Effect of Different Kernel Functions on Hazardous Liquid Detection Using a New Spectroscopy System and Support Vector Machines

Ebru Efeoglu and Gurkan Tuna

Abstract—**Spectroscopy methods have become widespread in many applications including liquid classification. In this study, a new spectroscopy system that can classify liquids without opening the lid of their containers is proposed. Thus, the operators are prevented from being exposed to harmful substances and wasting time. Everyday liquids such as carbonated drinks, fruit juices, shampoo, cream and alcoholic beverages and hazardous liquids were characterized remotely by the method in which spectroscopic signatures of a total of 52 liquids were used. In order to be able to classify liquids with the highest accuracy, it is also important to determine the most suitable measurement system as well as the correct selection of the classification algorithm and algorithm parameters that show the best performance. In this study, Support Vector Machines algorithm, which is a very successful algorithm in separating binary classes, is used. In addition, the effects of the algorithm on the classification performance have been examined using different kernel functions and cross-validation technique has been used for the performance analysis. As a result of the performance analysis, it is seen that up to 100% success can be achieved when linear or polynomial kernel functions have been preferred.**

Index Terms—**Hazardous liquids, Support Vector Machines, Kernel functions, Accuracy.**

I. Introduction

SOME FLAMMABLE liquids that are readily available can be used to make explosives. Examples of these liquids are acetone and alcohol types. By mixing acidic drinks with acetone, a very powerful handmade explosive substance called TATP (Tricycloacetonperoxide) can be obtained. Bottles, which are part of our daily life, can be used to store such liquids. For this reason, methods for non-contact detection of liquids in any container are of great importance. Many methods have been developed to detect hazardous liquids at security checkpoints. The relationship between ethanol concentration in alcohol-water solutions at different concentrations and terahertz reflection signals was demonstrated using terahertz (THz) time domain spectrometer [1], and the detection of flammable and explosive liquids was realized [2][3]. The THz transmission spectra of explosives and recent developments in spectroscopic techniques for detection of explosives were investigated using a THz-TDS and Optical Parametric Oscillator based system in [4]. Similarly, Nuclear Magnetic Resonance (NMR) method was used to analyze unknown liquids together with infrared (IR) spectroscopy and classical chemical color tests in [5]. As given in [6].NMR method was also used to detect and classify liquid explosives. On the other hand, in [7] Raman spectroscopy method was proposed for non-contact detection of hazardous liquids stored in glass and plastic containers. Similarly, to classify liquids in glass bottles the use of a low energy X-ray transmission system was proposed in [8].

Microwave spectroscopy methods are more practical and less costly than other methods [9]. These features of the method have recently increased the interest in the method. Dielectric properties of liquids can be analyzed with the method of dielectric spectroscopy. Different measurement techniques have been developed for this purpose and several research studies have been carried out in this domain in recent years. Simulation studies were carried out to measure the permeability of liquids using an open-ended microwave waveguide [10]. Static dielectric permittivity ($\varepsilon 0$) and relaxation time (τ) was acquired by the least-square-fit method in [11]. Dielectric relaxation mechanisms and the temperature dependence of complex permeability of water were calculated in [12]. The relationship between water molecules and dielectric was deduced in [13]. An optimized rectangular waveguide cavity resonator was designed for compositional analysis of liquid solutions in [14]. Cooking oil classification was made using dielectric spectroscopy at 8.2-12.1 GHz microwave frequencies [15]. Microwave spectroscopy method was used not only in liquid classification but also in determining the quality parameters of tomato paste [16] and silicone [17]. Coaxial probe method was the most commonly

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used microwave measurement method is the past and it was used for different purposes including the dielectric measurement of biological [18] in the diagnosis of breast cancer [19]. However, in recent years remote and non-contact measurement and machine learning methods have been gaining interest. Machine learning techniques were used in toxic liquid detection with a thick film gas sensor [20]. Performance analysis of a 2% Fe2O3-added thick film gas sensor was performed in toxic liquid detection using machine learning techniques [21].

