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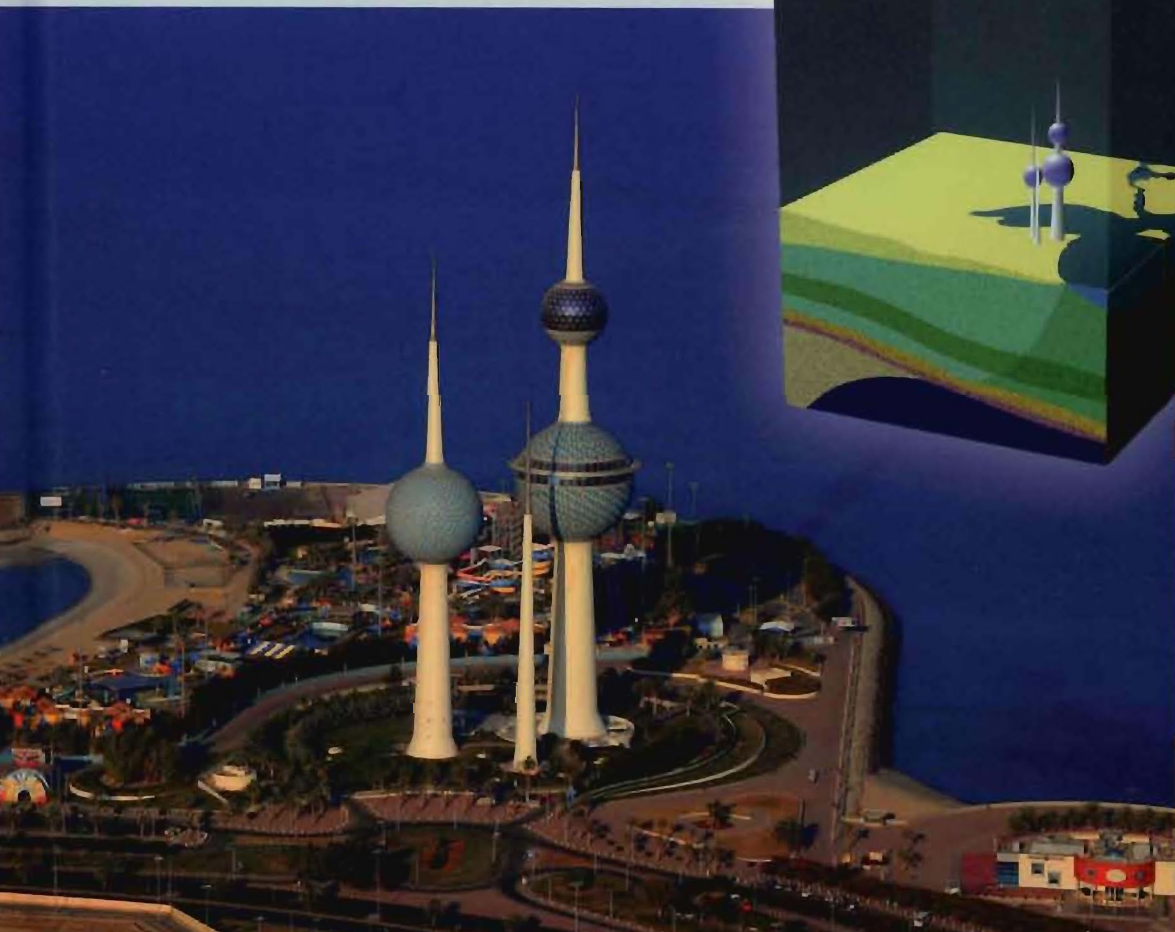

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Groundwater Modeling and Management under Uncertainty – Hadi & Copty (Eds)

Coupling of unsaturated and saturated soil zone models to estimate groundwater recharge in mining areas

