BALANCING OF POLLUTANT TRANSPORT IN THE SUBSOIL

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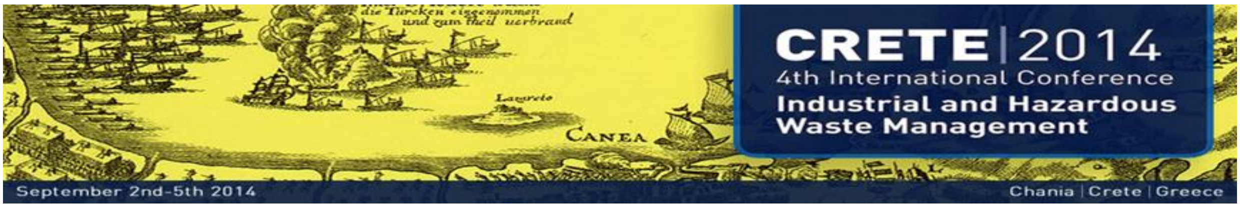
SUMMARY: The transport of heterogeneous contaminants in the subsurface is a very complex process and is influenced by a variety of factors. One approach to model such complex processes, as e.g. the pollutant transport, is by using simplified equivalent models. Under an equivalent model, a model with a simplified approach is to be understood, which considers only the essential aspects of processes, describes them abstract and still delivers realistic results. With an abstract representation of the processes it should be allowed to accept boundary conditions that lead to a simple solution of the problem. As an outcome, the complex process can be described qualitatively and despite the simplified assumptions the results should deliver realistic values. A statement on the actual processes taking place cannot be made here, since these actions are described equivalently. Based on the underlying physical and chemical processes equivalent models are created for particular cases to describe the transport of pollutants in the subsoil.

1. INTRODUCTION

By using the equivalent mathematical models it will be attempted to obtain meaningful predictions about the spread of pollutant loads due to different occurring processes. The goal is to provide the application of analytical solutions by suitable abstraction of the actual processes involved in the model area. This approach has the advantage of exact mathematical solutions for which results can be achieved more quickly. An extensive variation of various parameters, in the context of quasi-sensitivity analysis in the imaged model area (chemical and physical substance-/ground parameters), can be carried out in this way efficiently.

Requirement for the usability of such methodological approaches is to provide a suitable description of actual processes in the study area, with the necessary assumption of simplified geometric boundary conditions and homogeneous conditions in the model area, which is a prerequisite for analytical solutions.

Here two models are presented that differ in the modes of action of contaminant transport.



2. THERMAL-HYDRAULIC IN-SITU REMEDIATION

The described model is being applied in the context of an experimental field. In this experimental field the saturated area of the subsoil is contaminated with hydrocarbons (tar). By using a thermal-hydraulic remediation action, the pollutant is mobilized and so the subsoil is cleaned. The description of this process is carried out by means of a combination of different model assumptions. In focus there is an equivalent model, which allows describing the mass transfer of the pollutant as a one-dimensional transport. For this case analytical solutions are found and integrated in the simplified model. For determining temperature distribution and the flow conditions in the experimental field, the simplified model is based on a numerical simulation model. The equivalent flow and transport model for the thermal-hydraulic in-situ remediation is evaluated on the basis of a pilot test.

2.1. Numerical model for determining the temperature and flow conditions

For determining the temperature and flow conditions a numerical model with a length and width of each 100 m and a depth of 50 m was created. Based on exploratory drillings the layers in the subsoil were modelled in a way to consider the spatial extensions. Also the properties of the subsoil like porosity and permeability were determined. As part of a parameter study the arrangement of infiltration and extraction wells was chosen.

Figure 1 shows the arrangement of the experimental field consisting of 7 infiltration and 3 extraction wells. The depth of the wells is 13 meters with filter sections from bottom 8 meters upwards.

This arrangement was a result of the following considerations:

- The flow distance between infiltration and extraction wells should be small to achieve the mobilisation of the contaminants.
- The heat spreading downstream should be as low as possible.
- The area should be heated up to over 50 °C with a minimum of power losses.

