-.5}\sigma_z^{-1}\exp(-z^2/2\sigma_z^2)] \quad (40)$$
$$q(t+\Delta t)=q(t)\exp(-\Lambda\Delta t) \quad (41)$$
$$q(t+\Delta t)=q(t)\exp(-\lambda\Delta t) \quad (42)$$

where $\lambda=\ln(2/T)$, T being the half life of the pollutant.

1.7 Validation

ARCO has been first tested in constant and uniform conditions, for which the agreement of the results with the solution provided by the simple Gaussian plume model has been verified.

As stated in the introduction, ARCO retains some features of the ADPIC code (Lange, 1978 and 1989), which has been extensively tested against a number of tracer experiments in different meteorological and terrain conditions (see, for validation over Italy, Desiato and Lange, 1985, and Desiato, 1991).

ARCO as a whole has been tested against the SIESTA dataset (Desiato and Lange, 1991), in near neutral and moderately complex terrain conditions. This kind of studies is particularly interesting for comparing different methods for the evaluation of turbulence parameters (fig. 2), as those described in 1.2. New model validation studies in complex terrain and different stability conditions are foreseen for the next future.

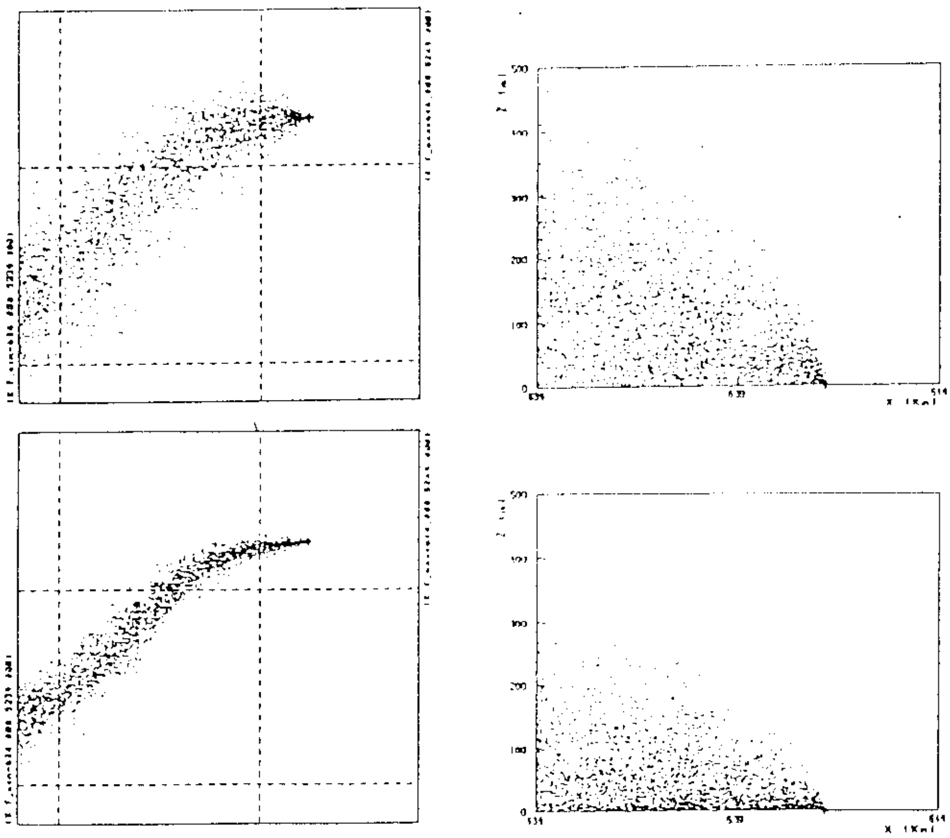

Fig.2 - Particle display on x-y (left) and x-z (right) planes, for two ARCO runs with different turbulence parameterizations, SIESTA experiment n. 1.

2 - The code

2.1 General features

ARCO is written in FORTRAN 77 language and consists of a program main and fifteen subroutines. The execution time on the VAX 6300 computer is of the order of five minutes for each hour of simulation.

ARCO is linked with a wind field model that provides a sequence of three-dimensional matrixes containing the three components of the computed wind in terrain following coordinates. The time interval between two consecutive wind fields is flexible, a time interpolation is performed in ARCO each time step.

Meteorological parameters like Monin-Obukhov length, mixing height and precipitation, can be specified in input as a time sequence of uniform values over the model domain or as two-dimensional grids. In both cases, if direct measurements are not available, they must be derived with some methods based on primary meteorological data available. For this purpose, ARCO is optionally linked with a meteorological preprocessor (PAD: Preprocessor for Atmospheric Dispersion models) (Mikkelsen and Desiato, 1992).

2.2 Input

Apart from the files containing the grids of wind fields and eventually other gridded meteorological data, such as precipitation and mixing height, the input to ARCO is divided into four files: SITE, METEO, REL, SAMP. SITE contains geographical data, source size, pollutants characteristics and code parameters. METEO contains time dependent meteorological data. REL contains release data. SAMP contains the coordinates of extra receptor points where concentration and deposition are calculated in addition to the standard grid. In the following a list of the input variables for each file is given.

