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# Support Vector Machine Techniques for Polar Liquid Categorization

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**ABSTRACT**

The dispersive nature of polar liquids creates ambiguity in their identification process. It requires a long time and effort to compare the measured values with the available standard values to identify the unknown liquid. Nowadays machine learning techniques are being used widely to assist the measurement techniques and make predictions with great accuracy and less human effort. This paper proposes a support vector machine (SVM) based classification model for the identification of six polar liquids-butan-1- ol, dimethyl sulphoxide, ethanediol, ethanol, methanol and propan-1-ol for a temperature range of 10 °C–50 °C and frequency range of 0.1 GHz–5 GHz. The model is constructed using the data from the National Physical Laboratory (NPL) report MAT 23. The identification of unknown liquid is based on complex permittivity measurement. If the measurement error in complex permittivity is less than ±6% of the standard value in NPL report, the proposed model identifies the liquids with 100% accuracy in the entire temperature and frequency range. The performance of the model is validated by testing the model with data external to the dataset used. The findings show that the proposed model is a useful and efficient tool for identifying unknown polar liquids.

## 1. INTRODUCTION

Material characterization plays a major role in many applications like material processing, bioengineering, medical treatment and food industry. Materials can be characterized based on their electromagnetic properties like permittivity, permeability and conductivity. Measurements in the microwave frequency range focus on the complex permittivity (ε*) rather than the permeability and conductivity. Complex permittivity gives insight into the structure of the material, the temperature in the surroundings and the number of impurities in it. The real component of complex permittivity reflects the dielectric medium's ability to retain energy, whereas the imaginary part describes the medium's energy losses. Dispersion is the fluctuation of ε* with frequency. At microwave frequencies, the effect of orientation polarization is responsible for dispersion [1]. In the case of dispersive materials, repeated measurements at different temperatures and frequencies are required to study the dielectric dispersion characteristics [2]. This work looks at polar liquids that are dispersive in nature. These liquids are utilised in specific absorption rate (SAR) metrology because their complicated permittivity is comparable to that of biological tissue metrology [2], [3]. Polar liquids in their pure form can be employed as an excellent calibration material in the field of dielectric instrumentation. National Physical Laboratory (NPL) of UK has conducted a detailed study on the dispersion

characteristics of commonly used polar liquids using coaxial cell permittivity measurement technique. NPL report MAT 23 describes the ε* of polar liquids-butan-1-ol, dimethyl sulphoxide (dmso), ethanediol, ethanol, methanol and propan-1-ol for a frequency range of 0.1 GHz-5 GHz and temperature range of 10 °C-50 °C [2]. The dispersive nature of these liquids makes the identification process a complex task.

According to related studies, unknown liquids can be identified by measuring its properties like density, melting point, boiling point, solubility and then comparing the results to the values of known liquids. It takes lot of experimental procedures and is very time consuming. Nuclear magnetic resonance (NMR) spectroscopy followed by Fourier transform method has been used in the identification of unknown alcohols [4]. NMR spectroscopy is a non destructive technique but it is very expensive. Another method used to identify the liquids is using surface acoustic mode aluminum nitride (AlN) transducer [5]. This method is very useful to test small amount of liquids but the identification process is time consuming. Complex permittivity measurement is a powerful tool in the identification of liquids. The most popular measurement techniques are transmission and reflection line, open ended probe and resonant methods [6]. In the transmission and reflection line method, from the measured values of transmission and reflection coefficients the ε* is extracted with the help of Nicholson-Ross-Weir method. Open ended coaxial probe method uses rational function model to extract ε*. In resonant method, measurement of quality factor and shift in resonant frequency are used to extract ε*. In all these cases related to complex permittivity measurement, identification of an unknown polar liquid requires measured value of complex permittivity followed by manual search in the available standard report for close matching. This takes a lot of time especially in the case of polar liquids because of its dispersive nature.