In this study, an antenna was designed and it was connected to the Vector Network Analyzer (VNA) to collect spectroscopic signatures of liquids in the microwave frequency band. Then, Support Vector Machine (SVM) algorithm was applied to these spectra consisting of hazardous and everyday liquids to classify hazardous liquids. In addition, the effects of using different kernel functions on the success of the SVM algorithm were examined using various performance criteria.

II. EXPERIMENTAL SETUP AND METHODOLOGY

The complex dielectric permeability value varies depending on the chemical composition of the liquid tested in the proposed microwave spectroscopy method. This change in dielectric permeability affects the electromagnetic response of the antenna, and the different electromagnetic responses of liquids enable us to obtain information about the liquid. Measurement system used in this study consists of a VNA and a patch antenna, as shown in Fig.1. From the VNA, a signal is sent to the liquid in the 1.42-1.53 GHz frequency range of the microwave band and the amplitude of the signal reflected from the liquid is measured. The interaction between molecules and microwaves causes the molecules to rotate and align with the electromagnetic field. Polarization and depolarization of molecules in liquids with different dielectric permeability values, and energy loss due to friction of the directing molecules in the wave velocity cause a decrease in the magnitude of the wave. Dielectric loss factor measures the efficiency of energy loss [22]. The signal amplitude is a function of the dielectric constant of the sample and the change in dielectric loss factor [23]. The antenna was formed by placing a circular geometry conductive layer on a dielectric layer on a ground plane. This conductive layer provides the absorption or radiation of electromagnetic waves. Copper is used as the conductive layer. Rjadiation occurs between the conductive layer of the antenna and the ground plane and the most radiation occurs in the edge areas of the conductive layer. The reason why the circle patch was preferred is the symmetrical radiation characteristic of the circular patch which is not found in other types of patches. Another factor contributing to the circular patch selection was the use of a circular bottle for measurements. The thickness of the dielectric layer is directly proportional to the frequency bandwidth. The dielectric constant of the dielectric layer in the designed antenna is 4.4. Its dimensions are 10x10 cm and its thickness is 1.6 mm. The coaxial probe method was used as the feeding method for the designed antenna because the coaxial probe feeding method is more useful for antennas with thin layers. The inner conductor of the coaxial probe is connected to the radiation patch of the antenna and its outer conductor is connected to the ground plane of the antenna. The antenna illustrated in Fig.1 is feed by 50 Ohm SMA (SubMiniature version A) feed probe. The antenna diameter is calculated using Eq. (1) and Eq. (2). The antenna diameter is calculated using Eq. (1) and Eq. (2).

$$F = \frac{8{,}791x10^9}{f_r\sqrt{\varepsilon_r}} \qquad (1)$$

$$a = \frac{F}{\left\{1+\frac{2h}{\pi\varepsilon_r F\left[ln(\frac{\pi F}{2h})+1{,}7726\right]}\right\}^{1/2}} \qquad (2)$$

Here, ε_r represents relative permittivity of the substrate, f_r represents resonant frequency, h represents height of the substrate, and a represents radius of the patch.

