Application of Computational Fluid Dynamics (CFD) in Contaminant Monitoring and Analysis

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Abstract. Computational fluid dynamics can be used to simulate the diffusion of pollutants and estimate the pollution load. So we can monitor and analysis the pollution better, then find the solution in time. In this paper, we combine the explicit difference scheme with the implicit difference scheme to solve the concentration convection-diffusion equation. The result shows that the absolute error between the numerical solutions and analytical solutions is very small. So the actual environmental problems can be simulated by Computational Fluid Dynamics numerical calculation. According to Computational Fluid Dynamics in the practical application of the environment, it has the characteristics of low cost, time saving and accurate. Therefore, the Computational Fluid Dynamics plays an important role in the pollutant analysis and monitoring.

Introduction

With the rapid development of industry and the water transport, a large number of pollutants are discharged into water. It deteriorates the rivers, the lakes and the marine ecological environment. On the other hand, it also seriously affects the aquatic environment, the agricultural production, and our health. We can analyze and monitor the diffusion forms of pollutants by solving the definite solution problems of large-scale, high-dimensional partial differential equations. Such as the diffusion of pollutants in water[1], the emission of chimney exhaust gas[2], the weather forecasting, the detection and excavation of gas and oil reservoir, and so on, all of these can be analyzed by computational fluid dynamics. Therefore, it is very important for provide more effective protection and emergency measures to research the behavior and fate of pollutants in the water body by means of the Computational Fluid Dynamics, and it can provide a strong protection for the ecological environment and the health of human beings.

At present, the finite difference method and the finite element method are commonly used in Computational Fluid Dynamics, the finite difference method is currently used most, because most of the simulation area is fluctuating. In order to achieve a better simulation result, we need a more accurate difference scheme to construct the water quality model. The higher the precision is, the more accurate the analysis of pollutant diffusion is. We pay more attention on the pollutant movement rule in the convective diffusion equation, it involves hydrology, hydraulics, water chemistry, water biology, ecology, limnology and so on, it is a comprehensive interdisciplinary.

Numerical Examples

The following is for one concentration dimensional convection-diffusion equation with an initial condition[3]:

\[
\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2} + f(x) \quad 0 < x < m, t > 0
\]
\[ C(x,0) = \sin\left( \frac{\pi x}{m} \right) \exp\left( \frac{ux}{2D} \right) \quad 0 \leq x \leq m \]

(2)

and either the Dirichlet boundary condition

\[ C(0,t) = \phi(x) \quad C(m,t) = \phi(x) \quad t > 0 \]

(3)

the analytic solution of the problem is:

\[ C(x,t) = \exp\left( -\left( \frac{2\pi x}{m} \right)^2 + \left( \frac{u}{D} \right)^2 \frac{Dt}{4} + \frac{ux}{2D} \right) \sin\left( \frac{\pi x}{m} \right). \]

(4)

Here, \( D \) is diffusion coefficient; \( u \) is convection coefficient; \( C \) is concentration; \( x \) and \( t \) represent space and time variables respectively, \( m=1 \).

Combining the explicit difference scheme and the implicit difference scheme makes the positive and negative errors cancel each other. The difference scheme called the Crank-Nicolson difference scheme. The Crank-Nicolson difference scheme has the advantages of low computation time and high accuracy. So using the C-N method of computational fluid dynamics limited difference method to solve the problem Eq1 can obtain the absolute error, which is between numerical and analytical solutions. As shown in the figure.1: \( t=0.1 \), \( n=20 \)

![Figure 1. The absolute error of the numerical solution and exact solution.](image)

It can be seen from the Figure.1, from the beginning to the end of the simulation, the absolute error between numerical solution and analytical solution is very small. The max absolute error is 1.8e-9. Therefore, the numerical simulation method can be used to simulate practical problems. The simulation results are similar to the actual results.

The table.1 shows that the numerical solution is close to the exact solution. No matter how many discrete points, the numerical solution of each point is well matched to the analytical solution.

<table>
<thead>
<tr>
<th>Unit number(N)</th>
<th>The node (x)</th>
<th>Numerical Solution</th>
<th>Exact solution</th>
<th>Max absolute error</th>
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</thead>
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<tr>
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<td>0.264428426279091</td>
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</tr>
</tbody>
</table>

Table 1. Comparison of numerical solution and exact solution under different unit number (\( t=0.1 \)).
In summary, the absolute error between numerical solution and analytical solution is very small. Therefore, the diffusion of contaminant in water can be simulated by this method, and the diffusion of pollutant also can be monitored and analyzed.