Support vector machine (SVM) based classification model is proposed in this paper for the identification of the polar liquids. Complex permittivity (ε′ and ε″) of the liquid, frequency (f) and temperature (t) of the measurement system that are very relevant to all permittivity measurement techniques are used as the input features to identify the polar liquids. The paper is structured as: research method, results and discussion, graphical user interface and conclusion

## 2. RESEARCH METHOD

Machine learning (ML) algorithms have the ability to recognize data and separate them into categories. This process is known as classification. This can be used to identify the group membership of the new data instances. The workflow of the classification based ML model used in this work is shown in Figure 1. The data obtained from NPL report is used to develop the model. The parameters ε′, ε″, f and t which are very relevant in a permittivity measurement system are taken as the input features. Model is trained using training set and hyperparameters are tuned to get the best accuracy. The performance of different ML techniques is evaluated using performance measures and the most suitable one is selected. Complex permittivity can be measured using several techniques in which the most commonly used methods are coaxial probe, coaxial cell and planar sensors. Measurement using coaxial probe and coaxial cell are well suited for wide range of frequencies whereas planar sensors have limited frequency of operation. Since coaxial cell based complex permittivity measurement is used in NPL report, the ability of the model to identify the polar liquids based on other measurement techniques is also verified in this work.

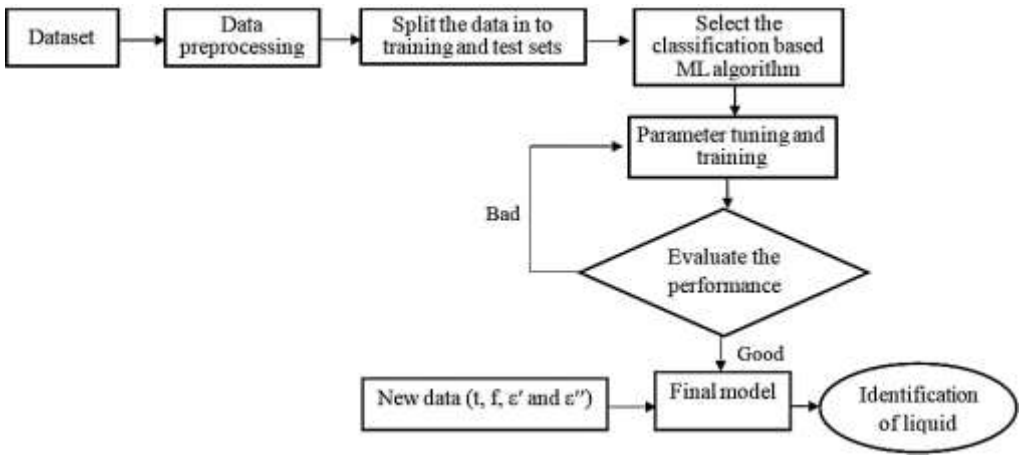



Figure 1. Workflow of the proposed methodology

### 2.1. Data gathering and pre–processing

The data for this work was gathered from NPL MAT 23 report. Table 1 shows the dataset description. The range of permittivity of six polar liquids for a temperature range of 10 °C-50 °C and frequency range of 0.1 GHz-5 GHz is shown in Table 2 [2]. This is a classification problem with multiple classes that includes the six polar liquids as the six classes. These classes are assigned with values from 1 to 6. For better use of the dataset of 1,000 samples, K–fold cross validation is performed on the whole data. This splits the dataset into subsets and performs training and testing on different parts of the dataset.

Table 1. Description of the dataset

| Dataset | | | |
|---|---|---|---|
| Inputs | | | |
| No | Features | | Values |
| 1 | Frequency (f) in GHz | | 0.1-5 |
| 2 | Temperature (T) in ℃ | | 10-50 |
| 3 | Permittivity (Real part) | | 3.23-78.5 |
| 4 | Permittivity (Imaginary part) | | 0.3-18.56 |
| Output | | | |
| No | Liquid | Number of samples | Class |
| 1 | Butan-1-ol | 140 | 1 |
| 2 | Dimethyl Sulphoxide | 140 | 2 |
| 3 | Ethanediol | 180 | 3 |
| 4 | Ethanol | 180 | 4 |
| 5 | Methanol | 180 | 5 |
| 6 | Propan-1-ol | 180 | 6 |

Table 2. Range of permittivity

| Polar liquid | Permittivity | |
|---|---|---|
| | Real part | Imaginary part |
| Butan-1-ol | 3.23-16.27 | 0.84-7.9 |
| Dimethyl Sulphoxide | 34.85-47.12 | 0.3-18.56 |
| Ethanediol | 6.93-43.48 | 0.94-18.3 |
| Ethanol | 4.93-26.18 | 0.82-11.13 |
| Methanol | 10.9-35.68 | 0.44-14.89 |
| Propan-1-ol | 3.66-20.35 | 1.1-9.35 |

