PUBLIC CUSTOMIZED TRAINING COURSE ON

Introduction to Geochemical and Reactive Transport Modeling

The **International School for Geoscience Resources** of KIGAM presents a public customized training course on **Introduction to Geochemical and Reactive Transport Modeling**. The course will take place at the Ara room of International School for Geoscience Resources of KIGAM in Daejeon (Korea) from **May 26 to 30, 2014** and will include the following topics.

Topics	Date	Instructor
Day 1. Modeling homogeneous and classical heterogeneous systems Topic 1. Introduction to geochemical modeling Topic 2. PHREEQC example problems Topic 3. Ion exchange Topic 4. Environmental mineralogy	May 26	James Davis (LBNL, USA) Douglas Kent (USGS, USA) Sung Pil Hyun (KIGAM, Korea)
Day 2. Modeling sorption Topic 1. Sorption Topic 2. Naturita field site talk Topic 3. Generalized composite sorption modeling Topic 4. Environmental microbiology and microbial processes	May 27	James Davis (LBNL, USA) Hee Sun Moon (KIGAM, Korea)
Day 3. Modeling oxidation-reduction Topic 1. Redox processes Topic 2. Cape Cod field site talk Topic 3. Modeling microbial processes Topic 4. Microbial processing of nitrogen in Ahumet Pond	May 28	James Davis (LBNL, USA) Douglas Kent (USGS, USA)
Day 4. Transport processes Topic 1. Transport processes Topic 2. PHREEQC transport problems Topic 3. Isotopic fractionation	May 29	Douglas Kent (USGS, USA) James Davis (LBNL, USA)

Day 5. Isotopic fractionation and non-ideal transport Topic 1. Modeling microbial redox reactions with isotopic fractionation Topic 2. Examples problems Topic 3. Discussion section	May 30	James Davis (LBNL, USA) Douglas Kent (USGS, USA)

COURSE INFORMATION

- **Agenda**
  - This course is intended to provide the participant with an introduction to geochemical equilibrium and 1-D transport modeling along with hands-on learning experience of PHREEQC and its applications.
  - The participant has an opportunity to apply their knowledge of geochemical principles and PHREEQC skills to practical geochemical problems of their own interest.

- **Course Covers**
  - Geochemical and biogeochemical processes
  - Geochemical modeling using PHREEQC v3
  - Application of PHREEQC to practical geochemical problems
  - 1-D transport modeling

- **Course Requirements: Prerequisite**
  - General knowledge of chemical equilibrium, aquatic chemistry and chemical reactions between minerals and groundwater such as sorption/desorption, precipitation/dissolution, oxidation/reduction
  - General knowledge of environmental microbiology

- **Who should Attend?**
  - Hydrogeologists and scientists/engineers in the related fields who are interested in the geochemical and microbiological processes occurring in groundwater and at the groundwater-sediment interface
  - Graduate students and advanced undergraduate students who would like to learn geochemical principles and thermodynamic modeling skills
  - Geochemists who are interested in the transport modeling

- **Summary of topics**

Day 1. Modeling homogeneous and classical heterogeneous systems

- Introduction to geochemical modeling
  * Water chemistry
  * Chemical reactions and equilibria
  * Activities; ionic strength
  * Thermodynamic functions, delta G, enthalpy, van Hoff
  * Gas solubilities
  * Acids and bases
  * Aqueous speciation
  * Mineral dissolution and precipitation; saturation index
  * Redox processes
  * Kinetics
- PHREEQC example problems
  * Introduction to PHREEQC; concept of KEYWORDS
  * How to enter solutions in PHREEQC; entering alternative/new master species
  * Calculating aqueous speciation; charge balance in PHREEQC; mixing solutions
  * Calculating CO_2 solubility as function of partial pressure
  * Calculating solution composition equilibrium solubility of $CaCO_3$ and CO_2
  * Calcite dissolution and precipitation; equilibrium and kinetics
  *Note: This introduces the KINETICS and RATES keywords
- Ion exchange
  * Theory, principles, activity conventions
  * PHREEEQC examples:
  * Solutions and exchangers: example with NH4
  * Solutions, exchangers, and minerals (e.g. calcite)
- Environmental mineralogy
  * XRD characterization
  * Microscopy
  * Spectroscopy

Day 2. Modeling sorption

- Sorption 1
  * Theory, principles, conceptual models, Kd, isotherms, surface complexation
  * PHREEQC examples with DDL model of Dzombak and Morel
  * Calculation of HFO surface charge as function of pH
  * Cation sorption on HFO,

- Sorption 2
  * PHREEQC examples with DDL surface complexation model of Dzombak and Morel
  * Anion sorption competition (chromate and sulfate)
  * Cation sorption with effects of nonsorbing complexing ligand
  * Cation sorption with sorbing ligand-metal complex
- Naturita field site talk
  * Plume description and uranium transport
  * Development of uranium GC model
  * In-situ Kd values
- Generalized composite sorption modeling
  * Zn sorption on Cape Cod sediments; GC model development
  * DDL versus GC models
  * Mineral buffering of pH
  * Sorption with complexation and mineral dissolution/precipitation (U(VI), CO_3, $CaCO_3$)
- Environmental microbiology and microbial processes
  * Processes; environments; microbial communities
  * Electron donors and acceptors
  * Fermenters and metabolizers in soils and aquifers (O_2, Mn(III/IV), N(V), * Fe(III), S(VI), CO_2)

