Limits of 3-D numerical flow and transportation modeling for the simulation of a vertical circulation flow system in the remediation of a research field site
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Abstract

Vertical circulation flows have become a well established in situ remediation technique. Their controllable flow field permits physical and biological remediation of the saturated as well as unsaturated subsoil. Large scale field experiments are carried out to systematically investigate the system efficacy and operation of groundwater circulation well in the remediation process. This paper is concerned with the realization of a 3-D numerical model of the field test site of the Institute for Hydromechanics in Karlsruhe - Knielingen. For the simulation of the 3-D flow field and transport, the numerical finite element model FRAC3DVS is used. The model has been calibrated with 3-D potential and transport measurements of multilevel monitoring wells. The problems related to mesh generation and error of discretization are discussed. The application is one of only few test sites with real 3-D field data for transportation simulation in a 3-D flow field.

Introduction

Artificially induced vertical circulation flows around wells with at least two screen sections known as groundwater circulation well (in German: Grundwasser-Zirkulations-Brunnen, GZB) are a widely applicable remediation tool (Herrling and Stamm1). Large scale field experiments are carried out to systematically investigate the system efficacy and operation of groundwater circulation well in the remediation process (Scholz and Stamm2). This paper is concerned with the realization of a 3-D numerical model of the field research site of the Institute for Hydromechanics in Karlsruhe-Knielingen. This site is located in the sandy gravel sediments of the upper Rhine valley in the south west part of Germany.
In the GZB of the Karlsruhe-Knielingen research site, the contaminated groundwater enters the GZB at the bottom which is stripped on site and clean water leaves the GZB at the top. In the vicinity of the GZB, an area of vertical flow circulation is created. The stripped air is transported by the blower across activated carbon filters, onto which the contamination is adsorbed and cleaned air escapes into the atmosphere. For the simulation of the 3-D flow and transport, the numerical model FRAC3DVS (Therrien and Sudicky) based on finite element method running on a series of HP9000 workstation is used. For pre- and post processing, the GMS (Groundwater Modeling System) is used which offers good visualization tools. The paper shows how an optimized 3-D finite element net with more than hundred thousand of elements is generated and possibilities of minimizing the error of discretization.

Description of the research site in KA-Knielingen

Figure 1: Map of the research site in Karlsruhe-Knielingen in the sediments of the upper Rhine valley in the south west of Germany with the remediation well (GZB) in the center and 51 single level and multilevel monitoring wells with total 111 sampling points. The research site is located in a PCE and TCE contamination plume. The remediation runs in the confined upper sandy gravel aquifer with a depth of about 7 meters.

The Institute for Hydromechanics operates a research site in Karlsruhe-Knielingen where experiments with a GZB have been carried out (Scholz and Stamm). Fig. 1 shows the GZB in the center of the site. The monitoring wells on the axis in direction of natural gradient allow the measurement of
contaminated influx and treated outflux of the GZB, and those on the cross axis through the GZB enable the control of circulation width.

From 9.5 to about 13 m, the aquifer material changes to medium and fine sand with a significant lower hydraulic conductivity. For this reason, the remediation experiments with the installed GZB were focused on the upper aquifer. The GZB in the Karlsruhe-Knielingen site always operates upwards, so the contaminated water is captured in the lower screen section and treated water leaves the GZB through the upper screen section.

Fig. 2 shows a 3-D view of the aquifer structure with different layers and sublayers. Even if the aquifer seems to be a homogeneous sandy gravel aquifer, Fig. 2 shows some of the heterogeneous structures as lenses, layers with different magnitude and ending layers.

**Numerical investigations**

To make use of the experimental results for future field applications, numerical modeling of the research site is very much essential. Fig. 3 shows the flow pattern for a case study with three layers around a GZB, in a vertical plain cross section for a horizontal stratified aquifer, calculated by
Herrling and Stamm\textsuperscript{1} with a radial symmetric finite element program. Water circulating around the GZB leaves through the upper screen section, turn downwards and turns on back to the pumping level at the bottom.

![Cross section of flow pattern for a GZB system with two screen sections in a stratified aquifer. The strongly curved flowlines near the GZB are obvious.](image)

As it is very difficult to represent the flow and transport phenomena around a GZB in a heterogeneous aquifer during remediation using 2-dimensional models, a 3-D steady state numerical modeling scheme was implemented to model the research field site. For the simulation of the 3-D flow field, the numerical model FRAC3DVS (Therrien and Sudicky\textsuperscript{3}) of the University of Waterloo, Canada, running on a series of HP9000 workstation, is used. The numerical model is based on finite element method. Prism elements are used for discretization. The 3-D mesh generation is carried out using GMS package (Groundwater Modeling Systems).

The requirements of a numerical discretization are, that it represent the hydrogeological structures, the number of elements should be a minimum to save computational time and the size of the elements must be fine enough to allow using linear shape functions to simulate curved flow paths. Especially in the circulation in the vicinity of a GZB, the radial divergent and horizontal infiltrated water has first to change its direction to a vertical flow and then to a radial convergent and horizontal flow to get into the pumping level. This require a fine horizontal and vertical discretization near the GZB and a more coarse discretization far away.