### 2.2. Support vector machine classifier

The purpose of the SVM classifier is to find the optimum decision boundary that can separate n-dimensional space into classes and accurately classify a new data point. For multi-class classification, the one-against-all technique is utilised. SVM creates models for each class in this way. The m$^{th}$ SVM is trained with all of the data in the m$^{th}$ class having positive labels and all other samples having negative labels when using S classes. [7], [8]. Thus with $l$ training data $(x1, y1), \dots (xl, yl)$, where $x_i \in R^n$ , $i = 1, \dots, l$ and $y_i \in \{0, 1, \dots, S\}$ is the class of $x_i$ and the m$^{th}$ SVM solves the following minimization

$$f = \min_{\omega^m, \xi^m} \frac{1}{2} (\omega^m)\, \omega^m + C \sum_{i=1}^{l} \xi_i^m \qquad (1)$$

such that $(\omega^m)^T \varphi(x_i) + b^m \geq 1 - \xi^m{}_i$ if $y_i = m$

$(\omega^m)^T \varphi(x_i) + b^m \leq -1 + \xi^m{}_i$ if $y_i \neq m$

$\xi_i^m \geq 0, \quad i = 1,2, \dots l$

The training data $x_i$ are mapped to a higher dimensional space by the function φ which is known as kernel. Here $\omega$ is the weight vector, b is the bias term, C is the penalty parameter and $\xi$ is the slack variable [9]. By minimizing $\frac{1}{2} (\omega^m)\, \omega^m$ SVM tries to maximize the margin $\frac{2}{\|\omega\|}$ between the data in different classes. The penalty term $C \sum_{i=1}^{l} \xi_i^m$ tries to reduce the number of training errors. For (1) there are S decision functions

$$(\omega^1)^T (x) + b^1, \dots, (\omega^S)^T \varphi(x) + b^S$$

$x$ is classified to the class that has largest value of decision function

Class of $x \equiv \text{argmax}_{m=1,2,\dots S} ((\omega^m)\, (x) + b^m)$.

In this work, for six polar liquids the number of classes is taken as S=6. K-fold cross validation is applied on the dataset and hyperparameters are tuned to get the best performance from the model [8], [10]–[13]. For reliable estimates and best results 5-fold cross validation is selected and the hyperparameter C is tuned to the value 21 and the kernel is the radial basis function (RBF). (φ) [14], [15]. At a time, the 5-fold cross validation on the 1,000 sample dataset creates a training set of 800 samples and a test set of 200 samples.

## 3. RESULTS AND DISCUSSION

The complex permittivity of polar liquids varies non-linearly with frequency and temperature. Several classifiers are applied to the dataset to learn the complex relationship among data. The performance of various classifiers is evaluated using performance measures (accuracy, error, specificity and sensitivity) and is presented in Table 3. It is observed that the hyperparameter tuning of SVM with RBF kernel and penalty parameter C=21 can separate the six polar liquids with 100% accuracy. The suitability of SVM is thus confirmed. The receiver operating characteristics curve (ROC) is shown in Figure 2. The ideal point on the figure is in the top left corner, where the false positive rate is 0 and the real positive rate is 1. The area under the curve for each class is obtained as 1 [16], [17]. This shows that all the six polar liquids are classified with an accuracy of 1.

Table 3. Performance comparison

| Model | Accuracy (%) | Error (%) | Specificity (%) | Sensitivity (%) |
|---|---|---|---|---|
| Naive Bayes | 59 | 41 | 91 | 59 |
| Decision Tree | 87 | 13 | 96 | 86 |
| KNN | 95 | 5 | 99 | 94 |
| Random Forest | 93 | 7 | 93 | 98 |
| SVM | 1 | 0 | 1 | 1 |