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ABSTRACT: Groundwater recharge is an influential factor on the water balance for the simulation and management of open pit mining areas. Regarding it in a process-oriented way will enable the consideration of changing climatic conditions. To achieve a process-oriented calculation of groundwater recharge models of the unsaturated and saturated soil zone are coupled. Two individual simulation tools are the basis of the coupled model: PCGeofim® which uses the finite volume method to simulate 3D groundwater flow especially for mining regions and PCSiWaPro®, a 2D model that simulates the water balance by solving the RICHARDS equation for transient flow in the unsaturated soil zone. For the coupling exchange, processes and parameters are defined, new routines for the calculation of groundwater recharge are implemented and the differing discretizations of the two simulation softwares are adapted. Evaluation using lysimeter data is conducted to verify the modelled groundwater recharge fluxes with measured data.

1 INTRODUCTION

Lignite is currently Germany's most important source of energy (AGEB, 2012). Following the energy transition of Germany, the use of nuclear power is declining and lignite is the resource bridging the demand of energy until renewable energy sources can fill the gap. According to the Federal Institute for Geosciences and Natural Resources, German resources of lignite sum up to 35.2 billion tons (BGR, 2006). The main deposits of lignite in Germany can be found in the Rhineland region and in Central Germany around Leipzig and in Lusatia.

The management of these areas imposes a wide number of challenges, one being the management of the water balance. During the operation of the open pit area the water table needs to be lowered in order to access the coal seam. Afterwards the area is recultivated and the water balance needs to be brought back into a sustainable and self-regulating state. The water balance during and after operating the mining area is managed with the help of simulation models.

Two of the most important goals of managing the mining areas are energy efficiency and sustainability. Water resources can be saved when less water needs to be pumped out while the groundwater table is lowered artificially. Less pumping also leads to a lower energy demand. The effect of the lowered groundwater table on neighbouring wetlands and other habitats needs to be evaluated. When managing recultivated mining areas the main points of interest are the raising of the groundwater table and the flooding of post-mining lakes.

For the simulation and the determination of the water balance one of the main components is groundwater recharge. This parameter is especially important for the forecast of the vertical position of the groundwater table which needs to be assessed in order to determine different mining water management strategies.

Groundwater recharge is highly dependent on the land use and plant coverage, the shape of the topographic surface, the heterogeneity of the soil structure in the unsaturated soil zone and on the intensity and variability of precipitation. To take this into consideration, transient time series of climatic conditions have to be used for water balance prognosis. Furthermore, modelling of mining areas is usually carried out by investigating the water balance over several decades. Considering climate change and its effects on different climatic measures therefore is a crucial factor for the management of mining areas.

For Central Germany, climate change is reported to result in more precipitation in the winter months and less precipitation in summer with longer dry periods and an increasing number of extreme rainfall events (SMUL, 2005). The effects of these climatic changes on groundwater recharge are still a matter of research. Some studies prognosticate a strong decrease of recharge rates for Saxony (Hattermann et al., 2004; LfULG, 2008).

However, open questions for mining areas that result from the changes are adaption of post-mining management, pit slope stability and interference of heavy stormwater events with open cast areas that are still in operation. Heavy rainfall can lead to saturated slope areas that allow landslides. Concepts of the filling up of post-mining lakes need to consider changing groundwater and river discharge regimes (Kaltofen et al., 2004).

To adequately simulate the complex processes of the water balance in mining areas models are needed that depict the system in a sufficient way. In the last decades a couple of models have evolved that describe the water balance in the groundwater zone with good accuracy for plenty of applications. MODFLOW (Harbaugh, 2005) is the most commonly used groundwater simulation tool. It shows, however, disadvantages in the spatial discretization of the soil zone as it uses finite difference method, which is geometrically inflexible due to its rectangular grid (Kinzelbach & Rausch, 2005). FEFLOW (Trefry & Muffels, 2007) is based on the Richards equation and the finite element discretization method. PCGEOFIM® (Sames et al., 2008; Müller et al., 2003) is used as the standard modelling tool in the open-cast mining regions of Central Germany. It regards the particular needs of mining by integrating the distinct time-dependent open cast mining phases (extraction, refilling, post-mining lakes). It is based on the finite volume discretization method. The software is equipped with a set of unique boundary conditions that are especially designed for mining areas, such as injection und pumping wells and surface water groundwater interaction (lakes, rivers).

