

Notes on the EQ3, EQ6 and EQPT CODES

1. EQ3 is used to model solubilities and aqueous speciation. It needs a file called **input** and a file called **data1** to run. It produces an **output** file containing the results of interest. It also produces a summary output file called **pickup**, which is used as part of the **input** file for EQ6.

2. EQ6 is used to model the progress of water-rock interactions and chemical mass transfer. It needs a file called **input** and a file called **data1** to run. It produces an **output** file containing the results of interest in great detail for each successive step of reaction progress, as measured by the reaction progress variable (z_i). It also produces a summary output file called **tab**, which is useful for taking a quick glance at the results of the model (and it produces a **pickup** file which can be used as part of another **input** file for additional EQ6 calculations).

3. EQPT is used to convert the primary data base file called **DATA0** to the file **data1** required by EQ3 and EQ6. It also produces an **Output** file indicating any errors in the original **DATA0** file. *EQPT must be run any time changes to the primary data file **DATA0** have been made.*