Development of a tool for efficient three dimensional reactive multicomponent transport modelling independent from the geohydraulic model system

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Abstract The groundwater in the Lusatian lignite mining district is extensively and sustainably affected by pyrite weathering. The geohydraulics at active mining sites and reclamation sites have been simulated for decades with user specific and well calibrated two- and three-dimensional regional groundwater flow models. Existing modelling software, which offers hydrogeochemical calculations in addition to geohydraulic calculations, requires the migration of existing regional groundwater flow models. This is costly and partially impossible due to special inner and outer boundary conditions. This paper shows the development of a reactive multicomponent transport model using PHREEQC and an existing geohydraulic groundwater flow model.

Key words geohydraulic modelling, hydrogeochemical modelling, groundwater, reactive multicomponent transport modelling, PHREEQC

Introduction

The groundwater in the Lusatian lignite mining district is extensively and sustainably affected by pyrite weathering. The processes of groundwater lowering at active mining sites as well as groundwater rising at reclamation sites have been simulated for decades with user specific and well calibrated two- and three-dimensional regional groundwater flow models. Increasingly, hydrochemical questions, such as the acidification of post-mining lakes, the inflow of iron-rich groundwater into watercourses and the discharge of contaminated water from dumps and piles are becoming more important. Reactive multicomponent transport modelling with hydrogeochemical functionality is the favoured tool to answer these questions. The use of modelling software, which offers hydrogeochemical calculations in addition to geohydraulic calculations, e.g. PHAST, requires the migration of the whole regional groundwater model including its inner and outer boundary conditions. The structures and limitations of the models are often incongruent or specific boundary conditions are not transferable. In the case of user-specific models, this transition is sometimes impossible because special boundary conditions are not transferable.

How can an existing regional groundwater model be used for reactive (hydrogeochemically based) multicomponent transport modelling? And is it possible to optimise these models for a large number of model cells and long-time predictions?

Initial situation

For decades, geohydraulic modelling has been an important planning tool in the Lusatian lignite mining area. In post mining rehabilitation for example, geohydraulic modelling plays a major role in the flooding of pit lakes and their interaction with watercourses. Geohydraulic modelling also provides a significant input for the long-term water resource planning and the management of mining-influenced river catchment areas.

There are several geohydraulic regional models in the Lusatian lignite mining district. The spatial extents of these models are mainly determined by the organizational units of the post mining (former open-cast mining sites or redevelopment areas) and the mining companies (active open-cast mines or production areas). The models are developed and operated by the companies themselves or on their behalf. The composition, the further development and the continuous adaptation of these models to changing boundary conditions and questions require a high personnel and financial effort. Therefore these models are also an economic investment and new developments would cost a lot of time and resources.

With the rise of the groundwater table in the Lusatian lignite mining area, hydrochemical questions play an increasingly important role in the planning proceedings of the mining and post mining companies. For example, predictions on the development of the water quality in pit lakes, the discharge of contaminants from dump sites and the contaminant inputs into watercourses are necessary. The required models are usually developed and applied separately for the specific issues. The hydrogeochemical model system PHREEQC is predominantly used. The PHREEQC model system is a highly flexible tool for hydrogeochemical calculations (Parkhurst et al. 2013).

In the Lusatian lignite mining district, PHREEQC is frequently used for hydrogeochemical modelling to predict the water quality in watercourses and lakes. The necessary water balances for the PHREEQC modelling are derived from hydraulic models for rivers, from water management models for catchment areas and from groundwater flow models. For the groundwater itself, hydrogeochemical modelling has so far only been carried out at a very low level of abstraction, for example by one-dimensional models or conceptual multibox models.

There are numerous models (e.g. OpenGeoSys, Hydrogeochem, TOUGH, PHT3D, PHAST), which combine geohydraulics with hydrogeochemistry. These models have the disadvantage that the geohydraulic part would have to be completely rebuilt and adapted for the respective questions of lignite mining. This would require a complex migration of the whole regional groundwater flow model including its specific inner and outer boundary conditions into the new model. The model structures and limitations of the respective models are often not identical. In the case of models developed for very specific questions in lignite mining, this transition is even impossible because their special boundary conditions are not transferable. A further disadvantage of the abovementioned models is that they often handle only a specific part of the hydrogeochemistry. This raises the question, how existing regional groundwater models could be used for reactive multicomponent transport modelling with the entire functionality and high flexibility of PHREEQC?