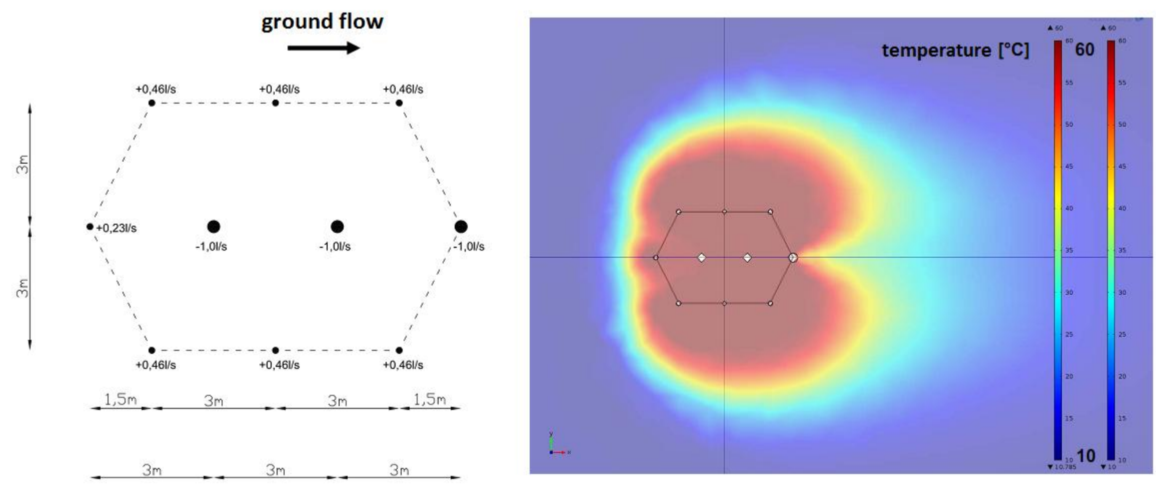


Figure 1. Left: Ground view of infiltration wells (external) and extraction wells (internal) as well as rates of infiltration and extraction of the wells. The ground water flow is from left to right. Right: Temperatures after 5 months in the area of the experimental field (horizontal sectional view in a depth of 10 meters).

Figure 1 (right) shows the result of the coupled thermal-hydraulic simulation after a time period of 5 months. It can be seen that the desired temperature of 50 °C could be reached in the whole experimental field area. The spreading of the thermal front in the groundwater flow is especially limited by the downstream extraction well.

For the analysis of the flow conditions on each infiltration well 80 massless particles were positioned in order to follow the fluid flow. Based on the flow paths it can be seen, that the preferred flow inner the experimental field is from an infiltration well to the nearest extraction well. This is a desired effect to mobilize the contaminants and bring them out on a direct way. However, some flow particles are moving away from the field and are captured from the outer ground water flow. Most of them can be captured by the last extraction well downstream and so a spreading of contaminants and temperature is minimized. Based on these calculations an analysis regarding the spatial path and speed of each flow particle was carried out. Those data finally formed the basis of the further transport model.

