Recovering and refurbishing of the SILNUC code, a tool to mitigate and prevent amorphous silica scaling

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Modelling the fate of silica in geothermal brines is of utmost importance to prevent and mitigate amorphous silica scaling both in surface installations and in the geothermal reservoir upon reinjection of spent fluids.

In principle, these theoretical predictions can be done using the software code SILNUC which was written by Weres and coworkers over thirty years ago. In practice, as far as we know, only the listing of this software is presently available in their report [1]. Thus, we decided to try to recover and refurbish this code.

SILNUC models the homogeneous nucleation and growth of colloidal particles of amorphous silica. It comprises three major algorithms.

The first one is the molecular deposition or particle growth algorithm. The Runge-Kutta approach is used to compute the particle radii and the dissolved silica concentration, both as a function of time. The second one is the nucleation algorithm, which simulates the generation of classes of colloidal particles. The third one specifies the temperature, pH, and fraction of water lost through steam separation as functions of time. Review of the recent literature is also planned during refurbishing of the SILNUC code.

[1] Weres O., Yee A., Tsao L. (1980) *Kinetics of silica polymerization*. Report LBL-7033, Lawrence Berkeley Laboratory, University of California.

The oxidation states of cerium and europium in silicate melts as a function of oxygen fugacity, composition and temperature

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Ce and Eu are the only rare earth elements (REE) to occur in oxidation states other than REE^{3+} under terrestrial magmatic conditions. The stability of Ce^{4+} and Eu^{2+} results in anomalous, chondrite normalised, abundances of these elements relative to the other REE due to the effect of oxidation state on trace element partitioning [1]. The link between oxidation state and oxygen fugacity (fO_2) means that fO_2 may be determined if Ce^{4+}/Ce^{3+} or Eu^{2+}/Eu^{3+} can be evaluated directly or inferred from the magnitude of an anomaly.

Ce and Eu L_{III}-edge XANES spectra were used to determine Ce^{4+}/Ce^{3+} and Eu^{2+}/Eu^{3+} in melts *in situ* [2], and quenched to glasses, as a function of fO_2 (from -14 to +6 log units relative to the quartz-fayalite-magnetite, QFM, buffer), composition (MORB plus ten Fe-free systems), temperature (1200-1500 °C) and pressure (1 atm and 1 GPa). Ce^{4+}/Ce^{3+} and Eu^{2+}/Eu^{3+} vary systematically with the thermodynamically predicted dependence on fO_2. For both elements higher oxidation states are favoured by less polymerised compositions (large values of optical basicity and NBO/T) and lower temperatures. Pressure appears to have a negligible effect. A general expression for Eu^{2+}/Eu^{3+} in geological melts has been derived. An fO_2 window, beginning near QFM, exists where both Ce^{4+} and Eu^{2+} are stable. Coexisting Ce and Eu anomalies in minerals such as zircon are thus not necessarily related to plagioclase fractionation. In Fe-bearing compositions, neither Ce^{4+}/Ce^{3+} nor Eu^{2+}/Eu^{3+} are preserved on quenching from a melt to a glass due to electron exchange reactions between Ce^{4+} and Fe^{2+} and Eu^{2+} and Fe^{3+}. This limits oxybarometry to estimates of Ce^{4+}/Ce^{3+} and Eu^{2+}/Eu^{3+} determined from partitioning derived anomalies.

[1] Burnham & Berry (2012) *GCA* **95**, 196-212. [2] Berry *et al*. (2003) *J. Synch. Rad.* **10**, 332-336.

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