# MODELLING OF CLEANING PLANT ELEMENTS FOR TCE-CONTAMINATED BERNAU PLACE, GERMANY

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#### 1 INTRODUCTION

During 1935-1990, two overlaying aquifers of the Bernau place (30 km northeastward of Berlin) have been polluted with TCE. It is a dense non aqueous liquid, sinking in groundwater until an aquitard is reached. Due to this feature, motion of TCE is controlled both by the hydraulic gradient of groundwater and by a top surface of the aquitard. In 2001, the German company INGAAS GmbH has started a pilot scale cleaning plant (CP) project for in-situ remediation of contaminated groundwater in high concentrations (75 - 300 mg/l). The accomplished part of CP (Fig. 1, Fig. 2) encloses an accumulator, which feeds a reactor where TCE gets dehalogeniated (Hein et al, 2002). The accumulator occupies an original TCE spill area, that is framed by a vertical wall. Within the accumulator, contaminated water is injected to uplift its table. Due to this additional hydraulic gradient, groundwater passes through the reactor.

For the full scale project, reactive walls, drains, and/or additional reactors may be used for in-situ cleanup of areas unreachable for the existing system.

Although general ideas of how CP should be developed and controlled are clear enough, there are questions to be answered if engineering details are considered:

- How does TCE spread out regionally? What are the optimal measures to stop this contaminant migration and to clean the place?
- What factors do control productivity of the existing system? What are its best groundwater pump-out and reinfiltration places and regimes?

To answer these questions, rather ample modelling has been accomplished. Its main results and methodologies used have been discussed in (Spalvins et al, 2001 and 2002) and (Burger et al, 2002).

In this paper, results of comparative regional modelling of tools that may be used for remediation are presented. Results on local modelling of the system accumulator  $\rightarrow$  reactor and dehalogenisation processes are not considered here. Because contamination processes at the Bernau are not investigated and understood enough, no final decision about the optimal full scale remediation is possible yet.



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Fig. 2. Vertical cross section NE - NW for the system accumulator  $\rightarrow$  reactor

## 2 SUMMARY ON HYDROGEOLOGICAL CONDITIONS AND MODELS, CONTAMINATION AND CLEANUP

In the Bernau area, two sandy Quaternary aquifers L2 and L3 (upper and lower ones, respectively) are TCE – contaminated. As it follows from the model schematization (Fig. 1), they are separated by the S2 aquitard. It includes a sand lens LS2 that divides this aquitard into two layers aS2 and bS2. A large hydrogeological window of the S2 aquitard provides a tight connection between the L2 and L3 aquifers. The confined L3 aquifer is bedded by the S4 aquitard that is assumed to be impermeable. The unsaturated part of the unconfined L2 aquifer is presented by the aeration zone aer that is conditionally treated as an aquitard including some fragments of the upper S1 moraine. Permeability of the principal aquifers is heterogeneous: 5.2 - 45.0 m/day and 7.0 - 28.0 m/day for the L2 and L3 ones, correspondingly.

For the initial spill area, thicknesses (confirmed by boreholes) of the LS2, bS2 and L3a layers are far for being uniform. For example (Fig. 3.), the bS2 aquitard ceases to exist just under the reactor pit and the accumulator. It is expected that other unexplored areas may also be geometrically heterogeneous.

For the L2 aquifer, the groundwater flow (Fig. 1) is more intensive then for the lower L3 aquifer (Fig. 4): for the contaminated area, the hydraulic gradient is  $\sim 0.0025$  and  $\sim 0.001$ , correspondingly (Fig. 3).

For the L2 aquifer, the Teufel pool is the main natural sink area. The pool collects TCE and it is carried out through the Southern ditch. This dangerous outrun of TCE occurs when large amount of surface water enters the pool (rainfall, melting of snow).



Fig. 3. Local HM. Piezometric head [m asl] for the vertical cross section SW – NE. Isoline step is 0.04 m



Fig. 4. Regional HM. Piezometric head [m asl] for the L3 aquifer

For the L2 and L3 aquifers, correspondingly, the TCE plumes are located at depths of 8 and 40 metres under the ground level (UGL). The plumes have been originated by leaking tanks of TCE. Intensity of this leakance at time is unknown. Exact configurations of the plumes are not detected, especially, for the L3 aquifer. A rather scarce set for pointwise observations of TCE concentrations are available, mainly for the original spill area at the L2 aquifer. For both aquifers, the plumes are located at their bottom parts, on surfaces of the aS2 and S4 aquitards. Recently (2002), high TCE concentrations (~ 250 mg/l) have been detected at the Teufel pool vicinity. Probably, TCE has pooled here, in some pits of these aquitards.