Methodological approach

For the coupling of a geohydraulic model with a hydrogeochemical model to a reactive multicomponent transport model the following basic methodological principles were defined:

- The coupling of the geohydraulics and the water quality is done offline. A feedback of hydro- and geochemical processes on the groundwater flow (e.g. density driven effects, buoyancy) are excluded. In the large spatial scales in which the model is to be applied, these effects are mostly negligible.
- The multicomponent transport model uses the model geometry of the geohydraulic model and the steady state or transient water balance calculated by it. Therefore the geohydraulic model must work according to the finite difference method (FDV) or the finite volume method (FVV) in order to maintain the water and mass balance in each model element. The geohydraulic model must provide the flow rates and the water level for each model cell in each time step.
- The full functionality of PHREEQC has to be available in every model cell to represent the hydrogeochemical processes. Therefore it must be possible to formulate and execute a specific PHREEQC script for each model cell.

By adopting the geometry and the water balance of the geohydraulic model, the complete congruence of the models with regard to geohydraulics is ensured and the construction of the multicomponent transport model is thereby simplified and accelerated. Using an appropriate pre-processor, the necessary structures of the multicomponent transport model are generated from the geometry and the water balance of the geohydraulic model. In this way changes in the geohydraulic model are automatically reproduced by the multicomponent transport model.

The solute transport is calculated by an explicit method. However, this method requires a time step limitation according to the Courant-Friedrichs-Lewy criteria. The calculation time step is then dependent on the spatial model discretization and the flow velocity.

The incorporation of PHREEQC into the multicomponent transport model is carried out using a template approach. The problem-specific PHREEQC scripts written by the user can be stored in the model and freely assigned to the model cells. For the calculation, the scripts are then supplemented with the water balance data and executed.

Technical implementation

The development of a corresponding software solution was necessary for the technical implementation of the above described methodological approach. The programming language C# was used for this.

First, a pre-processor was developed that imports the model geometry and the water balance of the geohydraulic model and forms the model structure of the multicomponent transport model (Figure 2). An Application Programming Interface (API) was implemented in the pre-processor to adapt to data structures of various geohydraulic models. Currently, the model geometry and water balance of the geohydraulic model PCGEOFIM® (Sames et.al. 2010) can be imported. This geohydraulic model is widely used in the Lusatian lignite mining district.

In the second step, the initial and boundary conditions for the quality of the groundwater, the geochemical declarations (phase models and kinetics) and the user defined PHREEQC scripts required for the calculation are imported by the pre-processor and assigned to the model cells by grid files (Figure 1, Figure 2).

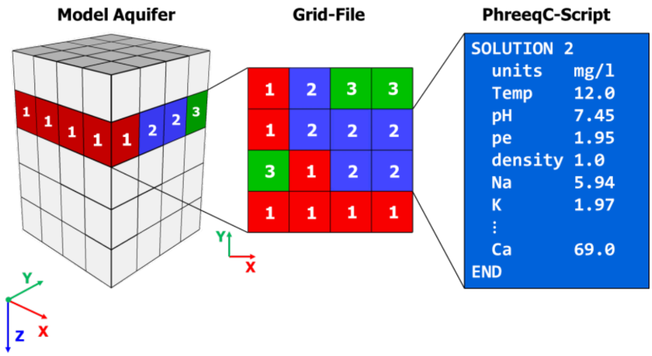

***Figure 1**: Assignment of PHREEQC scripts and the initial and boundary conditions to the cells of the multicomponent transport model using grid files*

The methodological approach for the multicomponent transport model is to calculate the water quality in each model cell with PHREEQC. However, the PHREEQC scripts can only be executed sequentially and single threaded. For models with several ten thousand model cells and long-term predictions of more than a hundred years this results in an immense calculation effort and thus a long calculation time. The calculation speed can be increased only within narrow limits by using powerful computer hardware. In order to carry out the model calculations in an acceptable time and at reasonable costs, an approach to parallelize the PHREEQC calculations has been developed.

For parallelization, the multicomponent transport model is split into segments at each time step. These segments are then distributed and calculated in a computer cluster (Figure 2). The computer cluster is set-up according to a client-server concept and can consist of one or more calculation servers connected via a network. Depending on the performance of the hardware, several PHREEQC instances can be used for the calculations on each calculation server. When the calculations for a time step have been completed, the results for the individual model segments are transferred from the calculation servers to a management client and reassembled to a complete model (Figure 2). The system developed for parallelization is very flexible due to the client-server concept and can be adapted to different structures. For example, the via a computer network connected office computers in a company or a university can be used for the calculations.

The computing speed achieved by the parallelization of the calculations cannot be increased infinitely. When the size of the computer cluster increases, the effort for cluster management, disassembling and reassembling of the model as well as sending and receiving data increases correspondingly (Amdahl, 1967). At a certain size of the cluster, the administrative expense exceeds the increase in computing speed. The optimum size of the computer cluster depends on the calculation tasks to be performed and cannot be reliably determined in advance. Therefore tuned benchmark tests are necessary for each problem.