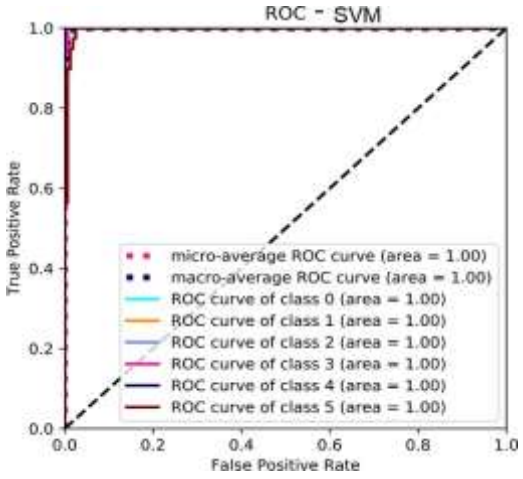
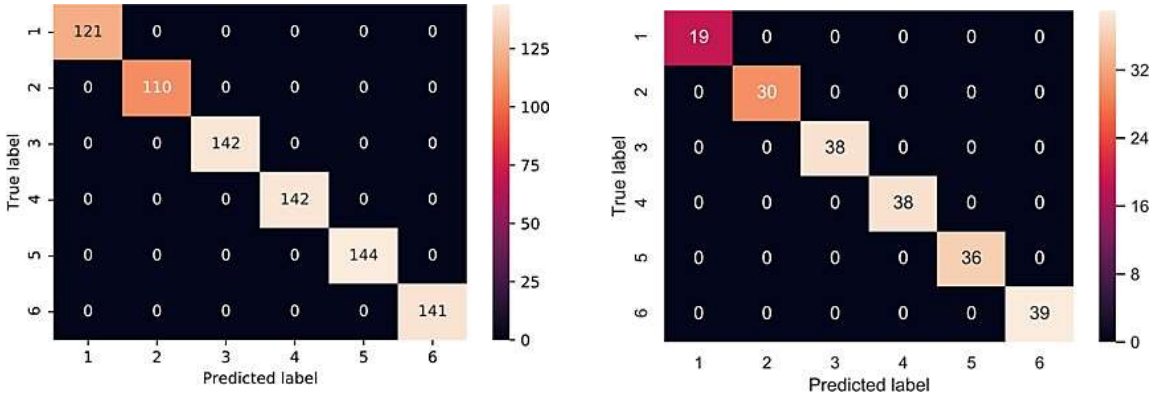



Figure 2. ROC for the proposed model

The accuracy of the proposed SVM model for 5-fold cross validation is obtained as 100% in all the 5 sets. This confirms the stability of the proposed model. The overfit condition is tested using three different methods. Firstly, the confusion matrix of both the training set and test set of the SVM classification is shown in Figure 3(a) and Figure 3(b) respectively. The diagonal elements indicate the correct predictions [16]–[18]. This shows that the SVM classifier performs well in both the training and the test set and the model is not overfitted. Secondly, the accuracy of the model is plotted for the training and test set by varying the penalty parameter C as shown in Figure 4. It shows that the model performs well in both the training set and test set and the accuracy is one when C=21. This also indicates that the model is not overfitted. Finally, the support vectors for each of the six classes have been identified and are shown in Table 4. The number of support vectors in each class is substantially smaller than the number of samples in each class [11]. This confirms that the model is not overfitted. All codes are written in the programming language Python 3.5 with the associated Scikit-learn library [10]. The average training time is 0.02s and the average time taken to test a

new data is 0.002s in a computer with an Intel Core i5 processor running at a clock speed of 1.6 GHz and equipped with 8 GB of RAM.




(a) (b)

Figure 3**.** Confusion matrix (a) Training set, and (b) Test set

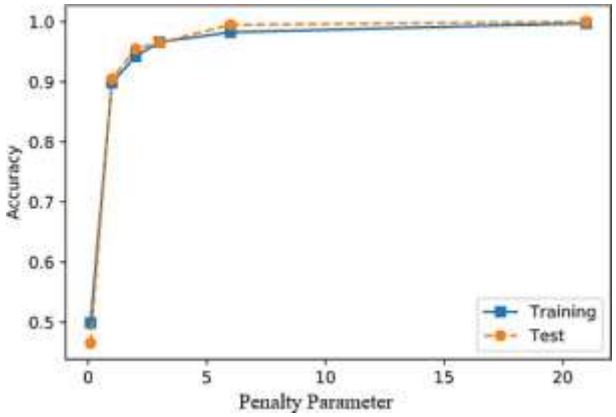



Figure 4. Accuracy vs penalty parameter (C)

Table 4**.** Support vectors for the proposed model

| Class | Polar liquid | Number of samples in the dataset | Number of support vectors |
|---|---|---|---|
| 1 | Butan-1-ol | 140 | 29 |
| 2 | DMSO | 140 | 17 |
| 3 | Ethanediol | 180 | 44 |
| 4 | Ethanol | 180 | 42 |
| 5 | Methanol | 180 | 32 |
| 6 | Propan-1-ol | 180 | 42 |

