

Final report for the ESF-funded FIMIN workshop on

“Modelling of surface reactions of ferric (hydr)oxides”

University of Bayreuth
Oct 8 – Oct 12 2012

Organised by Professors Stefan Peiffer (Bayreuth) and Thilo Behrends (Utrecht)

1) Summary

Iron is the 5th most abundant element in the Earth's crust. It occurs naturally as either ferrous or ferric iron and forms a wide variety of minerals, some of which are highly reactive in the environment. Iron tends to coordinate with a large number of organic and inorganic ligands, and this in turn exerts a strong impact on its redox properties. Our understanding of the chemical and biological fundamentals of surface processes and iron mineral transformation reactions is, however, still surprisingly incomplete. Improvement of our knowledge on the function of this abundant element in biogeochemical cycles is therefore a goal in many scientific disciplines. Moreover, it will significantly contribute to obtaining a better understanding of processes that are crucial to human and societal development such as the supply of clean water, remediation of contaminated sites or the regulation of CO₂ emissions.

The FIMIN Research Networking Programme supports a cross-disciplinary approach to understanding the role of iron in the environment, aiming to make the ensuing knowledge, expertise and relevant instrumentation available to researchers throughout Europe. This Research Networking Programme addresses this need through an intensive training and education programme. The ultimate goal of the FIMIN project is to elucidate the functionality of iron minerals through understanding cycling of electrons and matter through iron minerals, encompassing contrasting disciplines in the environmental sciences, including geochemistry, biogeochemistry, microbiology, soil and hydrological sciences, and biotechnology.

As part of these activities, the Steering Committee of FIMIN decided to organize a residential workshop covering the fundamentals and recent advances in describing and quantifying the interaction between surfaces of ferric (hydr)oxides and the solution. Professor Thilo Behrends from Utrecht University (Netherlands) and Prof. Stefan Peiffer from University of Bayreuth (Germany) organised a 5-day residential course in Bayreuth. The concept of this workshop was to link theoretical concepts of surface complexation with modelling approaches using the computer code PHREEQC and to apply this tool to problems of the participants.

The course started with an Introduction into the use of PHREEQC by Prof. Planer-Friedrich from University of Bayreuth on the first day. At days 2 and 3 Prof. Behrends introduced the

concept of surface charge and surface complexation in the morning sessions. Its implementation into PHREEQC was taught by Prof. Peiffer in the afternoon sessions with the opportunity to discuss own research problems of the participants. On Day 3 late afternoon a poster session was held where participants introduced their research. At Day 4 the multi site charge distribution concept and its implementation into PHREEQC was introduced by Dr. Lützenkirchen from Karlsruhe Institute of Technology. On day 5 experimental considerations for the determination of surface properties were discussed by Prof. Behrends and Dr. Lützenkirchen.

The course was aimed at researchers working on all aspects where mineral surfaces are involved in the Fe cycle including microbiologists, and attracted 15 exceptional early stage researchers as participants. The meeting was delivered on budget, and from course feedback was judged an overwhelming success by the attendees.

2) Description of the scientific content and discussion at the event

All attendees arrived in Bayreuth on the evening of Sunday 7th October, and the course started formally on the morning of Monday the 8th.

Day 1: Introduction into PHREEQC by Prof. Planer-Friedrich

The geochemical computer code PHREEQC provides the opportunity to perform calculations on surface complexation and surface charge. Hence, Day 1 served as a general introduction into the use of PHREEQC

Day 2,3 morning sessions: The formation of Surface Charge on Metal Oxides by Prof. Behrends

In this part of the workshop participants were introduced in the fundamental physicochemical concepts of surface charge formation, including diffusive double layer and triple layer models, points of zero charge, the effects of ionic strength on surface charge and the formation of surface complexes.

Day 2,3 afternoon sessions: Modelling surface complexation using PHREEQC by Prof. Peiffer

PHREEQC has implemented the tools to perform calculations on surface complexation phenomena. The principles and in particular the use of the corresponding keywords was taught and problems were discussed. Participants had the opportunity to ask for solutions to their own research problems.

Day 3 late afternoon: Poster Session

The participants were encouraged to bring Posters about their own research, which they briefly presented orally during the Poster Session. The Posters were then discussed by the audience.

Day 4, morning and afternoon sessions: Introduction of the CD-MUSIC approach by Dr. Luetzenkirchen

CD-MUSIC stands for **Charge Distribution – MultiSite Ion Complexation** and denotes a model that attributes specific charge to functional surface groups according to the coordination of the central atom. Through that each crystal plane of a certain oxide has different but specific charge distributions. The fundamentals were taught and its implementation into a PHREEQC module discussed.

Day 5, morning session: Practical considerations when determining mineral surface properties by Prof. Behrends and Dr. Lützenkirchen

Determination of mineral surface properties, such as point of zero charge, is of paramount importance when dealing with mineral surface chemistry. In this session, experimental aspects were discussed that need to be considered when setting up experiments in this regard. Advices were given in order to minimize errors during titrimetric approaches.

Attendee participation. There was plenty of opportunity throughout the workshop for the early-stage researchers to interact with the teaching staff. On each day, there were coffee and lunch breaks attended by the staff, with considerable mixing at each opportunity. On day 2 a joined dinner was organized with all participants and instructors. The lectures were also informal, with attendees (and members of the teaching team) encouraged to ask questions throughout.

3) Assessment of the results and impact of the event on the future direction of the field

The following template was used to obtain feedback on the course. The overwhelming response was exceptionally positive, with a cumulative total against each question shown in the table below. There was little negative feedback, although one respondent did note that more time for exercise would be beneficial! Several attendees praised the breadth of information provided, the quality of lectures, the usefulness of the practical sessions (PHREEQC), as well as the organisation.

Evaluation

FIMIN Workshop ***Modelling of surface reactions of ferric (hydr)oxides***
7 Oct – 12 Oct 2012

Attending the workshop was useful for performing my research project.	agree				disagree
	8	6	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
The content of the workshop fulfilled my expectations.	agree				disagree
	10	3	1	<input type="checkbox"/>	<input type="checkbox"/>
I feel confident that I can model surface reactions at ferric (hydr)oxides now by myself using PHREEQC	agree				disagree
	4	6	4	<input type="checkbox"/>	<input type="checkbox"/>
I would have preferred that more time had been dedicated to exercises using PHREEQC	agree				disagree
	3	2	5	<input type="checkbox"/>	4
Lectures on theories and concepts used to describe surface complexation were useful	agree				disagree
	10	1	3	<input type="checkbox"/>	<input type="checkbox"/>

I understood the underlying theories and concepts used for describing surface complexation.	agree 5	5	4	<input type="checkbox"/>	disagree <input type="checkbox"/>
I would have preferred that more time had been dedicated to theories	agree 1	2	4	1	disagree 6
Level of the lectures	too high 2	7	5	<input type="checkbox"/>	too low <input type="checkbox"/>
The Workshop gave me the opportunity to discuss my research questions.	agree 7	6	1	<input type="checkbox"/>	disagree <input type="checkbox"/>
Attending at the Workshop was useful to expand my professional network.	agree 10	4	<input type="checkbox"/>	<input type="checkbox"/>	disagree <input type="checkbox"/>
The workshop was well organized	agree 12	2	<input type="checkbox"/>	<input type="checkbox"/>	disagree <input type="checkbox"/>
The most profitable aspect of the Spring School for me was...					
The Spring School could have been more profitable if...					
(Please use the back of the page if you need extra space)					