For the contaminated area, a small head difference  $\sim \pm 0.1$  metres exists on the S2 aquitard. However, contamination of the underlying L3 aquifer cannot be explained by this hydraulic factor only. It is possible that the TCE plume from the L2 aquifer has steady penetrated the S2 aquitard, due to the gravity force caused by the difference between densities of water and TCE. Probably, some undetected local windows of the S2 aquitard are mainly responsible for pollution of the L3 aquifer.

Regional and local steady state hydrogeological models (HM) have been created by the team of the Environment Modelling Centre (EMC) of the Riga Technical University. Areas of  $1.2 \text{ km} \times 0.8 \text{ km} = 0.96 \text{ km}^2$  and  $0.23 \text{ km} \times 0.17 \text{ km} = 0.039 \text{ km}^2$ , correspondingly, are covered by them (Fig. 1). For regional and local HM, uniform approximation grid plane steps are 10 metres and 2 metres, accordingly. In HM, the L2 and L3 aquifers are split in four (L2a, L2b, L2c, L2d) and three (L3a, L3b, L3c) parts, respectively. Such a fine schematization enables to account for heterogeneity of aquifers and to simulate the TCE-transport spatially. Specialists from the University of Tuebingen (UT) have used regional HM to optimise funnel and gate type reactive walls.

The MT3D'99 code (Papadopulos, 1999) was used by the EMC team to simulate mass transport processes for various remediation tools (wells, reactive walls, drains). The code was driven by HM supported by the MODFLOW system (McDonald, 1988). The Groundwater Vistas environment was used for coordination of the MT3D and MODFLOW systems (Environmental Simulation, 1997).

The system accumulator  $\rightarrow$  reactor is located at the L2 aquifer (Fig. 2). Within the accumulator, contaminated water taken from the upper and lower aquifers can be injected in various amounts by controlling pumping rates. A pore volume ~ 250 m<sup>3</sup> is available for holding lifted groundwater at its peak value ~ 2.0 m above the groundwater table outside the accumulator. The rectangular reactor pit (19 m × 11 m) has a basement of concrete (1.0 m thick) positioned 4.5 m UGL. On the basement, 18 modules are arranged side by side. The modules are connected with variable piping that enables to operate them in serial, parallel or combined modes. Various arrangements are possible and they are being tested. Cleaned water is reinfiltrated into the L2 aquifer and its quality is monitored by a multi-level screened well. In case of insufficient dehalogenation, water can be returned back to the accumulator. For high TCE input concentrations, the best experimental results have been obtained for the reactor flow 20 – 25 m<sup>3</sup>/day. Technically, much higher flow rates (120 m<sup>3</sup>/day) have been tested.

### 3 RESULTS AND DISCUSSION

The described above pilot scale system deals mainly with the initial spill area and also serves as a tool for developing dehalogeniation technologies. For the full scale project, the following main tasks must be solved to remediate the L2 aquifer:

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- to clean the TCE flow emitted by the initial spill;
- to prevent entering of TCE into the Teufel pool;
- to collect TCE accumulated in the area of the pool.

Water of the Southern ditch should also be cleaned, to prevent fast outspread of TCE via the hydrographical network of the place.

For the L3 aquifer, not enough field data are available yet, to formulate its full scale remediation strategy.

There are three main methods of remediation:

- water to be cleaned is pumped out from aquifers and then treated by central reactors;
- reactive walls for treating water are installed into aquifers;
- bioremediation is applied where contaminant concentrations are small enough.

For the L2 aquifer, combinations of the above methods are possible. Probably, remediation by the pump and treat method is the only realistic choice for the L3 aquifer.

In this paper, no general optimization of the full scale remediation system is considered. Only main elements of the system are examined by modelling their use for cleaning of the place. To investigate the elements, hypothetical TCE plumes have been created by accounting for the observed concentrations, advection and dispersion processes.

For the L2 aquifer, two and three dimensional (2D, 3D) versions of plumes were created. The simplest 2D plume is located at the L2d aquifer (Fig. 5, Fig. 7), as the initial concentrations for modelling. The 3D plume (Fig. 9) occupies all four layers of the L2 aquifer. Total TCE mass of plumes is  $\sim 2300$  kg and  $\sim 2100$  kg, accordingly, for the 2D and 3D ones. They obtain their final simulated shape after  $\sim 2500$  days (Fig. 9, Fig. 10 for 3D plume). About 85% of the 3D plume total mass belongs to the L2d aquifer. Therefore, the 2D plume is a rather good approximation for modelling purposes.