Groundwater recharge can be indicated as constant, dependent on the groundwater table height and as a given time series.

As groundwater recharge is one of the most important boundary conditions for the groundwater zone it is essential to model it in a process-oriented way instead of using constant average values. Not only does process-oriented modelling lead to more exact results considering different atmospheric and soil conditions but it also introduces the possibility of including climatic changes into mining management. To achieve this, the unsaturated soil zone and transient upper boundary conditions have to be regarded for modelling. The introduction of the RICHARDS-based unsaturated soil zone model PCSiWaPro® (Gräber et al., 2006) together with its associated weather generator WettGen (Nitsch et al., 2007) into mining management will result in a coupled model that is going to reflect the interactions between the unsaturated and the saturated soil zone and thus will lead to a better representation of the whole water balance in the modelling area.

2 MODELING OF SATURATED AND UNSATURATED SOIL ZONE PROCESSES

The saturated zone is defined as the soil zone beneath the water table where all pores are filled with water under pressure greater than atmospheric. The unsaturated soil zone describes the zone between the soil surface and the groundwater table. Pores may contain either water, gas or both. Due to these prerequisites, different aspects for modelling these areas of soil need to be regarded which leads to differing equations that describe these particular processes and hence differing models to simulate the processes.

2.1 *The saturated soil zone: PCGEOFIM®*

PCGEOFIM® is a 2D/3D simulation software for modelling groundwater flow. It solves the groundwater flow equation numerically with finite volume discretization.

$$S_0 \frac{\partial h}{\partial t} + \frac{\partial}{\partial x_i}\left(k_f \frac{\partial h}{\partial x_i}\right) = V_V \tag{1}$$

In Equation 1 the following terms are included: storage coefficient S_0, pressure head h, time t, hydraulic conductivity k_f and volumetric flow rate V_v.

The finite volume method integrates over a finite volume element. PCGEOFIM® uses a regular rectangular grid in the horizontal. For the case without local grid refinement, each cell has no more than six neighbours. Cells at the top, the bottom or the side of the model domain have fewer neighbours. Figure 1 gives a visual impression of a typical discretization. There can be missing elements in the vertical direction as indicated in Figure 1 with the arrow labelled "hydraulic connection". For this connection a leakage coefficient can be specified that controls the flow between the two neighbouring cells. This provides an alternative for representing aquitards by a leakage coefficient rather than by an own layer. If the flow in the aquitard itself is not of interest this method can help to save elements and therefore to speed up execution. Both approaches can be combined in one model as can be also seen in Figure 1.

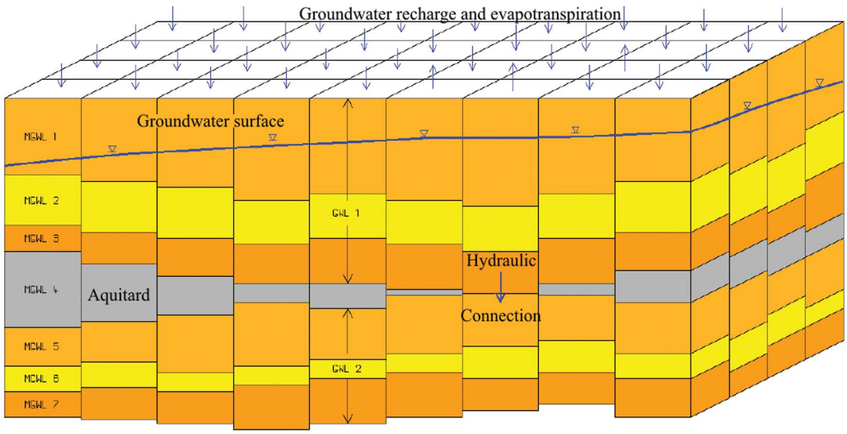

Figure 1. General discretization of a PCGEOFIM® grid.

