

FT-MS

The FT-MS Laboratory at SREL

Mass spectroscopy (MS) has been employed widely in environmental research and monitoring studies for both organic and inorganic contaminants. Gas chromatography-mass spectrometry (GC-MS) is the most commonly applied MS technique and is a powerful tool for the analysis of volatile (e.g., TCE, benzene) and semivolatile (e.g., PAHs, PCBs) organic compounds of interest in environmental, geochemical, and ecological studies. However, many compounds are not amenable to analysis by GC-MS because they are either too large, contain chemical groups that are too polar, or degrade at the elevated temperatures needed for analysis. The Fourier transform-ion cyclotron resonance-mass spectrometer (generally referred to as FT-MS) overcomes many of these limitations and is an important component among the array of cutting-edge analytical tools within SREL's Advanced Analytical Center for Environmental Sciences that are used to address complex environmental problems.

The Savannah River Ecology Laboratory's (SREL) FT-MS system provides not only the standard GC-MS capabilities but also includes a variety of other MS techniques which allow analysis of a broad range of organic compounds in different sample matrices. These expanded capabilities include liquid chromatography-mass spectrometry (LC-MS) and matrix-assisted laser desorption/ionization (MALDI). Both of these techniques are particularly suited for the MS analysis of biological molecules such as proteins, DNA fragments, and metal chelates. There is considerable interest in using many of these compounds as biomarkers to directly measure the impacts of environmental contaminants on organisms. Biomarkers are likely to play a role in EPA's plans for developing alternative endpoint criteria for cleanup of contaminated sites as well as in developing improved models for assessing ecological risks. LC-MS is also useful for determining the metabolic products of organic compounds resulting from biological processes. These products generally differ significantly in mobility and toxicity when compared to their parent compounds and may have an important bearing in calculating environment risks. In addition, different metabolic pathways often produce different transformation products. For example, the array of degradation products of TCE generated by plants (phytoremediation) will differ from those produced by soil bacterial (bioremediation).

What is mass spectrometry?

Mass spectrometry is a powerful analytical tool that has been widely used in environmental research to identify and quantify organic compounds in complex geological and biological materials such as water, sediments, biota, and air. Mass spectrometry measures the mass of molecules and molecular fragments in substances that have been converted into positively or negatively charged ions. Using the mass of the intact (unfragmented) molecule as a reference, the elemental composition of a substance can be calculated. By applying various techniques, a molecule can also be induced to break apart into component ions that provide a characteristic distribution, or spectrum, of the mass of these ion fragments in the original molecule.



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Thus, FT-MS will be an important tool in advancing our understanding of the fate of organic contaminants in ecosystems under conditions of both engineered remediation and natural attenuation.

