Steady-state modelling of biogeochemical processes in an aquifer

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Biogeochemical processes occurring in groundwater were studied using a laboratory column filled with aquifer sand. As carbon source for the microbial processes, lactate was introduced with the inflowing aqueous solution. To describe the quasi-steady-state conditions of the experiment, kinetically controlled biogeochemical processes and chemical equilibrium reactions were modelled simultaneously. The column was treated conceptually as a series of six boxes according to the position of the sampling ports used for the chemical analysis.

In the first part of the study, the model calculations were based on a single sampling event and focused on the turnover of carbon and sulphur that are closely related to calcium and iron, respectively. The comprehensive approach allows the quantification of all important processes and the verification of the stoichiometries of the reactions considered. The electrons provided by lactate and its reaction products amount to approximately 4 meq/L, which are consumed mainly by the electron acceptors oxygen (0.8 meq/L), nitrate (1.3 meq/L) and sulphate (1.9 meq/L). Since all oxygen and nitrate was reduced in the first centimetre, most of the carbon dioxide was formed in this section of the column, leading to a lower pH (7.45) and to undersaturation with respect to calcium carbonate. In the rest of the column, the pH was approximately 7.65 and $CaCO_3$ saturation was attained. Hydrogen sulphide, which was produced by 'reduction of sulphate', reacted mainly with iron(III) oxides in order to form FeS(s). A systematic sensitivity analysis was used to quantify the influence of the rate coefficients on the acid-base behaviour of the system. According to these
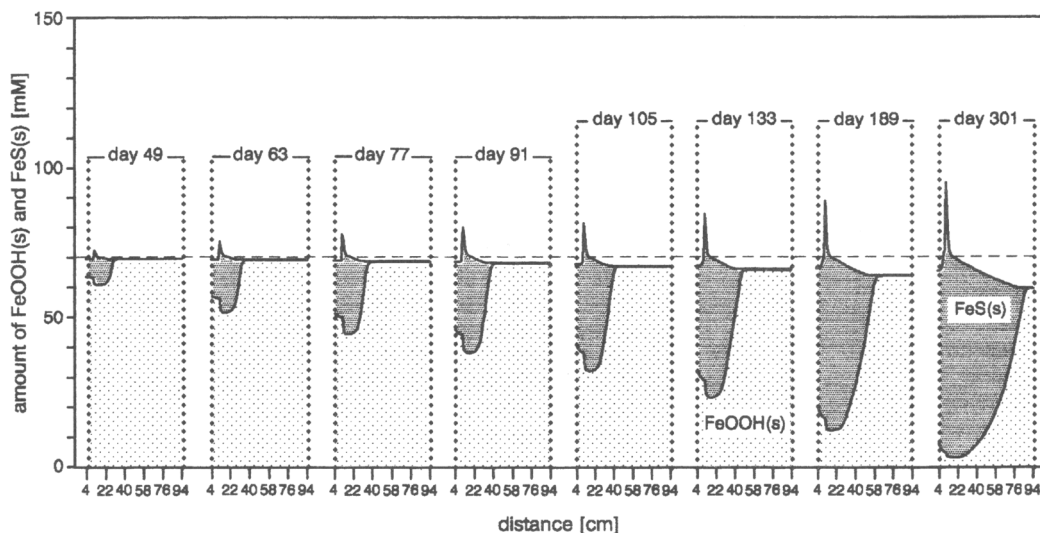

FIG. 1. Long-term behaviour of the solids FeOOH(s) and FeS(s) in the time span of 301 days and in the flow distance of 94 cm. As a function of operation time, the FeS(s) fraction of the total iron gradually increases and the front of FeS(s) moves towards the end of the column, reflecting the extent of the overall sulphide-immobilisation capacity of the aquifer sand.

calculations, the pH is most sensitive with respect to 'disproportionation' of lactate into propionate, acetate and bicarbonate as well as to the processes 'aerobic respiration' and 'denitrification'.

In the second part, time-dependent serial data from the column experiments were used to develop a dynamic model to describe the evolution of concentration profiles of the redox-sensitive chemical components iron(II), sulphate/sulphide, FeOOH(s), and FeS(s). The turnover rates of the slow processes 'reduction of sulphate', 'reduction of FeOOH(s)', 'formation of FeS(s)' and 'precipitation of FeS(s)' were determined by using an extended version of the program STEADYQL in combination with the parameter optimisation program SUFI. The major sink for sulphide appeared to be FeOOH(s) that is gradually transformed into FeS(s). Under the prevailing experimental conditions with a flow velocity of approximately 1 meter per day and a dissolved sulphate concentration in the inflow of 200 µM, the calculated sulphide front migrates in the order of 1 meter per year (Fig. 1).

In conclusion, it is possible to carry out prognostic modelling on the propagation of a sulphide plume in an anaerobic aquifer if the average surface characteristics of the aquifer matrix are known. A possible environmental problem may be derived from such information for aquifers that exhibit reducing conditions. Sulphide immobilisation may lead to a sulphide-free groundwater even if strongly reducible conditions are predominant. However, as soon as the binding capacity for sulphide is used up, a sudden increase in the sulphide concentration may result and affect the quality of a nearby water supply.

References

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