THE RAMS HYBRID PARTICLE AND CONCENTRATION TRANSPORT MODEL (HYPACT)

1 Introduction

The RAMS HYbrid Particle And Concentration Transport model (HYPACT) is a code developed to simulate the motion of atmospheric tracers under the influence of atmospheric flow, including turbulence. Although the RAMS atmospheric model can perform a similar function with any number of Eulerian tracer fields, HYPACT has certain advantages because of its Lagrangian component. The advantage is greatest near a source region for the tracer when the source is of small scale and unresolvable on the Eulerian grid. A completely Eulerian treatment would necessarily represent the source by a volume no smaller than one grid cell, and would immediately begin diffusing the tracer to the adjacent cells. A Lagrangian approach, on the other hand, is fully capable of representing a source of any size, and of maintaining a concentrated, narrow tracer plume downwind of the source until atmospheric dispersion dictates that the plume should broaden. In contrast, at large distances from a source, where the tracer plume is typically broad and well mixed, representation of the plume by Lagrangian particles can be inefficient due to the large number of particles required to achieve a smooth characterization of the plume concentration, and the Eulerian formulation is preferred. The hybrid Lagrangian and Eulerian approach used in HYPACT represents a tracer by Lagrangian particles near the source region where concentration gradients are large, and converts particles to Eulerian concentrations where appropriate at large distances downwind, thus utilizing the advantages of both schemes.

Although HYPACT can run from meteorological data from any source, including observational and hypothetical fields, it is most often driven by wind and potential temperature fields simulated in the RAMS atmospheric model, and will be described in that capacity here. HYPACT is currently run as a post-processing step, using a time series of datasets previously output from the atmospheric model. In the future, the option will exist to run HYPACT as part of a RAMS meteorological simulation, such that it will utilize simulated atmospheric fields each timestep and may interact with the simulated RAMS fields through parameterized responses to the HYPACT concentration fields.

The Eulerian component of HYPACT is primarily a subset of the RAMS code which performs the same advection, diffusion, and updating of scalar fields as done in RAMS. If HYPACT is run as a post-processing step, that code is executed apart from the main RAMS code. However, in the planned interactive type of run where HYPACT is run as an integral part of a RAMS simulation, the scalar prognosis will be performed by the standard RAMS code. In such cases, the Eulerian concentration field(s) may influence the meteorology, as for example, radiatively in the case of a dense smoke plume. Source and sink terms may include surface deposition, evaporation and condensation, precipitation scavenging, chemical interactions, and of course the source by conversion from Lagrangian particles. Description of the RAMS atmospheric model, including its treatment of scalars, have appeared in many journal articles and reports.

The Lagrangian part of HYPACT is by contrast the major component, and will be described here in considerable detail. Its basic function is to define a release configuration of one or more particle sources as a function of up to 3 spatial dimensions and time, to advect the particles under the influence of local atmospheric model resolved and subgrid turbulent winds, and optionally to add or subtract numbers of particles, or attributes of particles such as mass, in order to represent any particle-to-particle interactions, deposition, conversion to Eulerian concentration, etc. This latter conversion is performed in regions of the domain where (1) accurate concentrations can be computed from a sufficiently dense particle distribution, and (2) the particle plume is well resolved on the local Eulerian grid. Achievement of both conditions may require a large number of particles to be released.

The atmospheric model fields are determined at each particle location by interpolation, in space alone where HYPACT runs as part of an atmospheric model simulation, and additionally in time from a more temporally sparse set of model output fields. In order to achieve optimal efficiency in the spatial interpolation, and in addition to utilize the highest resolution atmospheric data locally available in the RAMS multiple nested grid configuration, a special HYPACT grid, called the "h-grid", is defined which has everywhere a resolution equal to or greater than the maximum local atmospheric grid resolution. The h-grid has a single monotonic grid cell indexing system in all 3 direction, so that particle locations can be easily defined (in grid cell index space), and atmospheric fields, which are assigned and interpolated to the h-grid from the atmospheric model are easily interpolated to each particle location. Index arrays are defined on the h-grid which contain mapping information relating location on the h-grid to location within, and the number of, the finest local RAMS grid. This facilitates locating particles on a complex system of nested atmospheric model grids, each of which has its own separate indexing system. Thus, the particles are freed from requiring direct knowledge of the current finest grid on which there are located.

Pollution dispersion in the Lagrangian part of the HYPACT is simulated by tracking a large set of particles. Subsequent positions of each particle are computed from the relations

$$X(t+\Delta t) = X(t) + (u+u')\Delta t \quad (1)$$

$$Y(t+\Delta t) = Y(t) + (v+v')\Delta t \quad (2)$$

$$Z(t+\Delta t) = Z(t) + (w+w'+w_p)\Delta t \quad (3)$$

where u, v and w are the resolvable scale wind components, which are obtained directly from the mesoscale meteorological model, u', v', and w' are the turbulent wind components, and w_p is the vertical velocity resulting from external forces.

Each particle represents a discrete element of pollution mass, m_p, which can vary in time due to

- deposition processes
- chemical or radiological decay
- evaporation if droplets are considered.

If the dispersion of heavy particles or droplets is considered, each model particle represents a subset of real particles with the same properties, e.g., density or diameter. Some aspects of physical parameterizations developed for the HYPACT are discussed in (Uliasz, 1993) from the point of view of mesoscale applications.

2 Dispersion of a passive tracer

The turbulent velocity components of particles representing a passive tracer are derived from a first order Markov chain scheme under the following assumptions which are consistent with the second-order turbulence closure applied in the mesoscale meteorological model:

- particles are assumed to take up the same distribution of velocities as the air;
- turbulence is nonhomogeneous in the vertical but is locally homogeneous in the horizontal;
- turbulence is Gaussian: turbulent components of wind have normal distributions with zero mean values and variances σ_u^2, σ_v^2 and σ_w^2 (the second order-closure scheme does not provide information on higher order moments);
- particles are assumed to move independently (one-particle model), so the results are applicable only to ensemble-averaged diffusion.

