Numerical simulation of the spread of bacteria in water flow considering the process of reproductions

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Abstract: In this paper, a simple approach for modelling the reproduction of bacteria in water flow is presented. Firstly, the basic mathematical model for simulating the advection-diffusion of pollutions in water flow is reviewed and validated. Then, a solution strategy of doubling the concentration at regular intervals by the basic model is proposed. This approach is easy to be implemented in the existing flow field solver and is proved to be feasible by simulating a standard example. Finally, the spread of the bacterial pollution in a pool is simulated. The result shows that the water quality variation in the pool can be attributed to both the flow patterns of the water flow and the reproduction characteristics of the bacteria. The recirculation region limits the spread of the bacteria, which induces the continuous deterioration of water quality when considering the reproduction of the bacteria.

1. Introduction

Water has tremendous impact on life health, but its quality is from bad to worse with the evolution of the modern society, which has become the global problems. In the last few decades, more advanced theories and methods have been developing not only to analyse the water quality, but also to predict its developing trends[1].

Numerical simulation, which uses to solve problems numerically, has been widely employed in the field of water environment. With the help of high-speed computers, this method can give comprehensive and visual results of complex problems, which is more economical than the traditional experimental analysis and especially suitable for studying the harmful conditions. The basic mathematical models and numerical methods for modelling water environment can be found in the publication of Peng et al.[2]. In recent years, researches in this area are growing very fast both in
theories and applications. Chen et al.[3] presented a new numerical approach by coupling the one-dimensional and two-dimensional shallow water models to accurately predict the water environment in large watersheds. Xu et al.[4] proposed a new hybrid approach of genetic algorithm and fuzzy simulation to solve the water quality management problem. Wang et al.[5] developed a new method for evaluating the water quality in the watershed with limited data and studied the water pollution of a watershed by the Hydrological Simulation Program-Fortran model. Ding et al.[6] provided a simple approach to simulate the dynamic diffusion and migration process of pollutions and apply it to a practical project. These researches offer us various options to solve different problems about water quality.

However, the existing work for simulating the water quality just considered the physical and chemical factors, such as the formation and diffusion of pollutions, while ignoring the biological factor, such as the population growth of microbes. In ideal conditions, bacteria can increase their population by a factor of two in dozens of minutes. That means a small number of bacteria can easily grow to millions in several hours. Therefore, the increase in population must be considered when the simulation involves microbe contaminates.

In this paper, a simple approach for modelling the reproduction of bacteria in the simulation of water quality and its application is presented. This approach can be easily implemented in the flow solver by the help of an external program, which provides an effective tool to solve these problems.

2. Numerical method

The first step of numerical simulation is to establish the mathematical models among different physical variables. Before the discussion of bacteria, the convective-diffusion model of the general pollution in water flow should be mentioned, which includes the mass conservation, momentum conservation equations and the transport equation of the pollution are need. These equations can be written as follows[2]:

Equation of mass conservation:

$$\frac{\partial p}{\partial t} + \text{div}(\rho \overline{u}) = 0$$

Equation of momentum conservation:

$$\frac{\partial (\rho u)}{\partial t} + \text{div}(\rho u \overline{u}) = -\frac{\partial p}{\partial x} + \text{div}(\mu \text{grad} u) + S_u$$
$$\frac{\partial (\rho v)}{\partial t} + \text{div}(\rho v \overline{u}) = -\frac{\partial p}{\partial y} + \text{div}(\mu \text{grad} v) + S_v$$
$$\frac{\partial (\rho w)}{\partial t} + \text{div}(\rho w \overline{u}) = -\frac{\partial p}{\partial z} + \text{div}(\mu \text{grad} w) + S_w$$

Transport equation of the pollution:

$$\frac{\partial (\rho C)}{\partial t} + \text{div}(\rho \overline{u} C) = \text{div}(\Gamma \text{grad} C) + S_C$$

where $p$ is the pressure, $u$, $v$ and $w$ are the velocity components, $C$ means the concentration of the pollution, $\Gamma$ is the diffusion coefficient of the pollution, $\rho$ is the water density, $t$ is the time, $x$, $y$ and $z$ is the coordinate component, $S$ indicates the source term. In this study, these equations are solved by the
computational fluid dynamic solver Ansys Fluent 13.0, more details about the theories of this solver can be found in reference [7].

To validate the above models in simulating the convective-diffusion process of the pollution, a two-dimensional computational domain is built, as shown in figure 1. In this case, a rectangular region, which is 5m wide and 15 m long, is defined as the source of pollution in a channel. The initial concentration of the pollution is defined as 450 g/m$^3$, the diffusion coefficient is set to 0.64 m$^2$/s, and the inlet velocity is 0.5 m/s.

