

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 #2

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The international unification of the standard methods to calculate calcium carbonate saturation and precipitation potential is a must. Making the underlying models more accessible via the program PHREEQC really is a nice job.

It is obvious that the tolerances for SI and CCPP in DIN are too small, because of uncertainties in K values and the details in the chemistry that affect the SI and CCPP calculations. The result of a calculation with a given composition of the water could be exact, but right or wrong.

Authors semi-quantitative point out that the analytical uncertainty in the calculated results is far greater than the tolerance specified in DIN. Given the program PHREEQC it

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is easy to calculate the influence of the analytical uncertainty on the calculated results for SI and CCP, assuming for instance an uncertainty of 0,10 mmol/L for alkalinity and calcium and 0,10 for pH. I think it is wise to do so and integrate it in the paper; it will explain a lot.

Scientifically the thermodynamic database used and its consistency is the fundament of the calculations. The question whether a calculated result is right or wrong depends hereon. In past Plummer and Busenberg amongst others elucidated the calcium carbonate system very well. For this reason modelling in operational practice, using the calcium carbonate system, clarifying significant trends is possible and useful. Bear in mind that the analytical uncertainty dictates the significance of a trend. It also dictates the conditions preventing rigid regulation.

With respect to the DIN approach, giving the composition of water samples and results for SI and CCP, I agree with my colleague Referee #1 who clearly stated “the values of SI and CCP cannot be known unambiguously”. The reason for using the DIN approach is probably comparing the results of different calculation methods for one underlying scientific model and not comparing calculated results from different scientific models. Posing a question like this in the discussion would be nice.

In authors Table 5 the water quality data set from DIN is presented. Although it seems a detail, according to me sample 5 is not a regular drinking water sample because of the pH (5,60). Perhaps it is bottled water. Moreover the water quality data set lacks the composition of a softened drinking water where alkalinity en calcium have been lowered and pH is in the range of 8,00 to 8,80, perhaps 9,00. In the introduction it is stated that the regular pH of drinking water ranges from 5,5 tot 8,5. Because of the suggested upper pH limit of 8,5 some assumptions have been made tot get to equation 1. In practice a pH of drinking water between 8,5 and 9,5 is rare, but you don't handle it in the paper.

I have no more comments.

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