TOUGHREACT V3-3-OMP

Training Course

February 17-19, 2020

Energy Geosciences Division
Lawrence Berkeley National Laboratory
Berkeley, CA 94720

Instructors

Eric Sonnenthal and Nicolas Spycher

Lawrence Berkeley National Laboratory
Energy Geosciences Division
1 Cyclotron Road, 84R0171
Berkeley, CA 94720

This course will provide a hands-on introduction to the latest shared-memory parallel release of TOUGHREACT (V3.3-OMP). Sample problems include simple reactive transport in batch and flow-through systems, equilibrium and kinetic reactions, hydrothermal experiments, followed by more complex problems on geological sequestration of CO_2 and subsurface nuclear waste storage. These problems serve as prototypes for creating input files for new applications. The course will also include discussions of the underlying physical and chemical processes, as well as the mathematical and numerical approaches used.

AGENDA

Monday, February 17, 2020

Afternoon Session

9:00   *Welcome, safety, introductions, overview of course (refreshments served)*

- Course objectives and outline
- TOUGHREACT V3.3-OMP installation on participant laptops

10:15   **TOUGHREACT basics**

- Overview of TOUGHREACT V3.3-OMP
- Multicomponent geochemical computations

11:30   **Problem No. 1** – *Introduction to Setup of a Simple Reactive Transport Problem (lunch served)*

- Discussion of flow input and output files
- Discussion of chemical input and output files
- Discussion of thermodynamic data file
- Simple aqueous transport with NaCl solution
- Aqueous transport with calcite, gypsum and dolomite: Batch and flow-through *(refreshments served)*
- Different mineral zones
- Problem variations

18:30   *Guest Speaker Presentation (Dinner served, Restaruant/location: TBD)*

Tuesday, February 18, 2020

9:00   **Problem No. 2** – *1-D Plug-flow reactor experiment (refreshments served)*

- Calculation of various input data, setup of input files
- Time discretization (Courant limitation)
- Mesh generation (1D Cartesian)
- Simulations with one (quartz) and more minerals (volcanic tuff) *(lunch served)*

13:00   **Problem No. 3** – *1-D radial CO_2 injection problem (Sample Problem 5 in manual)*

- Baseline simulation
- Flow-only simulation (no reaction)

- Simulations with/without CO_2 reaction feedback on flow
- Restart option
- *2D X-Z mesh* problem definition
- Setup of the chemical input files
- Local equilibrium versus kinetics
- Linear versus radial mesh *(refreshments served)*
- Connecting chemical zones to grid blocks
- Preparation of initial water composition
- Problem variations

17:00   *Adjourn*

Wednesday, February 19, 2020

9:00   ***Problem No. 4*** *– Geologic disposal of nuclear waste (refreshments served)*

- Problem conceptualization
- Setup of the chemical input files
- Local equilibrium versus kinetics
- Problem variations *(lunch served)*

12:30   *Concluding Remarks and Open Discussion*

1:30   *Adjourn*

Meals and Refreshments will be served after the meeting begins, while work is being performed.
Attendance is required during these times.