

Interactive comment on “Assessment of calculation methods for calcium carbonate saturation in drinking water for DIN 38404-10 compliance” by P. J. de Moel et al.

Anonymous Referee #1

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Given the standard methods related to calcium carbonate saturation and precipitation potential, it is a good idea to provide databases that allow for the stipulated calculations of DIN, SM, and NEN with the program PHREEQC. PHREEQC is easily available and can do the calculations as opposed to generating many single purpose programs to do the same calculations.

I might not go so far as to say "internationally accepted" (perhaps "widely used") with regards to the databases of PHREEQC. More work is needed to develop thermodynamically consistent databases; the current databases are to some extent collections of thermodynamic data from a variety of sources, without thorough documentation of

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those sources or demonstration of the accuracy. However, the work of Plummer and Busenburg on the carbonate system is relatively consistent and is better than for other chemical systems.

I agree wholeheartedly with the authors that the tolerances for DIN are too small. As stated, there are many more uncertainties in K_1 , K_2 , K_{calcite} , the identity and equilibrium constants for ion pairs and complexes that affect the SI and CCPP calculations than can be accommodated by the small tolerance given. The authors rightly point out that uncertainties in the analytical data are far greater than the specified tolerance.

The approach of DIN of giving results of SI and CCPP for 10 water analyses is not the best because the values of SI and CCPP cannot be known unambiguously. It would be better to base the method on reproducing solubility experimental data under a variety of temperatures and chemical conditions. That is what the authors hint at in the conclusions, but I think the argument could be made more strongly.

The only technical comment is that $f(i)$, $g(i)$, A , B , and DK need to be defined in the text.

Minor editorial comments are in the annotated manuscript.

Please also note the supplement to this comment:

<http://www.drink-water-eng-sci-discuss.net/6/C60/2013/dwesd-6-C60-2013-supplement.pdf>

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