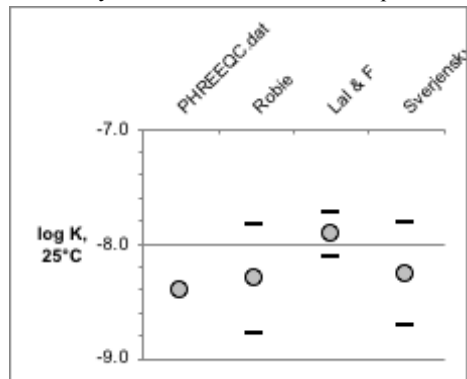


The Effect of Using Impure Calcite to Calculate Saturation States

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The calcite saturation state is an important fundamental property that affects assessment of corrosion, scaling, and chemical weathering. Calcite should be near saturation in most settings, unless it is absent, considering its relatively rapid reaction kinetics. However, the variation in some commonly used sources of calcite equilibrium constants is



relatively large (fig. 1; [1], [2]), and most speciation models use stoichiometric calcite, despite its near absence in the real world.

The impact of trace elements such as Mg and Sr on thermodynamic data is significant. Comparison of results using equations from Sverjensky [3] and La Iglesia and Félix [4] (fig. 1) show that the trace elements tend to increase the equilibrium constant, making solutions appear to be oversaturated with pure calcite. A comparison of calcite saturation states of groundwater from a long term (more than two decades) database using impure and pure calcite shows that the groundwater is much closer to saturation using the thermodynamic data for impure calcite. If this is a representative relationship, then the inverse could be applied, using calcite saturation states of pure calcite to estimate trace element content of limestone.

[1] Robie et al. (1979), *U.S.G.S. Bulletin 1452*.

[2] Woods & Garrels (1987), Oxford University Press.

[3] Sverjensky (1984), *Geochimica et Cosmochimica Acta* 48, 1127-1134.

[4] La Iglesia & Félix (1994), *Geochimica et Cosmochimica Acta* 58, 3983-3991.