The Markov chain scheme is defined by

$$u'(t) = R_u u'(t-\Delta t) + (1-R_u^2) r_u \quad (4)$$

$$v'(t) = R_v v'(t-\Delta t) + (1-R_v^2) r_v \quad (5)$$

$$w'(t) = R_w w'(t-\Delta t) + (1-R_w^2) r_w \quad (6)$$

where r_u, r_v, and r_w are purely random uncorrelated components, σ_u^2, σ_v^2, and σ_w^2 are variances of wind velocity components, R_u, R_v and R_w are Lagrangian autocorrelations of wind velocity components for lag time Δt assumed to be simple exponential functions:

$$R_u(\Delta t) = \frac{\overline{u'(t)u'(t-\Delta t)}}{\sigma_u^2} = \exp\left(-\frac{\Delta t}{T_{Lu}}\right) \quad (7)$$

$$R_v(\Delta t) = \frac{\overline{v'(t)v'(t-\Delta t)}}{\sigma_v^2} = \exp\left(-\frac{\Delta t}{T_{Lv}}\right) \quad (8)$$

$$R_w(\Delta t) = \frac{\overline{w'(t)w'(t-\Delta t)}}{\sigma_w^2} = \exp\left(-\frac{\Delta t}{T_{Lw}}\right) \quad (9)$$

and T_{Lu}, T_{Lv} and T_{Lw} are Lagrangian integral time scales.

If σ_w^2 is a function of height, the random component r_w of the vertical velocity w' (6) must have a nonzero mean value

$$\overline{r_w} = w_d = [1 - R_w(\Delta t)] T_{Lw} \frac{\partial \sigma_w^2}{\partial z} \tag{10}$$

to prevent spurious accumulation of particles in regions of low turbulence (Legg and Raupach, 1982; Thomson, 1984). w_d is called the drift velocity. A Gaussian distribution of vertical wind fluctuations does not imply a Gaussian r_w in inhomogeneous turbulence. The use of a Gaussian r_w is permissable whenever

$$\left| \frac{T_{Lw}}{\sigma_w} \frac{\partial \sigma_w^2}{\partial z} \right| \ll 1, \tag{11}$$

i.e., when fractional change in σ_w^2 over the length $\sigma_w T_{Lw}$, a measure of the inhomogeneity, is small (Thomson, 1984). The fulfillment of this condition is assumed in the present model. Distributions of r_u and r_v are Gaussian with zero mean values. The variances of r_u, r_v and r_w are equal to the variances of wind velocity components, σ_u^2, σ_v^2, and σ_w^2, respectively. The random fluctuations are generated at each time step as

$$r_u = \sigma_u \eta_u, \qquad r_v = \sigma_v \eta_v, \qquad r_w = \sigma_w \eta_w + w_d \tag{12}$$

where η_u, η_v and η_w are random numbers picked up from a standard Gaussian distribution.

The following meteorological variables are required as an input by the above formulated Lagrangian part of the HYPACT:

- u, v, w - resolvable wind velocity components;
- σ_u^2, σ_v^2, σ_w^2 - variances of wind components;
- T_{Lu}, T_{Lv}, T_{Lw} - Lagrangian time scales.

3 Turbulence parameterization

The turbulent variables required by the model are calculated diagnostically from available meteorological information using a simplified second-order closure technique developed by Mellor and Yamada (1974, 1982):

- A so-called level 2.5 scheme modified for a case of growing turbulence (Helfand and Labraga, 1988) is applied if the fields of wind, u, v, potential temperature, ϑ, and turbulent kinetic energy, e, are provided by the meteorological model which uses the same turbulence parameterization. This scheme is based on the prognostic equation for the turbulent kinetic energy solved in the meteorological model.

- A simpler level 2.0 scheme is applied if only wind and potential temperature fields are available from the meteorological model or observations. This scheme assumes an exact balance between production of turbulent energy and dissipation.

The wind and temperature enter these calculations in the form of nondimensional vertical gradients:

$$G_u = \frac{l}{\sqrt{2e}}\frac{\partial u}{\partial z}, \qquad G_v = \frac{l}{\sqrt{2e}}\frac{\partial v}{\partial z}, \qquad G_m = G_u^2 + G_v^2, \qquad G_h = -\beta\frac{l^2}{2e}\frac{\partial \vartheta}{\partial z} \tag{13}$$

The turbulent length scale, l, is assumed after Mellor and Yamada (1982)

$$l = \frac{\kappa\,(z+z_0)}{1+\kappa\,(z+z_0)\,/l_\infty}, \qquad l_\infty = 0.1\frac{\int_0^H z\sqrt{e}dz}{\int_0^H \sqrt{e}dz} \tag{14}$$

with an upper limit for l in stable conditions proposed by André et al. (1978):

$$l \le 0.75\left[\frac{2e}{\beta\partial\vartheta/\partial z}\right]^{1/2} \tag{15}$$

The above condition implies the constraint: $G_h \ge -0.75^2$.

