10.2 Outline of the Model to Estimate Atmospheric Diffusion

Up to the present, numerical solution solving the differential equation of discussion and the plume and the puff model, both offering an analytical solution are used to estimate the atmosphere diffusion. Furthermore, the particle method in which many particles released and traced in the compute to estimate diffusion is recently developed the computer calculates the value.

10.2.1 Plume and Puff Models

The plume model supposes that the concentration of the smoke diffusion takes a logarithnic profile during a windy condition, and the concentration is calculated by giving plume width. In the atmosphere, the smoke diffuses up and down, left and right floated by wind. Assuming that the distribution of the concentration both in the vertical and horizontal directions takes a logarithnic profile, then the concentration of the smoke can be shown by the Eq. (4).

$$C(x,y,z) = \frac{Q}{2\pi\,\sigma_y \sigma_z U}\ exp\{-\frac{y^2}{2\sigma_y^{\,2}}\}[exp\{-\frac{(z+He)^2}{2\sigma_z^{\,2}}\} + exp\{-\frac{(z-He)^2}{2\sigma_z^{\,2}}\}] \quad \cdots\cdots \quad (4)$$

The symbols for this formula are;

C (x, y, z) : The concentration at the point of downwind of emission source. x, y, z

σ_y, σ_z : Plume width in y and z direction respectively

Q : The emission rate of pollutants per unit of time (m^3/s)

U : Wind velocity (m/s)

He : The height of the plume axis above ground and is called the effective source height (m).

Because z is 0 when considering the concentration at the ground surfaces, the plume formula is simplified as shown in Eq. (5).

$$C(x,y,z) = \frac{Q}{\pi\,\sigma_y \sigma_z U}\ exp\{-\frac{y^2}{2\sigma_y^{\,2}}\}\ exp\{-\frac{He^2}{2\sigma_z^{\,2}}\} \quad \cdots\cdots \quad (5)$$

Eq. (6) gives the ground surface concentration by the puff model which assumes a regular concentration profiles describing diffusion in a calm condition. The puff model is temporarily discontinuous model, assuming smoke is released serially for same time duration.

$$C(x,y,z) = \frac{q}{\pi^{\frac{3}{2}}\sigma_y \sigma_z}\ exp\{-\frac{(x+y)^2}{2\sigma_y^{\,2}}\}\ exp\{-\frac{He^2}{2\sigma_z^{\,2}}\} \quad \cdots\cdots \quad (6)$$

By giving the plume widths σ_y and σ_z in the above plume model, the concentration profile in the horizontal direction can be computed. However, in estimating the pollution of an industrial area with many the emission sources, a simplified diffusion model is used because the long term average for an annual average is the object of the estimation. For an estimate of a long-term average concentration, the wind is divided into 16 directions, and it is assumed that the concentration perpendicular to the wind is uniform in each wind sector. This equal to replace σ_y to π x/8 and is equal to integrate the concentration profile with y.

The diffusion formula for this can be written as in Eq. (7).

$$C(x,0) = \left(\frac{1}{\pi}\right)^{\frac{1}{2}} \frac{Q}{\frac{u\pi x \sigma_z}{8}} exp\left(-\frac{He^2}{2\sigma_z^2}\right) \quad \cdots\cdots (7)$$

For the puff model, it gives the concentration by a single puff, therefore, it is necessary to use the puff formula to sum up all of the puffs which are floating in space from the continuing source at one time. The plume widths σ_y and σ_z are given in floating time t and represented by Eq.(8), and integrating all of the puffs which were discharged by that time.

$$\sigma_y = \alpha t$$
$$\sigma_z = \beta t \quad \cdots\cdots (8)$$

When integrating with the time, the ground surface concentration is given by Eq. (9).

$$C(R, 0) = \frac{2Qp}{(2\pi)^{\frac{3}{2}}} \left\{\frac{1}{R^2 + \alpha^2 He^2/\gamma^2}\right\} \quad \cdots\cdots (9)$$