For the flow calculation between cells an average hydraulic conductivity is used. It is determined by the harmonic mean. Therefore, the smaller values determine the resulting conductivity. The groundwater balance is calculated for each finite volume cell. The numerical implementation allows stable rewetting of cells that contained water in the previous time step. This is especially useful for the high amplitudes of changes in groundwater level which are typical for mining regions.

PCGEOFIM® provides a wide array of boundary conditions. Dirichlet, Neuman, and Cauchy boundary conditions are implemented in different variations. They can be constant or variable in time. According to the specified constrains, boundary conditions can switch between Dirichlet and Neumann boundary conditions. If given upper or lower limits of q or h are reached the behaviour of the boundary condition changes. All of the variability provides flexible boundary conditions that can represent a wide range of natural and anthropogenic conditions such as vertical and horizontal wells, or pipes with a limited flow capacity. Hydraulic conductivity parameters as well as geometric dimensions can be made time-dependent to account for changes in flow conditions and in model geometry due to mining activities. Two boundary conditions are implemented to include influences from surface waters onto the groundwater zone.

Lakes can be represented by a dynamic Cauchy boundary condition. For each lake one balance equation is added. A specified water table/volume function for the lake is used to calculate the current lake water table from its current volume, which in turn is calculated from all subsurface and surface flows including evaporation. Groundwater elements can be coupled to the lake in the vertical or horizontal direction. The balance equations are solved together with the linear system of equations for the flow problem.

Rivers can be represented in the model as Cauchy boundary conditions. They can enter each other in a hierarchical fashion. Required data includes a water table-discharge relationship, river-bottom elevation, initial water table, and inflow of the river at spring or at the outer model boundary if the river enters from outside the model. Different values can be specified for the colmatation coefficient, depending on the direction flow. Thus, infiltration can be made much smaller than exfiltration. The calculated discharge of the river at the outflow from the model can be used as additional criteria for verification of the model accuracy, if measured discharge values are available. Unlike the lake boundary condition, the river boundary condition is solved in a separate system of equations. Iterations are performed between river and the groundwater system of equation until convergence is reached.

2.2 *The unsaturated soil zone: PCSiWaPro®*

PCSiWaPro® simulates water flow in variably saturated soils under both steady-state and transient boundary conditions. The flow model can be described by the RICHARDS Equation 2.

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x_i}\left[K\left(K_{ij}^{A}\frac{\partial h}{\partial x_j} + K_{iz}^{A}\right)\right] - S \qquad (2)$$

The equation contains the volumetric water content θ, pressure head h, spatial coordinates x_i, time t, and $K_{ij}{}^{A}$ as components of the dimensionless tensor of anisotropy **K**. S is a source/sink term, which includes root water uptake. The equation is a strongly nonlinear partial differential equation which requires a numerical solution of the equation system. This relationship between water content and pressure head can be described by the soil water retention curve. This function can be parameterized by the VAN-GENUCHTEN-LUCKNER (Luckner et al., 1989) Equation 3.

$$\theta = \theta_{r,W} + \frac{\phi - \theta_{r,W} - \theta_{r,L}}{\left[1+\left(\alpha * h_c\right)^n\right]^{1-\frac{1}{n}}} \tag{3}$$

Φ is the porosity of the medium, h_c characterizes the pressure head difference between the wetting and non-wetting phase. α and n are empirical VAN-GENUCHTEN parameters. The simulation tool PCSiWaPro® implements this relationship to solve the RICHARDS equation in the vertically-plane dimension with transient or steady-state boundary conditions, using a numerical finite element approach. For the solution of the nonlinear system of equations originating from discretizing the RICHARDS equation an iterative preconditioned conjugate gradient solver is used.