SITE

X0WIN, Y0WIN
X-Y coordinates of the origin of the wind fields (km).

DELXWIN,DELYWIN

X-Y spacing of the wind field grids (km).

NXWIN, NYWIN, NZWIN
X-Y-Z number of wind grid points

X0CON, Y0CON
X-Y coordinates of the origin of the output concentration grid (km).

DELXCON, DELYCON
X-Y spacing of the concentration grid (km).

NXCON, NYCON
X-Y number of concentration grid points.

RGH
Roughness height (m).

X0Z0, Y0Z0
X-Y coordinates of the origin of the roghness grid (km). If set to 0, RGH is valid over the whole domain.

DELXZ0, DELYZ0
X-Y spacing of the roughness grid (km).

NXZ0, NYZ0
X-Y number of roughness grid points.

X0RAIN, Y0RAIN
X-Y coordinates of the origin of the precipitation grid (km). If set to 0, RAIN (see file METEO) is valid over the whole domain.

DELXRAIN, DELYRAIN
X-Y spacing of the precipitation grid (km).

NXRAIN, NYRAIN
X-Y number of precipitation grid points.

X0TURB, Y0TURB
X-Y coordinates of the origin of Monin-Obukhov length and mixing height grids (km). If set to 0, SMOLI and HMIX (see file METEO) are valid over the whole domain.

DELXTURB, DELYTURB
X-Y spacing of Monin-Obukhov length and mixing height grids.

NXTURB, NYTURB
X-Y number of Monin-Obukhov length and mixing height grid points.

XSOU, YSOU
X-Y coordinates of the release point (km).

SIGXSOU, SIGYSOU, SIGZSOU
X-Y-Z standard deviations of the initially assumed Gaussian source distribution (m).

XR, XL, YR, YL
X-Y right and left cutoff of the source, referenced to the source center.

ZT, ZB
Top and bottom cutoff of the source, referenced to the source center.

FRKERNX, FRKERNY
X-Y standard deviation of the Gaussian density distribution of the particles for computing the concentrations, expressed as fraction of the X-Y linear dimension of the concentration domain (X1CON-X0CON, Y1CON-Y0CON).

SKERNZ
Z standard deviation of the Gaussian density distribution of the particles for computing the concentrations (m).

ISTYEA, ISTMON, ISTDAY, ISTHOU, ISTMIN
Year, month, day, hour, minutes of the beginning of the release.

KALTT(I),I=1,20
Elapsed times from the beginning of required output (min).

DELT
Time step of a cycle for particle motion (s).

ELEM(I),I=1,5
Strings identifying the pollutant species.

VDEP(I),I=1,5
Deposition velocities (m/s).

THALF(I),I=1,5
Half lifes (s).

WASH
Washout coefficient (s^{-1}).

NGEN
Number of particles to be generated at each time step.

ITURB
Flag for the selection of the method for evaluating σ_v (see 1.2).
1: σ_θ measurements for horizontal; Hanna (1982) for vertical.
2: σ_θ measurements for horizontal; σ_ϕ measurements for vertical.
3. Hanna (1982).
4: Gryning et al. (1987)
5: Carruthers et al. (1987).

ITLAG
Flag for the selection of the method for evaluating T_L (see 1.2).
2: Stability category.
3: Hanna (1982).

SDIA
Source diameter, for plume rise calculation (m).

XSIGT, YSIGT
Coordinates of points where σ_θ and σ_ϕ are eventually measured (km).

METEO

ITIMWIND(I),I=1,20
Elapsed times from the beginning of wind fields produced by wind model (min).

HMIX(I),I=1,20
Mixing height (m).

ITIMHMIX(I),I=1,20
Elapsed times from the beginning of HMIX observations (min).

SMOLI(I),I=1,20
Inverse of Monin-Obukhov length (m^{-1}).

ITIMSMOL(I),I=1,20
Elapsed times from the beginning of SMOLI observations (min).

RAIN(I) I=1,20
Accumulated rainfall over the time interval ITIMRAIN(I)-ITIMRAIN(I-1). If I=1, ITIMRAIN(I-1)=0.

ITIMRAIN(I),I=1,20
Elapsed times from the beginning of rainfall observations (min).

SIGTHETA(K,I),K=1,5,I=1,20
Horizontal wind fluctuation measurements at heights ZSIG(K) (degrees).

SIGHPHI(K,I),K=1,5,I=1,20
Vertical wind fluctuation measurements at heights ZSIG(K) (degrees).

ITIMSIG(I),I=1,20
Elapsed times from the beginning of SIGTHETA and SIGPHI observations (min).

ZSIG(K),K=1,5
Heights of wind fluctuation measurements (m).

ITIMSIG(I),I=1,20
Elapsed times from the beginning of wind fluctuation observations (min).

TAIR(I),I=1,20
Air temperature, for plume rise calculation (°C).

ITIMTAIR(I),I=1,20
Elapsed times from the beginning of air temperature observations (min).

