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MODELLING AND PREDICTION OF THE QUALITY OF MINE DRAINAGE WATER USED FOR THE DRINKING WATER SUPPLY IN THE GDR

Luckner, L. and Hummel, J.

Research Group for Open-Cast Mine Dewatering of the Großräschen Institute for Lignite Mining and the Dresden Technical University, GDR

ABSTRACT

The necessity of the use of mine drainage water from lignite mining for the supply with potable water in the GDR derives from an analysis of the use of water resources. Problems of the supply with drinking water arise especially due to the varying mine drainage water quantity and quality in space and time depending on natural and technological factors of mining. The design and the later operation of waterworks using such drainage water as raw water require applicable models for the prediction (simulation models) of the available water quantity and quality as to spatial distribution and time. The state of research and development work reached in the GDR is explained.

NECESSITY OF THE UTILIZATION OF MINE DRAINAGE WATER

The average yearly precipitation in the GDR amounted to 607 mm a^{-1} for the period of 1901 - 1970. At an average evapotranspiration rate of 447 mm a^{-1} a run-off rate of 160 mm a^{-1} remains for use. For the whole area of the GDR we assume the rate of underground run-off (equal to the rate of groundwater recharge) to be about 80 mm a^{-1}, which yields the stable water resource of approximately $9 \cdot 10^9$ m^3 a^{-1}. Nowadays, this resource can be increased by water from reservoirs and controlled lakes by approximately $1 \cdot 10^9$ m^3 a^{-1}. To attain an additional increase is very difficult. This means, the stable and regulated water resources in the GDR total about $10 \cdot 10^9$ m^3 a^{-1} today and also in the future.

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For the balance year 1975 the water demand of the main users was as follows /1/:

User	Surface water demand	Groundwater demand
Population	$0.2 \cdot 10^9\ m^3\ a^{-1}$	$0.6 \cdot 10^9\ m^3\ a^{-1}$
Industry	$5.4 \cdot$ "	$1.0 \cdot$ "
Agriculture	$0.9 \cdot$ "	$0.2 \cdot$ "

The water losses of the stable and regulated water resources amounted to about $2 \cdot 10^9\ m^3\ a^{-1}$ in industry (caused especially by open cooling systems) and in agriculture (caused ~~by~~ especially by the evapotranspiration in crop production).

The water demand in the GDR is steadily increasing due to the rising living standard of the population, the highly developed industry and the industrialized agriculture. The demand amounted to $8.3 \cdot 10^9\ m^3\ a^{-1}$ in 1975, $9.5 \cdot 10^9\ m^3\ a^{-1}$ in 1980 and is predicted to rise to about $11 \cdot 10^9\ m^3\ a^{-1}$ in 1985. The rate of drinking water demand increase is expected become 3 per cent every year in the future /2/.

From this balance of water supply and demand the necessity of multiple uses of water resources can be derived. In industrial centres of the GDR already today water is used 7 to 8 times. The widespread pollution of the surface water resources led to a relatively high degree of utilization of the groundwater resources for the drinking water supply. But the groundwater resources are very limited in the GDR. It is predicted that only 35 % of the additional drinking water demand to be met in the next time can be covered by groundwater resources which will be newly explored. This means, the largest part of the additional drinking water supply in the GDR is to be covered directly from rivers or lakes or indirectly by the artificial groundwater recharge. But these possebilities are expensive and involve health hazards, especially caused by the permanent changes of the surface water quality due to new chemical substances (often unknown in the waterworks). Such changes and their consequences are very hard to predict. For that reason in the GDR a large part of the additional drinking water supply should be met from the open-cast mine drainage.

The annual output of lignite by open-cast mining in the GDR amounts to more than 250 million tons. It is necessary to pump out about $1.5 \cdot 10^9\ m^3\ a^{-1}$ mine water using about 7000 dewatering wells. For 1990 an output of about 300 million tons of lignite is planned.

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Then it will be necessary to pump out more than $2 \cdot 10^9$ m^3 a^{-1} mine water.