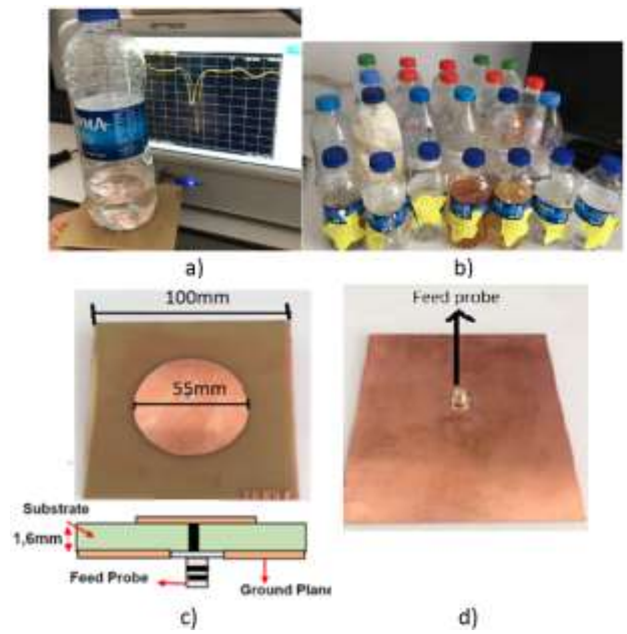

Fig.1. a) Measurement system used in this study b) Samples c) The geometry of the antenna and front view of the antenna d) Back view of the antenna.

A. *Support Vector Machines (SVM)*

SVM is an algorithm based on statistical learning theory [24]. This algorithm was originally developed for binary classifications [25]. The algorithm is based on the principle of classifying data by finding the best hyperplane that distinguishes the data of a class from those of the other class [26]. A decision function derived from training data is used to find the optimum hyperplane. In a classification problem that can be linearly divided into two classes, k is a training set showing the number of samples, if $x \in$ is an N-dimensional space, $y \in \{-1, +1\}$ is class labels and b is the trend value, then the support vectors are the points that make up the hyperplanes and they are expressed as in Eq. (3). Hyperplane inequalities are given in Eq. (4) and Eq. (5).

$$w.x_i + b = \pm 1 \quad (3)$$

$$w.x_i + b \geq +1 \quad \text{for each y=+1} \quad (4)$$

$$w.x_i + b \leq +1 \quad \text{for each y= -1} \quad (5)$$

where *w* is the normal of the hyperplane and is known as the weight vector [27].

According to the algorithm, the limit of the optimum hyperplane must be maximum. In this case, finding the most suitable hyperplane is possible with the solution of the limited optimization problem given in Eq. (6). Constraints due to this are as shown in Eq. (7) [24]. If this problem is solved by Lagrange equations, Eq. (8) is obtained. For data that can be divided into two classes linearly, the decision function is as given by Eq. (9) [27].

$$min \frac{1}{2}\|w\|^2 \quad (6)$$

$$y_i(w.x_i + b) - 1 \geq 0 \;\; ve \; y_i \in \{1, -1\} \quad (7)$$

$$L(w, b, \alpha) = \frac{1}{2}\|w\|^2 - \sum_{i=1}^{k} \alpha_i y_i (w.x_i + b) + \sum_{i=1}^{k} \alpha_i \quad (8)$$

$$f(x) = sign\left(\sum_{i=1}^{k} \lambda_i y_i (x.x_i) + b\right) \quad (9)$$

In some cases, a linear hyperplane that can categorize data cannot be found. In this case, the data in the feature space is moved to a higher dimensional kernel space and a classification is made by finding a hyperplane in the kernel space [28]. Some of the data that cannot be separated linearly remain on the other side of the optimal hyperplane. This problem is solved by defining a positive variable (ξ). The C correction parameter is used to check incorrect classifications. Thus, the problem can be expressed as in Eq. (10). The limitations related to this are as given in Eq. (11).

$$min\left[\frac{\|w\|^2}{2} + C.\sum_{i=1}^{r} \xi_i\right] \quad (10)$$

$$y_i(w.\phi(x_i) + b) - 1 \geq 1 - \xi_1$$
$$\xi \geq 0 \text{ and } i = 1, \ldots, N \quad (11)$$

The kernel function used to separate data that cannot be separated linearly is defined mathematically as given by Eq. (12). With the help of this function, data can be classified by making nonlinear transformations. The decision rule for this is as given by Eq. (13) [27].

$$K(x_i, x_j) = \phi(x_i).\phi(x_j) \quad (12)$$

$$f(x) = sign\left(\sum_{i=1}^{k} \alpha_i \, y_i \phi(x).\phi(x_i) + b\right) \quad (13)$$

The accuracy of SVM algorithm depends on the selected kernel function [29]. The kernels used in this study are Linear, Polynomial, Radial Basis and Sigmoid. Linear kernel is the simplest kernel function. It is as given in Eq. (14). Polynomial kernel is as given by Eq. (15).

$$K(x_i, x_j) = x_i^T x_j \quad (14)$$

$$K(x_i, x_j) = (x_i^T x_j + d)^P \quad (15)$$

where, *d* is constant term and *p* is polynomial degree.