REL

RATE(N,I),N=1,5,I=1,20
Release rate of species N at time interval I (g/s or Ci/s).

IRTIM(I),I=1,20
Elapsed times from the beginning of release rate interval (min).

SHEIGHT(I),I=1,20

Source height at time interval I (m).

RTEMP(I),I=1,20
Release temperature at time interval I, for plume rise calculation (°C).

RWEX(I),I=1,20
Release vertical exit velocity, for plume rise calculation (m/s).

2.3 Output

The output of ARCO consists, for each considered pollutant species, of five types of analysis at the required output times: instantaneous air concentrations, time integrated concentration, time averaged concentrations, total ground deposition and wet deposition. The values are provided on a standard grid for successive contour lines plotting, and on extra receptor points specified in the input file SAMP.

References

Carruthers D.J., Holroyd R.J., Hunt J.R.C., Weng W.S., Robins A.G., Apsley D.D., Smith F.B., Thomson D.J., and Hudson B. (1991): UK atmospheric dispersion modelling system, Proceedings of the 19th NATO/CCMS Int. Technical Meeting on Air Pollution Modelling and its Application, Ierapetra, Greece.

De Baas A., Van Dop H., Niewstadt F.T.M. (1986): An application of the Langevin equation for inhomogeneous conditions to dispersion in a convective boundary layer. Quart. J. R. met. Soc., 112, 165-180.

Desiato F. and Lange R. (1985): A sea breeze tracer study with the MATHEW/ADPIC transport and diffusion model, Proceedings of the IAEA Int. Symp. on Emergency Plsnning and Preparedness for nuclear facilities, Roma.

Desiato F. (1991): A dispersion model evaluation study for real-tome application in complex terrain. J. Appl. Meteor., 30, 1207-1219.

Desiato F. and Lange R. (1991): An intercomparison of atmospheric turbulence parameters and their application to a tracer experiment using a Monte Carlo particle model. Proceedings of the 19th NATO/CCMS Int. Technical Meeting on Air Pollution Modelling and its Application, Ierapetra, Greece.

Desiato F. and Maggi M. (1991): Incidenti tecnologici. Sapere, n. 4, 46-55.

Gryning S.E., Holtslag A.A.M., Irwin J.S., and Sivertsen B. (1987): Applied dispersion modelling based on meteorological scaling parameters. Atm. Env., 21, 79-89.

Hanna S.R. (1982): Applications in air pollution modelling, in "Atmospehric Turbulence and Air Pollution Modelling", F.T.M. Niewstadt and H. van Dop ed., D. Reidel Publ. Comp., Dordrecht/Boston/Lancaster.

Lange R. (1978): ADPIC - A three-dimensional particle-in-cell model for the dispersal of atmospheric pollutants and its comparison to regional tracer studies. J. Appl. Meteor., 17, 320.

Lange R. (1990): A comparison of the Monte carlo and the flux gradient method for atmospheric diffusion. Proceedings of the 18th NATO/CCMS Int. Technical Meeting on Air Pollution Modelling and its Application, Vancouver, Canada.

Legg B. J. and Raupach M.R. (1982): Markov chain simulation of particle dispersion in inhomogeneous flow: the mean drift velocity induced by a gradient in Eulerian velocity variance. Bound. Lay. Met., 24.

Ludwig F.L. (1988): Combined objective wind analysis and adaptive volume plume model codes for microcomputer use, in "Computer techniques in environmental studies", P. Zannetti ed., Computational Mechanics Publ., Southampton/Boston.

Mikkelsen T. and Desiato F. (1992): Atmospheric dispersion models and pre-processing of meteorological data for real-time application, to be presented at the Third Int. Workshop on Real-time computing of the environmental consequences of an accidental release to atmosphere fom a nuclear installation, Schloss Elmau, Bavaria.

Moussiopoulos N., Flassak T., and Knittel G. (1988): A refined diagnostic wind model. Envir. Soft., 3, 85-94.

Neumann J. (1978): Some observations of the simple exponential function as a Lagrangian velocity correlation function in turbulent diffusion. Atm. Env. 12, 1965-1968.

Sherman C.A. (1978): A mass-consistent model for wind fields over complex terrain. J. Appl. Met., 17, 312-319.

Sutherland R.A. and Hansen F.V. (1986): A quantitative method for estimating Pasquill stability class from windspeed and sensible heat flux density. Bound. Lay. Met. 37, 357-369.

Thomson D.J. (1984): Random walk modelling of diffusion in inhomogeneeous turbulence. Quart. J. R. Met. Soc., 110, 1107-1120.

Turner D.B. (1985): Proposed pragmatic methods for estimating plume rise and plume penetration through atmospheric layers. Atm. Env. 19, 1215-1218.

van Ulden A.P. and Holtslag A.A.M. (1985): Estimation of atmospheric boundary layer parameters for diffusion application. J. Clim. Appl. Met. 24, 1196-1207.

Weil J.C. and R.P. Brower (1984): An updated Gaussian plume model for tall stacks. J. Air Poll. Contr. Ass. 34, 818-827.