Eleanor

Aqueous speciation modeling has historically focused on specific, well defined systems, and is ideal for laboratory settings or the study of a small number of real-world systems. Standard tools such as Geochemist's Workbench and EQ3/6 exist to fill this niche, alongside more recent additions such as the WORM Portal. However, existing tools are not ideal for the study of systems that are underspecified (e.g. have incomplete composition), have high degrees of uncertainty (e.g. imprecise characterization), or for understanding the broader equilibrium landscape of systems of interest (e.g. serpentinizing systems in general). Eleanor is a powerful open-source modeling framework based on EQ3/6 which fills this gap, providing the process and data orchestration features necessary to facilitate large-scale aqueous speciation modeling. Eleanor includes a standalone executable which accepts a problem specification in YAML, TOML or JSON format, samples fully-defined systems for speciation via the EQ3/6-based "kernel", validates the results, and stores the data in a Postgres. Eleanor's modular design allows the user to swap the EQ3/6-based kernel with one of their own.