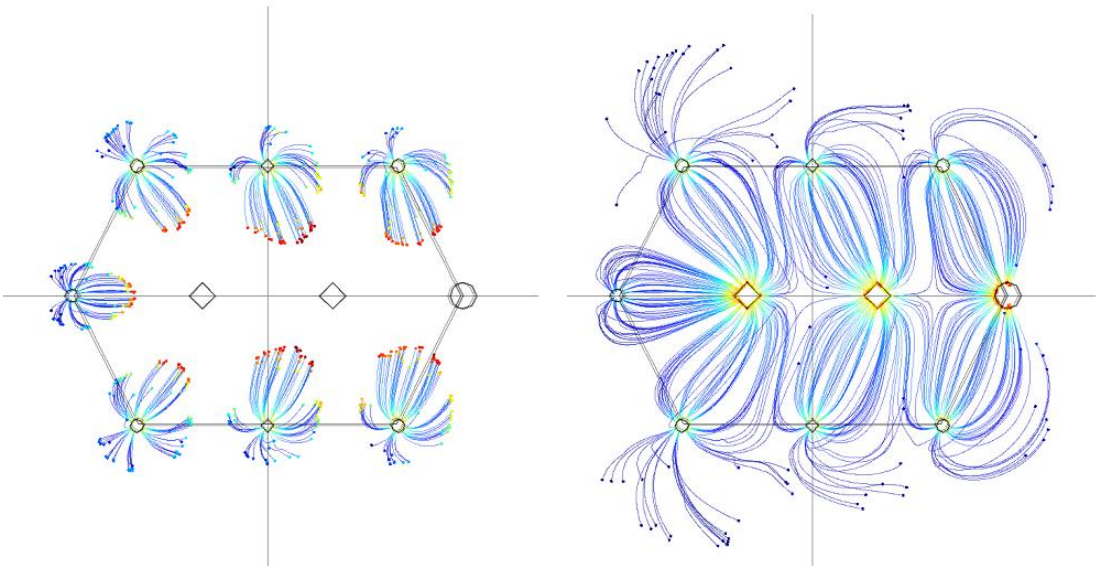


Figure 2. Layout of the experimental field with the flow paths of 80 massless particles per infiltration well (left: after one day; right: after eight days).

2.2. Equivalent flow model

The flow in the experimental field can be described by means of the potential theory. This allows an allocation of tubes which may be regarded as one-dimensional transport path. The geometry of the stream tubes is defined by the positioning of the wells. In summary all flow tubes together have to reproduce the flow pattern. Furthermore every flow tube has to get an assigned velocity. By means of the results of the numerical simulation a relation between the length of a flow tube and its middle velocity inside could be found. Because the cross-sections of the tubes are not constant, the velocity is varying also inside. For this the areas in the tubes gets respective lengths. The result is an equivalent flow tube with a constant cross-section and velocity, but a modified length (see figure 3).

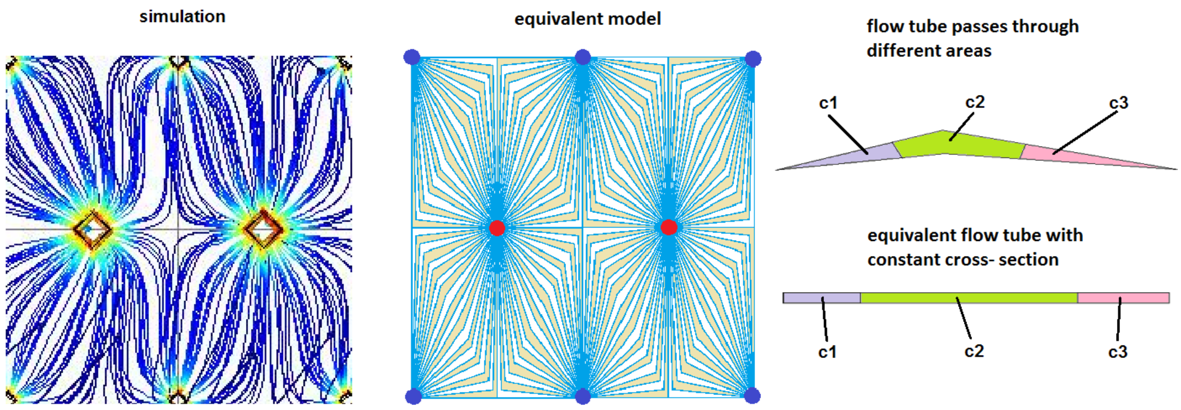


Figure 3. Formation of the equivalent flow model.

2.3. Transport model

In order to describe the mass transport of the contaminants, particles with a middle diameter are assumed which go into solution during their advective transport. The mass transfer due to solution can be described by using a potential approach for the Sherwood number. This allows determining the area-specific mass flow of the contaminants passing into solution. An existing pollutant concentration can be associated with a corresponding mass transfer area which depends on the particle size of the pollutant. Thus it is possible to calculate the amount of pollutant going into solution. The trend of the exit concentration depends only on the initial conditions. At the same time, the particles themselves are transported in the direction of flow. This disperse-advective transport occurs at a much lower speed than the flow rate of the water and is strongly temperature dependent. This disperse-advective transport is defined based on the one-dimensional mass transport equation.

