Quantification of Competitive Sorption of Chemical Species onto Activated Carbon: Unlocking the Modelling of Complex Mixtures

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Background/Objectives. The migration of contaminants in groundwater can be mitigated through injection of activated carbon reagents into the subsurface. The approach offers significant design flexibility in strategies ranging from source area containment to barrier configurations. It is applicable to a wide range of groundwater contaminants.

Numerical contaminant fate and transport models are used widely as predictive / descriptive tools in plume management. There is conceptually a natural synergy between the use of these and the use of in situ of activated carbon, as the latter - from a modelling perspective - is in essence a means of retardation-factor manipulation.

Contemporary models predominantly address single contaminant species. In the field however, contaminants are present in mixtures. When a mix of contaminants is present there is competition between species for sorption sites on the activated carbon. Compounds that sorb more strongly will tend to dominate and weaker-sorbing species may be competitively displaced. This can lead to significant predictive inaccuracies if the interactions are not accommodated within the model.

Approach/Activities. This talk presents a mathematical approach to predicting competitive sorption interactions between contaminant species present in simple and complex mixtures. The practical significance of this is the enabling of accurate modelling of the impact of in situ activated carbon applications in mixed contaminant plumes.

Predictive data are evaluated against laboratory results for mixtures of common groundwater contaminants including major plume-forming classes such as VOCs and PFAS. Correlations between predicted and actual performance are statistically analyzed, and performance limits of predictive confidence are presented.

The practical utility of the approach is illustrated using examples from laboratory feasibility studies, field remediation designs, and project performance analyses. The predictive integration of the approach into a wide range of contaminant fate and transport models to aid in concept evaluation, performance-prediction and engineering design is discussed.

Results/Lessons Learned. Competitive sorption and displacement are not absolute. There is instead an adjusted equilibrium for individual species. Using the present model, this can be mathematically predicted with reasonable accuracy based on physical parameters. Practical applications of this are manifold.