The results of each time step are stored by the model and are available for analysis during the model runtime. The results of each time step can also be used as initial values for a new calculation. Thereby it is possible to calculate long-term predictions in shorter subsections. A postprocessor was also developed to evaluate the model results. The results can be displayed and evaluated as maps or videos, or for single points as time series.

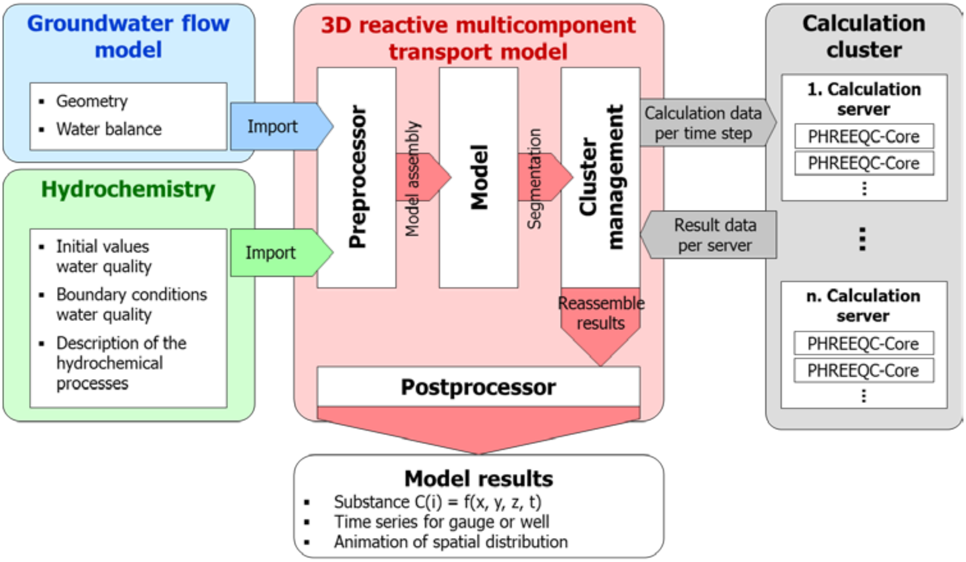

***Figure 2**: Structural scheme of the reactive multicomponent transport model*

Model test

A first test of the developed multicomponent transport model was carried out on a real problem. The question was, when and in what amount the discharge of contaminants from an opencast mine dump reaches a drinking water well gallery located north of the opencast mine.

The multicomponent transport model was constructed for an approx. 11x13 km subarea of an existing geohydraulic model. The model geometry and the steady state groundwater balance were imported unchanged from the geohydraulic model. The horizontal model discretization is 100x100 meters. In the vertical, the model is divided into seven aquifers. The tested multicomponent transport model consists of a total of 104,000 active model cells.

The conceptual geochemical model incorporates a set of 20 relevant chemical components (e.g. pH-value, alkalinity, anorganic carbon, sulphate, iron, calcium, magnesium). The model includes homogeneous and heterogeneous equilibrium reactions, such as complex formation and acid-base reactions as well as cation exchange, surface complexation, mineral solution and mineral precipitation. In addition, homogeneous and heterogeneous kinetic reactions are included, of which sulphate reduction is particularly important in this specific model application.

With the model test, the solute transport from the opencast dump was examined. For the results presentation, the parameter sulphate was chosen as an example. Sulphate concentrations of 1,400 and 200 mg/l were assumed for the groundwater in the dump of the opencast mine and for the groundwater in aquifers beside the opencast mine respectively. The exfiltration of the watercourses was assumed with 400 mg/l, the exfiltration of the lakes with 600 mg/l and the groundwater recharge with 0 mg/l sulphate.

From the model geometry and the steady state water balance, a calculation time step of 18 hours was determined taking the Courant-Friedrich-Lewy criterion into account. For a prediction of 100 years, the calculation of 48.700 time steps was therefore required. For the calculation, ten normal office computers with a total of 60 processor cores were connected via gigabit network. With this hardware configuration, the model calculation took about 20 days.

Figure 3 shows the predicted distribution of the sulphate concentration in the model aquifers along a vertical north-south section through the model at the beginning of simulation, after 50 years and after 100 years. In this illustration, it is clear that the sulphate discharge from the opencast dump in the direction of the well gallery occurs mainly in the upper three aquifers. In the lower aquifers, the solute spread is restricted by geological dislocations with low hydraulic conductivity. In addition, the dilution of the sulphate concentration in the dump by the groundwater recharge can be recognized.