In both options, the variances of wind components, and Lagrangian time scales are expressed in the same form:

$$\left\{\begin{array}{c}\sigma_u^2\\ \sigma_v^2\\ \sigma_w^2\end{array}\right\} = 2e\left[\frac{1}{3} - 2A_1(S_mG_m + S_hG_h) + 6A_1\left\{\begin{array}{c}S_mG_u^2\\ S_mG_v^2\\ S_hG_h\end{array}\right\}\right] \tag{16}$$

$$T_{Lu} = c_t\frac{l}{\sigma_u}, \quad T_{Lv} = c_t\frac{l}{\sigma_v}, \quad T_{Lw} = c_t\frac{l}{\sigma_w} \tag{17}$$

The constant c_t is assumed to be 2 in order to obtain a good agreement between Lagrangian time scales simulated in the model and given by empirical formulae (Hanna, 1982) for an idealized case of horizontally homogeneous atmospheric boundary layer.

In the level 2.5 scheme, the functions S_m, and S_h (nondimensional eddy diffusivities), depend on nondimensional gradients of wind and potential temperature, G_m, and G_h:

$$S_m = \frac{A_1\left\{1-3C_1-3A_2\left[B_2\left(1-3C_1\right)-12A_1C_1-3A_2\right]G_h\right\}}{1-3A_2\left(7A_1+B_2\right)G_h+27A_1A_2^2\left(4A_1+B_2\right)G_h^2+6A_1^2\left[1-3A_2\left(B_2-3A_2\right)G_h\right]G_m} \tag{18}$$

$$S_h = A_2\frac{1-6A_1S_mG_m}{1-3A_2\left(4A_1+B_2\right)G_h} \tag{19}$$

Empirical constants are assigned values following Mellor and Yamada (1982):

$$(A_1, A_2, B_1, B_2, C_1, S_e, a_\epsilon) = (0.92, 0.74, 16.6, 10.1, 0.08, 0.20, 2^{3/2}/16.6) \tag{20}$$

The solution of the level 2 model can be derived from the level 2.5 expressions under assumption of the balance between production of turbulent energy and its dissipation which leads to the following diagnostic equation for turbulent kinetic energy:

$$(e)_r = \frac{B_1}{2} l^2 \left[(S_m)_r \left(\left(\frac{\partial u}{\partial z}\right)^2 \left(\frac{\partial v}{\partial z}\right)^2 \right) - (S_h)_r \beta \frac{\partial \vartheta}{\partial z} \right] \tag{21}$$

All variables obtained from the level 2 scheme are denoted by $()_r$ signifying equilibrium values.

The functions $(S_m)_r$ and $(S_m)_r$ take the form (e.g., Yamada, 1975) :

$$(S_h)_r = C_h \frac{R_{fc} - R_f}{1 - R_f} \tag{22}$$

$$(S_m)_r = C_m \frac{R_{f1} - R_f}{R_{f2} - R_f} S_{h,r} \tag{23}$$

They depend on only one parameter, the flux Richardson number:

$$R_f = -\frac{S_h G_h}{S_m G_m} \tag{24}$$

The critical flux Richardson number, R_{fc}, and R_{f1}, R_{f2}, C_h, C_m are numerical constants which are determined explicitly from the previously cited empirical constants:

$$R_{fc} = E_1/E_2, \qquad R_{f1} = E_3/E_4, \qquad R_{f2} = E_1/E_5 \tag{25}$$

$$C_h = \frac{A_2}{B_1} E_2, \qquad C_m = \frac{A_1}{A_2}\frac{E_4}{E_5} \tag{26}$$

where

$$\begin{aligned} E_1 &= B_1 - 6A_1 \\ E_2 &= 12A_1 + B_1 + 3B_2 \\ E_3 &= B_1(1 - 3C_1) - 6A_1 \\ E_4 &= B_1(1 - 3C_1) + 12A_1 + 9A_2 \\ E_5 &= B_1 + 3A_1 + 3B_2 \end{aligned}$$

It may be shown that R_f is related to the gradient Richardson number

$$R_i = \frac{\beta \frac{\partial \vartheta}{\partial z}}{\left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2} = -\frac{G_h}{G_m} \tag{27}$$

by a quadratic equation from which the solution may be expressed as

$$R_f = \frac{1}{2}\frac{A_2}{A_1}\frac{E_5}{E_4} \left\{ R_i + \frac{A_1}{A_2}\frac{E_3}{E_5} - \left[R_i^2 + 2\frac{A_1}{A_2}\frac{E_3E_5 - 2E_1E_4}{E_5^2} R_i + \left(\frac{A_1 E_3}{A_2 E_5}\right)^2 \right]^{1/2} \right\} \tag{28}$$

This relation allows one to determine the functions $(S_m)_r$ and $(S_h)_r$ diagnostically.

In some circumstances, use of the level 2.5 closure can lead to non-physical results. The physical realizability of this closure scheme is discussed by Mellor and Yamada (1982), Hassid and Galperin (1983), Flatau (1985), Galperin et al. (1988) and Helfand and Labraga (1988). In the present model, the modification of the level 2.5 closure method proposed by Helfand and Labraga (1988) is implemented. They suggest the following modification of the nondimensional eddy diffusivities (18-19), wind velocity variances (16) in the case of growing turbulence when $e < (e)_r$:

$$S_m = \sqrt{e/e_r}(S_m)_r, \qquad S_h = \sqrt{e/e_r}(S_h)_r \tag{29}$$

$$\sigma_u^2 = e/e_r(\sigma_u^2)_r, \qquad \sigma_v^2 = e/e_r(\sigma_v^2)_r, \qquad \sigma_w^2 = e/e_r(\sigma_w^2)_r \tag{30}$$

where the equilibrium values $(\ )_r$ are obtained from the level 2 closure. The above modification of the level 2.5 scheme is used for growing turbulence only. There is no need to introduce any modifications into the original level 2.5 scheme for the case of decaying turbulence, when $e > e_r$.

