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A Study on Numerical Methods for Air Quality Simulation

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Abstract

The numerical method for the advection equation may be the most important factor in comprehensive atmospheric models. Since an inappropriate numerical methods cause a fatal effect on numerical simulation, it is very important to choose a suitable scheme. The Galerkin-type numerical method may be recommended based on this comparative study. However, it sometimes produce a great deal of computational ripples. Forester filter is useful to compensate the numerical noise, but the substantial peak is also scattered. The most appropriate value for the Forester coefficient is varied depending on the testing method. Even if the substantial peak is a little scattered, the use of these filters may be better choice to avoid the appearance of negative values.

1. INTRODUCTION

Air quality simulation models (AQSM's) may be the most important tools when making a decision on air pollution prevention program for regional or global scale. The numerical method for the advection equation is the most important factor in numerical atmospheric models. As the AQSM's are used for a wide range of applications, more accurate models are required to operate under severe conditions, e.g. long-period time integration. Since an inappropriate discretization of the advection terms can sometimes cause a fatal effect on numerical simulation, it is very important to choose the most suitable numerical method in comprehensive AQSM's. This study is aimed to evaluate and choose the most suitable numerical method for a three-dimensional air quality simulation model applicable to a site over complex terrain.

There are so much numerical methods that we cannot say the exact number of methods developed up to now. Literature survey on this field shows such excellent review papers as McRae et al.[1], Rood[2], and so on. There are many evaluation studies on the comparison of these methods; Chock and Dunker[3] and Chock[4]. Rotating cone method is the most popular testing method concerning the numerical schemes for advection equation, and almost all comparative studies employed this testing method. Recently other testing methods have been introduced by many researchers. The testing method by Siebert et al[5] uses the deformational flow field and evaluates the other aspects of the numerical methods by rotating cone test. The numerical filter to compensate some computational noises was also

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considered here.

2. NUMERICAL METHODS

In this study the performance scores of the five numerical methods by using the rotating cone and the deformational flow test were compared. A brief summary of the four methods had been already mentioned in our previous paper[6]. Here, one method was added and more extensive evaluations were carried out. The candidate numerical methods chosen in this evaluation study are five methods as follows.

2.1 Upwind differencing method

The up-wind differencing is one of the most popular numerical methods. Although this method has relatively large numerical diffusion, it has an important advantage that it is very easy to understand and that it is suitable for easy computer programming. The second order accuracy of the up-wind differencing of a space derivative has been chosen here, and is shown by eq.(1).

$$\left(\frac{\partial C}{\partial x}\right)_{\mathrm{i}} = \frac{1}{2\Delta x}\left(3C_{\mathrm{i}} - 4C_{\mathrm{i-1}} + C_{\mathrm{i-2}}\right) \qquad (1)$$

where, C is the concentration, and x is the variable of a space.

2.2 Particle method

The dispersion process can be simulated by using a large number of particles, and the atmospheric turbulence is modeled by a pseudo-random number generated by a computer. This method is known as particle method or random-walk method. This method was selected as a candidate because it can be used to solve the advection and diffusion equations. However, in order to evaluate only the advection term, the diffusion process was eliminated and displacement of a particle was calculated by using only the mean wind field. The initial number of particles was set proportionally to the initial concentration field.

2.3 Quasi-Lagrangian cubic spline method

In the field of air quality simulation, the quasi-Lagrangian cubic spline method was introduced by Pepper et al.[7]. This method uses the following basic concept; the concentration of place x_i at time $(n+1)$ is identical to that of place x_{i-1} at time $n\Delta t$. In order to estimate the concentration of place x ($x_{i-1} < x < x_i$), the cubic spline interpolation scheme was used. Details are explained in Pepper et al.[7] and Okamoto et al.[6].