Alcohols like methanol and ethanol are highly volatile and evaporate rapidly. This changes the liquid temperature and hence the permittivity. Polar liquids like DMSO and ethanediol are hygroscopic, absorb water from atmosphere leading to variation in permittivity. Values of complex permittivity obtained from the NPL report are based on the coaxial cell measurement technique. Complex permittivity can be measured using different measurement techniques. Robustness of the proposed model needs to be tested for data obtained using other measurement techniques as well. The most widely used permittivity measurement techniques for liquids using coaxial probe, planar sensors and transverse electromagnetic cell (TEM) are considered for this purpose. It has been noted that the measured values of ε* differ from the standard value in NPL report and the variation depends on the measurement technique, temperature, frequency and the liquids used [19]–[29]. The measurement errors in ε* associated with different measurement techniques are

calculated for all the six liquids and shown in Table 5. This variation is expressed as the maximum percentage of error (E) in measured value with respect to the standard value. The measurement error is found to be minimum in the case of TEM cell because of the closed structure. A new test set is formed considering these measured values and the response of the proposed model is noted. The number of samples in the new test set is 40. While preparing the new test set, focus is given to those values in which considerable variations occur with respect to the standard value. The proposed model is able to predict all the liquids with 100% accuracy. The confusion matrix for the new test set is shown in Figure 5.

Table 5. Robustness of the proposed model

| Liquid [Ref.No] | Measurement Technique | T (°C) | F (GHz) | Maximum error in permittivity E (%) | | | Number of samples supplied to the model | Number of samples identified |
|---|---|---|---|---|---|---|---|---|
| | | | | Real part (ε′) | Imaginary Part (ε″) | F (GHz) | | |
| Butan-1-ol [20] | Probe | 30 | 0.1-1 | -16.72 | -0.62 | 0.1 | 10 | 10 |
| DMSO [22] | Sensor | 25 | 1.58 | 2.88 | -37.6 | 1.58 | 1 | 1 |
| Ethanediol [23] | TEM Cell | 24.2 | 0.1-4 | 0.07 | 0.3 | 1 | 6 | 6 |
| Ethanol [24] | Probe | 25 | 1-5 | 10.15 | 8.04 | 5 | 10 | 10 |
| Methanol [24] | Probe | 25 | 1-5 | 10.49 | -0.75 | 1.5 | 9 | 9 |
| Propan-1-ol [25] | Probe | 30 | 0.1-1 | -3.68 | 4.55 | 0.4 | 4 | 4 |
| | | | Total | | | | **40** | **40** |

