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## CHLORINATED SOLVENTS TRANSPORT AND NATURAL ATTENUATION MODELING IN GROUNDWATER

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### INTRODUCTION

The purpose of this study is to compare natural attenuation models to predict transport and fate of chlorinated solvents in saturated groundwater systems. This work was realised within the framework of the research program TRANSPOL. This program was created in order to bring a better and common practice of the use of transport models concerning various pollutants the most encountered. Real case study, Real Case 3, concerns chlorinated solvents fate and transport in groundwater.

### SITE DESCRIPTION

This real case is based on a contaminated alluvial aquifer in northern Spain, which has been studied since 2000 by ENVIROS. The site (Fig. 1) has a length of 1000 meters along the direction of groundwater flow (S-N) and is 600 meters wide. A river crosses this site. The aquifer thickness is 16 meters including a 6 meters thick vadose zone. The sedimentary materials are unconsolidated and very heterometric (from clay to rolling cobbles), with very heterogeneous composition (from limestone and sandstone to metamorphic and igneous rocks).

Perchloroethene (PCE) is the primary solvent contaminant that was originally disposed at this industrial site. However, concentrations of chlorinated solvent degradation products such as trichloroethene (TCE), cis-dichloroethene and trans-dichloroethene (cis-DCE, trans-DCE) were observed in the monitoring wells located downstream from the source location. The kinetics of all the degradation reactions are assumed as first order kinetics. Flow conditions are assumed to be at steady state. The groundwater hydraulic head values at the model boundaries were based on measured data on 19 piezometers of which 6 are pumping well.

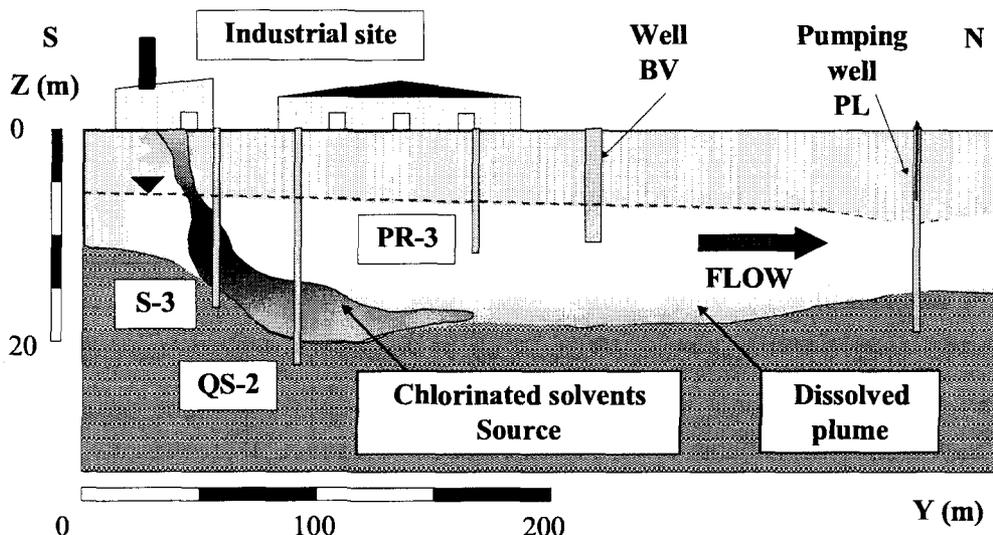


Fig. 1 South – North cross-section of the site.

## RESULTS

Numerical models described the aquifer as a single, continuous, unconfined unit with spatially variable transmissivity values. The different transmissivity zones used in the models were based on pumping tests results and calibration of head values.

Transport parameters are estimated by the concentrations calibration process as on many other field sites. The total amount of PCE mass discharged into the aquifer is unknown.

The model inter-comparison methodology was based on comparisons of flow and transport calibration results, calibrated parameter values, respected hypotheses and natural attenuation phenomena considered (particularly sorption and degradation).

In a first step, four teams studied this case and different codes have been employed (Table 1). Inter-comparison of results show differences, especially : source definition ; injection rate of PCE ; choice of piezometer used for calibration process ; taking into account sorption and dechlorination.

Table 1 Teams and codes used in the inter-comparison benchmark (FE : finite elements; FD : finite differences; TVD : total variation diminishing (Zheng et al. 2001)

	ANTEA	École des Mines de Paris		INERIS
3D Flow Modeling	MARTHE - DF V. 6.3 (déc. 2002)	METIS - EF V1 (mars 2004) and MODFLOW 2000 - DF V. GMS 4.0	TRANSIN - EF V. IV	MODFLOW 2000 - DF V. GMS 5.0 (mai 2004)
3D Transport Modeling	MARTHE - DF V. 6.3 (déc. 2002)	Metamodel - kriging and RT3D - TVD V. GMS 4.0	TRANSIN - EF V. IV	RT3D - TVD V. GMS 5.0 (mai 2004)

In a second step, to improve models, investigations were performed on site to test the consistency of results between new observed concentrations and calculated concentrations, in order to valid simulations. Moreover sorption and degradation parameters were evaluated by laboratory tests (on one sampling, PCE Sorption coefficient  $K_d$  (ml g<sup>-1</sup>) : 1,46 and PCE First order degradation constant  $\lambda$  (day<sup>-1</sup>) :  $1,7 \cdot 10^{-3} - 1,7 \cdot 10^{-2}$ ).

