Journal of Hazardous Materials 363 (2019) 309–315

Contents lists available at ScienceDirect

Journal of Hazardous Materials

journal homepage: www.elsevier.com/locate/jhazmat

Classification of measured unsafe liquids using microwave spectroscopy system by multivariate data analysis techniques

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ARTICLE INFO

Keywords:
Classification of liquids
Free space measurement
Hazardous materials
Multivariate data analysis

ABSTRACT

To identify hazardous (illegal and explosive) materials, microwave measurement (free space reflection type method) method has been tried to find best results in different frequency ranges. The main goal is to cluster some materials which are mainly preferred by passenger for aircraft travel. Therefore, the multivariate data analysis methods have been preferred to classify or distinguish the measured liquids. Thus, the abilities of used techniques have been shown to make the classification process easier and more responsive, while determining the convenient measurement method that can reflect the unique properties of the liquids. The desired success has been achieved magnificently by self-organizing maps algorithm.

1. Introduction

Recently, many researchers are focused on industrial waste and hazardous materials in order to contribute for environmental protection and human life. The recognizing of hazardous liquids effects has crucial significance on every living thing. These effects are seen in many applications such as health, security, military, and industry. Most of all, the security is needed more attention and care to safe the buildings such as airports and concert halls. The illicit and explosive substances can have transported by handling and storage or these materials can be carried by passenger in travelling duration.

Microwave measurement methods has been widely preferred in many applications such as industry, security, and military. Alternatively, microwave systems are used such as a remedial technique for waste, contaminated soils, and sludge. In detail, these applications are sorted as sample drying, measurement and monitoring of moisture, solvent extraction, and sample clean up etc. Moreover, this radiation has applied to sewage sludge stabilization [1]. The advantages of microwave radiation have emerged as higher speed of reaction and reducing the reaction time for environmental applications which are refinement of hazardous waste water and soil remediation [2].

Electromagnetic waves were started to be used in classification or identifying some materials as solid or liquid forms [3]. In this regard, a microwave radiation was used to remove the ammonia nitrogen in waste water [4]. Nevertheless, the nitrogen can be removed using proposed continuous microwave system to treat toxic waste water. The microwave treatment was used to recover the valuable metals for dust and PVC materials which were composed with different rates [5]. While a microwave radiation was used as a heat source in applications of pyro metallurgical, a reductive roasting of microwave system was preferred for Greek red mud treatment [6]. Furthermore, a microwave thermal process is useful in treating studies even for contaminated solids. This process can be explained as physical and chemical analysis using heat treatment method which is assisted by microwave radiation [7,8].

As mentioned above, microwave measurement method is increasingly becoming a useful instrument for materials characterization. A Vector Network Analyzer (VNA) can provide measurement of phase and magnitude of materials in wide frequency range. In addition, it can calculate the complex permittivity of materials with technological developments. Therefore, VNA is preferred for characterizing of materials to obtain the dielectric properties which are ε (complex permittivity), $tan\delta$ (loss tangent), and n (refractive index). Nevertheless, VNA has some disadvantages such as high cost, large bulk and unportable type [9,10].

The different types of liquids, which are in the baggage or underwear, can be recognized using microwave spectroscopy system and multivariate data analysis algorithm frequency depended of their scattering parameters in dB. The important thing is the interaction between of electromagnetic field and liquids at high frequencies. Previous studies have been applied to determine the properties of liquids using complex permittivity, while the scattering parameters in dB were used to estimate the complex permittivity of measured liquids [11]. Furthermore, the dielectric properties of liquids were achieved using different type microwave spectroscopy systems which are open metal cavity and dual mode resonator as well as Josephson spectrometer and Hilbert spectroscopy [12,13]. Moreover, the unsafe liquids

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https://doi.org/10.1016/j.jhazmat.2018.09.092
Received 25 May 2018; Received in revised form 4 September 2018; Accepted 30 September 2018
Available online 02 October 2018
0304-3894/

were detected by using nuclear magnetic resonance method [14]. The results of microwave spectroscopy measurement system in millimeter wave frequency range were supported with multivariate data analysis to benefit from the difference of the reaction of the liquids to the electromagnetic radiation unlike these studies. Thus, it is aimed with the proposed method to reduce the cost, shorten the measurement time and make the identification better.

The clustering problem emerged in many applications such as pattern classification, pattern recognition, vector quantization, data compression, and data mining. These techniques are based on summarizing or minimizing which is an objective function [15]. Various methods have been used to analyze multivariate data. These methods produce a solution to the problem of multiple linear connections. A hidden variable is revealed using the relationship of inputs values. These are sorted as Principal Component Analysis (PCA), K-means, and Self Organizing Maps (SOM). The classification method can be run using many tools or packet program. These are sorted as Minitab, Matlab, and JMP (SAS Instute). The proposed methods can have implemented by JMP program since its user interface is very simple.