The turbulent variables can be calculated diagnostically from the known wind and temperature fields using the level 2 scheme by the following iterative algorithm:

1. The turbulent length scale, l, is specified as a simple function of height prior to iterations.

2. The gradient and flux Richardson numbers, R_i and R_f, are evaluated from (27) and (28).

3. The equilibrium values of nondimensional eddy diffusivities, $(S_h)_r$ and $(S_m)_r$ are calculated from (22) and (23).

4. Turbulent kinetic energy $(e)_r$ is next calculated (21).

5. The turbulent length scale, l, is recalculated as a function of turbulent kinetic energy (14).

6. If the convergence condition is not satisfied the iteration process returns to step 3.

7. Finally, the wind velocity variances, and Lagrangian times scales are calculated from (16), and (17), where the equilibrium turbulent energy $(e)_r$ is used.

The algorithm used to calculate the turbulent variables from the known wind, temperature and turbulent energy field with the aid of the modified level 2.5 scheme can be summarized as follows:

1. The turbulent length scale, l, is calculated as a function of turbulent kinetic energy (14).

2. The nondimensional vertical gradients of wind and potential temperature, G_u, G_v, G_m, G_h, are evaluated (13).

3. The gradient and flux Richardson numbers, R_i and R_f, are evaluated from (27) and (28).

4. The equilibrium values of nondimensional eddy diffusivities, $(S_h)_r$ and $(S_m)_r$ are calculated from (22) and (23).

5. The equilibrium turbulent kinetic energy $(e)_r$ is calculated from (21).

6. For the decaying turbulence when $e > (e)_r$, the nondimensional eddy diffusivities, S_m, and S_h, are calculated from (18-19), and finally the wind velocity variances, and Lagrangian times scales are determined from (16), and (17).

7. For the growing turbulence when $e > (e)_r$, the nondimensional eddy diffusivities, S_m, and S_h, are calculated from (29), and finally the wind velocity variances, and Lagrangian times scales are determined from (16), and (17) where the equilibrium turbulent energy $(e)_r$ is used.

4 Chemical transformation and radiological decay

Chemical or radiological decay of a pollutant is taken into account by decreasing the mass of each particle at each time step:

$$m_p(t + \Delta t) = m_p(t) \exp(-\alpha \Delta t) \tag{31}$$

where $\alpha = \ln 2/\tau_{1/2}$ is the rate of transformation, and $\tau_{1/2}$ is the half life time. Transformation rates may vary with time and space.

Linear chemical transformations can be also easily included in the model. In this case, the particle represents multiple chemical species. Let us consider a case of two species with concentrations, c_1 and c_2 respectively, which transformations are given by a simple chemistry mechanism (e.g., SO_2 $\rightarrow$ particulate sulfate):

$$\frac{dc_1}{dt} = -\alpha_1 c_1, \qquad \frac{dc_2}{dt} = \alpha_1 c_1 - \alpha_2 c_2 \tag{32}$$

With the aid of the analytical solution of the above equation set at a given time step the mass of each particle is expressed as a sum of masses of two species $m_p = m_{p1} + m_{p2}$ which vary in time:

$$\begin{aligned} m_{p1}(t + \Delta t) &= m_{p1}(t) \exp(-\alpha_1 \Delta t) \\ m_{p2}(t + \Delta t) &= m_{p1}(t) \frac{\alpha_1}{\alpha_1 - \alpha_2} [\exp(-\alpha_2 \Delta t) - \exp(-\alpha_1 \Delta t)] + m_{p2}(t) \exp(-\alpha_2 \Delta t) \end{aligned} \tag{33}$$

The transformation coefficients, α_1 and α_2, may depend on local meteorological variables, e.g., temperature, humidity, solar radiation. A proper treatment of nonlinear chemistry may be very difficult or impossible within a Lagrangian framework (Zannetti, 1992).

5 Dispersion of heavy particles

Dispersion of gaseous species or fine particles with diameter $D_p \leq 1\ \mu m$ can be represented by the dispersion of the passive tracer as described in section 2. For larger particles the assumption that the turbulence characteristics of the tracer fluid or particle are similar to those of the surrounding fluid is no longer valid. The effect of gravitational forces on the mean particle motion should be included in the dispersion model by the addition of the mean particle settling velocity, v_t in equations (3). The particle attains its terminal settling velocity $v_t = T_p g$ for $t >> T_p$. The relaxation time, T_p, which is extremely short, can be determined for spherical aerosol particles as

$$T_p = \frac{D_p^2}{18\nu f(Re)} \frac{\rho_p}{\rho} \tag{34}$$

where ρ_p and ρ - densities of particle and air, g - gravitational acceleration, ν - kinematic molecular viscosity. The empirical correction factor $f(Re)$ is introduced to account for the drag force acting on the particle over entire range of Reynolds number beyond the Stokes law region (Seinfeld, 1986):

$$f(Re) = \begin{cases} 1 & Re < 0.1 \quad (Stokes\ \ law) \\ 1 + 0.188Re + 0.0563Re^2 \ln(2Re) & 0.1 < Re < 2 \\ 1 + 0.15Re^{0.687} & 2 < Re < 500 \\ 0.0183Re & 500 < Re < 2 \cdot 10^5 \end{cases} \tag{35}$$

where $Re = D_p v_t/\nu$ is the Reynolds number, and ν is the kinematic viscosity of air.

Since the dynamic response of a heavy particle to turbulent flow is different from that of a fluid element, two additional effects must be taken into account (Yudine, 1959; Csanady, 1963):

- Inertia effect. A particle with inertia does not respond to all frequencies of atmospheric turbulence but only to those with a period much greater than its relaxation time, T_p. This selective response means that there will always be some relative motion between the particle and the surrounding air. The effect of inertia can be neglected for small particles up to 400-500 μm diameter.