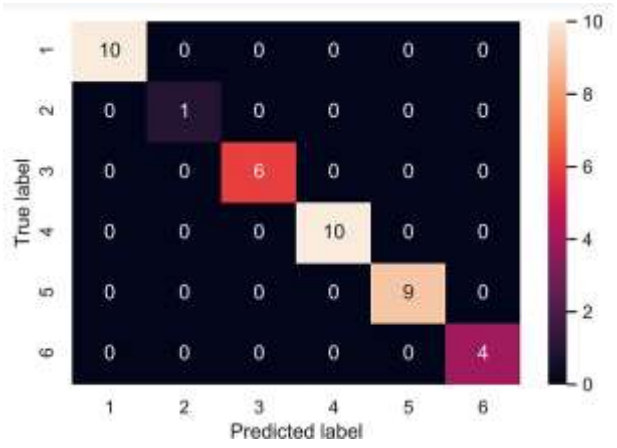



Figure 5. Confusion matrix for the new test set

Permittivity plot of the six liquids in the frequency range of 0.1GHz to 5GHz and room temperature 25 °C is shown in Figure 6. Real part of permittivity is shown in Figure 6(a) wheras imaginary part is shown in Figure 6(b). While the real part of permittivity (ε′) decreases with increasing frequency, the imaginary part (ε″) increases with frequency, reaches a peak at a frequency known as the relaxation frequency ($f_r$) and then decreases. In the case of DMSO $f_r$ is 8.32 GHz which is above the frequency range specified in Figure 6. Since the identification of these liquids are based on the measured value of complex permittivity (ε′ and ε″), the error in measurement leads to misclassification. For varied temperatures in the range of 10 °C to 50 °C, a modified test set is created by manually incorporating the measurement error that might occur in the entire frequency range (0.1 GHz to 5 GHz) during the permittivity measurement as a step variation of ±0.5% of the standard value of both ε′ and ε″. The performance of the model in each step is evaluated and the maximum measurement error in ε* that the model can accommodate without any misclassification is found out. For a particular temperature, this test set consists of 120 samples with 20 samples for each liquid. It is observed that if the measurement error introduced in both ε′ and ε″ is equal to 6% of the standard value, the first misclassification occurs in the case of butan-1-ol at 10 °C and 0.1 GHz as seen from row 1 of Table 6. The accuracy of the model drops to 99 %. For all other temperatures and frequencies the measurement error that the model can accommodate without misclassification is greater than 6%. The details of first misclassification observed at different temperatures are shown in Table 6. Since most of the measurements happen at room temperature 25 °C, the details of misclassification observed is also found out and presented in row 4 of Table 6. At 25 °C the first misclassification is observed at 0.1 GHz when the measured value of

both ε′ and ε″ decreases by 7.5% of the standard value. The complex permittivity plot at 25 °C and 0.1 GHz with a measurement error of -7.5% incorporated is illustrated in Figure 7 and the confusion matrix for the same is shown in Figure. 8. These results indicate that if the identification of an unknown liquid is to be carried out using the proposed model, well calibrated complex permittivity measurement systems with measurement error less than ± 6% is to be used to eliminate the chance of misclassification.

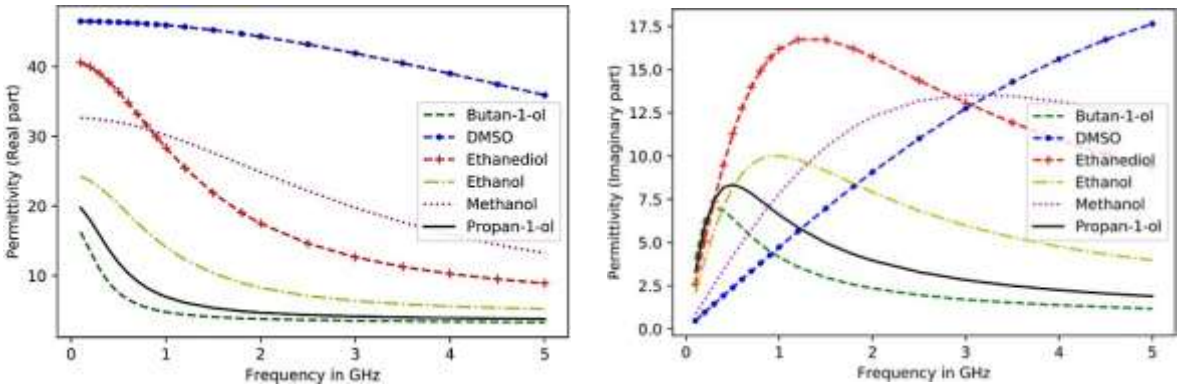



Figure 6**.** Permittivity plot at 25 °C (a) Real part, and (b) Imaginary part

Table 6**.** Misclassification test of the proposed model

| T (℃) | Error introduced in ε* (%) | Misclassification first observed Frequency (GHz) | Liquid | Misclassified result | Accuracy of the proposed model (%) |
|---|---|---|---|---|---|
| 10 | + 6 | 0.1 | Butan-1-ol | Propan-1-ol | 99 |
| 15 | -9 | 0.2 | Ethanol | Propan-1-ol | 98 |
| 15 | -9 | 0.1 | Propan-1-ol | Butan-1-ol | 98 |
| 20 | - 8 | 0.1 | Propan-1-ol | Butan-1-ol | 99 |
| 25 | -7.5 | 0.1 | Propan-1-ol | Butan-1-ol | 99 |
| 30 | + 10 | 0.1 | Butan-1-ol | Propan-1-ol | 99 |
| 35 | - 8 | 0.1 | Butan-1-ol | Propan-1-ol | 99 |
| 40 | -8.5 | 0.2 | Propan-1-ol | Butan-1-ol | 99 |
| 45 | -8 | 0.1 | Propan-1-ol | Butan-1-ol | 99 |
| 50 | -8 | 0.1 | Propan-1-ol | Butan-1-ol | 99 |
| 10-50 | Less than ±6% | _ | _ | _ | 100 |

