KIGAM Korea Institute of Geoscience and Mineral Resources

INTERNATIONAL SCHOOL FOR GEOSCIENCE RESOURCES (IS-Geo)
KOREA INSTITUTE OF GEOSCIENCE AND MINERAL RESOURCES (KIGAM)

PUBLIC CUSTOMIZED TRAINING COURSE ON
Applied Reactive Transport Modeling

The **International School for Geoscience Resources** of KIGAM presents an intensive training course on **Applied Reactive Transport Modeling**. The course will take place at the Ara room of International School for Geoscience Resources of KIGAM in Daejeon (Korea) in **May 18 to 22, 2015** and will include the following topics.

Topics	Date	Instructor
Day 1. Fundamentals of solute transport modelling Topic 1. Fundamentals of advective-dispersive transport Topic 2. Introduction to solute transport modeling Topic 3. Numerical solution techniques Topic 4. Examples of conservative transport simulations	5.18	Henning Prommer (CSIRO, Australia) & DOUGLAS B. KENT (USGS, USA) & OLIVIER ATTEIA (ENSEGID, Australia)
Day 2. Geochemical and reactive transport modeling Topic 1. Introduction to geochemical modeling Topic 2. Introduction to reactive transport modeling Topic 3. Mineral dissolution and precipitation reactions	5.19	
Day 3. Cation exchange and surface complexation reactions Topic 1. Basics of cation exchange Topic 2. Surface complexation reactions Topic 3. Coupled reactive transport of metals and radionuclides	5.20	
Day 4. Reaction kinetics: Modeling the fate of organic pollutants Topic 1. Microbial kinetics and biodegradation Topic 2. NAPL dissolution Topic 3. Coupled reactive transport of organic pollutants	5.21	
Day 5. Advanced topics and team exercises Topic 1. Modeling of groundwater age Topic 2. Denitrification and pyrite oxidation Topic 3. Team exercises	5.22	

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Ministry of Science, ICT and Future Planning

COURSE INFORMATION

Agenda

- This course is designed to introduce the participants to the model-based quantification of groundwater quality problems from various industries and disciplines (contaminant hydrology, mining, water supply).

Course Covered

- Participants also will understand the basics of coupled geochemical transport modelling. They will learn how to apply state-of-the-art models to real-world water quality problems.
- Participants will apply the theoretical framework with hands-on experience in the computer lab. They will practise the use of the wisely used modeling tools MODFLOW, MT3DMS, PHREEQC-2 and PHT3D (which couples MT3DMS and PHREEQC-2) and spend approximately half of the course in the computer lab. Simplified exercises that are based on real-world problems will help participants to translate theory into practice.

Course Requirements: Prerequisite

- Understanding of hydrogeological concepts and groundwater flow processes
- At least basic understanding of geochemical processes
- Participants will benefit the most from this course if they have already some working knowledge of groundwater models (flow/transport)
- Basic skills to process and visualise data

Who should Attend?

- This course is mainly designed to train entry and intermediate-level hydrogeologists, geochemists, and civil/environmental engineers interested in anthropogenic and geogenic groundwater quality problems and on the quantification of these problems
- For scientists and postgraduate students who would like to analyse and perform a model-based interpretation of their laboratory- or fieldscale data

• Course contents and learning objectives

Related to the material of the course, the participants will be exposed to:

- The basics of advective and dispersive solute transport
- Development of conceptual models
- Numerical solution schemes
- Construction of MODFLOW/MT3DMS flow and solute transport models
- Overview of key hydrochemical processes (kinetically controlled degradation of organic substances, ion exchange, mineral reactions, surface complexation reactions)
- Principles of modeling biogeochemical processes such as complexation reactions, sorption, mineral dissolution/precipitation, ion exchange, NAPL dissolution, biodegradation, and microbial growth/decay
- Modeling of equilibrium and kinetically controlled reactive processes with PHREEQC
- Coupled modeling of transport and chemical reactions using PHT3D
- A wide range of model applications (case studies) for organic and inorganic pollution problems (e.g., natural attenuation of organic pollutants, fate of metals)

• Day 1. Fundamentals of solute transport

This segment will introduce the fundamentals of solute transport

- Advection
- Dispersion
- Dual-Domain Mass Transfer
- Multi-species transport model MT3DMS
- Graphical User Interface ipht3d
- Pollution plume behaviour

• Day 2. Introduction to geochemical and reactive transport modeling

This segment will provide and overview of geochemical processes and introduce participants to geochemical and reactive transport modeling.

- Geochemical processes
- Geochemical model PHREEQC
- Aqueous complexation reactions
- Mineral dissolution and precipitation
- Introduction to reactive transport modeling

- Application to modeling acid mine drainage

- **Day 3. Ion exchange and surface complexation reactions**

  This course segment will introduce the surface reactions ion exchange and surface complextion

  - Basics of cation exchange
  - Application to modeling the fate of an ammoniacal liquor pollution
  - Basics of surface complexation reactions
  - Surface complexation modeling
  - Application to modeling the fate of zinc at the Cape Cod site

- **Day 4. Kinetically controlled reactions**

  This unit will introduce reaction kinetics and its application to quantifying the fate of organic pollution plumes

  - Modeling kinetic reactions
  - Modeling microbial dynamics with PHREEQC
  - Modeling NAPL dissolution
  - Application to modeling the fate of a BTEX plume

- **Day 5. Advanced topics and team exercises**

  This segment will allow the students to test their new skills and apply them to translate their own or pre-defined conceptual hydrochemical problems into numerical models. Potential simulation problems include

  - Denitrifcation coupled to pyrite oxidation
  - Arsenic mobilisation by reductive dissolution of Fe-oxides
  - In situ leaching of uranium
  - Degradation of PCE and associated isotope fractionation

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About the instructor – *Dr Douglas B. Kent*

Doug is a hydrologist with the U.S Geological Survey. He received a BA in chemistry from the University of California, San Diego and a PhD from Scripps Institution of Oceanography. Doug's main research interest is the fundamental understanding of chemical reactions at mineral-water interfaces, understanding the coupling between these reactions and physical and biological processes, and to develop conceptual and quantitative models that are broadly applicable to understanding and predicting metal and metalloid transport, mobilization, and sequestration in groundwater across the range of spatial and temporal scales required in field applications.

About the instructor – *Prof. Olivier Atteia*

Olivier Atteia is professor at the ENSEGID polytechnicum Bordeaux (France). He obtained his PhD from EPFL Lausanne (Switzerland). His research specialises on groundwater contamination of industrially contaminated sites and on numerical modeling of the coupled physical and geochemical processes that govern contaminant fate at these sites. His work involves applied and theoretical aspects of modeling reactive transport. He is the developer of the ipht3d interface that will be used in this shortcourse.

About the instructor – *Prof. Henning Prommer*

Dr Henning Prommer is a Winthrop Research Professor in a joint appointment between the University of Western Australia (UWA) and CSIRO Land and Water (Australia). He obtained his PhD from the University of Western Australia. His main expertise is the development of (bio)geochemical transport models and their application to an integrated quantification of physical flow/transport processes and geochemical reactions. A strong focus of his research is the assessment and prediction of the variability of the redox zonation in aquifers, the corresponding impact on the fate of anthropogenic macro- and micro-pollutants, weathering reactions, and the mobilisation, fate and remediation of heavy metal(loid)s. He is the original developer of the reactive transport model PHT3D, which will be used in this shortcourse.

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