The Application

In the beginning, the Computational Fluid Dynamics is simply applied to the aerospace field. With the computer's rapid development, the CFD has been widely applied to various fields, such as marine [4], chemical, urban planning [5], construction and so on. Currently, the Computational Fluid Dynamics (CFD) is widely used in the environment, too. For example, it can be used to evaluate the city's air quality [6], the marine functional area division and many other environmental problems [7].

The early migration and transformation of pollutants in water are mostly determined by fluid mechanics and watermarking. If the pollutant can be accurately simulated and monitored at the initial stage of pollutant diffusion, the diffusion behavior of pollutants can be better understood, and then put forward countermeasures in time to solve the problem of pollution from the source, therefore, we do not need to follow up the complex water treatment. The problem of diffusion of flue gas can also be solved by CFD, such as the simulation of the velocity direction of the diffusion after exhaust emission through numerical simulation before the emission of exhaust gas, and then evaluate its possible impact. Finally, the solutions are proposed according to the simulation results, and then the problems of pollution from the pollution sources are solved.

The specific application is described below:

Application of oil spilling: In fact, the problem of Oil movement in the ocean is a "convection-diffusion problem", it can be calculated by computational fluid dynamics. So that the oil spilling in the sea can be studied by numerical prediction, the diffusion direction and velocity of oil spilling can be determined by simulation. Therefore, we can solve the problem promptly to avoid oil spilling on the marine ecology causing a large area of harm. The application of Computational Fluid Dynamics (CFD) in oceanography is described in the Bohai Sea, and a numerical example shows that the model can be used to predict the actual oil spilling [8].

Application of flue gas desulfurization: In the large scale coal-fired power plants, the power generation process is mainly using wet flue gas desulfurization[9]. This method requires a lot of experiments, its data is limited and high cost. But the Computational Fluid Dynamics simulation of flue gas diffusion can greatly reduce the physical experiment, it not only can get a lot of data but also save time and cost less.

Application of primary settling tank [10]: CFD technique can be used to simulate the two-phase flow in the primary settling tank. In particular, the numerical simulation method is used to research the flow condition of primary sedimentation tank under various boundary conditions and operating conditions, and the distribution of suspended particles inside the sedimentation tank. And then determine the sedimentation efficiency and effluent condition of the sedimentation tank. It can provide the basis for optimizing the design of the tank, and achieve the unity of the engineering economic and social benefits.

Application of nuclear power industry [11]: In recent years, with the rapid development of nuclear industry and nuclear technology, the establishment of nuclear facilities has gradually increased. During the production and operation period, it will inevitably discharge a large amount of radioactive waste liquid to the water body. It will do a great harm to the aquatic ecological environment. We can simulate the migration and diffusion of the waste-water by the CFD, it can provide a reasonable scientific basis for the design of nuclear power low-level discharge. Application of CFD can avoid the impact of nuclear power waste-water on the water ecological environment.

Application of Chemical Leakage: Maritime transport activities are increasing, marine chemical spill incidents occur frequently, causing great impact on marine ecology. Most chemicals are colorless and easily soluble, so when the chemical leakage can’t visually determine the direction of its diffusion, concentration and speed. Therefore, it is impossible to propose a solution in time. The
numerical simulation of the chemical leakage can be done by the numerical method of fluid mechanics, which can accurately determine the velocity, direction and concentration of the diffusion of the chemical. It is convenient to monitor and analyze the diffusion of the chemical and promptly propose the solution. To avoid causing a widely range of marine ecological pollution. Application of CFD on chemicals and other easy to leak contaminants to track monitoring, and the change of concentration during transportation was monitored and analyzed. Can be timely to determine whether a leakage problem happen, thereby avoiding leakage of contaminants.

Conclusions
At present, the numerical calculation of the CFD has been applied in many areas of environmental engineering. The nature of the contamination can be understood by computational fluid dynamics numerical modeling, which plays an important role in the pollution control and the pollution abatement. The numerical simulation by CFD has the characteristics of fast speed, high precision and low cost. We can get the diffusion mode of pollutants in the first time by computational fluid dynamics numerical simulation and analyze the spread of pollutants and monitor pollutants more effectively. In addition, we can deal with pollution in the most appropriate time and location. So the computational fluid dynamics can analysis and monitor the pollutant diffusion more effectively. Because of its powerful simulation capabilities, there will be more applications in water pollution and atmospheric governance.

References