**Figure 1.** The computational domain of the two-dimensional convective-diffusion model.

The simulated concentration distributions at different times are compared with the analytical solutions in figure 2. Note that the analytical solutions are obtained by the formula which is presented in reference [2] and has been validated by several methods. It is obvious that the two results agree well with each other, indicating that the models above are valid and accurate.

**Figure 2.** Comparisons between the simulated concentration distributions and the analytical solutions.

From the viewpoint of numerical modelling, bacteria can be treated as a kind of pollution which doubles its concentration at regular time intervals. To implement this, we just need to modify the existing flow field solver which is available for simulating the convective-diffusion process of the general pollution, and the detailed solution procedure is demonstrated in Figure 3. By applying this approach, the case above is simulated again and the doubling time interval is set as 20s. The results are illustrated in figure 4 and it can be seen that the doubling of the concentration of the pollution in the process of advection-diffusion is executed accurately, which shows the feasibility and practicality of this approach.
3. Application

In this section, the numerical treatment proposed above are employed to simulate the convective, diffusion and reproduction process of the bacteria in a pool. The computational domain of the pool is
depicted in figure 5. In the normal operation conditions, water enter into the pool at the inlet with a constant velocity of 0.05m/s and is drained out of the pool at the outlet.

Firstly, water flow without bacteria is simulated to obtain the preliminary hydraulic characteristics in the pool, the velocity vectors of the water are shown in figure 6. The flow can be divided into two patterns: the main flow and the secondary flow. The main flow, which runs along a narrow region, connects the inlet and outlet of the pool, while the secondary flow circulates around the centre of the pool. Obviously, the secondary flow region, especially near the centre of the pool, is not conducive to the spread of pollutants.

Figure 5. The computational domain of the pool.

Figure 6. The velocity vectors of the water flow.

Then the bacteria, which are put into the centre of the pool as a point source, are taken into consideration. The initial concentration of the bacteria in the point source is 20,000 per square metre of water and the diffusion coefficient is set as $8.3 \times 10^{-6}$ cm$^2$/s. To investigate the influence of reproduction on the spread of the bacteria, two cases are simulated. In case A, the bacteria is considered as a pollution which cannot reproduce, while in case B the generation time of the bacteria is 20 min. The developments of bacteria distributions over time are shown in figure 7, in which the colours represent the concentration of the bacteria. Figure 8 depicts the trends of both the bacteria concentration in the outflow and the relative area of water which is contaminated over time in case B. Note that the contaminated water is defined as the region where the concentration of bacteria is over 20,000 per square meter. In case A, although the bacteria are limited in the central region of the pool, their concentration decreases quickly and almost reaches to zero after about an hour. Additionally, there are hardly any bacteria in the outflow in the whole process, which means that the water quality is nearly unaffected. In case B, both the area of water which is contaminated by bacteria and the maximal bacterial concentration keeps increasing. After 5 hours, more than half of the pool is full filled with bacteria and about 99% of the water is contaminated after 14 hours. Moreover, the concentration of the bacteria in the outflow is also continue to increase, which means that the water quality is deteriorating irreversibly.
The development of bacterial pollution in the pool can be attributed to both the flow patterns and the reproduction of the bacteria. The bacteria source is located in the secondary flow region, so the bacteria circulate in the central area, see figure 6, and hardly flow out of the pool. As a result, in case A, the bacteria still gather around the centre of the pool in a few hours, but the concentration keeps decrease for the convective diffusion effect. In case B, the spreading characteristics of the bacteria is the same as that in the case A, but their concentration keeps increase, for the reproduction of the bacteria. Therefore, the pool is full of bacteria for some time and the quality of outflow water continues to deteriorate.

4. Conclusions
In this paper, a simple approach for modelling the reproduction of bacteria in water flow is presented and is employed to simulate the development of the bacterial pollution in a pool. This approach is easy to implement in the existing flow field solver and is proved to be feasible by simulating a standard
example. The application of this approach shows that the evolving characteristics of bacterial pollution in a pool can be attributed to both the flow patterns of the water flow and the reproduction of the bacteria. The recirculation region limits the spread of the bacteria and provides enough time for their constant reproductions, which induces the continuous deterioration of water quality in the pool.

Additionally, the approach in this study should be improved further, for bacteria will not maintain their exponential reproduction endlessly in reality. In addition, further studies should also be emphasized on the validation of this approach by experiments.

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