Figure 4 shows the distribution of the sulphate concentration in the 3rd model aquifer at the start of simulation, after 50 years and after 100 years. In the illustration, the dilution of the sulphate concentration in the open pit dump, as well as the discharge of sulphate from the dump towards the drinking water well gallery are clearly visible. After approximately 80 years, the sulphate concentration in the well gallery begins to increase and the sulphate concentration has approximately doubled after about 100 years.

With the model test, the usability and the manageability of the developed reactive multicomponent transport model have been proven. In addition, optimization potential for a further increase in terms of calculation speed was discerned. In further model tests more functions will be checked and the prognosis capabilities of the model system will be extended.

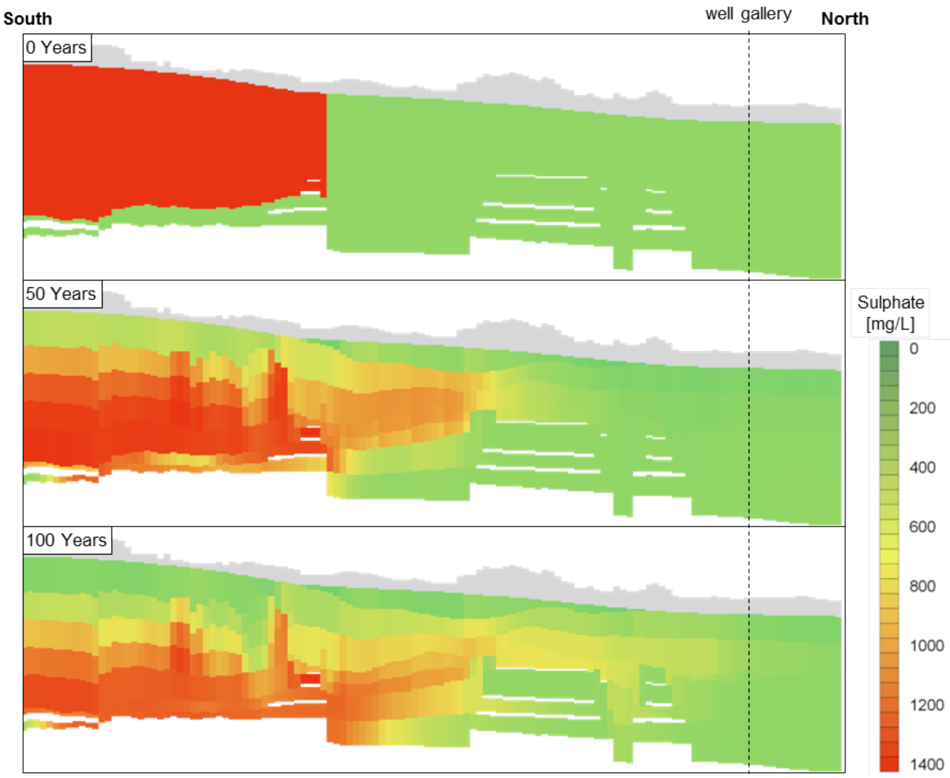

***Figure 3**: Distribution of the sulphate concentration in a vertical south-north section through the multicomponent transport model at the start of simulation (top), after 50 years (middle) and after 100 years (bottom)*

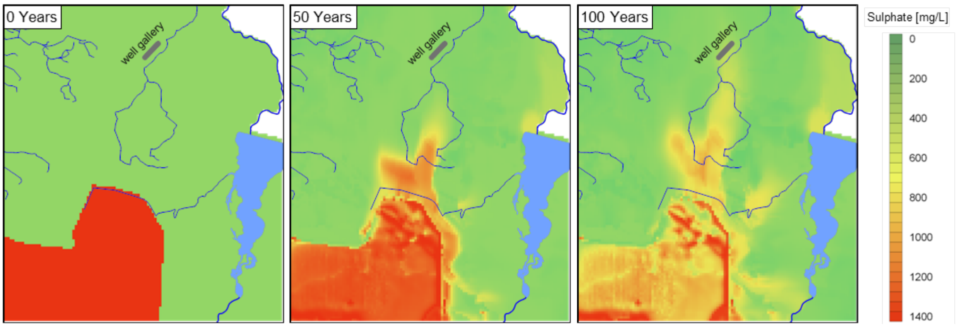

***Figure 4**: Distribution of the sulphate concentration in the 3rd aquifer of the multicomponent transport model at the start of simulation (left), after 50 years (middle) and after 100 years (right)*

Conclusions

With the first successful test of the reactive multicomponent transport model as an offline coupling of the geohydraulic model PCGEOFIM® with PHREEQC on the basis of a real problem, the practical feasibility of the developed model concept could be demonstrated. It has been shown that three-dimensional hydrogeochemical modelling with the full functionality of PHREEQC based on an existing geohydraulic model is possible in large areas for long prognosis periods with an acceptable calculation time.

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