Gaussian kernel expressed by Eq. (16) is an example of radial basis function kernel. For this kernel, σ determines the width of the Gaussian kernel and plays a major role for the kernel's performance.

$$K(x_i, x_j) = \exp(-\|x_i - x_j\|^2 / 2\sigma^2 \quad (16)$$

The Hyperbolic Tangent Kernel expressed by Eq. (17) is also known as Sigmoid Kernel and as Multilayer Perceptron kernel. Here, α represents slope and δ represents intersection constant.

$$K(X_i, X_j) = \tanh(\alpha x_i^T x_j + \delta) \quad (17)$$

III. Results

All liquids in the study were measured in pet bottles. 52 liquids were measured, including 23 hazardous liquids and 29 non-hazardous liquids. Liquids that contain alcohol-water solutions with an alcohol content of 70% or more can be hazardous; therefore, these solutions are classified as hazardous liquids [2]. With the proposed measurement system, spectra of liquids were collected in 56 steps in the 1.42-1.53 GHz frequency range and were used as input to SVM algorithm. Liquids used in this study are listed in Table I.

TABLE I
LIQUIDS USED IN THIS STUDY.

Hazardous liquids		**Non-hazardous liquids**		
Ethanol (70,80,90,100)%	Acetone	Peach juice	Vinegar	Turnip juice
Methanol (70,80,90,100)%	Cologne	Shower gel	Shampoo	Champagne
1-propanol (70,80,90,100)%	Toluene	Hair conditioner	Screen cleaning fluid	Tequila
Isopropanol (70,80,90,100)%	Butanol	Lens solution	Buttermilk	Whiskey
Gasoline	Octanol	Ketchup	Apricot juice	Cocoa milk
Thinner		Beer	Liqueur	Hair gel
		Baby food	Water	Liquid soap
		White wine	Red wine	Milk
		Cola	Tea	Gin
		Vodka	Raki	

The amplitude spectra of the aqueous alcohol solutions are given in Fig.2a, the amplitude spectra of the pure hazardous liquids in Fig.2b, and finally the amplitude spectra of the non-hazardous liquids in Fig.2c. Flowchart of the proposed approach is given in Fig. 3.