The symbols in Eq. (9) are as follows:

R : The distance from the point source to the computation point $(x^2 + y^2)^{\frac{1}{2}}$

Qp : Amount of pollutant in a puff for every time unit

α : The rate of increase of the time of the horizontal plume width

γ : The rate of increase of the time of the vertical plume width

10.2.2 The Numerical Simulation Model

The numerical simulation model for diffusion is used to the diffusion over complex terrain and the diffusion of the temporarily changing location of air currents. It is in adequate to use the usual plume model for logarithnic profile for diffusion over complex terrain and diffusion of unsteady state condition.

The numerical simulation model calculates the airflow first, using the Navier Stokes equation for the turbulent flow. The next step is to calculate the diffusion in the flow field.

The basic form of the Navier Stokes equation is shown in Eq. (10).

$$p\{\frac{\partial u}{\partial t} + u * \nabla u\} = - \nabla p + pg + \mu \nabla^2 u \quad \cdots\cdots (10)$$

The formula of mass conservation is given by Eq. (11).

$$\nabla u = 0 \quad \cdots\cdots (11)$$

Here, symbols are as follows:

∇ : $\frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}$

u : Vector flow velocity

ρ : Fluid density

g : Gravitational force

μ : Molecule viscosity coefficient

The air flow is normally a turbulent flow. Thus, the actual place of the flow is obtained by an equation rewritten from the Navier Stokes equation to meet the place of the turbulent flow.

Numerical simulation models of the turbulent flow are the model in which the turbulence structure is processed statistically. They are the k- ε model, the closure model which considers a higher turbulent structure, the Large-eddy simulation model which reproduces turbulence directly.

These models are used for the computation of the air flow over complex terrain, the simulation the of land and sea breezes, etc. and give the special structure of the air flow.

There are several numerical model for the simulation of diffusion such as solving the differential equation of diffusion by finite difference method, or the particle method in which particles are released and the transport and diffusion of them are traced.

The differential equation of discussion (the Fick equation) of diffusion in the turbulent boundary layer is given by Eq. (12)

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = kx\frac{\partial^2 C}{\partial x^2} + ky\frac{\partial^2 C}{\partial y^2} + \frac{\partial}{\partial z}(kz\frac{\partial C}{\partial z}) \quad \cdots\cdots (12)$$

Here, the symbols are as follows:

C : Concentration

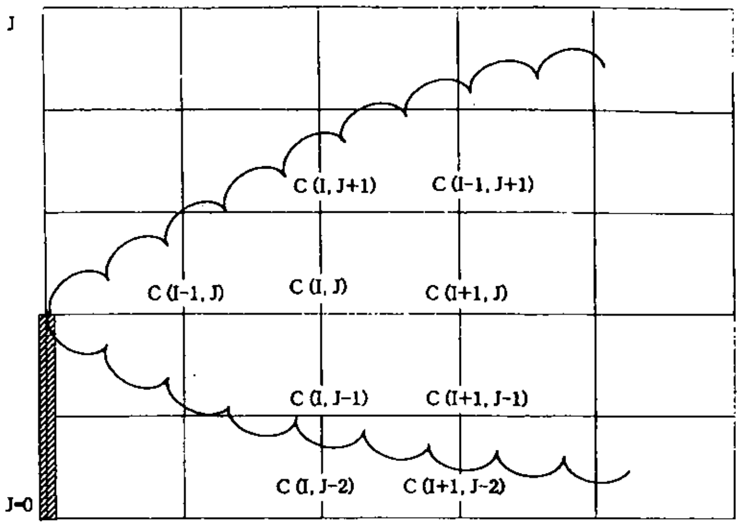
t : Time

x, y, z : Coordinate axis of the perpendicular coordinate

u, v, w : The components average flow in the directions of x, y, z

kx, ky, kz: The turbulent flow diffusion coefficient for the directions of x, y, z