The weather generator WettGen (Nitsch et al., 2007) has been implemented for the generation of synthetical climate time series. Measured time series in the vicinity of the investigation site are statistically analyzed. Through spatial interpolation of the statistical parameters to the location of the modeling site a set of local parameters is obtained, which is then used to sample local time series. Precipitation, potential evaporation and potential transpiration can be calculated taking site and vegetation characteristics into consideration.

2.3 *The combining factor: Groundwater recharge*

Groundwater recharge is the access of infiltrated water to groundwater (DIN 4049-3, 1994) and the shared boundary of the unsaturated and saturated soil zone. It is an important measure for the ability of groundwater resources to regenerate.

The main contributing factor to groundwater recharge is seepage water that arises from precipitation (N). Groundwater Recharge (GR) can be calculated as the residual of the water balance (Eq. 4) by considering the actual evapotranspiration ET_a and the fast runoff Q_D (surface runoff, interflow).

$$GR = N - ET_a - Q_D \tag{4}$$

This Equation 4 is used to calculate recharge rates for longer time periods as it doesn't consider fluxes to or from neighbouring aquifers or from lakes and rivers. Furthermore, runoff can be only quantified in defined catchment areas. The quantification of local groundwater recharge is therefore a subject of simulation tools.

3 COUPLING SCHEME FOR PCSiWaPro® AND PCGEOFIM®

After the evaluation of different coupling concepts (Sallwey et al., 2012) the first prototypical implementation was chosen to be a merging of the horizontal 2D model of the unsaturated zone with a 2D planar cross section of the PCGEOFIM® groundwater model (Fig. 2).

The common interface of both models is the groundwater table. As its depth can vary during the runtime of the simulation both the PCSiWaPro® as well as the PCGEOFIM® model have to cover the whole area in which the groundwater table can possibly lie during the simulation.

For the coupling particular focus lies on adjusting the different spatial and temporal discretizations. As shown in Figure 3 defined time steps have to be met by both models to exchange the transfer parameters.

The coupling between the two models will be online, meaning that for each time step of the predefined exchange time pattern the models will exchange three transfer parameters.

a. Groundwater recharge at the current groundwater table is calculated with the PCSiWaPro® model and transferred to PCGEOFIM®
b. Vertical position of the groundwater table is calculated by PCGEOFIM® and transferred to PCSiWaPro®

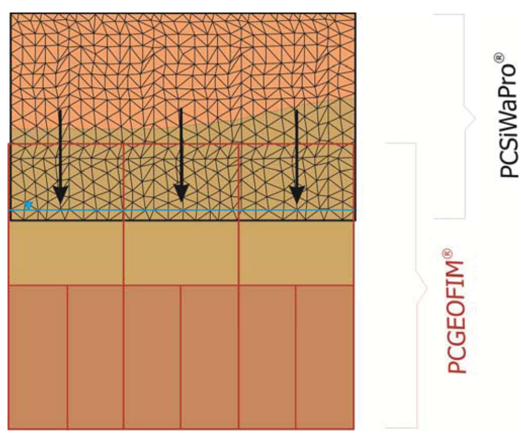

Figure 2. Coupling scheme in a soil section with three different soil types with overlapping discretizations of PCSiWaPro® (black) and PCGEOFIM® (red) to ensure the groundwater table (blue) lays always within both model domains.

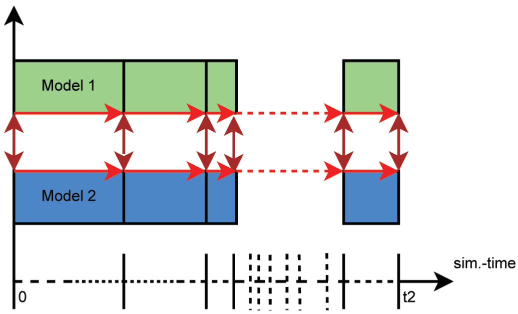

Figure 3. For the parallel interaction sequence both models compute simultaneously and exchange data at a predefined exchange time pattern. The exchange times have to be met exactly but not necessarily with the same amount of time steps.

c. Horizontal discretization of the PCGEOFIM® volumes which includes the current groundwater table is transferred to PCSiWaPro®.