Three teams participated to this second step (ANTEA, ENVIROS and INERIS).

This new data show notably an improvement of both conceptual model (ENVIROS and INERIS took into account sorption in this second exercise) and calculated concentrations (Fig. 2 and Fig. 3).

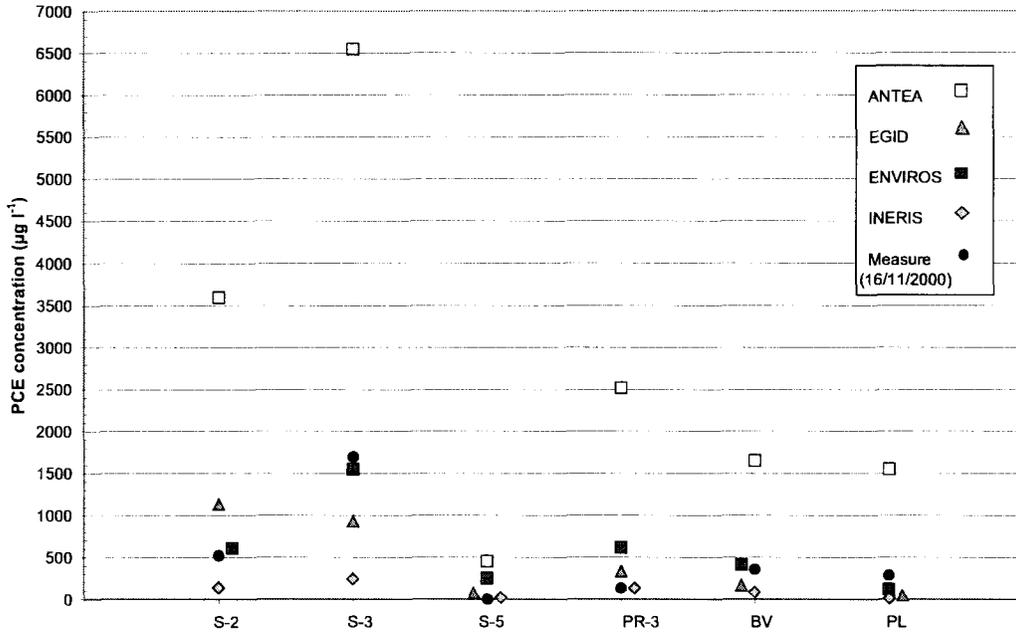


Fig. 2 First phase - PCE concentrations ( $\mu\text{g l}^{-1}$ ) at five years

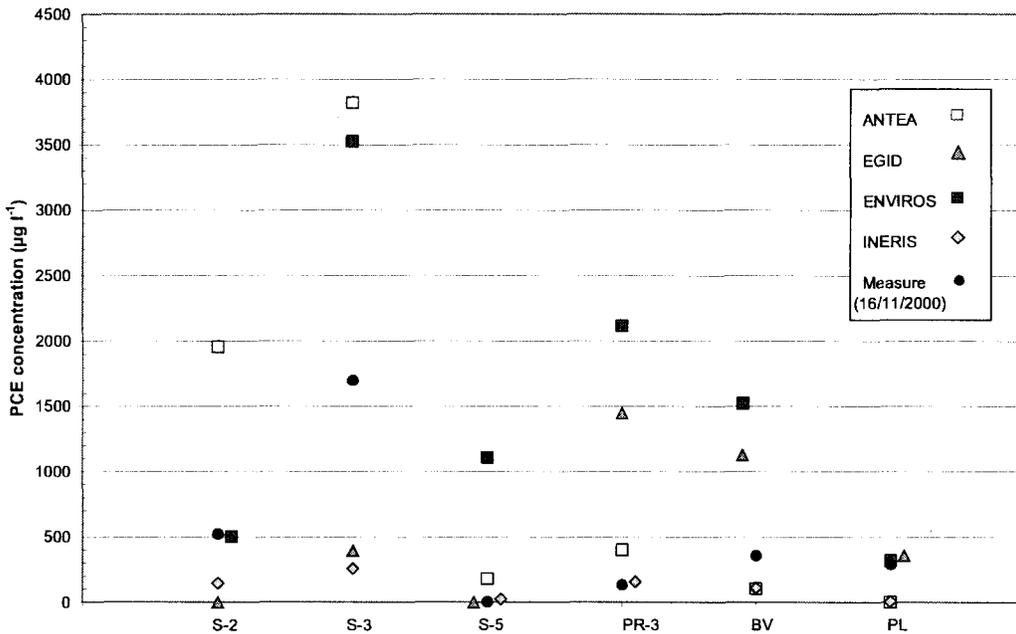


Fig. 3 Second phase - PCE concentrations ( $\mu\text{g l}^{-1}$ ) at five years

## CONCLUSIONS

Multi-species models were used to model transport and natural attenuation processes occurring at a chlorinated solvent release site. Different codes were used by four modelling teams (ANTEA, ENSMP, ENVIROS and INERIS). First results show the difficulty to estimate source concentration and to simulate sorption/degradation. A more accurate diagnosis was lead in order to reduce the uncertainty of model parameters and improve the conceptual model. Thus, more accurate data were acquired concerning the presents distribution of pollutants and the degradation and sorption rate of PCE. These new data show an improvement of results (conceptual model and concentrations simulated).

All TRANSPOL results are presented on the website : <http://transpol.ineris.fr/>

## ACKNOWLEDGEMENTS

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