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Heat Flux Based-Estimates of Petroleum NSZD Rates: Uncertainty Analysis Using a Modeling Approach

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Background/Objectives. Petroleum biodegradation reactions (often referred to as natural source zone depletion, or NSZD) are exothermic. Field temperature data suggest that there is a thermal signature to these reactions. E-Flux has developed BioTherm, a web-based first principles-based model to account for heat transfer in soils and microbial Monod-based degradation rates to explore these processes. The basic BioTherm output consists of location-dependent soil temperatures and biodegradation rates. The later are temperature-adjusted (per laboratory empirical data) to account for the sensitivity of microbial activity to temperatures. Local soil temperatures depend on boundary conditions (time-dependent ambient and groundwater temperatures), heat conduction processes, and local heat generation from biodegradation reactions. This virtual system of interdependent local temperatures and soil contaminant degradation rates allows to test different scenarios and conduct virtual experiments that obey basic laws of physics and microbiology.

Approach/Activities. BioTherm is a transient, one-dimensional model of heat transfer and generation in the vadose zone upon petroleum biodegradation. Based on geochemical zones observed at field sites and the location of the contaminant within these zones, BioTherm assumes either aerobic biodegradation at near ground contaminant locations, or a methanogenic process at deeper (oxygen-limited) zones that results in methane and CO_2 production. Consistent with field observations, the model assumes that methane produced in this manner diffuses upward and readily oxidizes once it reaches the aerobic zone.
The model simultaneously solves the coupled heat and mass balance, estimating both contaminant concentration profile changes (NSZD rates) and local soil temperatures. The temperatures are then processed to measure thermal gradients and thermal-gradient based NSZD rates. Because NSZD rates directly calculated by the model are based on temperature-adjusted Monod kinetics parameters, we refer to these as $\boldsymbol{NSZD_{Monod}}$. The thermal-gradient NSZD rates are referred to as $\boldsymbol{NSZD_{TG}}$. Although the model is subject to uncertainties, the coupled model solution provides a self-consistent data set for both $\boldsymbol{NSZD_{Monod}}$ and $\boldsymbol{NSZD_{TG}}$ under the modeled local soil temperatures. Three variants of the $\boldsymbol{NSZD_{TG}}$ method were implemented: i) based on absolute soil temperatures, ii) background corrected temperatures (based on the difference between the contaminated location and one assumed uncontaminated), and iii) the long-term estimate based on time-integrated averages.

Results/Lessons Learned. Comparison of BioTherm predictions of $\boldsymbol{NSZD_{Monod}}$ and $\boldsymbol{NSZD_{TG}}$ provide the following findings: i) the $\boldsymbol{NSZD_{TG}}$ method (both for absolute temperatures and background-corrected ones) can be very sensitive to short-term changes in ambient temperatures depending on the location of the measured thermal gradient; ii) the background correction is very sensitive to differences in soil properties between impacted and impacted locations; iii) heat losses (fluxes) to groundwater are of similar order of magnitude than those to ambient surroundings, so both need to be accounted for by $\boldsymbol{NSZD_{TG}}$. A major finding is that calculating $\boldsymbol{NSZD_{TG}}$ based on a long term, time-integrated heat balance using high frequency measurements is consistent with the $\boldsymbol{NSZD_{Monod}}$ estimates. This approach effectively cancels out the noise related to short-term ambient fluctuations, irrespective of depth to measure thermal gradients located outside of the reactive zone. This is the basis for a patent-pending approach. Both BioTherm and this proprietary algorithm are available commercially.