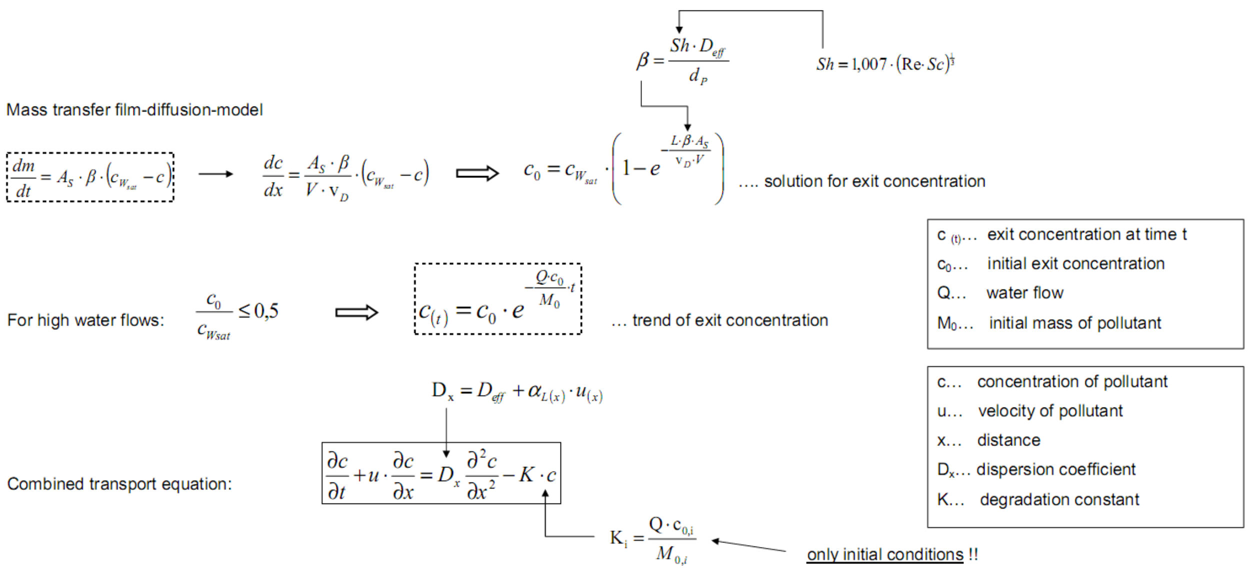


Figure 4. Formation of the combined transport equation.

The approach for combining the two mechanisms is the assumption that the solution of poorly soluble substances can be regarded as a first-order degradation process. The concentration of the disperse-advective moving pollutant is thus reduced by the amount going into solution (see Figure 4). For the analytical solution of the transport equation now an equivalent model is required, which allows to use assumable boundary conditions. For this purpose, a grid-like height-layered contamination model is coupled with the equivalent flow model. The flow tubes pass through on their way respective different contamination areas. Depending on their position, there are various path lengths, speeds, and also allocated lengths of areas of contamination. So it is possible to determine the time-depended trend of the concentration at each point along a flow tube. As for balancing the amount of discharged pollutants is interesting. For this the length coordinate of each stream tube is used as its coordinate on the exit. Thus, the time-varying discharge concentrations of pollutants in the extraction wells result as the summary of all flow tubes. The discharge by solving pollutants is obtained as the difference between the results of the calculation and a reference calculation (without solubility).

Figure 5 shows the results of the experimental field and the predicted trend of the combined equivalent model. As a further parameter the middle water temperature in the field is shown. Well visible is the kink of the trends when the temperature is reduced (day 42).