Horizontal drains and reactive walls with funnels and gates were investigated by using the 2D plume (Fig. 5 - Fig. 8). For the drain (Fig. 5, Fig. 6), concentration sources causing the plume remained active (emitted TCE) during the experiment. For the wall (Fig. 7, Fig. 8), the sources were taken out (no TCE emission).

The 3D plume was supported by a line of constant concentration sources 150 mg/l located at the L2d aquifer. The sources were active for the permeable wall test of Fig. 7.

In reality, TCE plumes may be very complex, because a long term TCE emission is possible from any polluted soil volume (especially, from the aS2 aquitard where the groundwater flow velocity is small).

Wells and horizontal drains are used to withdraw contaminated water for treating it by a reactor. The following contradicting targets are important for this system:

- to minimize amount of water to be cleaned, its TCE concentration should by high;
- to keep the processes within the reactor optimal, TCE concentration should be constant at time;
- energy and investments for development and maintenance of the system should be minimal.



Fig. 5. Remediation of the TCE plume for the L2d aquifer by a drain



Fig. 6. Computed TCE mass versus time for the test of Fig. 5 and when an extra drain at the Teufel pool is used



Fig. 7. Remediation of the TCE plume for the L2d aquifer by a reactive wall with the single gate



Fig.8. Computed TCE mass versus time for the test of Fig. 7, and when the Teufel pool is the only sink for TCE



Fig. 9. Initial concentrations [mg/l] of the spatial TCE plume for the L2 aquifer



Fig. 10. Computed mass versus time for the growing spatial TCE plume of Fig. 9



Fig. 11. Concentrations [mg/l] of the spatial TCE plume for the L2 aquifer after 1500 days when a permeable reactive wall is used



Fig. 12. Computed TCE mass versus time for the test of Fig. 11



Fig. 13. Concentrations [mg/l] of the spatial TCE plume for the L3 aquifer when a well MW (75 m<sup>3</sup>/day from the L3c aquifer) is used



Fig. 14. Graphs of recovered TCE mass versus time for the test of Fig. 13 and when the withdrawal rate  $25m^3/day$  is used

No real management can reach these targets simultaneously. However, the targets are helpful if elements and regimes of the clean-up system are to be chosen. For example, a horizontal drain possesses some advantages over a set of single wells:

- a rather constant TCE concentration for water collected from a large area;
- if a vertical TCE distribution at an aquifer is strongly uneven then the output TCE concentration of the drain can be considerably enlarged by separating water in clean and polluted flows;
- in same cases, a natural outflow of water from a drain is possible without pumping.

Horizontal drains have been modeled as the elements serving the full scale clean up system (Fig. 5, Fig. 6).

As it follows from Fig. 5, the drain of the length 90 m (60 m<sup>3</sup>/day from the L2d layer) manages the plume of the width ~ 200 m. By enlarging the pumping rate, even larger plumes may be controlled. To raise the TCE concentration on the reactor input, the drain should be separated into two parts: the upper and the lower ones located at L2a and L2d aquifers, respectively (Report 2002). From the upper drain, ~ 25 m<sup>3</sup>/day of almost clean water may be pumped out and infiltrated into the ground, without being treated by the reactor. From the lower drain, ~ 35 m<sup>3</sup>/day of contaminated water is pumped to the accumulator  $\rightarrow$  reactor. The TCE concentration for the lower drain is nearly twice than the concentration for the single drain located at the L2d aquifer.

It follows from Fig. 5, Fig. 6 that after  $\sim 2000$  days, if no preventive measures are taken, the part of the plume, downgradient the drain, is sunk by the pool. To prevent entering of TCE into the pool, an extra drain should be installed before the pool. It follows from the graph – a TCE mass versus time t (Fig. 6) then the system of two drains is effective. However, this system cannot collect TCE accumulated at the pool area, and the second extra drain should be applied here (Report 2003a). Probably, a second reactor will be needed for treating water provided by the both extra drains and by the L3 layer here. For the pool area, all four layers of the L2 aquifer are contaminated (Fig. 9), and no parting of water (taken from drains) into the clean and polluted ones is possible.

