

The Dark Arts of Perple_X and C-O-H Fluids

This 2-day course will cover less commonly used components of Perple_X. As the exercises make use of the programs at a “beginner” level it may be possible for users with no experience with Perple_X to participate. However, the course is not intended as an introduction to Perple_X, therefore new users are advised to install the programs and familiarize themselves with the interface prior to the course (see [WINDOWS](#)¹, [OSX](#)², and [LINUX](#)³ for brief installation instructions). The course will not cover details of controlling grid and compositional resolution that belong in a beginner course, some information on these details are discussed by [Caddick](#)⁴ and [Hirsch](#)⁵. Likewise, while some concepts will be reviewed, the lectures will assume a basic understanding of: Schreinemakers projections, i.e., how the reactions about an invariant point can be deduced from phase compositions; and familiarity with concepts such as chemical potential and thermodynamic activity.

Petrologic phase diagram software is commonly used to calculate isochemical phase diagram sections (a.k.a. “pseudosections”). The popularity of such software has obscured the value of Schreinemakers phase diagram projections (a.k.a. “petrogenetic grids”). Day 1 will review the application of petrogenetic grids to metacarbonate rocks ([Connolly & Trommsdorff 1991](#)⁶ and references therein). Specifically, the construction of petrogenetic grids for a system in which an H₂O-CO₂ fluid is a possible phase, the relation of such a grid to $T - X_{\text{CO}_2}^{\text{fluid}}$ and $p - X_{\text{CO}_2}^{\text{fluid}}$ section/projections. The practical will involve the calculation of $p - T$, $T - X_{\text{CO}_2}^{\text{fluid}}$, $\mu_{\text{H}_2\text{O}} - \mu_{\text{CO}_2}$ projections and composition (chemographic) diagrams for the CaO-MgO-SiO₂-H₂O-CO₂ system (programs [BUILD/VERTEX/PSVDRAW](#)¹⁰). These exercises will correspond to updated versions of the material outlined in chapters 2, 3, and 6 of the out-of-date [Perple_X tutorial](#)⁷.

Day 2 will cover C-O-H fluids (largely as in [Connolly & Cesare 1993](#)⁸ and [Connolly 1995](#)⁹): how speciation is calculated; why $X_{\text{O}}^{\text{fluid}}$ is a better variable than f_{O_2} for understanding devolatilization, why $p - T - X_{\text{O}}^{\text{fluid}}$ diagrams are no different than $p - T - X_{\text{CO}_2}^{\text{fluid}}$ diagrams for carbon saturated systems; and metasomatic systems (i.e., the possibility of moving on/off the carbon saturation surface). The practical will involve the more typical components of Perple_X and the students can choose from a smorgasbord of problems, e.g.: fluid speciation (program FLUIDS, plotting in Matlab or PSTABLE); (the minor) influence of graphite on the metacarbonate grid from Day 1 (BUILD/VERTEX/PSVDRAW); phase diagram sections (metasomatic) involving silicates, carbon, and metals ([BUILD/MEEMUM/VERTEX/WERAMI/PSSECT](#)¹¹).

¹www.perplex.ethz.ch/perplex/ibm_and_mac_archives/README_WIN_USERS.txt

²www.perplex.ethz.ch/perplex/ibm_and_mac_archives/README_MAC_USERS.txt

³www.perplex.ethz.ch/perplex/ibm_and_mac_archives/README_UNIX_USERS.txt

⁴www.perplex.ethz.ch/perplex/tutorial/Marks_C2C_workshop_Sevilla.zip

⁵serc.carleton.edu/NAGTWorkshops/petrology/teaching_examples/44110.html

⁶www.perplex.ethz.ch/papers/connolly_cmp_91.pdf

⁷www.perplex.ethz.ch/perplex/tutorial/tutorial.pdf

⁸www.perplex.ethz.ch/papers/connolly_jmg_93.pdf

⁹www.perplex.ethz.ch/papers/connolly_cmp_95.pdf

¹⁰www.perplex.ethz.ch/images/perplex_07_projection_flow_chart.jpg

¹¹www.perplex.ethz.ch/images/perplex_666_section_flow_chart.jpg