Up to now, only a small share of this water has been used /3/. So were used, e. g., only about 30 % of the 0.9 · 10^9 m^3 a^{-1} mine drainage water for water supply in the Lusatia area. The costs of this utilization are relativly low. They amount, for example, only to about 0.10 M/m^3 for the drinking water production in a waterworks of that area with a capacity of about 4 · 10^5 m^3/d. In contrast to that, the equivalent costs of the utilization of surface water in that area amount up to 1.50 M/m^3. A new regulation valid from the beginning of 1981 promotes the utilization of mine drainage water for the drinking water supply in the GDR. On this basis, the producer of drinking water gets 0.70 M/m^3 from the distributor and the distributor gets 0.90 M/m^3 from the consumer. This leads to an economic incentive for the liquite open-cast mines to produce drinking water.

PROBLEMS OF THE UTILIZATION OF MINE DRAINAGE WATER

The problems can be divided into two groups: problems of water quantity and problems of water quality.

Problems of Water Quantity

Up to now, in the GDR the principle has been followed to use the groundwater resources only to such an extent as they are naturally or artificially recharged. Groundwater recharge is referred to as dynamic groundwater resources, in contrast to the static groundwater resources. Only these are used in our groundwater works, because in doing so the ecology is disturbed to a minimum degree. Of course, the utilization of mine drainage water leads to the utilization of static groundwater resources to a large extent. Therefore, problems will arise when the static resources are used, and especially after closing down the mines when the groundwater table in the mined area is rising again.
In any case, the designing of a waterworks using mine drainage water requires a prediction of the amount of groundwater to be used during the period of mining as well as during the reclamation period.

The problems emerging during the mining period comprise especially the changes of the groundwater yield as to space and time. These changes are determined by the technology of mining. Of course, water is only an accompanying raw material in lignite mining and it is impossible to plan the groundwater pumpage on the basis of the water demand. Therefore, we see primarily the way to predict the mine drainage water yield on the basis of the optimal

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mining technology and to design such a waterworks on the basis of the so determined minimum mine drainage water output, which is regarded as the so-called "safe"mine drainage water output. Naturally, there are many possibilities to get a higher than minimum safe mine drainage water output. Most of them are based on the attempt not to optimize the mining technology alone but to optimize the lignite mining and water winning technologies together. Naturally, such an optimization necessitates very fast but also sufficiently detailed models for simulating the dewatering process as parts of the whole optimization procedure. In any case, it is a relativly easy possibility to use drainage water from several open-cast mines that are in operation over a long period of time, because the sum of the pumped water from all these mines is more equalized than that from a single one.

Problems of Quality

All groundwater resources which are utilized today or are to be used in the future for drinking water supply are protected in the GDR. Legal regulations stipulate the size of such protection zones (there are three zones) and the possibilities of their agricultural and other utilization and management.

Of course, it is impossible to comply with these regulations in open-cast mines. Up to now, it has been impossible in the GDR to pass a special legal regulation for protection zones in mined areas. This problem will play an important role in the future. But, independent of this fact, mine drainage water is and will be used for the drinking water supply in the GDR. In any case, the health hazards are less than in the case of the utilization of surface water from big rivers (for example from the river Elbe), as it is done nowadays and is planned for the future, too. Also for such rivers it is impossible to establish protection zones.
The pumped mine drainage water should be transported to the waterworks through closed pipes. Open canals involve too great risks of pollution.
At all times there have been many industrial activities and waste dumps in mining districts connected with contamination risks for mine drainage water from heavy metals, phenols, organic substances and other contaminants which are not unimportant. Only by means of reliable simulation methods it is possible to predict the migration of such contaminants from their sources to the pumping wells and,consequently, the mine drainage water quality to be expected during the process of dewatering of open-cast mines or in the phase of reclamation.
Another risk for the utilization of mine drainage water for the drinking water supply in the GDR is the salt water intrusion (salt water coning). In several lignite

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fields salt water is situated not very deep below the lignite seams, so that pumpage causes the risk of salt water intrusion (coning). The salt in the mine drainage water naturally causes many difficulties in the drinking water production in the waterworks, if such a raw water quality was not expected, or, if such a quality was expected at least the costs of drinking water production will be very high.