A reactive wall with a single gate (width of the gate -80 m, length of the impermeable funnel  $-2 \times 170$  m = 340 m, height of the wall  $\sim 8$  m) was tested nearly at the location where the drain of Fig. 5 was positioned. As expected, the part of the plume upgradient the wall gets cleaned. However, the wall changes the head of the L2 aquifer in such an unfavorable way that the TCE contaminated area considerably enlarges, downgradient the wall (Fig. 7). Probably, due to this side effect, the MT3D code stops computations when t > 1100 days.

Specialists from UT have found that the wall with two gates is the best cost effective choice of this kind of remediation tool. To ease the unwanted side effects of the wall, it should be positioned closer to the pool and/or extra elements (drains, walls) should be used to prevent the TCE inflow into the pool.

By using the 3D plume (Fig. 9, Fig. 10), the permeable reactive wall was investigated (Fig. 11, Fig. 12) as an alternative to the funnel and gate type one. This kind of wall contains no funnels. If the wall functions rightly (no blocking caused by chemical processes within the wall) it, unlike the wall of Fig. 7, does not deform the groundwater flow, and no side effects are present. The length of the wall should slightly exceed the width of the TCE plume (140 m).

If the wall is positioned, like the drain of Fig. 5 then its upper part may be set impermeable for the L2a, L2b layers, because practically no TCE is present here (Fig. 9). It follows from Fig. 11 (t = 1500 days) that the wall does not enlarge the polluted area. For such

a modified wall, the amount of the reactive materials needed for cleaning of water is reduced twofold. However, extra elements of TCE recovery are necessary for the Teufel pool area.

Hence the vicinity of the Teufel pool has not been investigated fully, it is hard to decide which combination of elements modelled should be applied for the full-scale project.

Is has been observed that no dehalogeniation is complete, especially, for high TCE concentrations (Hein et al., 2002). Some partly dehalogeniated intermediates, like cis - 1.2 dischlorethene (DCE) and vinylchloride (VC), may be present in water cleaned by a reactor or a wall. However, concentrations of these metabolites are low and natural or enhanced bioremediation of them seems possible (Report 2003b).

For the L3 aquifer, a hypothetical 3D plume of TCE has been created. A possible TCE emission was accounted for by lines of constant concentration 150 mg/l sources, located at the L3b, L3c layers. The spatial concentration distribution computed for t = 8000 days was applied as the initial TCE concentrations for numerical experiments. For tests on wells, the lines of concentration sources were switched out. Due to heterogeneous permeability and thicknesses of the L3 aquifer, practically no TCE entered the L3a layer. The L3b layer was considerably contaminated only at the vicinity of the TCE emission line (in Fig. 13, see initial concentrations for the L3b, L3c aquifers). The total mass of the 3D plume was ~ 3700 kg.

It follows from Fig. 13, Fig. 14 that a single well which intercepts the plume (withdrawal 75 m<sup>3</sup>/day from the L3c aquifer), considerably reduces its mass (~ 1650 kg of TCE recovered). However, for such a well, the TCE recovery decreases rather fast at time. If the withdrawal rate is ~ 25 m<sup>3</sup>/day then the TCE recovery is practically constant at time (Fig. 14). Moreover, the recovered ~ 1000 kg of TCE if far better than ~ 550 kg formally expected from the relation: 1650/(75/25).

This result shows that a set of wells possessing moderate withdrawal rates should be used for the L3 aquifer. The rates should be controlled by accounting for the observed TCE concentrations of water monitored at each well (the concentrations at wells should be kept high, as long as possible).

### 4 CONCLUSIONS

A system of hydrogeological models has been designed to investigate groundwater flows and contaminant migration for the Bernau place.

Mathematical modelling of various remediation tools has been accomplished by using the regional hydrogeological model as the driver for the mass transport calculations.

Results of modelling have been used by the INGAAS GmbH company for developing of a full scale remediation project.

More field data and extra modelling are needed for the final decision how to remediate the place by using cost effective technologies.

### REFERENCES

- Burger, C.M., Finkel, M. & Teutch, G. (2002): Technical economical evaluation of multiple gate funnel – and – gate systems under homogenous and heterogeneous aquifer conditions. *Proc. of the 4-th International Conference on Groundwater Modelling.*; Vol. II: 520-524. Prague, Czech Republic.
- 2. Environment Simulations, Inc. (1997): Groundwater Vistas. Guide to using.

