Evaluation study of numerical schemes for an air quality simulation model in complex terrain


1. Introduction

An air pollution prediction is a very important subject, and many models have been proposed to predict pollutant concentrations. Although these models can usually be applied to some emission sources on flat terrain, they are mostly not well applicable to sources located in an area of complex terrain. The underlying paper describes the results of first years efforts. The first stage of this development is the evaluation study on the numerical methods for the advection equation to incorporate the composite model.

2. Numerical methods for advection equation

The numerical method for the advection equation may be the most important factor in composite atmospheric models, because an inappropriate discretization of the advection terms can sometimes have a devastating effect to a numerical model. Therefore, it is very important to select the most suitable numerical method in our air quality simulation model. Although there are many review papers concerning the numerical methods, an evaluation study has been carried out to confirm their conclusions. The candidate numerical methods chosen in our evaluation study are four methods as follows.

1) Up-wind differencing method

The up-wind differencing is one of the most popular numerical models although it is largely concerned with numerical diffusion. Its advantage is that it is very easy to understand and that it suits computer programs. We therefore choose this method of the second order accuracy for our evaluation study.

2) Taylor-Galerkin method

Although the Galerkin finite element method using a chapeau function is an attractive scheme for the discretization of a space derivative, the combination with a time differencing makes the scheme unstable, because of computational pseudo-negative diffusion. The Petrov-Galerkin and

* Tokyo University of Information Sciences
** Chiyoda Engineering Consultants Co., Ltd.
Taylor-Galerkin methods were developed to overcome these defects. The Taylor-Galerkin method was proposed by Donea (1984). Chock (1991) carried out an extensive evaluation study for the numerical methods, and concluded that the Taylor-Galerkin method is one of the most excellent choices for use in solving the advection equation.

3) Quasi-Lagrangian cubic spline method

In the field of air quality simulation, the quasi-Lagrangian cubic spline method was introduced by Pepper et al. (1979). This method uses the following basic concept; the concentration of the place \( x_i \) at time \( (n+1) \Delta t \) is identical to that of the place \( x_{i+1} \) at time \( n \Delta t \). The concentration at the place \( x \) can be estimated by using cubic spline method.

4) Particle method

The dispersion phenomena can be simulated by the movement and distribution of a large number of particles, and the atmospheric turbulence is modeled by a pseudo-random number generated in a computer. This method is known as particle method or random-walk method. However, in order to evaluate only the advection term, the diffusion process was omitted and movement of a particle was expressed by using only the mean wind field. The initial number of particles was set proportionally to the initial concentration field.

3. Evaluation of methods

The computational performance of the numerical methods for the advection equation can be measured by the rotating cone problem. In this test, the initial concentration field is represented by cosine function and its center is biased from the center of the circulating flow field. Chock and Dunker (1983) have carried out an extensive evaluation study for the numerical methods, using the rotating cosine hill test in a \( 33 \times 33 \) grid. The rotating cone testing was carried out to reconfirm the evaluation results given by Chock. The experimental conditions including the initial concentration field, and wind field were the same as that of Chock (1991).

Seibelt and Morariu (1991) used the deformational flow field to test their semi-Lagrangian numerical advection methods. Their purely deformational flow field is expressed; \( u = -ax \quad v = ay \). In this flow field the calculated mass after time increment \( n \) can be analytically obtained and this analytical result suggests that a continuous growth of the total mass may occur in conventional case.

In order to evaluate the numerical methods, this deformational flow field was also used. The initial concentration field was set for a rectangular shaped block of central \( 8 \times 8 \) grid elements in the \( 32 \times 32 \) computational domain, which is the same as that of Siebert et al. (1991). The flow for the latter half cycle is in reversed direction. Therefore, the rectangular block is stretched along the \( y \)-axis. After that, the flow becomes reversed, stretched along the \( x \)-axis, and returns to the shape of initial conditions after one-cycle computation in the theoretical analysis.
4. Results

As for the rotating cone and deformation flow problems, the two-dimensional equation was numerically solved by operator splitting. In the rotating cone problem, the maximum Courant number \( \mu \) was set at 0.4 except for the up-wind differencing, because this scheme was not stable for \( \mu = 0.4 \). Therefore, the Courant number was set at 0.2 only for the up-wind differencing method. The number of particles used in our particle method was 500. The calculated concentration distributions of the rotating cone after two revolutions are examined. Good performance was obtained for cubic spline and Taylor-Galerkin methods, and the up-wind differencing method reveals the worst in our comparison, because the concentration field after two revolutions reveals a quite different shape from the initial condition. In the particle method, a little bias of the center position was observed.

5. Conclusion

An evaluation study on several numerical methods for an air quality simulation model applicable to the emission sources located in the complex terrain was carried out. The candidate numerical methods were chosen by our limited literature survey. The two-dimensional numerical tests showed that Taylor-Galerkin scheme exhibited a good performance in computing speed and accuracy, and is easy to use. The results indicate that the appropriate numerical scheme can provide the suitable concentration distributions. However, more extensive evaluation and refinement of the scheme may be necessary.

References