Geochemical Speciation Sofware Comparative Study and Development of a New Software

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Evolution in geochemical modelling for natural environments and the accuracy of experimental results are related to numerical techniques capable of solving complex mathematical problems as well as the improvement of computing capacity. To verify the distribution, mobility and availability of chemical species in geological environments [1], and to test the efficiency and accuracy of a code that we are developing called SHPECK, we performed a comparative study of geochemical speciation using our code, PHREEQC® and Geochemist's Workbench (GWB®). We modelled the chemical behaviour of the minerals compounds known for the water from the North Sea [2], and found the following mineral Saturation Index values at 25 degrees, for GWB, SHPECK and PRHEEQC, respectively: Anhydrite (-1.13, -0.44 and -0.91), Halite (-2.55, -2.52 and -2.46), Sylvite (-3.61, -3.49, -3.52). For the following minerals, we have results only for GWB and SHPECK: Thenardite (-3.32, -2.34); Arcanite (-5.26, -2.54); Hydrophilite (-15.56, -14.84); Chloromagnesite (-24.83, -24.27); $MgSO_4$ (-9.46, -9.01); Lawrencite (-18.19, -17,61), $FeSO_4$ (-13.43, -12.87); and $Al_2(SO_4)_3$ (-63.41, -29.75). One can observe that similar results were achieved with all of them, differences on the SI values being consequence of using different methods to calculate the activity coefficient of the solutes. GWB and SHPECK employ an integrated system to define when to use Davies, Debye-Huckel or B-Dot equation, according to the value of the solution ionic strength. On the other hand, PHREEQC requires human decision in order to use different solving methods.

[1] Baccar *et al* (1993) *App Geochem*. **8**, 285-295 [2] Morad *et al* (1990) *J. Sediment. Petrol*. **60**, 411-425