Last not least, in mining regions the quality of groundwater resources is strongly affected by the oxidation of pyrite. During mining the underground is aerated for a longer period of time. The flushout of the oxidation products with the percolation water in the aerated zone or the rise and fall of the groundwater table in such areas leads to discharges that are often very acid. Especially the acidity of drainage water in spoils is very high. The problems of the high acidity of the water from lignite open-cast mines in the GDR are caused by the low neutralization capacty (lime content) in the geological formations of lignite mining regions. Of course, many of these problems are avoidable by such a placement of the pyritic materials that oxygen cannot reach this material. Also top-soiling, liming and rapid replanting of spoils may be effective tools for the minimization of the acidity-generation.

MODELLING OF THE QUANTITY AND QUALITY OF MINE DRAINAGE WATER

The design and later operation of waterworks using mine drainage water as raw water for the drinking water production require applicable models for a reliable long-term prediction of the available water quantity and quality as to space and time. This detailed prediction therefore requires process-simulation models of a new quality as compared with models used for the design and control of classical groundwater works.
At the first stage, these models will be conceptional distributed parameter models. They have to be capable of taking into consideration all physical, chemical and biological reactions.
Of course, in the future it will be also necessary to transfer these models into conceptional block models, because only such models allow a fast operation at a reasonable computational expenditure. In any case, such models must allow the simulation of soil and ground water flow as well as of chemical characteristics (e. g. condentration of sulfates, iron, toxic substances and acidity). Such coupled models of flow-rate and water-quality are also termed migration models. Practically only computer models can meet the objectives mentioned above.

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The computer simulation of the flow processes in mining areas has reached a relatively high level in the GDR /4/, /5/, /6/, /7/. This is also true for the computer simulation of the water movement in unsaturated media /8/, /9/. Compared to that, the computer simulation of migration processes is still in the development stage /10/. Up to now, we have developed only the computer program SIMKA-2 D /10/ for practical investigations - all the other models serve only research purposes.
In SIMKA-2 D it is assumed that the groundwater or soil-water flow regime can be approximated by a two-dimensional (2 D) stationary flow field. That means, we can represent the non-stationary water flow process in the time period of interest (or a part of the whole period) by a stationary one with sufficient accuracy. Such a flow field has to be subdivided in to several stream tubes. In each of these tubes the one-dimensional migration process is simulated on the basis of the following mathematical model /11/, /12/:

$$D_{\xi\xi}\ \partial C^2/\partial \xi^2 + D_{\eta\eta}\ \partial C^2/\partial \eta^2 - v_\eta\ \partial C/\partial \eta = \alpha\ \partial C/\partial t + \beta C + \gamma \qquad (I)$$

Here η is the direction of the flow velocity and the ξ -axis is normal to it. The dispersion coefficients $D_{\eta\eta}$ and $D_{\xi\xi}$ are

$$D_{\eta\eta} = \delta_L v_\eta + D_M \qquad (Ia)$$

$$D_{\xi\xi} = \delta_T v_\eta + D_M. \qquad (Ib)$$

The flux oriented (perpendicular) transversal to the streamlines, caused by the transversal hydrodynamic dispersion, is taken into account in the source term determined by an iterative procedure or at the point of time $t - \Delta t$.

This model seems to be applicable to the prediction of the effects of point and also non-point pollution sources on the well water quality during the mining phase with sufficient accuracy. For such an investigation it is at first necessary to identify the pollution sources, including their causes, and possible generation-rates as well as the duration of pollutant disposal. On this basis, we can identify the potential pollutants, the main processes of their generation, their mobility in the saturated or unsaturated zones and also the mechanism of their movement from the source into the moving groundwater. Such pollution source analyses seem to be especially important. In the mathematical migration model these processes are described in the source-term for that point where the pollutant source is situated.

During the post-mining phase (with rising groundwater table) we can only seldom find representative stationary stream tubes over a longer time. Hence it is necessary

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to develop a real two- or three-dimensional non-stationary coupled flow-quality computer model for the purposes of the utilization of mine drainage water. Such a model is being tested in our basic research work. After each time step, for solving the flow-model the quality model is solved by the method of characteristics.
In this model the generation of acidity, its neutralization and transformation have to play an important role as the main source of the pollution of mine drainage water.

