Travel time-based modelling of nitrate reduction in a micritic fractured limestone aquifer

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Research question

How can nitrate be reduced if the bacterial activity is only possible in the fractures?

Fractured limestone aquifers (e.g., Triassic Upper Muschelkalk) provide an evidence of denitrification. The lithological properties (small pore size, porosity of 1%) limit bacterial activity to the fracture surface. Possible redox reactions include diffusion limited pyrite oxidation and iron bearing carbonate dissolution.

Approach

o Test different conceptual models of redox reactions to obtain the reaction function as a function of real time t and travel time (τ, C_r) t, τ.

o Nitrate concentrations, $C_{GW,i}(t)$, at sampling locations i is calculated by convolution (e.g., Cirpka & Kitanidis, 2000):

$$C_{GW,i}(t) = C_{GW}(t, \bar{\tau}_i, \alpha) = \int_0^\infty C_r(t, \tau)\, f(\tau, \alpha, \bar{\tau}_i)\, d\tau,$$
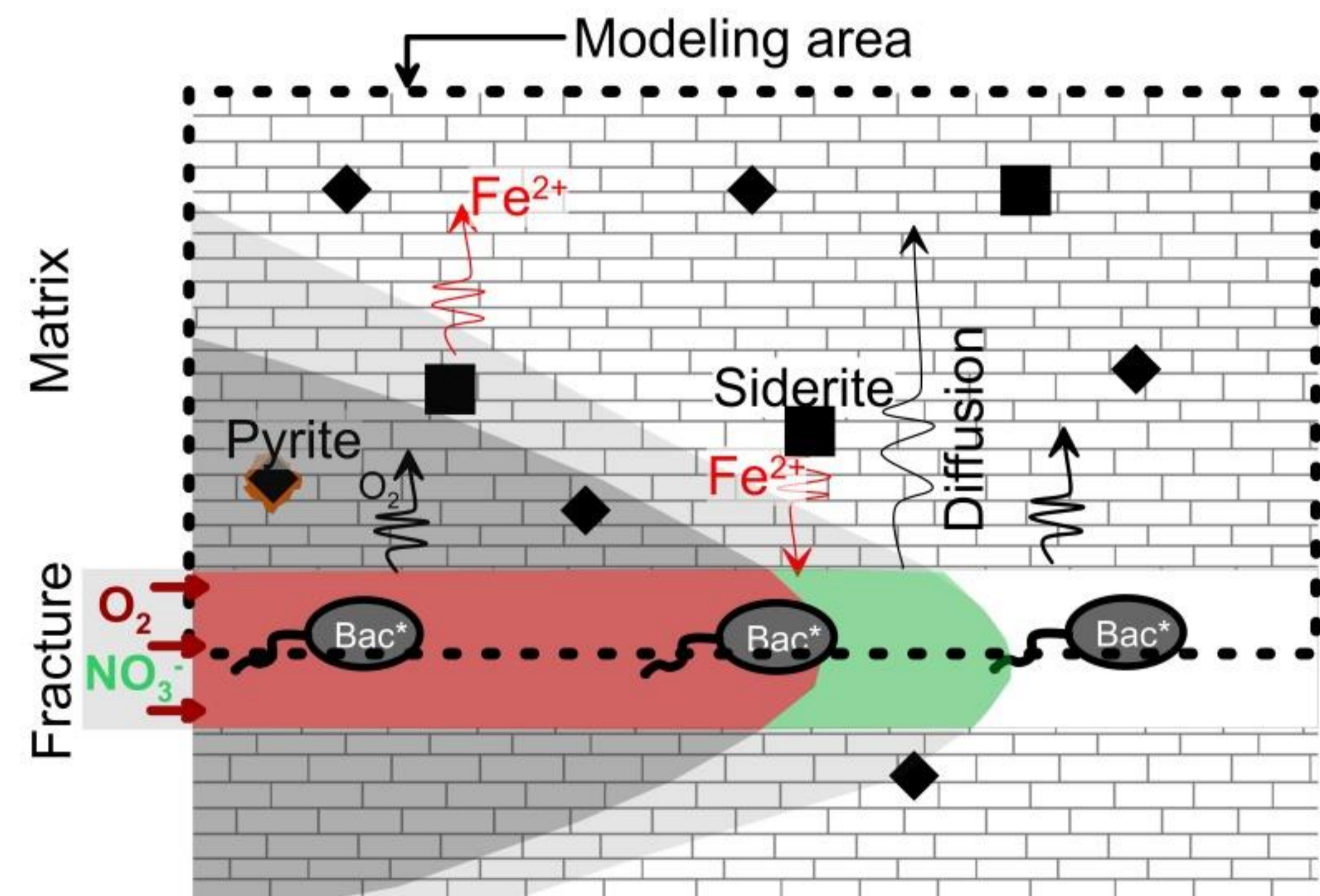

Figure 1. Conceptual model.