In the differential equation of discussion model of diffusion, the field of diffusion is divided into the meshes, and the concentration, at the points of intersection or at the mid-point of the mesh points are calculated. An example of the mesh division is shown in Fig. 10.2.1.



$$u\frac{\partial C}{\partial x} = Kz\frac{\partial^2 C}{\partial Z^2}$$

$$u_{i,j}\frac{C(i,j) - C(i+1,j)}{\Delta X}$$

$$= Kz\frac{C(i,j+1) - 2C(i,j) + C(i,j-1)}{\Delta Z^2}$$

Fig. 10.2.1 An example of the Mesh division for the finite difference method

10.2.3 The particle method model of diffusion

Next, diffusion simulation by the particle method is introduced. The conditions can be set to meet the statistical nature of the turbulent flow in the particle method. In other words, in a differential equation of discussion, the condition of the diffusion is dependent on the diffusion coefficient. Generally, in atmospheric diffusion, near the emission source, the plume width is proportional to the distance from the emission source and, on the downwind side, it is known to be proportional to the square root of the distance. This shows that the diffusion coefficients are dependent on the distance from the source. However, it is difficult to change the diffusion coefficients by distance in the Fickian equation. For the particle method, on the other hand, it is possible to simulate actual turbulent diffusion by reproducting turbulent structure and releasing particles in the flow field. To get a smooth concentration profile when using the particle method, however, several hundreds of thousands of particles must be discharged, therefore it requires long computer time. Therefore, a simpler particle method is also proposed.

The velocity $v\,(t)$ of a particle in the particle method is give in Eq. (13).

$$v(t) = v + v'(t)$$
$$v'(t) = R(\Delta t)\,v'(t - \Delta t) + n(1 - R(\Delta t))\sigma v \quad \cdots\cdots\cdots (13)$$

Here, v is the average velocity, $v'(t)$ is the turbulent component and n is a random number with an average value of 0 and a standard deviation of 1. In the particle method, the diffusion condition can easily be grasped visually by expressing the distribution of particles like a cloud.

10.2.4 The model of the plume rise

Smoke which is discharged into the air, rises up the atmosphere because of its own inertial force and buoyancy. In the diffusion calculation of the actual smoke, the distance of the plume rise is calculated and it is assumed that the smoke is horizontally discharged from the maximum height that smoke reaches (effective source height *He*). Many models are proposed as a method to estimate the plume rise. Introduced here are the Briggs and CONCAWE (Conservation of Clean Air and Water, Western Europe) models which have been adopted by Japan in the manuals for the total emission control method.

The CONCAWE model gives the distance ΔH that the plume rises through Eq. (14)

$$\Delta H = 0.157\, Q_H^{\frac{1}{2}}\, u^{-\frac{3}{4}} \qquad \cdots\cdots (14)$$

Here, each symbol is represented as follows:

ΔH : Distance of the plume rise (m)

Q_H : Thermal effluent (cal/s)

u : Wind velocity (m/s)

where, Q_H is shown in Eq. (15).

$$Q_H = \rho C p Q \ \Delta t \qquad \cdots\cdots (15)$$

p : Exhaust gas density at 0℃ (1.298×10^3 g/m^3)

Cp : The specific heat at constant pressure (0.24 cal/kg/K)

Q : Exhaust gas quantity for unit time (m^{3}N/S)

Δt : The difference between the exhaust gas temperature (Tg) and the atmospheric temperature (Tg-15℃)

The Briggs model gives the plume rise under a calm condition with no wind in Eq. (16).

$$\Delta H = 1.4\, Q_H^{\frac{1}{4}} \left(\frac{d\theta}{dz}\right)^{-\frac{3}{8}} \qquad \cdots\cdots (16)$$

Here, $\frac{d\theta}{dz}$ is the heat gradient (C/m).

Also, the effective source height is a summation between the stack height and the plume rise.