The stoichiometric reaction equation for the acidity generation by the weathering of pyritite is:

$$4\ Fe\ S_2(s) + 14\ O_2 + 4\ H_2O \rightarrow 8\ SO_4^{\ 2-} + 4\ Fe^{2+} + 8\ H^+ \quad (1)$$

$$4\ Fe^{2+} + O_2 + 4\ H^+ \rightarrow 4\ Fe^{3+} + 2\ H_2O \quad (2)$$

$$4\ Fe^{3+} + 12\ H_2O \rightarrow 4\ Fe\ (OH)_3\downarrow + 12\ H^+ \quad (3)$$

$$\Sigma\ 4\ Fe\ S_2(s) + 15O_2 + 14\ H_2O \rightarrow 8\ H_2\ SO_4 + 4\ Fe\ (OH)_3\downarrow \quad (4)$$

The most important reaction for the acidity generation in aerated materials is the reaction equation (1). This reaction is slow and governs the velocities of the reactions (2) and (3), depending directly on the generation of H^+. For low ratios Fe^{3+}/Fe^{2+} ($< 0{,}3$) and a high O_2 concentration the pyrite oxidation by the reaction equation (1) greatly exceeds the pyrite oxidation rate by reaction (5), directly depending on (2) /13/.

$$Fe\ S_2(s) + 14\ Fe^{3+} + 8\ H_2O \rightarrow 15\ Fe^{2+} + 2\ SO_4^{\ 2-} + 16\ H^+ \quad (5)$$

The reaction rate of (1) depends on the type and particle size (specific surface) of pyrite, on the oxygen concentration , on temperature, on the part of the surface of the pyrite crystals which is in contact with water and on the pH of this water.
Test data in /14/ show that by halving the oxygen concentration the oxidation rate of pyrite is reduced by about 60 % of that occurring when the pyrite crystals are in contact with O_2 saturated water. In any case, the oxidation rate goes to zero in the absence of oxygen.
It is also shown in /14/, that the reaction rate of pyrite exposed to air of 100 % relative humidity is essentially the same as if the pyrite would be immersed in O_2-saturated water. In dewatered aquifers or in spoil banks we can always assume a humidity of the soil atmosphere of about 100 % .
As a typical chemically controlled reaction the reaction rate of pyrite is doubled for each 10 K increase of temperature.

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Finally the oxidation rate increases as pH increases (i. e., the solution in contact with pyrite becomes more alkaline, e. g. by liming) /14/, although the acid formed will then be neutralized by lime.
In general it is assumed that the microbiological activity does not play a significant role in the formation of acid mine drainage water.
Taking into account all the above mentinoned factors, we can summarize, that the oxygen concentration in the soil atmosphere is the most important rate-controlling factor of the pyrite oxidation. Then, the most important O_2 transport process is the gas diffusion

$$f_g = - D' \text{ grad } C = - D \text{ grad } p_g \qquad \text{(II)}$$

with $D = D'/(RT)$

f_g - rate of gas transport

C - O_2-concentration in the soil atmosphere

p_g - O_2-partial pressure in the soil atmosphere

D', D - diffusion coefficients

In unsaturated media the diffusion coefficient depends on saturation. It is about 10^4 times greater in well aerated soils ($\sim 10^{-1}$ cm^2/s) than in water-saturated ones ($\sim 10^{-5}$ cm^2/s). The best possibility for sealing the pyritic material from O_2 diffusion therefore is a saturated overlying material, like silt or clay, or the ponding of the pyritic material.
Of course, also the removal of oxidation products (sulfate-, iron-, and hydroxide-ions) controls the oxidation rate. The most important removal mechanism is the flushing of oxidation products by water percolating down through the overburden (natural or artificial infiltration).
Compared with this, the flushout by the rise and fall of the groundwater table is low in general. This process plays an important role only when the ground water tabel in the dewatered naturally lying or disturbed layers (in the spoil banks) rises again. If, e. g., SO_4^{2-} is regarded as the pollutant (migrant) in the mathematical migration equation, the source rate W_{SO_4} of SO_4^{2-} can be described for a specific pyritic material, temperature and pH by a first approximation as