- Crossing trajectories effect. As a consequence that a particle has a mean downward velocity the particle does not remain within a particular turbulent eddy but continuously drops out from the influence of eddies. The result is that a particle with a large enough terminal velocity crosses the trajectories of many eddies and loses correlation more rapidly that would a passive tracer. The crossing trajectories effect is important down to even quite small diameters.

The dispersion of heavy particles is simulated under the following assumptions:

- Particles have density, ρ_p, much greater than density of air ($\rho_p >> \rho$).
- Particles are spherical with diameter D_p. Non-spherical particles are represented by equivalent spheres of equal settling velocity.
- Since very fine particles are not considered, the non-continuum effects (Cunningham correction factor) on particle settling velocity are neglected.

Several authors proposed modifications to the particle dispersion model which take into account these two effects (Hunt and Nalpanis, 1985; Walklate, 1986; Walklate, 1987; Hashem and Parkin, 1991; Sawford and Guest, 1991). The inertia effect reduces the particle variance σ_{pi}^2 and increases the particle autocorrelation $R_{pi}(\Delta t)$ in comparison to the corresponding values of air velocity σ_i^2 and $R_i(\Delta t)$ while the cross trajectory effect reduces the particle autocorrelation only. It means that heavy particles may disperse faster than fluid elements if the inertia effect controls the dispersion. On the other hand, if the inertia effect is negligible, the dispersion of heavy particles is less than the dispersion of a passive tracer following fluid elements. A comprehensive analysis of heavy particle dispersion was recently presented by Wang and Stock (1993). Following Walklate (1986, 1987) the reduction of the particle variance σ_{pi}^2 and the particle autocorrelation $R_{pi}(\Delta t)$ due to the inertia effect can be parameterized as

$$\sigma_{pi}^2 = \sigma_i^2 \frac{1}{1 + C_1 T_p / T_{Li}} \tag{36}$$

$$R_{pi}(\Delta t) = \frac{R_i(\Delta t) - C_1 T_p / T_{Li} \exp(-\Delta t / C_1 T_p)}{1 - C_1 T_p / T_{Li}} \tag{37}$$

where $i = u, v, w$, and the value of the constant recommended by Walklate (1987) is $C_1 \simeq 4$. For small particles when $CT_p/T_{Li} \approx 0$, the inertia effect may be neglected. The particle autocorrelation in the vertical, $R_{pw}(\Delta t)$, must be further corrected due to the crossing trajectory effect

$$R_{pw}(\Delta t) = \frac{R_i(\Delta t) - C_1 T_p / T_{Li} \exp(-\Delta t / C_1 T_p)}{1 - CT_p / T_{Li}} \exp\left(-\frac{\Delta t}{T_{Lw}} \frac{v_t}{\sigma_w C_2}\right) \tag{38}$$

where C_2 is a constant in the range 1 to 2. If the inertia effect can be neglected, the above expression reduces to

$$R_{pw}(\Delta t) = \exp\left\{-\frac{\Delta t}{T_{Lw}}\left(1 + \frac{v_t}{\sigma_w C_2}\right)\right\} \tag{39}$$

6 Dry deposition

The interaction of the particle with the ground surface is parameterized following Boughton et al.(1987). Above a certain height h, the probability of particle deposition is negligible. If the particle comes below the height $z < h$, the probability that the particle is absorbed during time

Δt is computed from the transition probability density given by Monin (1959)

$$\begin{aligned} P(z,\Delta t) &= \phi\left[-\frac{z-v_t\Delta t}{\sqrt{2K\Delta t}}\right] + \frac{v_d}{v_d-v_t}\exp\left(\frac{v_t z}{K}\right)\phi\left[-\frac{z-v_t\Delta t}{\sqrt{2K\Delta t}}\right] - \\ & \frac{2v_d-v_t}{v_d-v_t}\exp\left[\frac{v_d z}{K}+\frac{v_d(v_d-v_t)\Delta t}{K}\right]\phi\left[-\frac{z+(2v_d-v_t)\Delta t}{\sqrt{2K\Delta t}}\right] \end{aligned} \quad (40)$$

where v_d is the deposition velocity, $\phi(x)$ is the standard Gaussian distribution, K is the eddy diffusivity, and z is the height of the particle above the ground surface. For particles with a zero settling velocity, v_t, this equation reduces to:

$$P(z,\Delta t) = 2\left(\phi\left[-\frac{z}{\sqrt{2K\Delta t}}\right] - \exp\left[\frac{v_d(z+v_d\Delta t)}{K}\right]\phi\left[-\frac{z+2v_d\Delta t}{\sqrt{2K\Delta t}}\right]\right) \quad (41)$$

The probability of absorption given by the above equations allows one to simulate a partial deposition of the pollutant, as well as the extreme cases of perfect reflection and perfect absorption. For a later case, the probability $P(z,\Delta t)$ is derived by taking the limit of equation (40) as $v_d \to \infty$. Two treatments of ground-level particles are possible:

- The particle which appears at $z < h$ is first moved as if no boundary were present. Then, if a random number from the uniform distribution on $[0,1]$ is less than $P(z,\Delta z)$, the particle is absorbed. Otherwise, the particle is moved as if the boundary were perfectly reflecting. This option is designed for heavy particles with a non-zero settling velocity.

- The ground-level particle is perfectly reflected from the ground surface and the particle mass is reduced by a fraction equal to the absorption probability $P(z,\Delta t)$. This option is applied for simulations with linear chemistry where each particle represents multiple species which may have different deposition velocities. For each species, the probability P is calculated separately and then a proper mass reduction is applied.

Both options can be used in the case of the passive tracer. Specification of the height h is not critical because the absorption probability falls off very rapidly as the particle moves away from the boundary.

