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Organic Modeling Issues and Problems - Dr. Chen Chiang

Chen Chiang, Equilon Enterprises, an environmental engineer and the technology lead for Equilon's fate and transport modeling group, discussed the issues and problems associated with modeling the leaching behavior of organic constituents. A copy of Dr. Chiang's presentation materials is available through the following link: chiang1.pdf. He began his presentation by emphasizing that successful leaching tests must be both practical and site specific, and that successful mathematical models must incorporate time-dependent leachate characteristics and NAPL issues. He suggested that modeling approaches that strive to predict leaching over a 100-year time frame may be unrealistic, and that instead, it may be possible to take a tiered approach to modeling, providing realistic predictions based on critical, fundamental thermodynamic parameters.

Dr. Chiang reminded the audience that the goal of a waste leaching modeling exercise is to estimate the concentration of the constituents of interest in the leachate (C_L) or in the waste (C_T) that will give you an acceptable concentration in the receptor (C_R) . The model must consider any interaction between leachate and waste concentrations, fate and transport through the groundwater (e.g., biodegradation and dispersion), and derived dilution and attenuation factors. Other parameters and processes that must be considered in the model include volatilization of the waste, infiltration from rainfall, and waste specific issues. One example of a waste-specific issue is the standard practice in the petroleum industry of centrifuging oily wastes before disposal, so at the time of disposal you have a residual NAPL, but not a mobile NAPL. Therefore, the need for multi-phase flow modeling needs to be evaluated. He also pointed out that leachate will preferentially partition into NAPL, so actual leachate, in the presence of residual NAPL, will be small.

Dr. Chiang noted that a lot of fundamental information can be derived from a simple batch for Tier 1 analysis and simple modeling, such as time-dependent leachate concentrations. The current batch testing approach (TCLP) assumes equilibrium partitioning between soil and water, and further assumes that the leachate concentration (C_L) and waste concentration (C_W) are constant over time. An improved approach to this type of finite source modeling might include partitioning between air, soil, water and residual NAPL, and should also consider kinetics, and the movement through the subsurface system.

It is also important to account for the finite nature of the source. For example, one may find temporal changes in the bulk waste as a result of losses due to leaching and volatilization. We can accommodate these factors by employing source zone modeling coupled with groundwater transport modeling, using appropriate measured leaching parameters. Refer to Dr. Chiang's presentation materials for source zone modeling equations.

The question can then be asked, where does a batch test fit in when we are modeling dynamic processes? Batch tests can be used to generate C_{Lo} (the leachate concentration at a leachate/waste ratio extrapolated to zero) and K_w (the partition coefficient.) if equilibrium conditions exist, and for nonequilibrium conditions or when losses (other than leaching) occur, calculations using acceptable default values or separate tests are needed.

Reiterating the original goal of a waste leaching modeling exercise as estimation of the concentration of the constituents of interest in the leachate (C_L) or in the waste (C_T) that will give you an acceptable concentration in the receptor (C_R) , Dr. Chiang outlined a potential procedure for determining acceptable C_L and C_T :

- Batch tests for C_{Lo} and K_w for equilibrium leaching (in the absence of other losses).
- Use separate procedure to measure kinetics when important.
- Use default values or separate tests for volatilization, degradation, etc. when important.
- Use default or measured values in coupled source zone & groundwater transport model to determine acceptable C_L and C_T values.

He concluded his presentation by noting that batch tests can be used to obtain equilibrium leaching parameters for organic compounds, but that separate estimation methods/tests are recommended for accounting for other loss processes, such as volatilization and degradation. Kinetics can be accounted for by using default values or separate test methods.

At the end of his presentation, Dr. Chiang addressed a question from Greg Helms, OSW, who asked Dr. Chiang to elaborate on the terms "residual NAPL" and "mobile NAPL". Dr. Chiang responded that he had empirical data that showed that, to mobilize a residual petroleum hydrocarbon, you need to have a hydraulic gradient of 7 (typical hydraulic gradients are usually on the order of 0.001). He conducted a 7-month long pumping test, covering 4 wells; the estimated residual NAPL volume was 5,000 gallons, and they recovered 34 gallons (mobile NAPL).