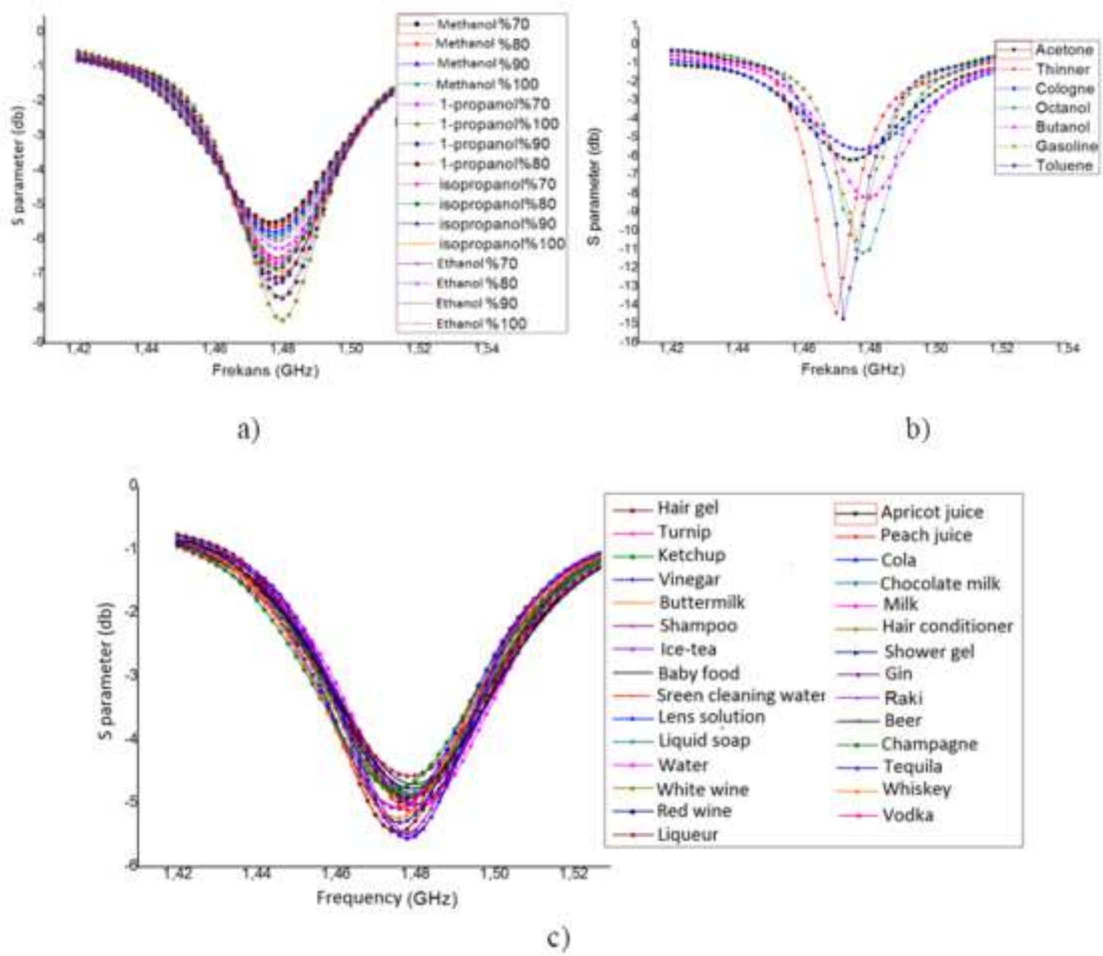

Fig.2. Amplitude spectra of liquids a) Aqueous alcohol solutions b) Hazardous liquids c) Non-hazardous liquids.

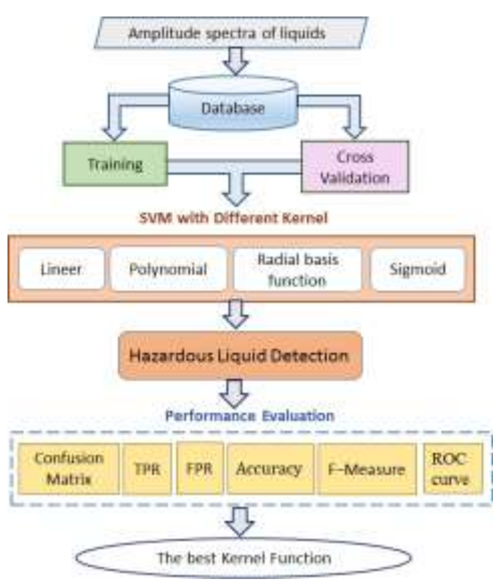

Fig.3. Flowchart of the proposed approach

A. Performance Evaluation

Since kernel functions can affect the performance of the algorithm, to analyze its effects a classification was made using four different kernel functions. K-fold cross validation technique was used in the performance evaluation of this study. In this technique, a dataset is divided into parts and some of it is used as training data and the remaining is used as test data. In this way, it is understood how the model performs on a dataset that it has not seen before. Therefore, a successful algorithm must be able to make an accurate prediction even about a liquid type it does not know at all.