The deposition velocities are computed with the aid of the resistance-model approach (Walcek et al., 1986):

$$v_d = (r_a + r_b + r_c)^{-1} \quad (42)$$

The atmospheric resistance r_a is parameterized using surface layer similarity theory, the boundary resistance r_b is related to molecular transfer across a thin laminar sublayer immediately adjacent to the surface, and the surface resistance r_c is a function of land use and vegetation physiology.

This parameterization of dry deposition in the Lagrangian particle model was compared against prediction of the high resolution K-theory dispersion model. A very good agreement was found for deposition fluxes calculated by the Markov-chain versions of the particle model and the K-theory model. The simplified random-walk versions of the particle model did not perform as well. This is due to the time step used to move particles being too long for a proper treatment of the interaction of particles with the ground surface.

7 Buoyancy phenomena

Several modelers suggested different approaches to simulate buoyant plumes with Lagrangian particle models (Zannetti and Al-Madani, 1984; Cogan, 1985; Gaffen et al., 1987; Shimanuki and Nomura, 1991; Van Dop, 1992; Luhar and Britter, 1992; Anfossi et al., 1993; Hurley and Physick, 1993). The most promising seems to be a model proposed by Van Dop (1992) where the additional stochastic equation describes the buoyancy evolution for each particle. However, even simpler approaches which derive an additional vertical velocity for each particle from an analytical plume rise model may still be acceptable in applications. In our implementation, two options for treatment of buoyant plumes are considered:

- particles are released at an effective stack height, z_{eff};
- particles are released at stack top, z_s, and an additional vertical velocity, $w_p = w_b$, due to buoyancy is applied to each particle until the particle reaches the effective stack height, z_{eff}.

Plume rise calculations are based on an analytical model developed by Netterville (1990) for point emission sources. This model is based on the momentum and buoyancy conservation equations written as:

$$\frac{dM}{dt} = F - fM, \qquad \frac{dF}{dt} = -N^2 M - fM \tag{43}$$

where $M = UR^2 w_b$ and $F = UR^2 g(T_s - T_a)/T_a$ are the downwind fluxes of vertical momentum and buoyancy, U is wind velocity, T_s and T_a are temperature of exit gases and ambient atmosphere, R is a plume radius, $f = T_{Lw}^{-1}$ is a frequency of atmospheric turbulence, and N is the Brunt-Väisälä frequency defined as $N^2 = g/T_a\, d\vartheta/dz$. The above equations may be solved analytically for atmospheric layers with constant U, N^2, and f in order to obtain height of the plume centerline above the stack, $Z(t)$, and its vertical velocity, $w_b(t)$, in each layer. For the i-th layer starting at height Z_i above the stack the following expressions for plume momentum, buoyancy and height can be obtained:
stable atmosphere ($N^2 > 0$)

$$M(\Delta t) = \exp(f\Delta t)\left[M_i \cos(\sqrt{s}\Delta t) + \frac{F_i}{\sqrt{s}}\sin(\sqrt{s}\Delta t)\right] \tag{44}$$

$$F(\Delta t) = \exp(f\Delta t)\left[F_i \cos(\sqrt{s}\Delta t) - M_i\sqrt{s}\sin(\sqrt{s}\Delta t)\right] \tag{45}$$

$$Z(\Delta t) = \left\{\frac{3}{\beta^2 U(f^2+N^2)}\left[F_0 + fM_0 + \left\{NM_0\left[\sin(N\Delta t) - \frac{f}{N}\cos(N\Delta t)\right]\right.\right.\right.$$

$$
\begin{aligned}
&-F_0\left[\cos(N\Delta t)+\frac{f}{N}\sin(N\Delta t)\right]\Bigg\}\exp(-f\Delta t)\Bigg]\\
&+\left(\frac{R_0}{\beta}\right)^3\Bigg\}^{1/3}-\frac{R_0}{\beta}
\end{aligned}
\tag{46}
$$

neutral atmosphere ($N^2 = 0$)

$$F(\Delta t) = \exp(f\Delta t)F_i \tag{47}$$

$$M(\Delta t) = \exp(f\Delta t)(M_i + F_i\Delta t) \tag{48}$$

$$
\begin{aligned}
Z(\Delta t) = &\left\{\frac{3}{\beta^2 U f^2}\left[F_0 + fM_0 - \{fM_0 + F_0(f\Delta t+1)\}\exp(-f\Delta t)\right] + \left(\frac{R_0}{\beta}\right)^3\right\}^{1/3}\\
&-\frac{R_0}{\beta}
\end{aligned}
\tag{49}
$$

unstable atmosphere ($N^2 < 0$)

$$
\begin{aligned}
M(\Delta t) = &\frac{1}{2}\Bigg[(M_i + \frac{F_i}{\sqrt{-s}})\exp((\sqrt{-s}-f)\Delta t)\\
&+(M_i - \frac{F_i}{\sqrt{-s}})\exp(-(\sqrt{-s}+f)\Delta t)\Bigg]
\end{aligned}
\tag{50}
$$

$$
\begin{aligned}
F(\Delta t) = &\frac{1}{2}\Big[(M_i\sqrt{-s}+F_i)\exp((\sqrt{-s}-f)\Delta t)\\
&-(M_i\sqrt{-s}-F_i)\exp(-(\sqrt{-s}+f)\Delta t)\Big]
\end{aligned}
\tag{51}
$$

$$
\begin{aligned}
Z(\Delta t) = &\Bigg\{\frac{3}{\beta^2 U(f^2+N^2)}\Bigg[F_0 + fM_0 - \Bigg\{NM_0\left[\sinh(N\Delta t)+\frac{f}{N}\cosh(N\Delta t)\right]\\
&+F_0\left[\cosh(N\Delta t)+\frac{f}{N}\sinh(N\Delta t)\right]\Bigg\}\exp(-f\Delta t)\Bigg]\\
&+\left(\frac{R_0}{\beta}\right)^3\Bigg\}^{1/3}-\frac{R_0}{\beta}
\end{aligned}
\tag{52}
$$

where $N = \sqrt{|N^2|}$, $\Delta t = t - t_i$, index i refers to values at height z_i.