Groundwater recharge is applied as an upper boundary condition to the groundwater flow model. The depth of the groundwater level cannot be used directly as a lower boundary condition in PCSiWaPro® since the groundwater table is generally situated at a depth somewhere within the model domain and boundary conditions only apply to model boundaries.

The implementation of the groundwater table into the unsaturated soil zone model is therefore carried out by using a variable pressure head boundary condition at the bottom of the model and adjusting the nodal values of the pressure head in the area that is covered by groundwater according to exchange parameter (b).

This approach, however, interferes with the way the water balance is calculated in a PCSiWaPro® model. To level out the water balance equation, an artificial term has to be introduced to account for the manually added or removed amount of water. This term is determined by calculating the volume of water before and after the manual adjustment of the pressure heads. The difference between the two quantities is then interpreted as an artificial influx into or outflux out of the model.

While PCSiWaPro® uses a discretization of finite elements to numerically solve its differential equations; PCGEOFIM® deploys the finite volume method. Exchange parameters (a) and (b) have to be calculated separately for every single PCGEOFIM® volume. This calls both for an individual groundwater recharge calculation for each volume, as well as for a volume-dependent (and therefore x-coordinate-dependent) adjustment of the pressure head values inside the PCSiWaPro® model. Depending on the current depth of the groundwater table the mapping of PCSiWaPro® nodes onto PCGEOFIM® volumes can change. It is necessary to exchange the corresponding horizontal discretization of the two models at the current groundwater table for each data exchange time step.

3.1 *Calculating groundwater recharge in PCSiWaPro®*

To date fluxes were only calculated over model boundaries and internal fluxes have not been considered in PCSiWaPro®. As the groundwater table lies somewhere within the model domain a new routine has to be implemented to calculate groundwater recharge at any point inside of a PCSiWaPro® model.

At first the nodes which form the groundwater table at the current time step are determined (Fig. 4). The groundwater table is distinct by identifying the set of nodes whose pressure head is equal to or greater than zero and who have at least one neighbouring node whose pressure head is below zero. Since due to infiltration and ponding effects an identical scenario can also occur in the upper parts of the unsaturated soil zone model that do not belong to the groundwater table, the depth of the water table that is received from PCGEOFIM® in the previous time step is used as a first estimate for the vertical coordinate to find the corresponding nodes.

The calculation of nodal fluxes q for the nodes of the current groundwater table is carried out by using the pressure heads h at the node itself and at the neighboring nodes, combined with geometry data of the finite elements (Eq. 5).

$$q_z = -\frac{K_n}{N_e}\sum_{e_n}\left[\frac{\gamma_i^z h_i + \gamma_j^z h_j + \gamma_k^z h_k}{2A_e} + K_{zz}^A\right] \qquad (5)$$

$$\gamma_n^z = K_{xz}^A b_n + K_{zz}^A c_n$$

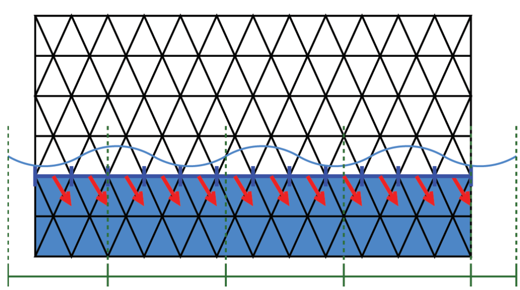

Figure 4. Schematic visualization of groundwater recharge calculation in PCSiWaPro® (black lines) and the mapping onto PCGeofim® volumes (green lines). The actual groundwater table (light blue line) is approximated by the closest mesh nodes (dark blue line). The arrows represent groundwater recharge fluxes.