![Plan zoom view of the mesh discretization for the research site near the GZB. The element size in the well is about 5 cm and 500 cm near the boundary.](image)

As in Fig. 2, the aquifer consists of 8 layers with many sublayers so that there are total 52 layers. Each layer is discretized into 2590 prism elements so that there are in total 133680 elements and 70702 nodes. To simulate the 3-D flow around the circulation well, the size of the elements vary from 5 cm near to GZB and 500 cm near to boundary, in horizontal direction. In
Figure 5: Vertical plain cross section of the KA-Knielingen Aquifer with GZB/UVB remediation well in the center and multilevel monitoring wells. The natural gradient is from left to right. The aquifer is discretized in 6 layers with total 60 sublayers. In the vertical direction, the element size vary from 7.5 cm near to the screen sections and 21 cm at other places. Fig. 4 shows a plan view of the discretization near the GZB. The vertical discretization is shown on a slice in Fig. 5. As can be seen, a very fine mesh is provided near to the GZB.

Results and discussion

Sensitivity analysis

Stamm showed the importance of the horizontal as well as the vertical discretization in the vicinity of the GZB. He showed that the dimensionless parameter $\Delta h/H$ is a sensitive value to estimate the error of discretization in relation to the element size. $\Delta h$ is the hydraulic head difference between the upper and lower filter section of a GZB and $H$ the magnitude of the aquifer. Therefore an analysis has been carried out with various sets of element sizes. A GZB (well radius 0.2 m, two screen section of 1.0 m at the
top and the bottom of an aquifer, $H = 10$ m) was simulated in a homogenous aquifer. The horizontal net was fine (element size < 8 cm) near the GZB and coarse far away and had 987 nodes and 1908 triangular elements. In one series of calculations, the number of layers was homogeneously extended. Fig. 6 shows the influence of the discretization to the dimensionless parameter $\Delta h/H$. Even with 100,000 elements the discretization has an influence on the calculated flow field and also on the transport, which is not shown here. So for the simulation of a GZB the vertical discretization must be as fine as the horizontal discretization. Fig 6 also shows, that an optimization can be achieved by variable layer thickness with fine layers near the filter screen sections and thicker layers between the filter sections.

With a workstation (HP9000, 180 MB RAM) the calculation up to 180,000 prism elements was possible, but the maximum number of elements for post processing with GMS software on a PC (64 MB RAM) was about 100,000 elements. Therefore an optimized vertical discretization was developed for the Karlsruhe-Knielingen model which is shown in Fig. 5.

**Calibration of the model**

The numerical model described is calibrated with respect to the field measurements in the research field site. In the field, the GZB has operated for different pumping rates (discharge = infiltration) and piezometric heads have been measured at different monitoring wells. Fig. 7 shows the potential variation at different points for a pumping rate of the GZB of $4 \text{ m}^3/\text{h}$. The targets in Fig. 7 show the differences between the measured and the calculated data in one of the calibration steps. The positive and negative differences are obvious. The problem of the calibration is, that in a radius of only 10 m around the GZB, the changes of the water heads due to the pumping activity of the GZB get less than 1 cm. But tracer tests show obviously that, the radius of influence of the GZB is more. Therefore the model was not only calibrated with the measurement of the waterheads but also with the tracer measurements.

**Transport simulations**

For the Karlsruhe-Knielingen research site, several tracer tests have been simulated. Infiltrating the tracer in upgradient monitoring wells and simulating the transport into the GZB or downgradient was not a numerical problem. But tracer simulation with tracer adding into the GZB infiltration filter caused oscillating concentrations in the GZB well and less oscillation in a larger radius. Even a reduction of the time steps to values less than one second (Courant number lower than 0.2) did not solved the problems. One of the reasons of these numerical problems may be, that the GZB well pipe was
Figure 7: Potential variation at the Karlsruhe-Knielingen research site with the GZB in the center. The figure shows one of the calibrations steps. The calibration targets of GMS visualize the errors of the calculation to field data at the monitoring wells. Always the potential line at the top and at the bottom of the aquifer is plotted. The model has a length of 100 m and a width of 80 m. The waterheads are in cm above a reference level of 90 m above sea level.

simulated with only four element columns in the radius. So strongly curved flow inside the well is not simulated good enough. Adding the tracer not directly in the center of the GZB well, but in a radius of 20 cm reduced this problem.

Transport simulations for tracer transport and the simulation of the remediation process have been carried out (Fig.8). After several days, a tracer, injected in the upper filter screen section of the GZB, is spread all over the vertical circulation cell. Only some of the tracer travels downgradient. After some weeks, a
downstream plume of the tracer is obvious. As Stamm$^4$ calculated for homogeneous aquifers, the width of the downstream plume at the upper aquifer is larger than at the bottom.

Conclusions

Here the 3-D numerical model of the flow and transport simulation in a groundwater circulation well (GZB) flow field at a research site in the southwest of Germany is presented. It shows the complexity of 3-D modeling for natural aquifers to include the different layers, heterogeneity and anisotropy. A sensitivity analysis has been carried out to show the effects of discretization to obtain accurate results for the special flow field in the vicinity of a GZB. The results show that for the simulation of a GZB the vertical discretization near the two filter screen sections must be as fine as the horizontal discretization. Up to now, the available hardware is still a limitation to fulfill this rule for optimal 3-D numerical simulations.

Even if the aquifer seems to be relatively homogeneous, the model shows the effects of the complex natural structure. The calibration of the model with 3-D potential measurements of multilevel monitoring wells shows good agreement. Hence the model results can be upscaled for other field problems and further studies.

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References