$$W_{SO_4} = k_{SO_4} \, C_{O_2} \, (\max C_{SO_4} - C_{SO_4}) \qquad \text{(IIIa)}$$

k - rate coefficient

C - concentration

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For O_2 as a migrant the source rate of O_2 W_{O_2} then is

$$W_{O_2} = - k_{O_2} C_{O_2} (\max C_{SO_4} - C_{SO_4}) , \qquad \text{(IIIb)}$$

the ratio of k_{O_2}/k_{SO_4} being given by the stoichiometric equation.
This means that in any case we have to formulate two or more coupled migration equations.
Last not least, the neutralization mechanism plays an important role for the generation of the mine drainage water quality.
This is of course affected by the amount, reactivity, and distribution of the CO_3 minerals, especially calcite (Ca), dolomite (Ca, Mg) or siderite (Fe).
Hence, the most important and stoichiometrically typical reaction equation is

$$H_2SO_4 + CaCO_3(s) \rightarrow Ca\ SO_4 + H_2O + CO_2\uparrow \ . \qquad (6)$$

With increasing contents of Ca^{2+} and Mg^{2+} and under special conditions also with an increasing content of Fe^{2+} the pH value will increase, too.
Predominantly Ca- and Mg-saturated clay minerals (X) support an ion - exchange, which may provide the same effect as the reaction (6):

$$Ca\text{-}X + 2H^+ \rightarrow H_2\text{-}X + Ca^{2+}. \qquad \text{(7a)}$$

For illite this reaction is, e. g.

$$10H_2SO_4 + 2KAl_3Si_3O_{10}(OH)_2 \rightarrow$$

$$3Al_2(SO_4)_3 + K_2SO_4 + 6H_2SiO_3 * H_2O \qquad \text{(7b)}$$

Following /13/ we can assume the "transformation reactions" as buffering, since the H^+ consumed in the original reactions is immediately regenerated on an equivalent basis:

$$Al^{3+} + 3H_2O \rightarrow Al(OH)_3 + 3H^+, \text{ and} \qquad \text{(8a)}$$

$$Fe^{3+} + 3H_2O \rightarrow Fe(OH)_3 + 3H^+. \qquad \text{(8b)}$$

Thus, both Fe and Al transport H^+ ions through and out of the aerated zone.

SUMMARY

The utilization of mine drainage water from lignite opencast mines for the drinking water supply is absolutely necessary in the GDR. Therefore, the main question to be answered is: how can such mine systems be managed so that the negative effects on the mine drainage water quality in its utilization for the drinking water production are avoided or at least minimezed.

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Of course, two general alternatives can than be distinguished:

1) Finding of effective measures for controlling potential pollution sources or

2) finding of effective processes for treating the polluted water.

Both ways require a sufficient knowledge about the kinetics of the pollution generation process. Mathematical modelling and process simulation are important tools for the process analysis, for prediction and therefore also for the optimization of all economic measures. We believe that the best way for doing this is to build up a conceptional coupled quantity-quality model with distributed parameters, which should be reduced to a conceptional block model in future. The research work on this, which is based on the groundwater flow simulation, is still at the beginning in the GDR. Our way is directed to the mathematical formulation of the main reaction processes. The models developed in this process have to be tested first in the laboratory, then in pilot plants (e. g. lysimeters) and finally in field test-facilities. An effective monitoring system has to be developed together with the field tests, which is naturally necessary for the model of the utilization of mine drainage water for the drinking water supply.
We regard the ground water monitoring as a scientifically designed program of continuous surveillance on the basis of process models. Then, the monitoring of the water quality includes the direct sampling and remote quality measurements, the recording of existing and potential causes of changes (hence, pollution source monitoring should be included), and the analysing of the causes of past quality changes and the predicting of the nature of future quality changes /16/. Also this work is still at the research stage in the GDR and at the very beginning in its practical implementation. Therefore, much is still to be done in order to guarantee an effective and sufficiently safe utilization of mine drainage water for the drinking water supply in our country.

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