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Implications of using inappropriate fate descriptors for engineered nanoparticles

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There has been a lot of debate in recent years regarding appropriate fate descriptors for engineered nanoparticles (ENPs), needed to predict ENP concentrations and transport in different environmental compartments. It is tempting to simply apply concepts for conventional organic pollutants, such as the use of equilibrium partition coefficients (e.g. Kow, Kd) in fate and risk assessment of ENPs. However, due to their fundamentally different properties compared to organic chemicals, equilibrium partition coefficients lack a fundamental physical definition for ENPs and a fate assessment based on such coefficients is essentially meaningless. Here we present a few short case studies to demonstrate the implications of using any sort of ill-defined distribution coefficient in fate predictions for ENPs. We demonstrate the results of using operationally defined partition coefficients in different types of model preditions to exemplify why such coefficients cannot be used in the same universal manner as equilibrium partition coefficients are used in fate models for organic contaminants. Currently, model validations with field measurements of ENP concentrations in complex environmental matrices are not yet feasible, making it particularly important to carefully design environmental fate models for ENPs based on a strong theoretical understanding of the underlying processes to avoid making meaningless model predictions.

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