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Opinion

Theoretical Investigation of Groundwater pH

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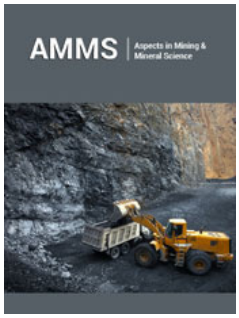

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The different ways of pH calculation are described. The systematic errors and problems of experimental and theoretical correlation are discussed the best way of water properties calculations are proposed – mass balance numerical calculation. Behaviour prediction of groundwater properties is important at day-to-day life in the fields of oil companies, civil engineering and so on. The different types of assumptions were applied for the prediction of properties by researchers. At the same time, empirical parameters numbers have some portion of inaccuracy due to methods precession. The general method of water properties calculation is proposed to combine researchers and increase the efficiency of development. There are two great assumptions known so far for highly diluted solutions: pH is dependent on strong base (or acid) concentration or water equilibrium prevails [1]. The next step of calculation methods improvement is the precise calculation of all anions and cations in the solution. The dissociation equilibriums have taken place. The constant of the equilibrium may be calculated by approximation [2]. The other problem of the direct calculation is the activity coefficient, which is usually calculated by the extended Debye-Huckel equation. Activity coefficient can be calculated by different methods [3]. So currently, no method can be calculated of pH without any assumption. Even the ionization constant depends on the pH [4]. The general method is the charge neutrality equitation method. In this method, all inions and cations, including H+ and OH– are taken into account. The equitation is calculated numerically by different methods such as the quadratic interpolation method or Golden section [2]. Accuracy pH calculation checking is challenging due to the accuracy of pH measurement. Measurement of pH may have systematic errors due to CO_2 dissolution in water. Correction of errors is however hampered by a lack of correct understandings of error sources and magnitudes [5].

The parameter pH is also a part discussion. Originally pH was a negative logarithm of concentration. Currently, the pH number term is changes toward using hydrogen ion activity instead of calculation. The Langelier saturation index is still in use [6]. The development of the wide using method is a key to progress in calculation prediction methods. The direct method of mass balance should be used as a standard one [2]. The equitation should be neutral regardless of the number of anions or cations that take place. Equilibrium constant should be taken regardless of pH. calculation of the equitation should be done with the desired accuracy regardless of the method of solution (Golden section, half of the range and so on) It can be applied to different types of water from all over the world to check the possibility of accurately calculation of pH based on the chemical composition. All deviations between experimental and calculated parameters give us a map where we can find systematic errors. All systematic errors may be eliminated in a future investigation.

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