A three-dimensional numerical model for the calculation of complex flow and transport phenomena

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Abstract

This paper presents a real three-dimensional numerical model for the calculation of complex flow and transport phenomena in reservoirs, coastal lakes and lagoons. The turbulent processes are simulated with the large-eddy technique. Finite elements of arbitrary shape and with unstructured mesh topology are used to approximate spatial operators. The model is verified by the calculation of a straight channel flow and the comparison to data from the literature. Additionally a physical model experiment is recalculated for a validation of the model. Further applications of flow and transport in a real reservoir are shown in an accompanying paper by Bergen et al. [1].

1 Introduction

The flow and transport phenomena in large natural geometries such as lakes and lagoons are very complex and in most cases totally three-dimensional. This is due to the irregular boundaries, the large volume of the water body and the variability of the external forces on the water body. Numerical models that claim to be capable of simulating flow and transport in such reservoirs correctly, must therefore at least be able to model the large scale eddies in three dimensions. A wind driven flow in a reservoir can not be modeled two-dimensionally, also density dependent flow and the influence of the Coriolis forces are difficult to be modeled exactly with a two-dimensional model. A numerical model is needed which is able to fit the irregular boundaries of natural reservoirs. The finite element method seems to be the best possibility to fulfill this requirement.
Another problem is the large spectrum of the turbulences that exists in large natural geometries. For a standard statistic turbulence model based on the Reynolds-equations it is very difficult to model the whole spectrum, which is changing from reservoir to reservoir and with the boundary conditions. Another theoretically possible approach is the direct numerical simulation of the total eddy spectrum, but this would require far more computer capacity than available.

A very promising approach is therefore the large-eddy simulation technique. Table 1 shows the range of accuracy and computational costs between the three different general approaches. A large-eddy model simulates only the large scale quantities of the eddy spectrum directly on a relatively fine discretization level and models the small (subgrid) scale turbulences with a suitable turbulence model. This turbulence model can then be very simple, because the modeled energy spectrum of the eddies is limited. Only few statistical turbulence parameters are necessary which are transferable to other applications. In this paper we therefore present a large-eddy approach for the simulation of turbulent flow and transport phenomenas in complex geometries with the finite element method.

<table>
<thead>
<tr>
<th>averaging or filtering grade</th>
<th>simulation type</th>
<th>averaging procedure</th>
<th>smallest simulated eddies</th>
<th>accuracy of calculation</th>
<th>computational costs</th>
</tr>
</thead>
<tbody>
<tr>
<td>high</td>
<td>Use of the Reynolds-equations with statistical turbulence models</td>
<td>temporal average (spatial average not necessary)</td>
<td>non turbulent flow structures</td>
<td>small</td>
<td>small</td>
</tr>
<tr>
<td>medium</td>
<td>large-eddy simulation and/or temporal</td>
<td>very large eddies</td>
<td>small</td>
<td>medium</td>
<td></td>
</tr>
<tr>
<td>small</td>
<td>large-eddy simulation</td>
<td>medium large eddies</td>
<td>high</td>
<td>high</td>
<td></td>
</tr>
<tr>
<td>very small</td>
<td>direct numerical simulation</td>
<td>smaller eddies</td>
<td>very high</td>
<td>out of range</td>
<td></td>
</tr>
<tr>
<td>without averaging</td>
<td>—</td>
<td>dissipative eddies</td>
<td>very high</td>
<td>out of range</td>
<td></td>
</tr>
</tbody>
</table>

Table 1: Simulation model types and their accuracies and computational costs
2 Mathematical background

Flow

The spatially filtered Navier-Stokes equations are

\[ \frac{\partial \bar{v}_i}{\partial x_i} = 0 \]  

(1)

and

\[ \frac{\partial \bar{v}_i}{\partial t} + v_j \frac{\partial \bar{v}_i}{\partial x_j} = - \frac{\partial \bar{P}}{\partial x_i} + v \frac{\partial^2 \bar{v}_i}{\partial x_j^2} - \frac{\partial \tau_{ij}}{\partial x_j} + \bar{F}_i \]  

(2)

with the subgrid scale stresses

\[ \tau_{ij} = v_i v_j - v_j v_i . \]  

(3)

In these equations \( v_i \) represents the three velocity components in x, y, z-direction, \( P \) is the kinematic pressure and \( v \) is the kinematic viscosity. \( F_i \) includes all internal force terms like buoyancy and Coriolis forces. The overbar denotes a spatially filtered variable. The filtering functions used in equations 1 and 2 depend on the numerical approximation functions (see also chapter 3).

All subgrid scale turbulences are modeled with a Smagorinsky [10] turbulence model

\[ \tau_{ij} - \frac{2}{3} k \delta_{ij} = - 2 \nu_t \bar{S}_{ij} \]  

(4)

with the eddy viscosity

\[ \nu_t = (c_s \Delta)^2 \cdot (\bar{S}_{ij} \bar{S}_{ij})^{1/2}, \]  

(5)

the filtered deformation tensor

\[ \bar{S}_{ij} = \frac{1}{2} \left( \frac{\partial \bar{v}_i}{\partial x_j} + \frac{\partial \bar{v}_j}{\partial x_i} \right) \]  

(6)

and the filter width

\[ \Delta = \left( \frac{1}{n_k} \sum_{i=1}^{n_k} (\Delta_k)_i^2 \right)^{1/2} \]  

(7)

\( n_k \) is the number of the element edges at each finite element node, \( (\Delta_k)_i \) is the length of an element edge. \( c_s \) is the statistical turbulence model parameter with \( c_s \approx 0.1 \). Germano et al [5] and Lilly [8] have developed a method to calculate the value of \( c_s \) as a spatial and temporal variable by
introducing a double filtering approach. This method is also implemented in the turbulence model, but is not described here in detail.