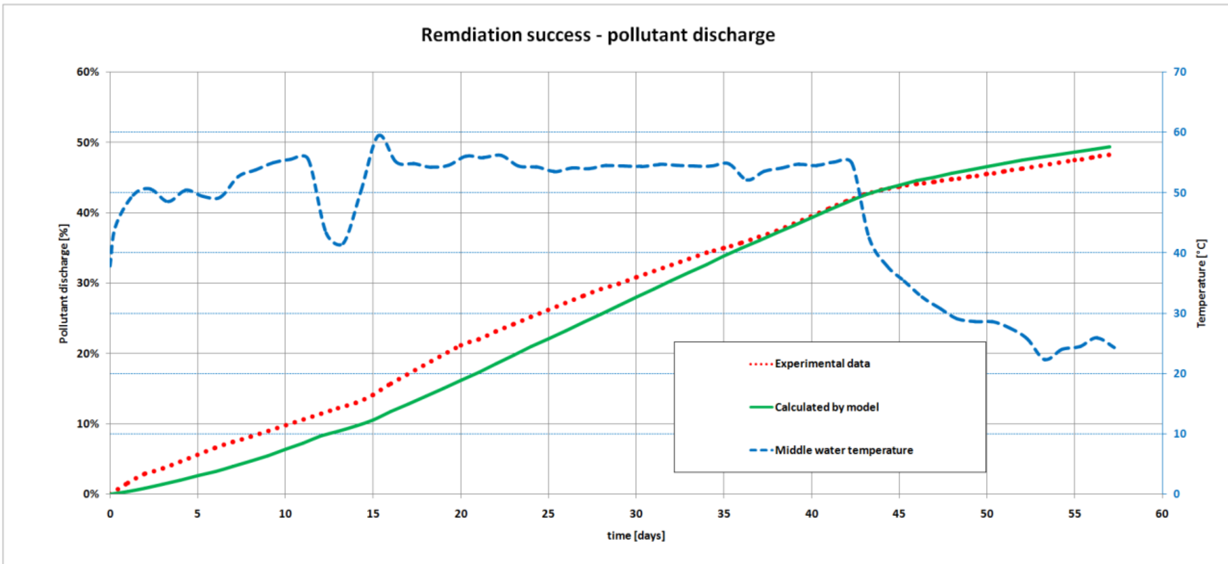


Figure 5. Pollutant discharge trend measured and predicted by model.

The precision of the calculation also depends on the knowledge of the amount of contamination. This is one of the most difficult ascertainable parameter. In the course of this experiment the field was investigated very well. In summary 133 measurement values were used to feed the contamination model which consists of 220 “contamination”-cells.

3. PHASE REMOVAL (SCOOPING) OF DNAPL AND LNAPL

As part of a redevelopment project organic phases LNAPL (**L**ight **N**on-**A**queous **P**hase **L**iquid) and DNAPL (**D**ense **N**on-**A**queous **P**hase **L**iquid), present in the soil, should be removed. This should mainly be done by removal of the phases only. In order to obtain an estimate of the discharge and to determine the respective impact factors, this process of removal is represented by simulations. To perform a wide variety of settings in the foreseeable future, the calculation time for the simulation should be small.

Here also a simplified Excel-based model brings out results quickly. By varying the extraction wells, in arrangement and shape (vertical, horizontal), the different effects can be represented. The results serve as a decision support for the selection of arrangement and shape of the wells. With the help of a pilot experiment "real" parameters should be obtained from the surroundings. With these parameters the simulation model then can be adapted. So decisions regarding the further approach, arrangement and design of the facilities can be made. To obtain an indication of the accuracy of the approach, the model is compared with a CFD simulation.

3.1. CFD-model

To perform a wide variety of settings in the foreseeable time, the calculation time for the simulation should be small. Therefore for the variation of settings a simplified Excel-model is used. To obtain an indication of the precision of the approach, the model is compared with a CFD simulation.

The CFD model used for the comparison with the equivalent model is a Volume of Fluid (VoF) solver for which the two existing VoF Solver from the software package Open FOAM (http://www.openfoam.com/) were combined. These solvers are MultiphaseInterFoam which can describe multi-phase flows, and PouroseInterFoam can describe what a two-phase flow inside and outside porous media. This gives you a solver which describes multi-phase flows inside and outside a porous media.

At first a 3-dimensional model with one well and about 3.5 million cells was created. This includes all occurring phases, air, LNAPL, water and DNAPL. At the bottom of the well, which is shown in black in Figure 6, on that spot a velocity outlet was defined using “groovy boundary conditions” (http://openfoamwiki.net/index.php/Contrib_groovyBC). The velocity is transient set to a value were the face of the well contains 95% DNAPL.

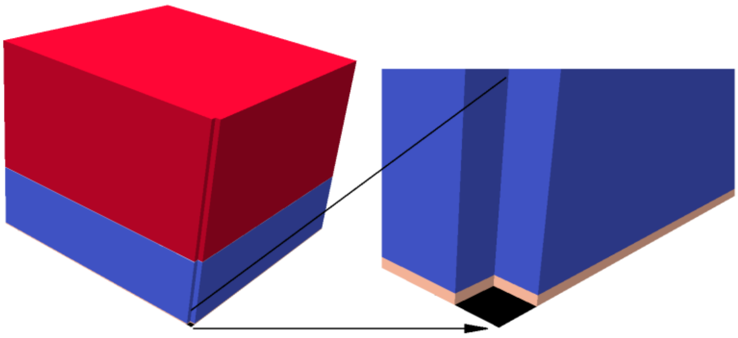


Figure 6. Structure of the model.