2.4 Taylor-Galerkin method

The Galerkin finite element method using a chapeau function is an attractive scheme for the discretization of a space derivative. However, the combination with a first-order time differencing makes the scheme unstable, because of computational pseudo-negative diffusion. Donea[8] proposed the Taylor-Galerkin method and this method can mitigate these situations. An extensive evaluation study for the numerical methods was carried out by Chock[4], and it was concluded that the Taylor-Galerkin method is one of the most excellent choices for solving the advection equation. The one-dimensional advection equation descretized by the Taylor-Galerkin method is shown in eq.(2), in case that the wind speed is uniform for the whole computational domain.

$$\left(1-\mu^2\right)C_{i-1}^{n+1}+\left(4+2\mu^2\right)C_i^{n+1}+\left(1-\mu^2\right)C_{i+1}^{n+1}=\left(1+3\mu+2\mu^2\right)C_{i-1}^{n}+4\left(1-\mu^2\right)C_i^{n}+\left(1-3\mu+2\mu^2\right)C_{i+1}^{n} \tag{2}$$

where, μ is the Courant number ; $\mu = u\,\Delta t / \Delta x$.

2.5 Taylor-Galerkin with Forester filter method

The Galerkin-type numerical methods are useful for solving the advection equation. However, these methods produce a great deal of computational noise in highly steep gradient area of the values (concentrations). In order to smooth the computational values, Forester[9] proposed an iteration smoothing process, and Chock[4] called it the Forester filter. This filter is identical to the diffusion calculation to compensate computational-generated ripples. In this study this filtering method was combined with the Taylor-Galerkin method. The filtering procedure in each calculation step is expressed by eq.(3)

$$C_i^{k+1}=C_i^k+\frac{\nu}{2}\left\{\left(C_{i+1}-C_i\right)\left(\phi_{i+1}+\phi_i\right)-\left(C_i-C_{i-1}\right)\left(\phi_i+\phi_{i-1}\right)\right\}^k \tag{3}$$

where Φ is a function , and its value is one or zero depending on the existence of the numerical ripples. The coefficient v plays a similar role to the diffusion coefficient. The superscript k means the number of iterations.

3. NUMERICAL CALCULATIONS

The two-dimensional advection equation is shown by eq. (4)

$$\frac{\partial C}{\partial t}=-\frac{\partial}{\partial x}(uC)-\frac{\partial}{\partial y}(vC) \tag{4}$$

where C is concentration, and u and v are wind components for x and y directions, respectively. This two-dimensional equation was numerically solved by operator splitting[1]. In these calculations, the maximum Courant number μ was set at 0.4 except for the up-wind differencing. Since the up-wind differencing method was not stable for $\mu = 0.4$ in the rotating cone test, the Courant number was set at 0.2 only for this test. Five hundred particles were used in the particle method.

The most popular testing methods to measure the computational performance of the numerical methods for the advection equation may be the rotating cone test. In this test, the initial concentration field is represented by a cosine-hill function and its center is biased from the center of the circulating flow field as shown in Fig.1. Chock and Dunker[3] and Chock[4] describe an extensive evaluation study for the numerical methods, using the rotating cosine hill test in a 33 x 33 grid. The initial peak concentration is assumed to be 100.0 of an arbitrary unit. The experimental conditions, including the initial concentration field and wind field, were the same as those of Chock[4].

Seibelt and Morariu[5] proposed an evaluation method by using the deformational flow field. Their purely deformational flow field is expressed by eq. (5).

$$u = -\alpha x \qquad v = \alpha y \tag{5}$$

In this case, the deformation F cannot be zero, even though the divergence becomes zero.

$$F = du / dx - dv / dy = -2\alpha \tag{6}$$

In this flow field the calculated mass after time integration, in which the first order difference of wind field is employed, can be analytically obtained and this analytical result suggests that a continuous growth of the total mass may occur. This deformational flow field was also used to evaluate the numerical methods. The initial concentration field was set for a rectangular shaped block of central 8 x 8 grid elements in the 32 x 32 computational domain, which is the same as that of Siebert et al[5]. The initial concentration of the block-shaped hill is assumed to be 100.0. The flow field for the former half computational cycle is shown in Fig. 2, and the flow for the latter half cycle is the same as the former half 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. EVALUATION