N_e is the number of subelements e_n that are adjacent to node n. Each boundary segment γ_i^z that is connected to node n can be determined with geometrical shape factors b_n, c_n and components of the dimensionless anisotropy factor K_{ij}^A. A_e is the area of the triangular element. The computation of q_x is carried out analogously to Equation 5.

By multiplying the nodal fluxes with the length of the element edges that form the groundwater table, the values of groundwater recharge for the whole length of the groundwater table are calculated. Since the horizontal length of one PCGEOFIM® volume element usually comprises more than one groundwater table element edge in the PCSiWaPro® model, the calculated edge fluxes have to be grouped and added to determine the final groundwater recharge value for each PCGEOFIM® volume.

3.2 *Validation of groundwater recharge calculation*

To ensure that the calculation of the groundwater recharge delivers consistent results benchmark testing was conducted.

As direct measurements of the groundwater recharge are not easily accessible, lysimeter data was used. The investigated lysimeters are 3 m high soil columns with several soil profiles from different regions in Germany. These lysimeters are situated in Brandis, Germany and measurements of the soil water balance and climatic measures have been undertaken since 1980 (Haferkorn, 2000).

Measured values of the seepage water, pressure heads and climatic factors were used to validate the simulated model results against the measured lysimeter data.

Figure 5 exemplarily shows the results of a 3 m column of undisturbed eroded cambisol. The PCSiWaPro® model consisted of a 3,5 m column, with a groundwater table lying in 3 m depth. The comparison between the simulated and measured values shows that the new routine for calculating groundwater recharge can predict the time variation of the outflux very well. The exact flow values of the peaks could not be reached.

For one the VAN-GENUCHTEN soil parameters, which drive water flow in the unsaturated soil zone, were determined with the help of the VEREECKEN pedotransfer function (Vereecken et al., 1989). As pedotransfer functions are empirical functions, they introduce inaccuracies into the model results. A laboratory distinction of these parameters would improve their accuracy.

Furthermore, the PCSiWaPro® model does not consider macropores. As the lysimeters are planted with the same crops that surround the lysimeter station, it can be assumed that because of the

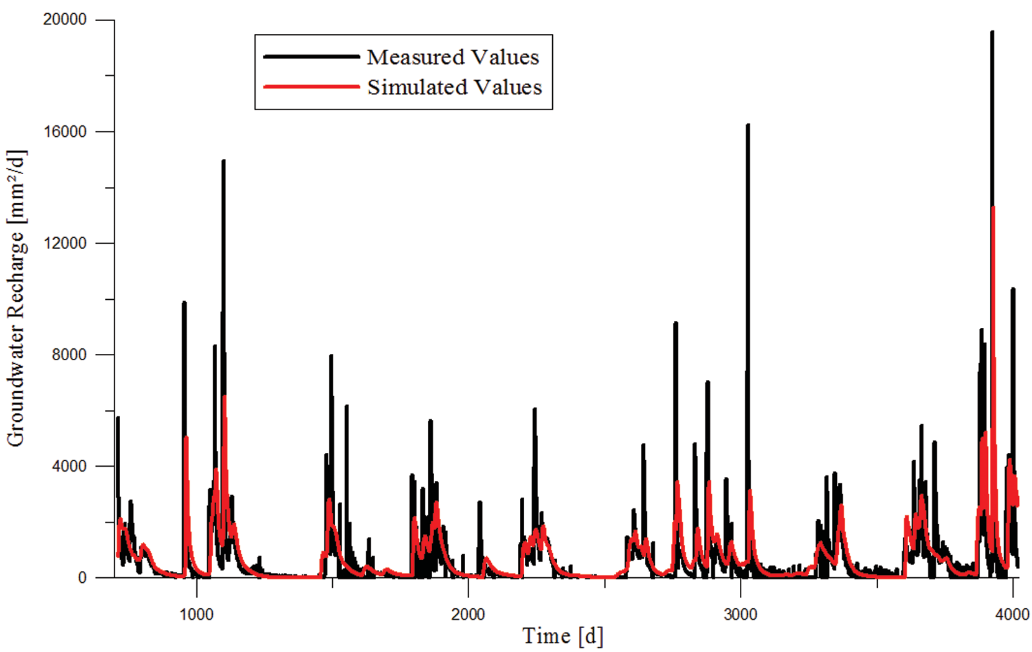

Figure 5. Comparison of measured values of the groundwater recharge (seepage water from lysimeter) and groundwater recharge values obtained from the new computation routine implemented into PCSiWaPro®.