In this 3D model, there was a mixture between the DNAPL phase and the water. This mixture simply means that both, DNAPL and water are present in a cell. This can be attributed to two causes. For one, it comes to numerical mixing effects; these can be suppressed with a finer computational mesh and better discretization method. On the other hand the separation of the phases can be affected by the surface tension.

Furthermore the knowledge from the 3D model could be gained, that only the first few centimeters of water have an impact on the flow of the DNAPL phase and all phases overlying can be neglected.

3.2. Simplified Excel-model

The simplified Excel-model which is based on a finite difference approach should allow a sufficient precision for the investigation of different arrangements. The two-phase flow of the water-DNAPL flow is simplified set by a 1-phase flow with the differential properties of the two phases and adjusted by a correction factor. Illustrating the removal of the phase and the comparison facility with the simulations, a section is selected which is configured rectangular. The length of a 0.1 m wide channel section is 22.5 m and the DNAPL is located on the bottom resting phase with a height of 0.1 m. Over this phase water is located to saturate the channel which has a constant porosity. On one side an extraction well is located (always completely filled with water) to remove the phase at a constant level.

Now the time trends of the discharging DNAPL phase were investigated and compared. Figure 7 shows the results of the calculations. The two important parameters, the height of the phase surface level and the flow velocity, are plotted for the first 2.5 meters nearest the extraction well for the time of 12 hours after the start of the discharging process.

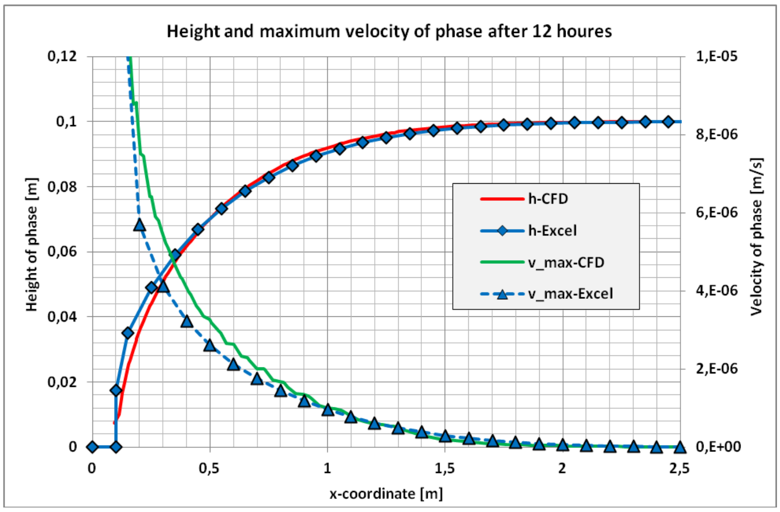


Figure 7. Phase borderlines and velocities after 12 hours.Geben Sie Text oder eine Website-Adresse ein oder lassen Sie ein Dokument übersetzen.Abbrechen

In summary the relationship from phase height and velocity results in an approximately equal temporal discharge of the phase. Also similar results provide comparisons of the two phase profiles after longer periods of time.

Now the different influences to the phase removal should be found and displayed. On the one hand the phase itself determines the trend of the removal because of its properties like density and viscosity. On the other hand, the position of the phase affect (if floating or underwater lying) the driving pressure gradient necessary for the removal.

The positioning and shape of the extraction wells have a great influence to the behavior of the removal. To find out the best positioning of the wells some variants have been calculated and compared. The residue phase after a time period of removal can give a statement about the removal success.