**Transport**

A similar approach is used for the conservative transport equation with the concentration of the transported solvent \( C \), the molecular diffusion coefficient \( D_m \), the subgrid scale dispersion \( E_i \), the sink/source term \( M_c \) and the transport dispersion parameter \( c_t \) depending on the corresponding flow turbulence parameter \( c_s \).

\[
\frac{\partial C}{\partial t} + \frac{\partial}{\partial x_i} (v_i \bar{C}) - D_m \frac{\partial^2 C}{\partial x_i^2} + \frac{\partial}{\partial x_i} E_i = M_c. \tag{8}
\]

with

\[
E_i = -2D_t \frac{\partial C}{\partial x_i}. \tag{9}
\]

and

\[
D_t = (c_t \Delta)^2 \langle \bar{S} \rangle. \tag{10}
\]

**3 Numerical approach**

The numerical model is based on a finite element model by Daniels [2] for the solution of the transient incompressible Navier-Stokes equations and the transport equation. Time-accurate solutions are obtained by using the 'projection 2' algorithm which was developed and analyzed by Gresho [6]. Modifications to the original algorithm were made where it was appropriate. The model consists of different time integration schemes (explicit, semi-implicit, implicit) to solve the momentum equations and the transport equation.

The element type is a hexahedron with a trilinear approximation function for the velocities and the concentrations and a constant pressure in the element. The numerical approximation functions lead to the so-called triangle filter for the velocities and to a box filter for the kinematic pressure (Forkel et al. [3] and Forkel [4]). Because of the arbitrary shape of the elements all integrations on the element level are obtained by full 2x2x2 Gauss point integration in the general case. For more details of the numerical model see Daniels [2] and Forkel [4].

**4 Verification examples**

**Straight channel flow**

As a first verification example the simulation of a turbulent straight channel flow was chosen. This example has been investigated thoroughly by
experiments, direct numerical simulations and large-eddy simulations and an abundance of data is available for the comparison with the results of the presented model. Out of many simulation runs for the verification of the model only one example will be shown here. The modeled geometry is shown in Figure 1, the discretization consists of 24*20*24 nodes in x,y,z-direction with constant spacing. The geometry and discretization is similar to a simulation by Piomelli et al. [9].

Figure 1: Model geometry by Piomelli et al. [9], Re\textsubscript{c}=640

At the walls we used the logarithmic law of the wall as proposed by Unger and Friedrich [11], the outflow boundary is described by zero pressure/stress boundary conditions. At the inflow boundary we used periodic boundary conditions with

\[ v_i(t, x = 0) = v_i(t - \Delta t, x = 2\pi b). \]  

The simulated area is extended in x-direction (additional 5 nodes with same spacing) to avoid the damping influence of the outflow boundary condition. The turbulent initial condition was calculated in a previous channel flow simulation. The temporal discretization should be explicit. Other temporal discretizations lead to unstable or overdiffusive results [4]. Similar stable results without extensive numerical diffusion could only be produced with the semi-implicit scheme of Leismann and Frind [7], but with very small time steps.

Figure 2 shows the velocity profiles of our simulations with the Smagorinsky (\(c_s=0.1\)) and the Germano-Lilly model in comparison to the profile of Piomelli et al. [9]. The velocities are averaged over time and over planes parallel to the walls. The comparison shows a rather good agreement between the three curves. The curve of Piomelli et al. [9] is smoother due to the fact that they use a much longer time interval for averaging. More results from other simulation runs and a more detailed evaluation of the presented verification is given by Forkel [4].
Recalculation of a model experiment
The previous verification example has shown that the new model is able to simulate turbulent flow in a relatively simple geometry correctly. As the model should be used for the simulation of laminar and turbulent flow and transport in complex geometries much more verification is needed. This is done by the recalculation of a physical model experiment. This experiment includes a turbulent tracer injection in an initially laminar flow through a very complex, threedimensional geometry (figure 3).

Figure 2: Comparison of simulated velocity profiles ($v_x^+$ is made dimensionless by the friction velocity $u_r$) with data from the literature

Figure 3: Model geometry of the tracer experiment (5* vertically enlarged)
The tracer movement is taped by a video camera through a plexi glass plate which is fixed on top of the model. The information is converted by digital image processing technique into digital data, the measured concentrations are evaluated by reference measurements and can then be compared with the results of the numerical model. Figure 4 shows the very good agreement between the calculation and the measured data at different times after the beginning of the tracer injection.

![Figure 4: Two-dimensional vertically averaged concentration distributions](image)

5 Discussion

The presented three-dimensional model can be used for the simulation of turbulent flow and transport processes in complex geometries. The large eddies are simulated directly, the smaller eddies are modeled with a simple turbulence model. A question is still whether the large energy spectrum that is filtered out by the discretization can be modeled with such a simple turbulence model or
not. Anyhow the verification examples show the applicability and accuracy of the method for simple and complex problems. More detailed applications of the developed code for the simulation of a reservoir are shown in a separate paper by Bergen et al. [1] which will be presented on the same conference.

6 Literature