Smart Notes

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How do isotope fingerprints support petrochemical investigations?

Our modern lifestyle depends on mobility and electricity. Oil and gas derivates are running our cars, planes, and trucks, but also providing important resources for production of asphalts, lubricants, pharmaceuticals, paints, fertilizers, pesticides, and plastics. It is impossible to imagine life without these commodities. With the raising demand, oil and natural gas play critical roles in today's energy and economic systems, with growing need to assure reliable and safe supplies. Oil exploration comes with a risk and a significant cost of millions of dollars. As exploration is expensive, petroleum companies use multiple criteria for source identification, such as chemical and isotope fingerprinting, to meet a decision on exploitation activities. Identification of sources can be achieved because petrochemical materials, just like other natural and synthetic materials, carry a unique chemical signature and we refer to this as the isotope fingerprint. To visualize this fingerprint, Isotope Ratio Mass Spectrometry (IRMS) is used. Application of isotope fingerprints in exploration and exploitation industry allows for differentiation of gas sources, migration, reservoir characterization, but also assessment of maturation and biodegradation processes. Isotope fingerprints of carbon, nitrogen, sulfur, oxygen and hydrogen are also used to address the influence of petrochemical exploration on environment.

Isotope fingerprints in petrochemical materials

Petrochemical material, such as crude oil and gas, have their origin in organic material. Organic material carries an isotope fingerprint derived from atmospheric CO_2 and H_2O it was exposed to during its lifetime. Once the organic material is deposited, a portion of it undergoes chemical and physical changes under extreme temperatures and pressure, resulting in oil and/or gas production.

This means that incorporation of isotope fingerprints, such as carbon and hydrogen, in petrochemical materials is related to botanical origin, geographical region and mineralization processes. By exploring isotopes in petrochemical materials, we can reveal information on original source materials, and maturation and biodegradation processes on different time scales, going all the way in deep past.

Hydrocarbon exploration

Crude oil and natural gas are made of hydrocarbons which can be used as geochemical markers for their migration and accumulation in the earth's crust. When the hydrocarbons are trapped under the Earth surface, an oil and gas reservoir is formed. By analyzing isotope fingerprints of oil and gas, the maturity and type of organic matter that acted as precursor for the hydrocarbons can be investigated.

These reservoirs of oil and gas potentially represent economically important accumulations of our sources of crude oil and gas. By drilling through the cap rock and into the reservoir, hydrocarbons can be pumped to the surface and analyzed using different technologies, including stable isotope ratio mass spectrometry.

Using the biomarkers and their respective isotopic values helps petroleum geochemist reconstruct the origin and history of the oil, providing better understand of the quality and quantity of newly discovered accumulations of oil, as well as the geological age of the oil.

The most commonly used stable isotopes in hydrocarbon exploration are those of carbon and hydrogen, supported by nitrogen, sulfur and oxygen isotope fingerprints. Multi-isotope approach offers higher levels of source differentiation and helps deliver conclusive answers to diverse petrochemical questions (see Table 1 for examples). Carbon isotopes are often used to distinguish between oils derived from marine and nonmarine organic matter, and to explore the level of maturation of oil. In respect to gases, high levels of maturity generally result in high levels of methane, however such high levels of methane may as well be consequence of biogenic activity at low levels of thermal maturity. Using isotope fingerprints allows to distinguish biogenic from thermogenic methane.

Table 1. Examples of isotope fingerprints in petrochemical investigations

Isotope fingerprint	What is the interpretation?	Example petrochemical interpretation	What sample types can be analyzed?
Carbon	Correlations oil–oil, oil–source rock, gas-source rock	Maturity, reservoirs compartmentalization, biodegradation, migration	Crude oil, natural gas, source rock
Hydrogen	History of thermal events	Maturity, source of water	Crude oil, water
Nitrogen	Origin of gases	Differentiation Thermogenic vs. Biogenic gas	Natural gas
Oxygen	Meteoric water detection	Distinguishing meteoric water vs. water trapped during formation	Water (exploited with oil)
Sulfur	Correlation oil-source rock	Investigating origin/source of oil	Crude oil, source rock

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Environmental forensics in petrochemical investigations

In the light of the growing environmental concerns and initiatives, it is also important to assess the risks that petroleum exploration, storage and transport carries. Such studies are part of the environmental forensics, where isotope fingerprints are used to correlate different fossil fuel derived pollutants or contaminants in the environment to their sources. Environmental forensics is associated with all stages of petroleum exploitation, from exploration over production to field abandonment. In the exploration stage isotopes are used to determine potential and maturity of the source, preventing unnecessary disruptions of the environment if the exploitation site would not be fruitful. In the later stages, analysis of isotope fingerprints can uncover influence of gas storage and crude oil leaks on ground water contamination, and link the spilled petrochemical product to its origin, such as pipeline. Further isotope applications are in detecting sediment or maritime environment contamination and allocating source of bird feather oiling to a tanker or similar. Also post-exploitation activities, such as proper sealing of the exploitation site, are critical to assure there are no leaks of petrochemical material and to protect our soil, air and water from contamination.

Analytical solution: differentiation of sources using isotope fingerprints

Using isotope fingerprints, it is possible to trace the origin of oil and gas across space and time. Isotope Ratio Mass Spectrometry (IRMS) works by detecting the “isotope fingerprint” of a sample, a unique chemical signature that changes from sample to sample. There are a number of approaches to processing sample materials for their isotope fingerprint depending on what question is being answered, however, the fundamental process for IRMS is the conversion of a solid or liquid sample to a gas at high temperature.

Samples can be introduced for analysis using a number of analytical peripherals, for example an elemental analyzer (EA-IRMS) or a gas chromatograph (GC-IRMS) both regularly used for analysis of petrochemical samples. In the case of EA-IRMS and GC-IRMS, the conversion of the sample to a gas is performed by two processes: combustion and pyrolysis. Combustion, burning the sample at around 1000 ˚C with oxygen, is used to evolve carbon, nitrogen and sulfur from the sample in the form of N_2, CO_2 and SO_2. Pyrolysis, breaking down the sample at around 1400 ˚C in a reductive environment, is used to evolve hydrogen and oxygen from the sample, in the form of H_2 and CO. Direct injection of sample gas in different volumes, depending on the concentration, is possible with GC-IRMS. After the gases are produced/injected, they are transferred in a continuous gas flow to a detector that measures the isotope fingerprint of the sample. Thermo Fisher Scientific provides dedicated Isotope Fingerprinting solutions with a portfolio designed to offer different capabilities and performances, with dedicated features for the coupling to the Thermo Scientific™ IRMS Systems, according to the varying analytical needs of the laboratory working for routine and research pollution source and environmental change applications:

- the Thermo Scientific™ EA IsoLink™ IRMS System, for analysis of bulk sample material;
- the Thermo Scientific™ GC IsoLink II™ IRMS System, for analyzing volatile compounds within a sample;
- the Thermo Scientific™ LC IsoLink™ IRMS System, for analyzing polar compounds within a sample;
- the Thermo Scientific™ GasBench II System, for the analysis of gas samples evolved from bulk sample materials.

Find out more at **thermofisher.com/IsotopeFingerprints**

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