Why NanoGeosciences are Necessary for Petroleum Engineering

TOSHIFUMI MATSUOKA

Environment and Resource System Engineering, Kyoto University, Kyoto 615-8540, Japan; and Fukada Geological Institute, Tokyo 113-0021, Japan (matsuoka@fgi.or.jp)

Petroleum Engineering is typical multi-disciplinary engineering and it needs to cover wide temporal-spatial areas such as Geological time and Basin-wide to Chemical reaction time and Molecule structures of hydrocarbons. In order to handle these disciplines, engineers in oil and gas industry have been developing computer simulations such as reservoir simulators, LBM simulation for multi-phase flow in porous media. Now, molecular dynamics (MD) simulations become unavoidable in oil and gas industry. I will highlight two examples of MD simulations: (1) Digital Oil Conception; and (2) Wettability Evaluation for CO2/water/rock, and how to up-scale these results into geological space and time

The initial objectives of digital oil are to understand and solve asphaltene problems through MD simulations. We have constructed a digital oil model (a full molecular model of crude oil) for a crude oil sample, of which the field actually confronts asphaltene problems, on the basis of analytical experiments and quantitative molecular representation (QMR) method. After constructing the digital oil model, we calculated association energies of asphaltenes by potential of mean force (PMF) using MD simulations. The data obtained in this work should be used in a thermodynamic model of phase behavior of asphaltene dealing with asphaltene association and precipitation. Furthermore, we propose that association energy of asphaltene can be criteria for selecting good asphaltene solvents.

CO2 Geo-Sequestration, that substantial quantities of CO2 can be injected into subsurface porous rock formations, has been well accepted as the most effective way to reduce the anthropogenic greenhouse gas CO2. Cappliary phenomenon is dominant in the CO2 injection to the underground, and it is the capillary pressure to maintain the CO2 under the caprocks. However, the wettability of CO2/water/rock exhibits different trends as function of pressure dependent on the type of the rock surfaces. Furthermore, it changes with sallt concentration. I'll show how we could address this problem using MD simulations. Finally, I show my perspectives of application of nanogeosciences to petroleum engineering in near future.

I would like to acknowledge the financial support from JAPEX, INPEX, JOGMEC, JST and JSPS, and thank to my colleagues at Kyoto University for their contributions.