Results

o The model is able to realistically describe changes in the nitrate concentration at the catchment scale.

o Pyrite and siderite provide enough denitrification potential.

o Applying the model to the catchment scale by convolution of the reaction curve with the probability density function of travel time.

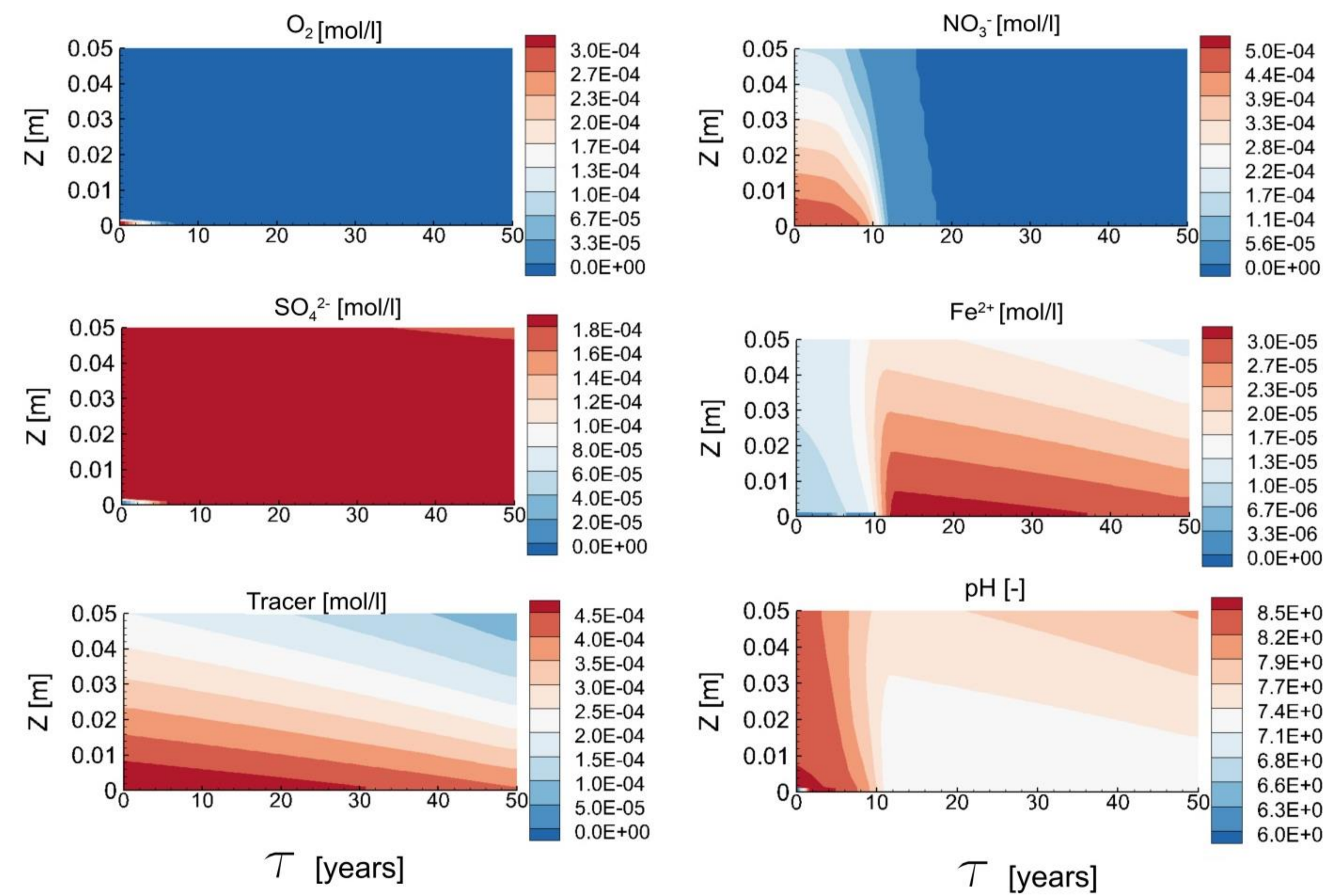o Mismatches are related to the uncertainty in parameters.

