

# Why High Resolution Mass Spectrometry is Sometimes a Desire – The Problem of Measuring Methane, Ammonia, and Water in a HDT Environment

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Methane, ammonia, and water are common gases in industrial processes and their production values are often desired to track performance of a process. However these gases can be difficult to analyze in a mass spectrometer because the mass spectral patterns overlap and the ammonia and water molecules tend to undergo exchange with surfaces that are encountered or can be produced by the ionization filament. The problem becomes increasingly difficult when values below 1% are required because the isotopic blends of  $^{12}\text{C}/^{13}\text{C}$ ,  $^{14}\text{N}/^{15}\text{N}$ , and  $^{16}\text{O}/^{18}\text{O}$  come into play. The measurement becomes extremely challenging when one has to also consider the possibilities of mixtures with hydrogen, deuterium, and tritium isotopes. There are 144 different mass fragments between masses 12 and 28 for a common 70 eV electron impact spectrum. To help solve this problem, one approach used at SRNL is to simulate the mixtures based on NIST fragmentation patterns and the trinomial distribution pattern for the HDT blends. The simulation helps the analyst identify the important mass fragments that should appear for an expected blend as well as visualize the expected pattern from mass spectrometry. The difference between the expected pattern and the measured pattern can often be used to rapidly identify what is happening in a process. An enhanced simulation takes the fragment numbers and converts them to a predicted mass peak shape according to the resolution and characteristics of the mass spectrometer. This allows one to observe the effect of resolution on the fragmentation pattern and the measurement.

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