Day 3. Modeling oxidation-reduction

- Redox processes
  * Theory and principles; redox ladder; pe-pH diagrams
  * Fe redox chemistry
  * Nitrogen redox chemistry
  * Coupled and uncouples nitrogen/Fe redox
  * Redox processes, PHREEQC examples
  * pe-pH diagram for nitrogen system
  * Nitrate + acetate equilibrium
  * Dissimilatory Fe(III) reduction, HFO + acetate using Kinetics and Rates
  * Nitrogen redox with Fe(II): uncoupling redox half-reactions
- Cape Cod field site talk
  * Plume development and description
  * Nitrogen cycling; nitrogen isotopes
  * Zinc plume; pH gradient
  * Cessation of effluent disposal
  * Flow modeling on Cape Cod
- Modeling microbial processes

* Rate expressions (0-order, 1-order, Michaelis-Menton, changes in biomass)
* Partial equilibrium approach
* PHREEQC examples:
* Batch titration of groundwater with dissolved oxygen, nitrate, Mn(III), Fe(III), sulfate, CO2 with CH2O without then with sorption of divalent cations
* Dissimilatory reduction of HFO with sorbed As(V)/As(III) in the presence of aquifer sediments

- Microbial processing of nitrogen in Ashumet Pond
  * Modern-day nitrogen cycle (if not already covered)
  * Sites with contrasting hydrologic conditions (discharge of anoxic; nitrate-contaminated groundwater; discharge of oxic "pristine" groundwater; recharge of lake water
  *Microbial populations and processes

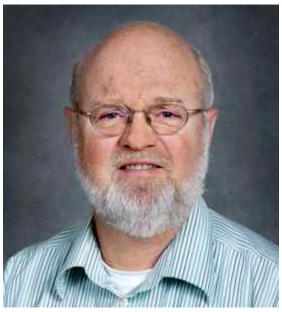
Day 4. Transport processes

- Transport processes
  *Advection
  * Diffusion
  * Dispersion and handling dispersion in PHREEQC
  * Transport and cation exchange (use NH_4 example)
- PHREEQC transport problems
  * Zn 1D transport at different/variable pH values
  * Naturita uranium 1D transport at different alkalinity values
  * Transport with cation exchange with ammonium, Fe(II)
  * Adding denitrification coupled to organic carbon as compared to Fe(II) oxidation with phosphate, As(III/V)
- Isotopic fractionation

Day 5. Isotopic fractionation and non-ideal transport

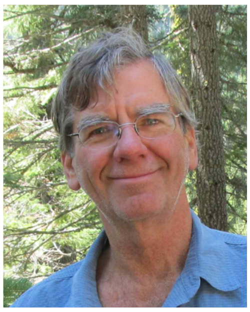
- Modeling microbial redox with isotopic fractionation
  * Denitrification in batch systems
  * Denitrification with fractionation during advective-diffusive transport
- PHREEQC example problems
- Discussion section

About the instructor – *Dr. James A Davis*



Dr. Davis is a Senior Scientist in the Earth Sciences Division at Lawrence Berkeley National Laboratory (LBNL). He got his Ph. D. in Environmental Engineering at Stanford University in 1972. Before he moved to LBNL, he worked with the US Geological Survey for 30 years. He has performed extensive experimental and field research on biogeochemical processes occurring at mineral surfaces and their effects on water and sediment mineralogical compositions in aquifers. The research has examined geochemical processes at multiple scales, from molecular-scale spectroscopic studies to large field-scale investigations. Current research is focused on the biogeochemistry of uranium and arsenic and their transport in engineered or natural groundwater systems.

About the instructor – *Dr. Douglas Kent*



Dr. Kent is a Research Hydrologist at the US Geological Survey. He received his Ph. D. in Oceanography at the University of California-San Diego in 1983. Since then he has conducted research targeted at understanding the coupled physical, chemical, and biological processes that influence the fate and transport of inorganic solutes in aquatic systems. Research is carried out over a range of spatial and temporal scales. Short-term, bench-scale laboratory experiments are used to identify biogeochemical reactions influencing transport and to quantify parameters for reactive transport modeling. Intermediate-scale natural- and forced-gradient transport experiments are conducted with inorganic and organic solutes that undergo adsorption, complexation, precipitation-dissolution, and oxidation-reduction reactions, including those driven by microbial metabolic processes. Large-scale natural-gradient transport experiments and plume-scale studies are conducted to test applicability of conceptual and quantitative models developed from laboratory and small-scale field experiments to the larger spatial and temporal scales typically encountered in groundwater contamination investigations. The research utilizes a wide range of laboratory instrumentation, analytical and spectroscopic techniques, and numerical models.

About the instructor – *Dr. Hee Sun Moon*

Dr. Moon is a Senior Researcher in the Groundwater Department at KIGAM. After receiving her Ph. D. in Environmental Engineering from Seoul National University in 2005, she did her Post-Doc at Princeton University. Then she took her position at Seoul National University as a Research Professor until she joined KIGAM in 2013. Throughout her career, her research has covered a wide range of topics related to biogeochemistry, including a biological reactive barrier, remediation of contaminated sites with uranium using biostimulation, phytoextraction of heavy metals, and biological treatment and energy production using solid wastes, and environmental bioengineering.

About the instructor – *Dr. Sung Pil Hyun*

Dr. Hyun is a Senior Researcher in the Groundwater Department at KIGAM. He received his Ph.D. in Environmental Mineralogy from Seoul National University in 2000. After that, he worked with Korea Atomic Energy Research Institute and the University of Michigan focusing on the mineralogical aspects of the geochemical processes at the mineral-water interface, including uranium sorption and reduction, arsenic redox chemistry, and dechlorination of chlorinated ethylenes. In his research, he combines the equilibrium geochemical modeling approach with his skills in microscopic and spectroscopic characterization techniques. He joined KIGAM in 2011 and has worked on the artificial groundwater recharge, biogeochemical processes influencing nitrogen transformation and transport at the groundwater-surface interface, environmental impacts of shale gas development, and assessment of the impact of chemical spills on groundwater and soil environments.