1) Performance metrics

Performance criteria used in this study consists of False Positive Rate (FPR), True Positive Rate (TPR), Confusion matrix, ROC curve, F-Measure, and accuracy. Confusion matrix is a matrix containing information about the actual classes and predicted classes of liquids and is given in Fig.4. The diagonal values of the matrix in green show the number of liquids that the algorithm predicts correctly (True Positive (TP) and True Negative (TN)), and the cells in pink show the number of liquids that it predicts incorrectly (False Negative (FN) and False Positive (FP)). When Fig. 4 is examined, it can be seen that all 52 liquids were correctly classified in both training and cross validation when linear and polynomial functions were preferred. Radial basis function classified 3 hazardous liquids incorrectly. Sigmoid function classified all of the hazardous liquids as non-hazardous.

TPR is the ratio of true positive samples. It is also called recall and is calculated using Eq. (18). FPR is the ratio of false positive samples and is calculated using Eq. (19).

$$TPR = \frac{TP}{TP+FN} \quad (18)$$

$$FPR = \frac{FP}{TN+FP} \quad (19)$$

Accuracy shows the overall performance of the model. It is the most popular performance evaluation measure and can be calculated using Eq. (20). F-Measure is a hybrid metric useful for unbalanced classes and is calculated using Eq. (21).

$$Accuracy = \frac{TP+TN}{TP+TN+FP+FN} \quad (20)$$

$$F-Measure = \frac{2TP}{2TP+FP+FN} \quad (21)$$

In a successful classification, F-Measure and TP values are desired to be as close to 1 as possible.

2) Experimental results

TPR, FPR, F-Measure metrics and accuracy values of all the kernels are listed in Table II. In a ROC curve, FPR is on the X axis and TPR is on the Y axis. As the remaining under the curve increases, the discrimination performance between classes increases. The ROC curves are given in Fig.5 for different kernels.

As it can be seen from the ROC curves of polynomial and linear functions, liquids were correctly classified. The areas under the ROC curves took the value of 1. On the other hand, as it can be seen from the ROC curves of Radial basic function, some misclassifications were done so the ROC area value was calculated as 0.93. Finally, as it can be seen from the ROC curves of Sigmoid function, the function did not classify any liquids correctly, so the ROC area value was calculated as 0.5. This indicates that Sigmoid function is not suitable for liquid classification when SVM algorithm has been preferred.

When Table II is examined, it is seen that the algorithm achieved 100% accuracy by correctly predicting all the liquids when Polynomial and linear kernels were used. Therefore, Kappa, F-Measure and TP values were 1. Moreover, Root Mean Squared Error value of 0 indicates that the algorithm made the classification error-free. When Sigmoid kernel function was used, the algorithm did not accurately predict any hazardous liquid. Therefore, F-Measure value was not computed.

TABLE II
AVERAGE VALUES OF PERFORMANCE METRICS OF DIFFERENT KERNEL FUNCTIONS.

Metric	**Linear**	**Polynomial**	**Radial basis function**	**Sigmoid**
TPR	1	1	0.94	0.55
FPR	0	0	0.07	0.55
F-Measure	1	1	0.94	---
Accuracy (%)	100	100	94.23	55.76

			TRAINING			CROSS VALIDATION		
			Predicted			Predicted		
			True Positive	True Negative	TOTAL	True Positive	True Negative	TOTAL
Linear	Actual	True Positive	23	0	23	23	0	23
		True Negative	0	29	29	0	29	29
		TOTAL	23	29	52	23	29	52
Polynomial	Actual	True Positive	23	0	23	23	0	23
		True Negative	0	29	29	0	29	29
		TOTAL	23	29	52	23	29	52
Radial basis function	Actual	True Positive	20	3	23	20	3	23
		True Negative	0	29	29	0	29	29
		TOTAL	20	32	52	20	32	52
Sigmoid	Actual	True Positive	0	23	23	0	23	23
		True Negative	0	29	29	0	29	29
		TOTAL	0	52	52	0	52	52

Fig.4. Performance of different kernel functions.