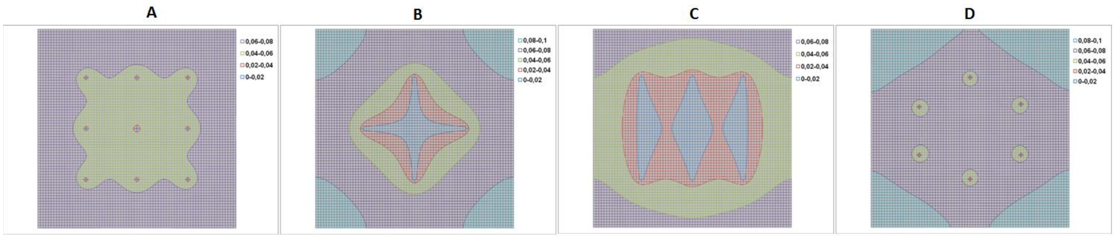


Figure 8. Different arrangements for DNAPL extraction wells and trenches.

In example “A” there are nine vertical extraction wells to remove a DNAPL. Also in example “D” vertical wells are used; in the shape of a hexagon. The examples “B” and “C” are showing an arrangement of horizontal trenches or wells (cross and parallel shapes), which can remove the phase over their whole length.

The results of the calculations are giving out the trends for the phase removal of the different arrangements of wells. The next figure 9 is shows the calculated removal success for four different positioning of wells.

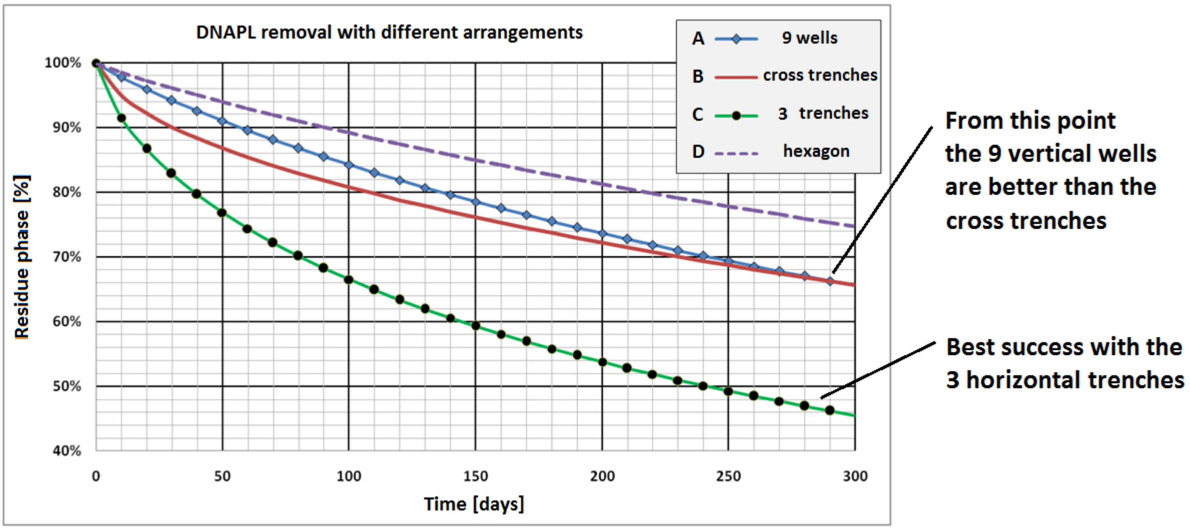


Figure 9. Phase removal success for different well arrangements.Geben Sie Text oder eine Website-Adresse ein oder lassen Sie ein Dokument übersetzen.Abbrechen

3. CONCLUSIONS

The presented methodological approaches could ultimately represent suitable practical planning tools for the prediction and interpretation of various remedial measures concerning the reduction or removal of contaminants from the subsurface.

The equivalent flow and transport model for the thermal-hydraulic in-situ remediation was evaluated on the basis of an experimental field and can be used subsequently for the design of a large-scale renovation.

For the phase removing (scooping) it could be shown, that the removal for the LNAPL could be done relative quickly and easily. An elaborate (and expensive) arrangement of horizontal trenches would not be necessary here. In contrast is the removal of the DNAPL. Here it will be necessary to use trenches in parallel arrangement. Trenches in cross shape will only remove the phase near the trenches properly. In bigger distance the removal of the DNAPL will deteriorate.

REFERENCES

Mohrlock, U. (2009) *Bilanzmodelle in der Grundwasserhydraulik*. Karlsruhe, Germany: Universitätsverlag Karlsruhe.

http://www.openfoam.com/

http://openfoamwiki.net/index.php/Contrib_groovyBC