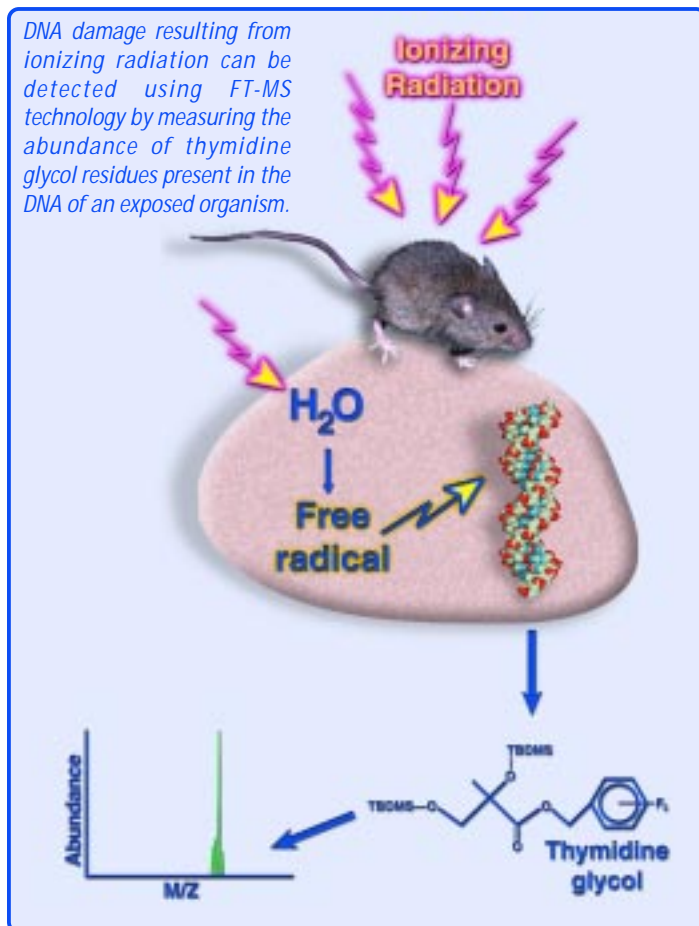
Environmental Studies

Assessment of Genetic Damage:

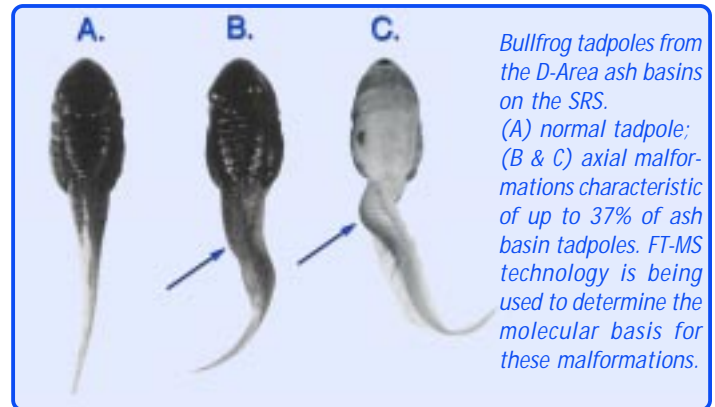
Damage to DNA can occur as a result of chemical reactions with free radicals, which are compounds that contain an unpaired electron and consequently are highly reactive. For example, ionizing radiation passing through cells will interact with water and produce hydroxy free radicals. Reaction of free radicals with the DNA base thymidine produces a cascade of reactions which result in the production of thymidine glycol as a stable end product. Measuring the amount of thymidine glycol residues provides a means of quantifying damage to DNA in organisms exposed to ionizing radiation. Studies are underway in the FT-MS laboratory to determine the levels of thymidine glycol residues in DNA extracted from small mammals collected at the site of the nuclear accident at Chernobyl, Ukraine.

Enhanced Degradation of Chlorinated DNAPL Contaminants:

Chlorinated hydrocarbons forming dense nonaqueous phase liquids (DNAPLs) are not only some of the most common



subsurface contaminants but also are among the most difficult to clean up. SREL researchers are investigating the natural reductive dehalogenation of PCE and TCE by chemically reduced iron and manganese associated with clays and mineral oxides in SRS aquifers. The FT-MS laboratory is assisting in the identification of polar products of PCE degradation such as chlorinated aldehydes and acids that are a result of natural degradation of these organic solvents.



Metal Binding Protein Biomarkers:

Metallothionein is a metal binding protein that is used by many organisms to detoxify certain heavy metal contaminants such as zinc, cadmium, copper, and mercury. Exposure to elevated concentrations of metal contaminants can induce the production of metallothionein and serve as an indicator of metal stress. The FT-MS laboratory is currently developing the methodology to determine the metallothionein concentrations in liver extracts of amphibians collected from the SRS D-Area coal fly ash basins. These studies will assist in determining the extent of contamination in the vicinity of the ash basins. In addition, previous studies have documented increased selenium concentrations in tadpole tissues and indicated that selenium may be replacing sulfur in structural proteins. Metallothionein contains a large number of sulfur-rich cysteine molecules, which play a primary role in metal binding. Thus, selenium substitution in the cysteine molecule will profoundly affect the ability of the metallothionein to sequester toxic metals. FT-MS analysis will be used to determine the extent of selenium substitution in the metallothionein extracts of tadpoles collected from the D-Area ash basins.

For more information on the FT-MS laboratory at SREL or potential uses of FT-MS technology, please contact Dr. Gary Mills; SREL; 803-725-5368; Mills@SREL.edu. 30 September 1999