Practical Applications of Petroleum Hydrocarbon Chemistry

Expanded Outline

Introduction

Review of key organic chemistry principles and processes

Review of nomenclature, molecular mass, density, vapor pressure, solubility and sorption.

Chemistry of Petroleum Mixtures

Description of composition of common petroleum products, including: Gasoline; #2 Fuel Oil/Diesel Fuel; Jet Fuel; #4/#6 Heating Oil; and petroleum naphtha. Chromatograms of each product, data on relative abundance of compounds of interest (BTEX, naphthalene, etc.,) and properties of each product will be described. Two main points will be:

1) Compare/contrast composition and properties between products. For example, gasoline is volatile and #6 isn't because of the vapor pressures of the component compounds; and
2) Variability of composition within each product description. For example, the variability of gasoline composition (additives, seasonal mixes, ethanol composition, proprietary markers and other performance enhancers) will be covered to demonstrate that gasolines differ and as a result, behavior at sites may differ.

Solubilization Case-Study

A site history and a site map, hydrogeochemical data (boring logs, monitoring well data and analytical data) and other supporting information will be provided for petroleum contamination from an unknown source or sources. Reviewers will develop a conceptual site model based on the data to explain the origin(s) of the groundwater plume(s) and soil contamination and, with this information, develop an approach to determine the source(s) of contamination.

Physical/Chemical Properties of Petroleum Mixtures

Description of properties of the different petroleum products, including co-solubilization (like dissolves like), density as a function of (temperature), viscosity (as a function of temperature), weathering and separation of products due to volatilization, solubilization in water and sorption to solids.

Volatilization Case-Study

Recent regulatory guidance from EPA, ITRC, and several states supports that petroleum hydrocarbons differs from chlorinated solvent vapor intrusion in their potential for vapor intrusion. Accordingly, shorter screening distances, differing attenuation factors, and/or a distance-based approach may be considered when petroleum hydrocarbons are present. The basis for these factors will be presented along with case studies as to when some of these approaches are and are not applicable.

Analytical Measurement Methods/Techniques

EPH/VPH/APH, GC-MS, etc. method descriptions, pointing out how the methods are designed to identify and measure target analytes in petroleum product of interest, based on the design of the given methodology. The discussion will also describe what potential analytes of interest (such as attenuation products) would NOT be measured by the common analytical methods. This section would identify some examples of how common methods would miss attenuation products and what methods may alternatively be considered (for example, measurement of CO_2, Redox potential, etc.)

Interpretation of Analytical Data Case-Study

Laboratory data, with supporting QA/QC documentation would be provided and the reviewer is asked to evaluation the adequacy of the data used to make an interpretation of site conditions. Some issues that would be considered would include detection limits, choice of analytical method(s) and comparison to applicable regulatory standards. Perhaps some aspect of the sampling methodology could be brought into the case study.

Thermodynamics, kinetics and biological reaction mechanisms

1) Spontaneous Reactions; Conservation of Energy; Entropy and the 2^{nd} Law of Thermodynamics; Heat and Work; Reversible/Irreversible Reactions; Entropy of Phase Change; Entropy of Chemical Reactions (combustion; microbial; and oxidation/reduction).
2) Gibbs Free Energy; Chemical Equilibrium/LeChatelier's Principle; Heats of Reaction; Exothermic/Endothermic Reactions; Temperature Dependence; Catalysis ; Concentrations and Physical States; Rate Laws (Zero, 1^{st}, 2^{nd} order reactions), relevant examples (microbial reactions, chemical weathering, etc.) and effects of changes in concentration with time; activation energy/catalysts (enzymes); effect of temperature; reaction mechanisms; phase change mass transfer coefficients.

Biological Degradation Case-Study

The case-study will look at microbial action on petroleum constituents from a well-documented release. Site data will be provided to illustrate the biological and inorganic chemistry and kinetics occurring. Information on reactants and products of reaction will be provided. Reviewers will review the data and make conclusions relative to contaminant fate and transport.

Wrap-up

Seminar Agenda

Course Outline		
Time	**Part**	**Topic**
8:00 – 8:10		Introduction
8:10 – 9:00	1	Review of Key Organic Chemistry Principles and Physical/Chemical Properties
9:00 – 9:45	2	Analytical Measurement Methods/Techniques
9:45 – 10:00		**Break**
10:00 – 10:45	3	Case Study: Data Interpretation and QA/QC Review
10:45 – 11:45	4	Chemistry of Petroleum Mixtures Physical/Chemical Properties of Petroleum Mixtures
11:45 – 12:30	5	Case Study: Fractional Solubilization
12:30 – 1:30		**LUNCH**
1:30 –2:45	6	Case Study: Volatilization and Vapor Mobility
2:45 – 3:15	7	Chemical and Biological Reactions
3:15 – 3:30		**Break**
3:30 – 4:00	7	Chemical and Biological Reactions (cont.)
4:00 – 4:45	8	Case Study: Biological Degradation
4:45 – 5:00		Review/Wrap up