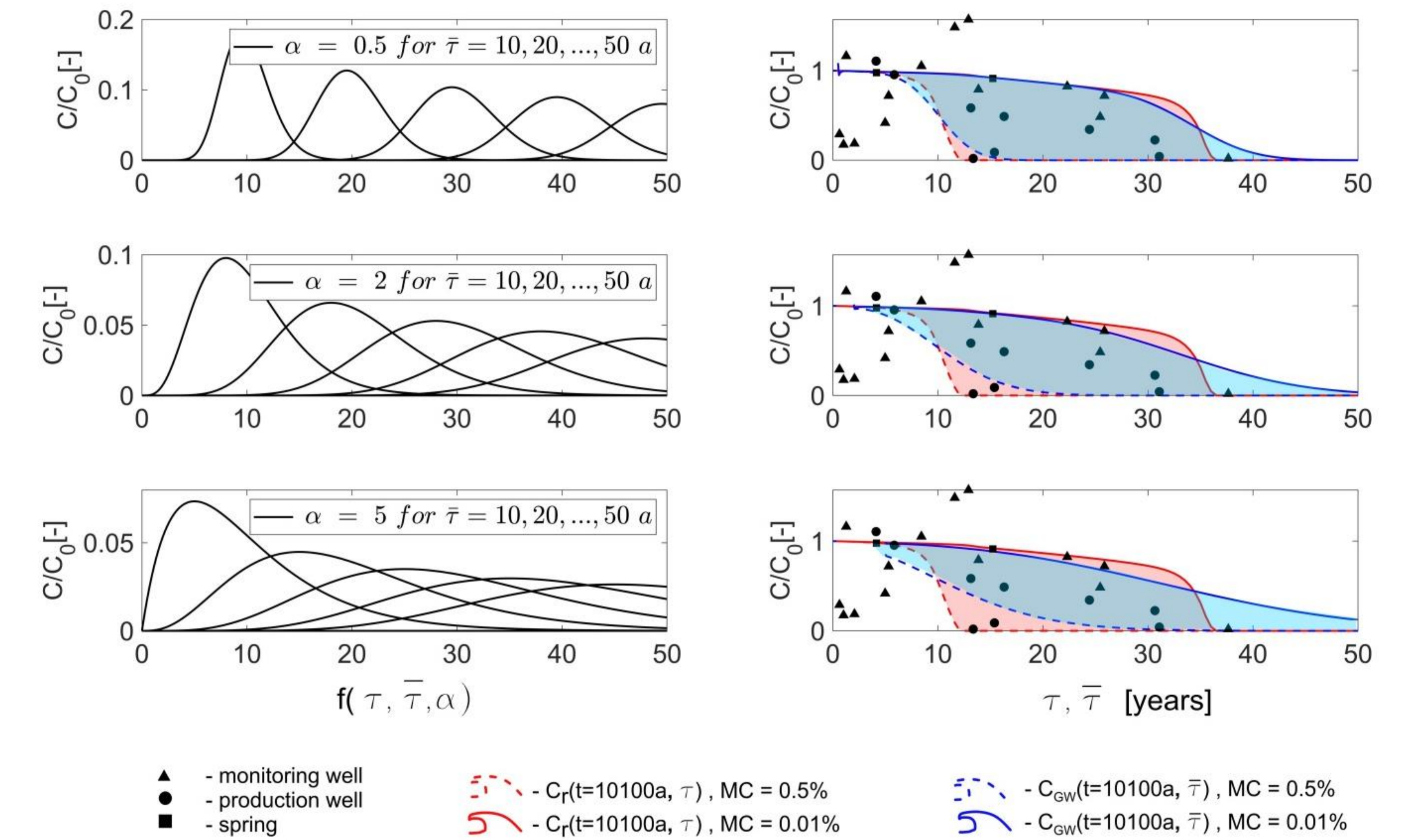Figure 2. Distribution of main water chemistry parameters close to the fracture over travel time.

Figure 3. Comparison of modelled and measured nitrate concentration in groundwater (right) for different travel time distributions (left). Reaction fronts for low and high mineral concentration (MC).

Conclusions

Measured nitrate concentrations in the catchment can be explained by the travel time-based, fully coupled reactive model accounting for pyrite and siderite involved redox processes. Unknown shape of travel time distributions result in large variability of model results.

Outlook

o Sensitivity analysis to investigate the influence of geochemical parameters.

o Reducing the uncertainty in the description of the travel time distribution.

Questions?

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