Modeling nitrogen species as a source of titratable alkalinity and dissolved gas pressure in water

LESLIE HARDY[1]

[1] Wood Environment & Infrastructure Solutions, Edmonton,AB, Canada, leslie.hardy@woodplc.com

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Alkalinity is a measure of the acid buffering capacity of water that is defined by an explicit chemical model of the acid-base processes involved. This paper presents an alkalinity speciation model using C1, C2 and N1 species to model the measured responses during alkalinity and acidity titrations. Charged species can contribute to alkalinity, and uncharged species can contribute to dissolved gas pressure which can be evaluated using the Ideal Gas Law. Groundwater monitoring programs have demonstrated the importance of dissolved gases and the resulting affects on aquifer properties when gas bubbles form. At one such site, there was more titratable alkalinity than could be produced by the total carbon in the sample if it was all present as bicarbonate. With the hypothesis that nitrogen species were contributing to titratable alkalinity, titratable acidity, and dissolved gas pressure in groundwater, an evaluation of the alkalinity and acidity titration curves was undertaken. Modeling of titration curves indicates the importance of charged and uncharged nitrogen species and the resulting reactions with CO_2 and acetic acid. Two models have been developed: Model 1 uses titration curve data and electrical charge balance to speciate total alkalinity or acidity using normal curves, and Model 2 provides limits on the possible contribution of titratable nitrogen based on total carbon and total alkalinity. These calculations use C1, C2, and N1 which provide limits on the missing electrical charge that could be provided by titratable nitrogen. The hysteresis seen between fast and slow alkalinity titrations is explained in terms of known reactions and degassing. Missing electrical charge calculated in Model 1 is within the limits provided by the ratio of C1:C2 species as evaluated in Model 2, and the maximum gas pressure that could be provided by N1 and C1 gases is within the limits imposed by the Ideal Gas Law. Alkalinity is a non-specific measurement, and the methods applied here are non-specific but provide a conceptual framework to be further developed as suitable specific analytical methods for these N species are applied to water samples.