This paper was prepared to show the ability of Microwave Spectroscopy system and multivariate data analysis methods are suitable for clustering the explosive and illicit materials in different frequency ranges. Furthermore, this process was repeated to understand behavior of the data collected by VNA such as complex permittivity, and transmission parameter (S_{21}). Firstly, the well-known parameter epsilon was used to identify the materials, since its grouping capability is dominant over others. Secondly, the distinctive feature was explored for S_{21} parameter and phase values to determine effective separation the different materials. Moreover, the classification techniques (PCA, K-means, and SOM) were compared to discover the explicit approach for recognition of the unsafe liquids. Measured liquids are classified whether liquids can be grouped with regard to difference and similarity between each liquid using these techniques. The best results have been achieved with SOM algorithm, although the all classification techniques have been showed a significant success. In brief, firstly, a new spectroscopy system is presented to measure and recognize the hazardous liquids; secondly, the most appropriate parameter is selected to definite the liquids as safe or unsafe; thirdly, a convenient multivariate technique is determined to classify the unsafe group. Thus, the recognition and detection of the liquid components that can be used in fabrication of improvised explosive devices will be easy using proposed method, particularly in security applications in the public places such as airports, shopping malls, railway stations, and concert halls.

2. Measurement method

There are many measurement techniques to obtain the dielectric properties of materials. The material form (gas, liquid, and solid), frequency range, and temperature (high or low) are important to choose the most appropriate measurement method [3]. A Free Space Measurement method, which is based on reflection type, can enable to measure magnitude of S_{21} and phase values simultaneously. This measurement system consists of two horn antennas, a sample holder, and a VNA. The receiving and transmitter antennas are set around the sample holder with different angles [16]. Three different containers were used as sample holder to put the determined liquids. The schematic view of reflectivity-free space microwave measurement method is shown in Fig. 1. The incident wave is sent by transmitter antenna and the interaction between radiation and material, which is the reflection signal, is retrieved by receiver antenna.

Nevertheless, the position of antennas should be determined carefully to obtain the reflected signal at different angles which is transmission parameter for receiving path [17]. A spherical wave is considered instead of a plane wave, since a signal does not propagate through the sample. Moreover, the antennas operate in close the container for reducing of diffraction effects. All measurement processes

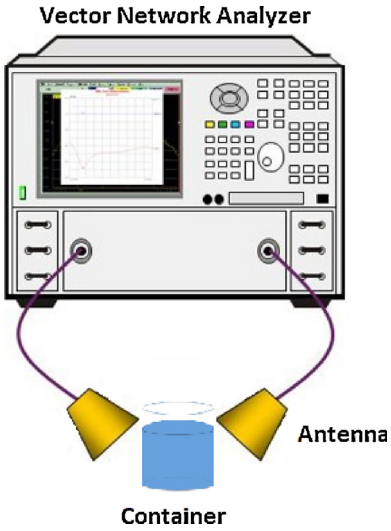

Fig. 1. Used measurement set-up.

were implemented at room temperature. In addition, the sizes of cylindrical container are r = 25.0 mm, and h = 30.0 mm, which are radius and height values, respectively. The amount of liquid to be analyzed was approximately 25 and 50 mL. When the container was half full and full, the same results were obtained while the transmission parameters were measured.

The determination of complex permittivity of liquid samples is very important due to multiple diffractions in the liquids. Therefore, the coaxial probe method is very suitable to characterize the liquids if the main aim is to obtain the complex permittivity value of materials. Furthermore, this method can allow to measure the complex permittivity at high temperatures. When this method is used, the electromagnetic wave must penetrate liquid with minimum reflection in frequency range [18]. The complex permittivity can be used by clustering techniques since it is a decisive feature for all materials. Therefore, when it is chosen to classify the measured liquids, a difference between the liquids can be seen immediately as shown in Fig. 2.

The showed liquids in Fig. 2a can be preferred by an airway passenger. Although all liquids are safe for travelling, only cologne samples have been used to show the big difference of it from other liquids. In Fig. 2b, the ethyl alcohol and methanol liquids were added to show these liquids can be grouped with cologne sample. It should be considered; the using of dielectric constant is easier to classify the liquids. But, there are two problems for Coaxial-Probe method: Firstly, it is not possible to measure all liquids by Coaxial Probe method and secondly, we should reduce the measurement and extracting processes times to make the classifying in a short time.

3. Classification techniques

In order to classify the materials, it is necessary to have determinative properties. Therefore, permittivity, transmission parameter, and phase values can be used as a fingerprint of a material. The demonstrating that the materials are different from each other using any of these values is very important to identify the explosive and illicit liquids.

3.1. Principal component analysis

Principal Component Analysis (PCA) is a statistical technique for multivariate data set. The multicollinearity problem can be solved, and number of predictive variable can be reduced using this technique. The goal of this method is to reduce the dimensionality of data without any loosing much information for determining the linear combinations. This