Temperature Effects on Petroleum NSZD Processes: Lessons from Coupled Heat Transfer and Heat Generation Modeling

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Background/Objectives. Reactions associated with petroleum biodegradation (often referred to as natural source zone depletion [NSZD]) are exothermic. Accordingly, field temperature data suggest that these reactions have distinct thermal signatures, which may be useful for studying NSZD in petroleum-impacted areas. In this work, we model heat conduction processes coupled with heat generation rates derived from NSZD rates in soils to shed light on NSZD soil processes. Further, we quantify the magnitude of thermal signatures of different biodegradation reactions. Together, these factors help develop our understanding of the potential and limitations of estimating NSZD rates using soil temperature measurements (i.e., heat fluxes).

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 within these zones. Either aerobic (at near-surface 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, similar to CO_2, is a stoichiometric reaction byproduct 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 the literature, and are based on empirical (microcosm) data. The model was calibrated to two different sites by adjusting input biodegradation rates until the model-predicted, depth-integrated biodegradation rates (R_{Monod}, based on mass balance) matched field-measured NSZD rates. Model solutions were used to i) estimate the effects of ambient and local soil temperatures on R_{Monod}, ii) estimate the magnitude of temperature increases caused by NSZD reactions, iii) compare with degradation rates calculated from soil temperature measurements, or thermal gradients (R_{TG}), and iv) analyze the effects of temperature measurement errors on R_{TG} by adding simulated noise to the model-predicted temperatures. This modeling approach of comparing both methodologies to estimate NSZD rates is subject to uncertainties. However, the coupled heat/mass balance solution provides a self-consistent data set for both modeled biodegradation rates and local temperatures.

Results/Lessons Learned. First, our model predicted that local soil temperatures, when adjusted for site-specific conditions, are strongly influenced by ambient temperatures. Second, the predicted increase in local soil temperatures is from 1.5 °C to 2 °C; these small temperature differences are seasonal, follow the dependence of NSZD reaction rates on local soil temperatures, and are consistent with previously published data. Third, comparison of NSZD rates from both mass (R_{Monod}) and heat (R_{TG}) balances reveal that the heat flux method is subject to noise (interference) due to short-term ambient temperature fluctuations. However, this noise can be reduced by averaging heat fluxes over different time scales; we present the results of analyzing heat fluxes based on instant, average monthly, and average annual soil temperatures. Fourth, the usefulness of soil temperature measurements depends on the measurement error of the temperature probes used.