Modeling Coupled Heat Transfer and Heat Generation: Lessons for Measuring NSZD Rates Using Thermal Gradient Methods

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Background/Objectives. Petroleum biodegradation reactions (often referred to as natural source-zone depletion, or NSZD) are exothermic, and field temperature data suggest that these reactions have distinct thermal signatures. These thermal signatures may be used to estimate the rate of these reactions through a heat balance (the so-called thermal gradient method). This work presents a model of heat conduction coupled with heat generation rates derived from NSZD rates in soils. The model is used to test the effects of implementing different variants of the thermal gradient method (such as the use of background-corrected temperatures, or the calculation of a long-term heat balance in what is called the "single stick method") on the NSZD rates calculated by the method.

Approach/Activities. A transient, one-dimensional model was developed to study processes related to heat generation and transfer upon petroleum biodegradation in the vadose zone. The model is based on geochemical zones observed at field sites and the location of contaminant mass within these zones. Either aerobic (at near-ground contaminant locations) or anaerobic/methanogenic (at deeper, oxygen-limited zones) biodegradation is assumed; anaerobic biodegradation results in production of methane and CO_2, and the methane is then oxidized to CO_2 when it reaches the aerobic zone. Both reactions are exothermic, and the produced heat is a stoichiometric reaction byproduct (similar to CO_2) that is measurable using soil temperatures.

The model simultaneously solves the coupled heat and mass balances, estimating temperature profiles and biodegradation rates based on microbial (i.e., Monod) kinetics adjusted for temperature-dependent effects. These temperature-dependent kinetic parameters are available in literature, based on empirical (microcosm) data. Thus, the model generates mass-balance predictions of contaminant biodegradation rates, as well as heat-balance predictions of soil temperature profiles that are in principle self-consistent. The biodegradation kinetics-based biodegradation methods (similar to the mass-balance based NSZD rate measurement methods) and the heat balance-based NSZD rate measurement methods (i.e., thermal gradient) were compared to identify the sources of error in the thermal gradient method.

Results/Lessons Learned. The model predicts strong effects of ambient temperatures on soil temperatures. A comparison of mass balance-based NSZD rates (i.e., based on biodegradation kinetics) to those of the thermal gradient method reveals that the heat flux method is subject to noise (interference) due to short-term ambient temperature fluctuations. This noise can be reduced by averaging heat fluxes over different time scales; this work presents the results of analyzing heat fluxes based on instant, average monthly, and average annual soil temperatures. The measurement error due to non-ideal deviations on the background location used, temporal averages at different time scales, and error due to heat sources extraneous to the heat of reaction due to NSZD processes will be presented.