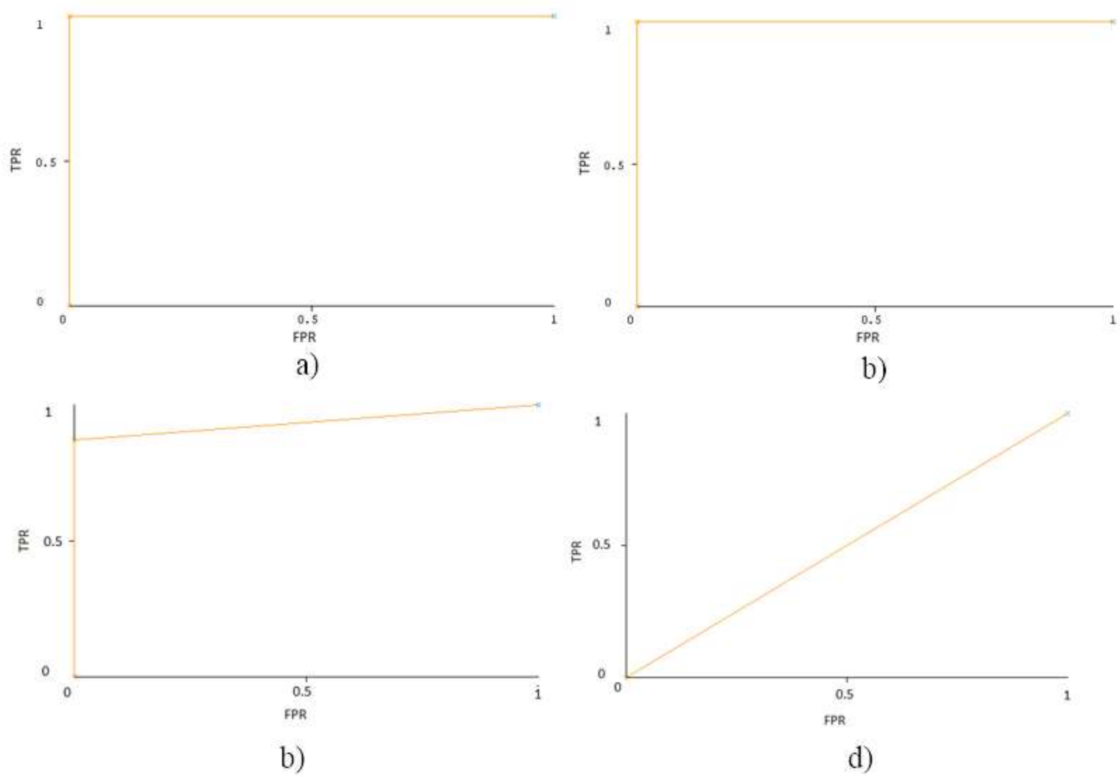

Fig.5. ROC curve of hazardous liquids with different kernel functions a)Linear b) Polynomial c) Radial basis d) Sigmoid.

IV. CONCLUSION

In this study, a system that can be used for non-contact detection of hazardous liquids is proposed. With this system, hazardous liquids can be evaluated independently of operator interpretation. Therefore, the obtained result does not vary from person to person. In addition, as the measuring system can scan liquids with a closed container, it prevents the operator from experiencing health problems caused by smelling these hazardous liquids and touching them.

When the measurement system and the embedded SVM algorithm are used, hazardous liquids can be detected quickly and with high accuracy. Kernel functions (Linear, Polynomial, Sigmoid or Radial) can be used to increase the success of the SVM algorithm. As a result of the classification made when Linear and Polynomial functions were used, the TPR value was 1 and the FPR value was 0. In addition, the accuracy rate was 100%. These values prove that the algorithm can classify all liquids correctly when Linear and Polynomial functions have been used. The confusion matrices and ROC curves presented in this paper support this conclusion. Consequently, it is recommended to use Polynomial or Linear kernel functions in the proposed system.

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