Defense Announcement

Size Exclusion Chromatography (SEC) Method Development to Investigate Natural Organic Matter (NOM) and Organic Contaminant Binding Interactions

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Organic contaminants are known to partition onto natural organic matter (NOM), which can, in turn, affect their fate, transport, and behavior in the environment. Characterizing and obtaining reliable data on NOM-organic contaminants interactions can be challenging. One of the most commonly used methods to investigate binding interactions is equilibrium dialysis, which can be limited by low recovery, poor separation, or slow equilibration times. The objective of this research is to evaluate size exclusion chromatography (SEC) methods to quantify NOM-contaminant binding interactions, validate the SEC methods against conventional equilibrium dialysis methods, and develop strategies to achieve a high-throughput SEC analysis. In the first study, humic acids (HA) were extracted from soils collected on eleven properties in Texas, and their binding interactions with a pesticide, alachlor, were investigated. Samples were analyzed using the pre-equilibrium SEC (PE-SEC) method, and it was found that three out of eleven HA extracts analyzed showed complete binding to alachlor. However, a mechanistic interpretation of these results was challenging, as the occurrence of alachlor binding did not correlate strongly with any of the measured properties of the HA, including aromaticity and molecular weight, across the field samples. Therefore, to validate the method developed in the first study, a second study investigated the interactions of standard NOM and HA extracts from two different sources (Suwannee River and Elliott Soil) with a suite of organic contaminants with varied hydrophobicity and charge, including four uncharged contaminants (carbamazepine, atrazine, and N,N-diethyl-meta-toluamide (DEET), alachlor) and two weak acids (sulfamethoxazole and mecoprop). Equilibrium dialysis showed binding of carbamazepine and atrazine to the Elliott Soil humic acid. When pre-equilibrating the NOM and contaminants followed by SEC separation (non-equilibrium conditions), no binding was observed, suggesting that rapid desorption occurs. Further SEC analyses following the Hummel Dreyer methodology to investigate equilibrium conditions were then performed and optimized to reduce sample analysis times. The resulting partitioning coefficients were comparable to those measured by equlibirum dialysis. Furthermore, the SEC method permitted evaluation of interactions with the lower molecular weight Suwannee River NOM, which was not feasible by equilibrium dialysis. Overall, the SEC method was successfully demonstrated as a reliable, high throughput method to investigate NOM-contaminant interactions.