The plume radius, R, is given by

$$R = R_i + \beta(z - z_i) \tag{53}$$

and the plume vertical velocity w_b is calculated from the momentum flux M. The downwind fluxes of source momentum and buoyancy are, respectively,

$$M_s = UR_s^2 W_s, \qquad F_s = UR_s^2 g(T_s - T_a)/T_a \tag{54}$$

where R_s, W_s, T_s are the stack diameter, exit velocity and temperature, and U and T_a are wind speed and atmospheric temperature at stack top. The initial values of plume momentum, buoyancy and radius after the plume has bent over are given by (Djurfors, 1983)

$$M_0 = M_s\frac{W_s}{U}\frac{T_a}{T_s}, \qquad F_0 = F_s, \qquad R_0 = R_s\left(2\frac{W_S}{U}\frac{T_a}{T_s}\right)^{1/2} \tag{55}$$

The model takes into account the vertical structure of the atmosphere (vertical changes of wind, thermal stratification and turbulence) but still assumes that all meteorological fields are horizontally homogeneous in the the area where plume rise takes place. The advantage of Netterville's model is that the plume rise is terminated by the effect of ambient turbulence in neutral or unstable conditions. Vertical profiles of wind, potential temperature and Lagrangian time scale, T_{Lw}, required by this algorithm are provided by the meteorological model.

The effective stack height and/or plume vertical velocity are calculated at each time when new meteorological fields are available. Then, the buoyant vertical velocity component can be picked from the calculated table at each time step of particle motion. Optionally, it is possible to take into account the effect of the plume internal turbulence following Anfossi et al.(1993). A spectrum of z_{eff} and/or w_b profiles is calculated for a range of F values. An initial buoyancy flux is assigned randomly for each released particle from a normal distribution with mean value F_s calculated from provided stack parameters and the standard deviation equal to $F/3$. At each time step the buoyant vertical velocity component is selected for each particle from a precomputed set of values according to its initial buoyancy and current height. If the first option of plume rise calculation is selected, the particle is simply released at the height, z_{eff}, corresponding to its initial buoyancy.

8 Concentration calculations

The initial mass of the i-th particle at release time is given by

$$m_{pi} = \begin{cases} \Delta t Q / r_p & for\ continuous\ releases \\ M / r_p & for\ instantaneous\ releases \end{cases} \tag{56}$$

where Q is the emission rate for continuous releases, and M is the total mass of pollutant for instantaneous releases. In the general case, when linear chemical reactions and removal processes are considered, the particle mass m_{pi} can vary in time. The particle release rate r_p specifies the number of particles n_p released per time step Δt. If r_p is set to a value $1/n_p$ then release of a single particle will be made every n_p time steps. Initial positions of particles are selected randomly or at prescribed nodal points within a box determined by location of the source center and three source dimensions. It allows one to simulate volume, area, line and point sources by a proper definition of dimensions of the emission box.

The pollution concentration, c, at a given time and location may be determined by counting the number of particles in an imaginary sampling volume centered at (x,y,z):

$$c(x, y, z, t) = \frac{1}{\Delta x_s \Delta y_s \Delta z_s} \sum_{i=1}^{N} m_{pi} I \tag{57}$$

where

$$I = \begin{cases} 1 & for \ |X_i - x| < \Delta x_s/2 \ and \ |Y_i - y| < \Delta y_s/2 \ and \ |Z_i - z| < \Delta z_s/2 \\ 0 & otherwise \end{cases},$$

and m_{pi}, X_i, Y_i, Z_i are the mass and coordinates of the i-th particle at time t. The computed concentrations depend on the size of the sampling volume $\Delta x_s \Delta y_s \Delta z_s$ and on the number of particles N used in the computations. Confidence in this statistical estimate increases with the increase of a number of particles found in the sampling volume and can be achieved by increasing N or by expanding the sampling volume dimensions. However, an increase in N results in a growth of computer time, while an increase of Δx_s, Δy_s, or Δz_s reduces the resolution of the dispersion model. To obtain a smooth and statistically steady concentration field it is usually necessary to release a large number of particles on the order of several thousands. In a rigorous concentration calculation, the contribution of each particle mass should be weighted by the total time spent by the particle inside the sampling volume during each time step (Lamb et al., 1979). However, this requirement seems to be unnecessary in most of applications where sizes of sampling volumes are usually much larger than distances traveled by the particle in one time step.

Computational efficiency of the particle model can be significantly improved by application of a kernel density estimator to calculate the concentration field from particle locations (Lorimer, 1986; Boughton et al., 1987; Yamada and Bunker, 1988; Grossmann, 1989; Uliasz, 1990; Zannetti, 1992). The kernel method requires no imaginary sampling volumes and produces a smooth concentration distribution with a much smaller number of particles. The concentration at a given point is calculated as the sum of contributions from all particles taking into account a reflection of particles from the ground surface:

$$c(x,y,z) = \sum_{i=1}^{N} \frac{m_{pi}}{h_{xi} h_{yi} h_{zi}} \left[K(r_x, r_y, r_z) + K(r_x, r_y, r_z') \right] \tag{58}$$

where the kernel K satisfies the condition

$$\frac{1}{h_{xi} h_{yi} h_{zi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} K dx dy dz = 1 \tag{59}$$

and $r_x = (X_i - x)/h_{xi}$, $r_y = (Y_i - y)/h_{yi}$, $r_z = (Z_i - z)/h_{zi}$, $r_z' = (Z_i + z)/h_{zi}$. The parameters h_{xi}, h_{yi}, h_{zi} are the bandwidths which determine the degree of smoothing in each coordinate direction. The bandwidths should not be kept constant, as is done in many applications, but they should be particle dependent and change in relation to a natural length scale. Various functional forms can be used for the kernel K. The concentration estimations are not very sensitive to the functional form of the kernel. However, they depend fairly critically on the bandwidths.

