Geophysical Research Abstracts, Vol. 7, 07370, 2005 SRef-ID: 1607-7962/gra/EGU05-A-07370 © European Geosciences Union 2005



## N-S-O heteroaromatic Compounds as potential 'NA-Killers' at Coal-Tar contaminated Sites:

## **Chemical Analyses, reactive Transport Experiments and Field Studies**

M. Piepenbrink (1), M. Krüger (1), T. Ptak (2), P. Grathwohl (1)

(1) Center for Applied Geoscience, University of Tübingen, Germany

(2) Geosciences Center, University of Göttingen, Germany

(matthias.piepenbrink@uni-tuebingen.de / Phone: ++49(0)7071-2977453)

N-S-O heteroaromatic compounds are toxic and potentially carcinogenic substances, which can typically be found in groundwater at tar oil contaminated sites. Most of these substances are not yet routinely monitored. Existing field studies (e.g. Zamfirescu and Grathwohl, 2001) show a relatively high persistence coupled with a high mobility, consequently resulting in extended contaminant plumes in groundwater.

Goal of the submitted paper is to present results of 1) an optimized chemical analysis of N-S-O heteroaromatic compounds, 2) transport experiments of selected compounds at laboratory scale and 3) the quantification of the in-situ natural attenuation-potential at field-scale.

The quantification of N-S-O heteroaromatic compounds in groundwater required the testing and improvement of existing analytical techniques. It finally turned out that sample preparation via SPE followed by measurement via GC-MS delivered the most stable/reliable results. Laboratory column experiments concerning the transport behavior of selected N-S-O heteroaromatic compounds (Methylbenzofuran, Dimethylbenzofuran, Benzothiophene, and Quinoline) were conducted with an online-monitoring set-up, which was able to detect the anticipated small retardation factors of the NSO compounds compared to a set of conservative tracers, and with varying aquifer materials from Borden and Southern Germany. Some of the selected N-S-O heteroaromatic compounds were transported like conservative tracers, some showed slight retardation, but all of them were less retarded than Acenaphthene, which was in former studies determined as the most persistent and mobile contaminant at the field site. Reactive transport parameters obtained from laboratory batch experiments were used to simulate the measured breakthrough curves, employing the Lagrangian stochastic transport model SMART (Finkel et al., 1997). The foreward modelled breakthrough curves (BTCs) e.g. of Dimethylbenzofuran fit well to the experimentally measured BTCs. The quantitative determination of the natural attenuation potential of NSO heteroaromatic compounds in groundwater at field scale is performed at a tar oil contaminated field site in southern Germany using an integral investigation approach at multiple control planes (integral-pumping tests, e.g. Ptak and Teutsch, 2000; Bockelmann et al. 2001) positioned downgradient of the source zone. The concentration time series determined during the integral-pumping tests already indicate that contaminants like BTEX and PAH almost vanished on their way to the most downgradient control plane, while NSO heteroaromatic compounds are still present. The minor losses in the determined mass flow rates further indicate that especially Methylbenzofuran and Dimethylbenzofuran are not only very mobile, but also highly persistent. These results indicate the need for more efficient remediation techniques e.g. ENA, to overcome the existing limitations of NA concerning the remediation of NSO heteroaromatic compounds (especially Methylbenzofuran and Dimethylbenzofuran).

## **References:**

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## Acknowledgement:

The authors greatly acknowledge the financial support of this study within the

KORA-framework of the German Ministry of Education and Science (BMBF), grant 02WN0361.