- 3. Hein, P. Tauchert, J., Freygang, M. & Vigelaghn L. (2002): Design and Construction of Horizontal ZVI-based Permeable Reactive Barrier (PRB) System for the In-Situ-Treatment of Halogenated VOC'S in Groundwater at the Bernau Site Near Berlin. *Proc.* of the Third International Conference on Water Recourses and Environment Research, ICWRER 2002; Vol. II: 173-179, Dresden, Germany.
- 4. McDonald, M. & Harbaugh, A. (1988). A Modular Three-Dimensional Finite-Difference Ground-Water Flow Model, U. S. Geological Survey, Open File Report Washington: 83-875.
- 5. Papadopulos & Associates, Inc. (1999). MT3D'99. Users Guide.
- 6. Report on Corrected HM. Drains for Remediation. (2003a). Agreement No 6476. *Modelling of Groundwater Flow Dynamics and Contaminant Transport Processes for the Bernau Area, Germany.* January 2003, Riga. 45 pages.
- 7. Report on Permeable Walls, Wells and Biological systems for Remediation. (2003b): Agreement No 6476. *Modelling of Groundwater Flow Dynamics and Contaminant Transport Processes for the Bernau Area, Germany.* February 2003, Riga, 64 pages.
- 8. Report on Walls, Drains and Wells for Cleaning of Groundwater. 2002. Agreement No 6476. *Modelling of Groundwater Flow Dynamics and Contaminant Transport Processes for the Bernau Area, Germany*. July 2002, Riga, 49 pages.
- 9. Spalvins, A., Slangens, J., Janbickis, R., Lace I., & Hein, P. (2002): Modelling of remediation tools for the contaminated Bernau place, Germany. *Scientific Proc. of Riga Technical University in series "Computer Science". Boundary Field Problems and Computer Simulation.*; Vol. 12 (44): 24 29, Riga.
- Spalvins, A., Slangens, J., Janbickis, R., Lace I., & Hein, P. (2001): Modelling of groundwater flow dynamics and contaminant transport processes for the Bernau area, Germany. Scientific Proc. of Riga Technical University in series "Computer Science". Boundary Field Problems and Computer Simulation.; Vol. 7 (43): 143 – 153, Riga.

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### Spalvins A., Slangens J., Janbickis R., Lace I., Eglite I., Skibelis V., Hein P. Modelling of cleaning plant elements for TCE-contaminated Bernau place, Germany.

The Bernau place is heavily polluted with trichlorethylene (TCE). To help in solving the remedy problem of the place, a system of hydrogeological models has been developed and applied for investigating elements of an insitu cleaning plant. Results of comparative regional modeling of tools (reactive walls, drains, wells) that may be used for remediation are presented. these results have been used by the INGAAS GmbH company for developing of a full scale remediation project. More field data and extra modeling are needed for the final decision how to clean the place cost effectively.

## Spalviņš A., Šlangens J., Janbickis R., Lāce I., Eglīte I., , Šķibelis V., Hein P. Attīrīšanas iekārtu elementu modelēšana ar TCE piesārņotajā Bernau vietā, Vācijā.

Bernau vieta Vācijā ir ļoti piesārņota ar trihloretilēnu (TCE). Lai palīdzētu risināt šīs vietas atveseļošanas problēmu, ir izstrādāta un attīstīta hidroģeoloģisko modeļu sistēma. Ar tās palīdzību pētīti attīrīšanas iekārtu elementi. Iegūti rezultāti par dažādu elementu (reaktīvās sienas, drenas, urbumi), kurus var izmantot attīrīšanai, piemērotību. Šos rezultātus izmantos firma INGAAS GmbH, lai izstrādātu plaša mēroga attīrīšanas projektu. Ir vajadzīga papildus informācija par vidi un modelēšana, lai varētu pieņemt galīgo lēmumu par efektīvas sistēmas izveidošanu.

#### Спалвиньш А., Шланген Я., Янбицкий Р., Лаце И., Эглите И., Шкибелис В., Хейн П. Моделирование элементов очистительных устройств для ТСЕ-загрязненной местности Бернау, Германия.

Местность Бернау очень загрязнено трихлорэтиленом (TCE). Создана и развита система гидрологических моделей, которая помогает решать проблему оздоровления этой местности. Модели использовались для изучения различных элементов (реактивные стены, дрены, скважины), которые могут быть применены в системе очистки. Результаты моделирования использованы фирмой INGAAS GmbH при разработке проекта широкомасштабной системы для очистки местности. Необходимо иметь дополнительную информацию относительно местности и работы по моделированию, чтобы можно было принять окончательное решение относительно создания эфективной системы очистки.