Yamada and Bunker (1988) used a Gaussian kernel with particle dependent bandwidths related to σ_x, σ_y, and σ_z calculated for each particle with the aid of Taylor diffusion theory.

However, this choice of the bandwidths leads to oversmoothing of concentration fields and values of these bandwidths must be limited, especially, in unstable conditions. A more computationally efficient three-dimensional parabolic kernel was discussed by Grossmann (1989). The application of the kernel density estimation to the Lagrangian particle model presented by Lorimer (1986) and Grossmann (1989) is a purely mathematical technique for estimating a probability density (concentration) from a sample (particle positions). It can not be interpreted physically in the context of the atmospheric dispersion problem. The bandwidths are dependent on the number of particles and are related to the standard deviations of the particle distribution. The same bandwidths are applied for all particles at a given time. The proposed method for selecting bandwidths is derived under the assumption that the concentration has a trivariate Gaussian distribution. It seriously limits applications of their approach in practice.

Since the problem of bandwidth selection for a kernel technique is not generally solved, a very simple uniform kernel is implemented in the HYPACT:

$$K(r_x, r_y, r_z) = \frac{1}{8} I_x I_y I_z, \qquad I_\alpha = \begin{cases} 1 & for\ \ r_\alpha^2 < 1 \\ 0 & otherwise \end{cases}, \qquad \alpha = x, y, z \tag{60}$$

The bandwidths are constant and proportional to the increments of the grid used in the calculations: $h_x = \alpha \Delta x$, $h_y = \alpha \Delta y$, $h_z = \alpha \Delta z$. Typically, $\alpha = 0.5$ is selected. Larger bandwidths can be prescribed if stronger smoothing of concentration field is desired. A given particle can contribute to the concentration in several cells of the concentration grid. For $h_x << \Delta x$, $h_y << \Delta y$, and $h_z << \Delta z$, the uniform kernel is practically equivalent to counting particles in a grid cell (57).

List of Symbols

c	pollution concentration (gm^{-3})
c_p	specific heat at constant pressure per unit mass of dry air ($1006 Jkg^{-1}K^{-1}$)
e	turbulent kinetic energy (m^2s^{-2})
e_r	equillibrium turbulent kinetic energy (m^2s^{-2})
f	Coriolis parameter (s^{-1})
F	buoyancy flux of source (m^4s^{-3})
M	momentum flux (m^4s^{-2})
g	gravitational acceleration ($9.81 ms^{-1}$)
h_x, h_y, h_z	bandwidths of kernel density estimator (m)
K	kernel density estimator
K_m, K_h, K_e	eddy diffusivities for momentum, heat (moisture), and turbulent energy (m^2s^{-1})
l	turbulent length scale (m)
L	Monin-Obukhov length scale (m)
m_p	mass of particle (g)
n_p	number of particles released per time step (-)
N	number of particles ($-$)
p	pressure (hPa)
q	specific humidity ($-$)
$q_{sat}(T)$	saturation specific humidity at a given temperature ($-$)
Q	emission source term ($kgs^{-1}m^{-3}$)
r_m	aerodynamic resistance for momentum (sm^{-1})
r_h	aerodynamic resistance for heat and moisture (sm^{-1})
Re	Reynolds number ($-$)
R_f	flux Richardson number ($-$)
R_i	gradient Richardson number ($-$)
R_u, R_v, R_w	Lagrangian velocity autocorrelation functions ($-$)
S_m, S_h	nondimensional eddy diffusivities for momentum and heat ($-$)
t	time (s)
T	temperature (K)
T_{Lu}, T_{Lv}, T_{Lw}	Lagrangian integral time scales (s)
T_p	particle relaxation time (s)
u, v, w	resolvable scale wind velocity components (ms^{-1})
u', v', w'	turbulent wind velocity components (ms^{-1})
u_*	friction velocity (ms^{-1})
v_d	depositon velocity for pollution (ms^{-1})
v_t	terminal settling velocity for heavy particles or droplets (ms^{-1})
V	volume flux $\div\pi$ (m^3s^{-1})

w_b	vertical velocity of particles resulting due to buoyancy (ms^{-1})
w_p	vertical velocity of particles resulting from external forces (ms^{-1})
x, y, z	terrain-following coordinates (m)
z_0	roughness length (m)
z_g	terrain height (m)
$\beta = g/\Theta_a$	buoyancy parameter ($ms^{-2}K^{-1}$)
Δt	time step (s)
Δt_p	time step of particle release (s)
$\Delta x_s, \Delta y_s, \Delta z_s$	sizes of sampling volume (m)
$\Delta X, \Delta Y, \Delta Z$	grid steps of computational mesh (m)
ϵ	dissipation of turbulent kinetic energy (m^2s^{-3})
ϑ	potential temperature (K)
ϑ_*	temperature scale (K)
Θ_a	reference potential temperature (K)
κ	von Karman's constant ($\simeq 0.4$)
ν	molecular diffusivity (m^2s^{-1})
ρ	air density ($1.23kgm^{-3}$ at sea level)
$\sigma_u^2, \sigma_v^2, \sigma_w^2$	variances of wind velocity components (m^2s^{-2})

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