Geophysical Research Abstracts, Vol. 6, 06015, 2004
SRef-ID: 1607-7962/gra/EGU04-A-06015

MODELLING BIOGEOCHEMICAL FLUXES USING A KNOWLEDGE-BASED REACTIVE TRANSPORT APPROACH. ANAEROBIC OXIDATION OF METHANE AS A CASE STUDY

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The rapid increase in observational data of biogeochemical transformation processes in natural environments requires efficient assimilation into predictive models. Reactive transport models provide a powerful tool for global cycle prediction, provided that the observational data are integrated into a robust and realistic model framework. To meet these demands, the Biogeochemical Reaction Network System (BRNS) has been developed from a knowledge base (KB) of physical and biogeochemical processes integrating reaction mechanisms and rates. A Graphical User Interface (GUI) on a web-based 'runtime' server allows the user to select any number of KB processes required for their modelling task. With this approach it is no longer the model itself, but an easily accessible, open resource element, the KB, which contains the conceptual and quantitative understanding of biogeochemical pathways and their interactions.

Our results demonstrate that the BRNS allows reaction networks of increasing complexity, evaluates alternative process formulations, and develops diagnostic indicators of biogeochemical pathways that can be measured in the field or in experimental set-ups. A case study of anaerobic oxidation of methane has been developed to highlight the main features of the BRNS.