The concentration distributions of the rotating cone after two revolutions were calculated, and relatively good performance scores were obtained for cubic spline and Taylor-Galerkin methods. The up-wind differencing method reveals the worst scores in this 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 and some spikes were also appeared. Figure 3 shows the calculated concentration distributions after five cycles of computation in the deformational flow field. The peak concentrations for the particle and Taylor-Galerkin methods are too high, and the total mass for cubic spline method is also large in this test.

For the quantitative evaluation, the mass conservation ratio R1 and the mass distribution ratio R2 were calculated.

$$R_1 = \sum C_{ij}(t) / \sum C_{ij}(0) \tag{7}$$

$$R_2 = \sum C_{ij}^2(t) / \sum C_{ij}^2(0) \tag{8}$$

may be the consequence of mass flow beyond the boundary. These scores suggest that there is not so much difference between the methods, except for the up-wind differencing method. However, the Taylor-Galerkin with Forester filter method may be slightly superior to other methods, and this result is similar to that of Chock[4].

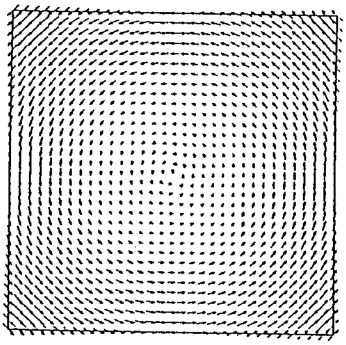


Figure1 Circulating flow for rotating cone test

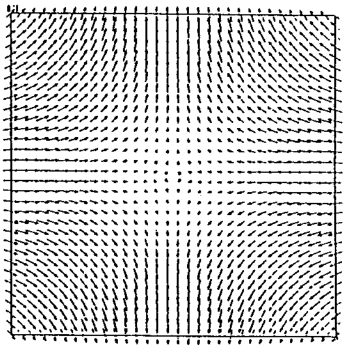
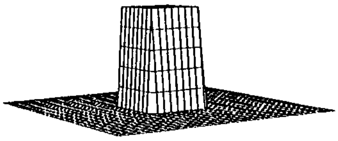
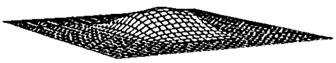


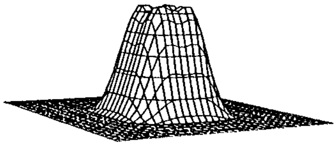
Figure2 Deformational flow of Siebelt et al[5]



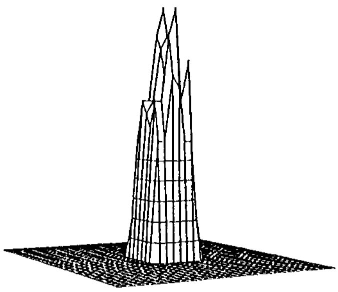
(a)initial



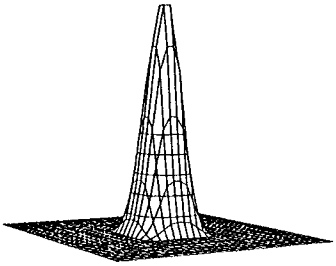
(b)up-wind differencing



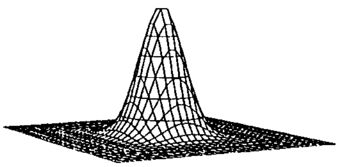
(c)cubic spline



(d)particle method



(e)Taylor-Galerkin



(f)Taylor-Galerkin with Forester filter

Table 1. Evaluation scores for the rotating cone test.

