

An Introduction to Perple_X

Perple_X is a collection of computer programs for calculating phase diagrams, equilibrium reactive transport models, and manipulating thermodynamic data. This two-part short course will consist of a mixture of theoretical lectures and practicals. The lecture for the first part (Tuesday, December 5, 10:30-13:30 Room 2G) will be devoted to explaining how Gibbs energy minimization, the essential tool of phase equilibrium calculations, is done in Perple_X and the consequences that this choice of algorithm have for the user. In the corresponding practical (Wednesday, December 6, 14:30-18:30; Room 2G), participants will compute phase diagram sections and learn how to extract physicochemical data from sections. Ideally the second part of the course (Monday, December 11, 14:30-18:30; Tuesday, December 12m 10:30-13:30; Room 2G) will be devoted to phase equilibrium topics and/or modelling problems suggested by the participants. In the absence of suitable suggestions, alternative topics include thermodynamic theory and the formulation of solution models and additional practical problems dealing with phase fractionation and reactive transport will be treated.

Participants should download and verify their installation of Perple_X as described at:

www.perplex.ethz.ch/perplex/tutorial/padova_phase_diagram_section_workshop_2023/