Development of quantitative detection method for mass spectrometry coupled to an infrared laser spectroscope (Picarro) to monitor in nitrogen matrix a complex gas mixture H2, He, CO, N2, Ne, O2, Ar, CO2, H2S, CH4, C2H4, C2H6, C3H6, C3H8, i-C4H10, n-C4H10 and C5H12

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Abstract

Within the framework of radioactive waste management, the evolution of the gaseous composition inside the underground repository structures must be understood. Indeed, chemical and microbial reactions and exchanges occur between the rock, the structures and the air. These processes are studied in the Andra's Meuse/Haute-Marne Underground Research Laboratory's (URL). Recently, a gas monitoring station "Flair soil" has been designed to monitor the gaseous composition inside this URL. This station is composed by two analyzers: a quadrupole mass spectrometer (QMS) which allows to follow the evolution of several gases and an infrared laser spectroscope (Picarro) providing simultaneous measurements of CH4, CO2 and CO. Thus, a multivariate calibration method for the quantitative detection of interfering and non-interfering gases in a nitrogen matrix has been developed for the QMS. The MS was calibrated from pure gases in a nitrogen matrix, with known concentrations and ion currents obtained from the measurement of each species of gas. This method uses matrix calculations to calculate the relative concentrations of an unknown gas mixture from the ion currents measured directly in the MS. The test gases T1 and T2 were used to assess the accuracy of the method. Daily ion currents are corrected from theoretical ion currents obtained from calibration coefficients and test gas concentrations. Some gases are less well quantified due to their low concentration in the test gases and interferences on the measured masses. One of the motivations of this study lay in developing an advanced measurement tool allowing to be low in sensitivity, and thus to improve the detection and quantification of gases at low concentrations. The objective of this paper is to propose an analytical method to measure the gaseous composition with several molecules. This method was able to detect hydrocarbons, noble gases, sulfides, greenhouse gases, oxygen, hydrogen, nitrogen in the same mixture.

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