	peak value	mass conservation ratio R_1	mass distribution ratio R_2	average absolute error	percent of meshes less than 0
Upwind differencing method	36.2	1.109	0.727	4.3	35
Particle method	92.6	1.000	1.000	2.9	0
Quasi-Lagrangian cubic spline method	79.2	1.001	0.835	0.5	48
Taylor-Galerkin method	74.7	0.999	0.790	0.7	49
Taylor-Galerkin with Forester filter method	73.5	1.000	0.778	0.7	49

Table 2. Evaluation scores for the deformational flow test

	peak value	mass conservation ratio R_1	mass distribution ratio R_2	average absolute error	percent of meshes less than 0
Upwind differencing method	21.9	0.225	0.022	6.2	32
Particle method	251.2	1.000	1.640	12.5	0
Quasi-Lagrangian cubic spline method	106.4	1.720	1.325	5.2	38
Taylor-Galerkin method	228.3	1.004	1.354	3.8	47
Taylor-Galerkin with Forester filter method	127.6	0.992	0.666	3.7	37

each numerical method are shown in Table 1 and 2. As for the rotating cone test, all methods show satisfied results for the mass conservation ratio R_1, but incredible mass growth was observed in cubic spline method in deformational flow test. The very small value R_1 for up-wind difference in this flow test may be the consequence of mass flow beyond the boundary. These scores suggest that there is not so much difference between the methods, except for the up-wind differencing method. However, the Taylor-Galerkin with Forester filter method may be slightly superior to other methods, and this result is similar to that of Chock[4].

5. FORESTER FILTER

The numerical filter is one of the most useful tools to suppress computational ripples. In air quality simulation the negative concentration produced by an inappropriate numerical method sometimes result in a fatal defect. Forester[9] proposed a numerical filter to mitigate the numerical error. Such a filter may be attractive for a Galerkin-type numerical method that has inherent numerical negative diffusion, and this characteristic is similar to the first-order centered difference. Forester's paper presented the basic concept of the Forester filter and examples of the one-dimensional test, but extensive evaluations for the two-dimensional calculations were not carried out. The rotating cone and deformational flow tests were carried out by using the Taylor-Galerkin with Forester filter method. In these tests the number of iterations and values of the coefficients were varied. Table 3 shows the relation between Forester coefficients and occurrence of the negative values and the calculated peak value for the rotating cone test. There are too much negative values, but almost all are very close to zero, and the percentage of the mesh number in which the calculated concentration is less than –1.0 is shown in Table

3. The initial peak concentration is 100.0, and this value decreases by the artificial diffusion in the numerical time integration. Although this filter can suppress the computational ripples, the substantial peak is also scattered by this filter. As for the number of iteration, only one iteration showed better results than two or more iterations. The smaller values for the Forester coefficient ν are preferred for the rotating cone test, but the deformational flow test suggest that larger value of ν is suitable to compensate the computational-negative diffusion in Galerkin-type schemes.

Table 3. Relation between Forester coefficients and occurrence of negative value and calculated peak values in the rotating cone test

Value of Forester coefficient	Peak value	Mass conservation ratio R_1	Mass distribution ratio R_2	Percent of meshes less than -1
None*	74.7	0.999	0.790	0.050
0.0007	64.1	1.000	0.647	0.019
0.00007	73.5	1.000	0.773	0.047
0.000007	74.6	0.999	0.790	0.050

* This method is same as Taylor-Galerkin method.

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6. CONCLUSIONS

Several numerical methods applicable to air quality simulation models were evaluated by the rotating cone and deformational flow tests. Although the Galerkin-type numerical method is an attractive scheme, it can produce a great deal of computational ripples. Forester filter is useful to compensate the numerical noise, but the substantial peak is also scattered. The most appropriate value for the Forester coefficient is varied depending on the testing method. Even if the substantial peak is a little scattered, the use of these filters may be better choice to avoid the appearance of negative values.

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