agricultural use macropores form up in the soil. Comparing investigations with the HYDRUS software package for dual porosity modeling (Šimůnek et al., 2012) showed that macropores are a highly sensitive parameter and are able to create outflux out of the lysimeter in the quantities that were measured.

However, even with the lack of exact soil parameters and modeling of macropores the results show that the calculation of groundwater recharge with the new routine is exact within characteristic uncertainty boundaries.

4 DISCUSSION

Both models have undergone changes to enable the input and output of the transfer parameters and to adjust the simulation code for the calculation of coupling-related values. First runs with the coupled model system have been conducted.

As the coupling with PCSiWaPro® will slow down the simulation runtime of PCGEOFIM® efforts have been made to decrease the individual computation times of the simulation tools. To achieve this parallelization of the codes has been undertaken, which achieved significant speed-up times (Meyer et al., submitted). Parallelized simulations of the unsaturated soil zone are of special interest for the computation of horizontal cross sections of mining areas. Their general measures of more than 1,000 m length are posing a challenge to computational solvers as the number of nodes rises to 100,000 and more. With the help of parallelization models with a high number of nodes can be calculated within reasonable time frames.

Validations with measured data have proven that the calculation of internal fluxes works well for the calculation of the groundwater recharge. The new routine uses values which are of lower precision than the simulated pressure heads, since these values are calculated after the numerical solution of the Richards equation is obtained. Using an individual routine to calculate the fluxes as a direct by-product of the solution of the Richards equation would result in an accuracy which is equal to the simulated pressure heads.

The adjustment of the groundwater table after each time step is necessary because the unsaturated soil zone model cannot depict the whole aquifer and therefore is not able to consider fluxes from or into other aquifers. The changing depth of the groundwater table entails the change of the pressure head values in the nodes surrounding the groundwater table. It is apparent that nodes that change from the unsaturated to the saturated zone obtain pressure head values of zero and above according to their distance to the groundwater table. However, it is not as straightforward to calculate the pressure head values for nodes that change from the saturated into the unsaturated soil zone after the groundwater table drops. The current solution is to linearly interpolate the pressure head values between the new groundwater table and a given point in the unsaturated soil zone. The resulting values are a good approximation but further research has to be put into the question if linear interpolation is the best method to calculate values in the capillary fringe.

5 SUMMARY AND OUTLOOK

As part of a research project to ensure energy efficient and sustainable mining water management a concept has been developed to couple a groundwater simulation model with an unsaturated soil zone model.

The basis of the coupled model is the merging of two-dimensional cross-sections. The groundwater table was identified as the common interface and the exchange of groundwater recharge values and the water table depth during the simulation runtime is considered.

First implementations have been carried out by calculating groundwater recharge for a groundwater table lying in an arbitrary depth inside the unsaturated soil zone model. This new routine has been successfully tested against measured lysimeter data. Implementations of data input and output routines into PCGEOFIM® and PCSiWaPro® have been successful. First runs of the coupled model have been conducted.

Further tasks lie in the testing of different data exchange formats, the ensuring of stable coupled model simulations and the validation of the results from the coupled model simulation. Software communication between the two models is currently carried out by text files. Tests with exchanging data by shared memory variables proved to be a faster and more stable approach in comparison to text or binary files. The applicability for this coupled model system will be tested and if successful shared memory variables will be integrated.

With the help of the coupled model, simulations are going to be undertaken that regard the unsaturated soil zone and show its importance for management of the water balance in mining areas. Case studies can be conducted that simulate the effect of different climate change scenarios on the management strategies.

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