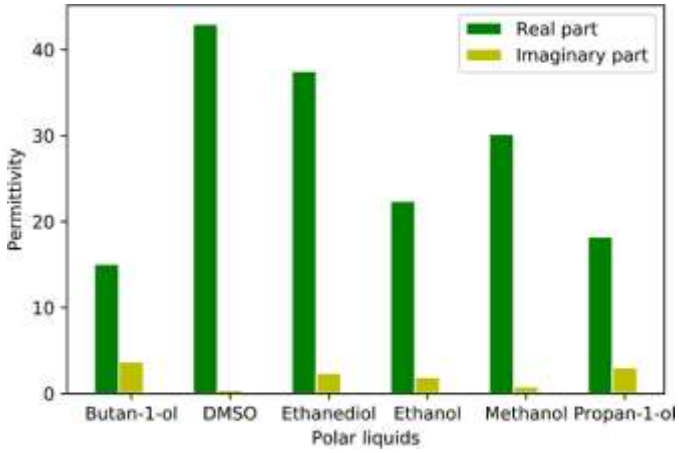



Figure 7**.** Permittivity plot at 25 °C and 0.1 GHz with a measurement error of -7.5%

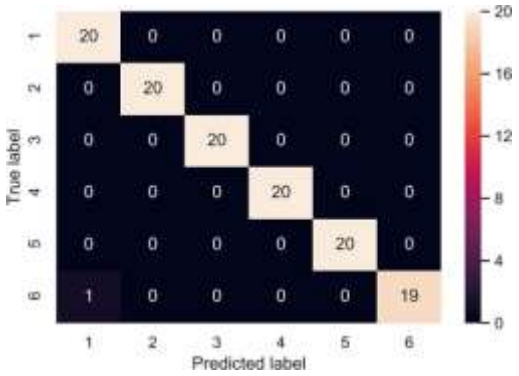



Figure 8**.** Confusion matrix for the modified test set at 25 °C and 0.1 GHz with a measurement error of -7.5%

## 4. GRAPHICAL USER INTERFACE

The proposed method is aimed to be used as a support tool to assist the measurement techniques. Graphical user interface (GUI) is designed for testing of unknown liquids. The inputs to the interface are the measured value of complex permittivity of unknown liquid, temperature and the frequency of the measurement system. The model identifies the unknown liquid within a fraction of a second. The front end of the GUI is designed using hypertext markup language (HTML) and the appearance is improved using cascading style sheet (CSS). The back end consists of the machine learning model and the web framework which are written in Python. Flask framework is used for the development of the interface [30]. It is a micro web framework that loads the machine learning model, takes the input from the front end and returns the predicted result. This GUI can be used for the temperature range of 10 °C to 50 °C, frequency range of 0.1–5 GHz. A warning message is displayed in the front end if the inputs exceed this range and also if the measured permittivity is not within the range of the dataset. The appearance of the GUI and an example of the predicted result are shown in Figure 9.


Figure 9**.** Graphical user interface

## 5. CONCLUSION

Measurements of complex permittivity in the microwave frequency range are well suited for the identification of unknown materials. But in the case of polar liquids, because of the dispersive nature, it is difficult to identify the liquid even though the permittivity is known or measured. In this work, SVM based classification model is implemented using Python for the identification of six polar liquids-Butan-1-ol, DMSO, Ethanediol, Ethanol, Methanol and Propan-1-ol for a temperature range of 10 °C-50 °C and frequency range of 0.1 GHz-5 GHz. The identification is done with minimum number of parameters. The input parameters are the complex permittivity, frequency and temperature, which are very relevant in a measurement system. The accuracy achieved is 100% for the specified temperature and frequency range. The performance of the model is validated to confirm that the model is not overfitted. The robustness of the model is tested using an external dataset and the performance of the model is found to be good. A GUI is

designed for the identification of unknown liquids. Probability of misclassification is also tested by manually introducing measurement error in complex permittivity to the standard NPL data. It is observed that the first misclassification happens when the measured values of complex permittivity deviates by 6% of standard value in the NPL report. All complex permittivity measurement techniques with measurement error less than ±6% can be incorporated with the proposed model to identify the unknown polar liquid for the temperature range of 10 °C-50 °C and frequency range of 0.1 GHz-5 GHz without any misclassification. The response is fast and the ambiguity in the identification process is eliminated. The model may be extended to identify polar liquid mixtures by suitably extending the dataset.

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