

A Brief Introduction to Perple_X

Perple_X is a collection of computer programs for calculating phase diagrams, equilibrium reactive transport models, and manipulating thermodynamic data. The program finds application primarily in petrology and geophysics. In geophysical applications it is used to provide an equilibrium model for caloric and elastic (e.g., seismic wavespeed) properties as a function of chemistry, pressure, and temperature. The course will consist of theoretical and practical parts. The theoretical part, ca. 2 hours, will present some applications and explain how Gibbs energy minimization, the essential tool of phase equilibrium calculations, is done in Perple_X. In the practical part, ca. 4 hours, participants will compute a phase diagram section for a metabasaltic lithology and learn how to extract information from the section. More advanced practical problems involving redox and/or electrolytic fluid will be provided for participants who are familiar with Perple_X.

Participants are advised to download and test Perple_X prior to the practical. Instructions are at www.perplex.ethz.ch/perplex/tutorial/iisc_tutorial/IISC_Perple_X_setup.pdf.

Since my arrival at IISc, together with Kizo Vipfezol and Koyomi Abe, I have been testing a method of inverting petrologic data for thermobarometric conditions and unmeasured chemistry, an important petrologic problem. The method, which relies on Perple_X, appears to work well. If there is interest, I shall be happy to present the method in the theoretical/practical format as the Perple_X introduction.