

EGU24-5822, updated on 23 Jan 2025

<https://doi.org/10.5194/egusphere-egu24-5822>

EGU General Assembly 2024

© Author(s) 2025. This work is distributed under the Creative Commons Attribution 4.0 License.



Pyrite and its role in the development of nitrate pollution and raw water quality in water catchment areas

Carsten Hansen¹ and Michael Kühn²

¹CONSULAQUA Hamburg Beratungsgesellschaft mbH, Germany

²GFZ German Research Centre for Geosciences, Fluid Systems Modelling, Potsdam, Germany

The assessment in accordance with the Water Framework Directive and the EU Water Framework Directive continues to show poor chemical status for around one third of groundwater bodies in Germany due to excessive nitrate concentrations. In many regions, this is due to high nitrogen fertiliser intensities that have been applied to agricultural land for decades.

Nitrate input and degradation processes in aquifers are modelled using step-by-step hydrogeochemical continuous stirred tank reactors (CSTR) sequences with PHREEQC. This makes it possible to show how the overall water quality is characterised by the interaction of hydrogeochemical sub-processes such as nitrogen and lime fertilisation, substance releases from grassland ploughing, denitrification via organic carbon (heterotrophic degradation) and most importantly pyrite (lithotrophic degradation) and sulphate reduction, but also nitrate breakthroughs and well clogging.

CSTR models are not discretised spatially or temporally; their focus is on identifying and quantifying the relevant hydrogeochemical reactions. The advantage of this method is much shorter and more manageable calculation times than with fully coupled reactive transport models. They provide the user with a comprehensive hydrogeochemical understanding of nitrate degradation by pyrite oxidation processes in groundwater. In addition to reaction kinetic aspects, this also includes the effects of a loss of nitrate degradation capacity [1]. In the focus is the dissolution of pyrite and its re-precipitation and a reaction front developing into the system [2]. Moreover, concentrations of pyrite dissolution products (iron, sulphate, trace metals) can be understood.

Hydrogeochemical modelling in this sense is initially retrospectively oriented based on measurements and the longest possible time series. However, a hydrogeochemical CSTR sequence has been checked for plausibility and validated with sensitivity and parameter studies can then also be used to forecast water quality [3]. This provides a "tool" with which the effects of anthropogenic interventions in a geosystem can be calculated with regard to the effects on groundwater and raw water quality.

[1] Wilde, S., Hansen, C. & Bergmann, A. Nachlassender Nitratabbau im Grundwasser und deren Folgen – abgestufte modellgestützte Bewertungsansätze. *Grundwasser* 22, 293–308 (2017). <https://doi.org/10.1007/s00767-017-0373-0>

[2] Kübeck, C., Hansen, C., König, C. et al. Ableitung der Reaktivität von organisch gebundenem Kohlenstoff in redoxzonierten Grundwasserleitern – Hydrogeochemische Modellierung kinetisch angetriebener Reaktionssysteme. *Grundwasser* 15, 103–112 (2010). <https://doi.org/10.1007/s00767-009-0136-7>

[3] Jesußek, A., Hansen, C. & Wilde, S. Identifikation und Regionalisierung von Nitratabbauprozessen in einem Grundwasserleiter – Möglichkeiten und Nutzen für die Wassergewinnung. *Grundwasser* 21, 333–344 (2016). <https://doi.org/10.1007/s00767-016-0337-9>