Public Customized Training Course on
'Introduction to Geochemical and Reactive Transport Modeling'

(Venue: Ara room)

Date/Time	Program Description	Remarks
5.26 (Mon)	**Registration and orientation**	**IS-Geo**
09:50-10:00		
5.26 (Mon)	**Modeling homogeneous and classical heterogeneous systems**	
10:00-11:00	Introduction to geochemical modeling 1 (Water chemistry, chemical reactions and equilibria, activities; ionic strength, Thermodynamic functions)	Dr. James Davis (LBNL, USA)
11:10-12:10	Introduction to geochemical modeling 2 (Gas solubilities, acids and bases, aqueous speciation, mineral dissolution and precipitation, redox processes, kinetics)	
12:10-13:10	Lunch (KIGAM cafeteria is available after 12:10 PM)	
13:10-14:10	PHREEQC examples problems 1 (Introduction to PHREEQC; keywords, how to enter solutions, calculating aqueous speciation; charge balance in PHREEQC; mixing solutions)	Dr. Douglas Kent (USGS, USA)
14:20-15:20	PHREEQC example problems 2 (Calculating CO_2 solubility as a function of partial pressure, calculating solution composition equilibrium solubility of $CaCO_3$ and CO_2)	
15:30-16:30	Ion exchange (Theory, principles, activity conventions, PHREEQC examples)	Dr. James Davis (LBNL, USA)
16:40-17:40	Environmental mineralogy (XRD, microscopy, spectroscopy)	Dr. Sung Pil Hyun (KIGAM, Korea)
5.27 (Tue)	**Modeling sorption**	
10:00-11:00	Sorption 1 (Theory, principles, conceptual models, Kd, isotherms, surface complexation)	Dr. James Davis (LBNL, USA)
11:10-12:10	PHREEQC examples with DDL (calculation of HFO surface charge as a function of pH, cation sorption on HFO)	
12:10-13:10	Lunch	
13:10-14:10	Sorption 2 (Anion sorption competition, cation sorption with effects of nonsorbing ligand and sorbing ligand-metal complex)	Dr. James Davis (LBNL, USA)
14:20-15:20	Naturita field site talk (Plume description and uranium transport, uranium GC model, in-situ Kd values)	
15:30-16:30	Generalized composite sorption modeling (Zn sorption on Cape Cod sediments, DDL versus GC models, mineral buffering of pH, sorption with complexation and mineral dissolution/precipitation)	
16:40-17:40	Environmental microbiology and microbial processes (Processes, environments, microbial communities, electron donors/acceptors, fermenters/metabolizers in soils and aquifers)	Dr. Hee Sun Moon (KIGAM, Korea)
5.28 (Wed)	**Modeling oxidation-reduction**	
10:00-11:00	Redox processes 1 (Theory and principles; redox ladder; pe-pH diagrams, Fe redox chemistry)	Dr. James Davis (LBNL, USA)
11:10-12:10	Redox processes 2 (Nitrogen redox chemistry, coupled and uncoupled nitrogen/Fe redox)	
12:10-13:10	Lunch	
13:10-14:10	PHREEQC redox example problems (pe-pH diagram for nitrogen system, nitrate+acetate equilibrium, dissimilatory Fe(III) reduction, nitrogen redox with Fe(II))	Dr. Douglas Kent (USGS, USA)
14:20-15:20	Cape Cod field site talk (Plume development, nitrogen cycling, Zn plume, cessation of effluent disposal, flow modeling on Cape Cod)	
15:30-16:30	Modeling microbial processes (Rate expressions, partial equilibrium approach, PHREEQC examples; batch titration of groundwater with dissolved oxygen, nitrate, Mn(III), Fe(III), sulfate, CO_2, dissimilatory reduction of HFO with sorbed As(V)/As(III))	
16:40-17:40	Microbial processing of nitrogen in Ashumet Pond (Modern day nitrogen cycle, sites with contrasting hydrologic conditions, microbial populations and processes)	
5.29 (Thu)	**Transport processes**	
10:00-11:00	Transport processes 1 (Advection, diffusion)	Dr. Douglas Kent (USGS, USA)
11:10-12:10	Transport processes 2 (Dispersion and handling dispersion in PHREEQC, transport and cation exchange with an NH4 example)	
12:10-13:10	Lunch (KIGAM cafeteria is available after 12:10 PM)	
13:10-14:10	PHREEQC transport problems 1 (Zn 1D transport, Naturita uranium 1D transport)	Dr. James Davis (LBNL, USA)
14:20-15:20	PHREEQC transport problems 2 (Transport with cation exchange with ammonium, Fe(II), adding denitrification coupled to organic carbon)	Dr. Douglas Kent (USGS, USA)
15:30-16:30	PHREEQC transport problems 3 (Transport with Fe(II) oxidation with phosphate, As(III/V))	
16:40-17:40	Isotopic fractionation	
5.30 (Fri)	**Isotopic fractionation and non-ideal transport**	
10:00-11:00	Modeling microbial redox with isotopic fractionation 1 (Denitrification in batch systems)	Dr. Douglas Kent (USGS, USA)
11:10-12:10	Modeling microbial redox with isotopic fractionation 2 (Denitrification with fractionation during advective-diffusive transport)	
12:10-13:10	Lunch	

13:10-14:10	PHREEQC example problems 1	Dr. Douglas Kent (USGS, USA)
14:20-15:20	PHREEQC example problems 2	Dr. James Davis (LBNL, USA)
15:30-16:30	PHREEQC example problems 3	
16:40-17:40	Discussion	

※ The working language is English