Estimation of Multi-Component Mixture Proportions using Regression Machine Analysis of Ultra-Wideband Spectroscopic Measurements

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***Abstract*—Ultra-wideband signals are used to examine multiple-constituent fluid mixtures in a semi-open system. A feedforward neural network operates on an array of easily computed signal properties, plus the weight and temperature of the fluid samples, to provide an estimate of the constituent proportions. The average performance of the neural network is tested by artificially increasing the test data sample size and repeatedly training neural networks of the same topology. Networks of differing topologies are compared. Statistical analysis is performed on these results and the 95% confidence interval of the data prediction is shown. The 95% accuracy averages around ± 6.9 percentage points for both oil and water.**

***Index Terms*—Microwave spectroscopy, dielectric sensing, complex permittivity, open system, neural network, oil/water mixture**

I. INTRODUCTION

MICROWAVE measurements have long provided a nondestructive method to determine the complex permittivity of various substances and simple mixtures. For mixtures of several constituents measurements over wide bandwidths are required to provide sufficient diversity to allow for separation of the responses of each material in the matrix. Analyzing these wideband measurements typically involves the task of separating the effects of complex interactions among the various material properties and the measurement geometry. Data processing strategies that rely on computation intelligence methods can be valuable in developing robust calibrations to determine the proportions of each constituent for pharmaceutical, food and chemical process monitoring and control applications.

II. MICROWAVE SENSING TECHNIQUE

Process materials can be characterized by their interaction with electromagnetic fields [1]. These interactions are delineated by the electrical permittivity and the magnetic permeability of the material. For most nonmagnetic natural materials, the magnetic permeability is close enough to that of free space that it can be approximated as such, leaving the electrical permittivity as the dominant variable in electromagnetic interaction.

A common method for estimating the complex permittivity $(\varepsilon' - j\varepsilon'')$ of a sample can be performed by transmitting a signal through a material sample and measuring the complex scattering parameters [1-8]. Jean [9] has shown that a simple system that measures only the forward scattering parameter S_{21} can provide a robust analysis of multicomponent mixtures that completely fill a wave guiding sample chamber with a constrained geometry and having a cutoff characteristic.

Composition analysis using simple S_{21} measurements for an open or semi-open system presents a more difficult measurement situation. The delay and attenuation of the signal through the sample material are directly related to the dielectric constant ε' and the dielectric loss factor ε'', but the unconstrained geometry introduces other factors which must be included in the analysis. In addition to delay and attenuation, measuring the dispersion of a signal will give further information about the test material's response across frequency. Fig. 1 shows an example time domain pulse

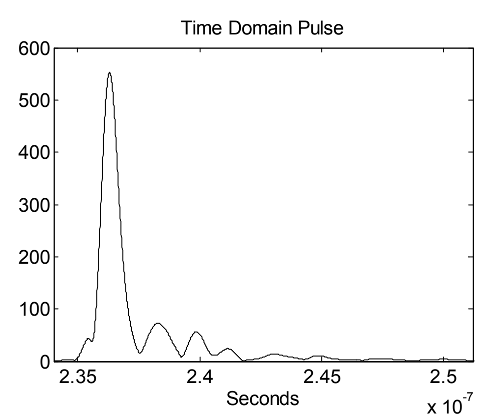

Figure 1: Time domain pulse exhibiting delay, attenuation and dispersion effects for a typical measured sample.

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received from a measurement that exhibits dispersion due to both geometry and material properties.

III. Materials and Methods

A semi-open measurement setup was devised that consists of a vector network analyzer, pseudo bowtie antennas for signal transmission and reception, and a cylindrical borosilicate glass sample container surrounded by microwave absorbing material (Eccosorb AN-75).

The antennas were chosen for their broadband characteristics and low dispersion. The microwave absorbing material was used to create an iris in which the sample can be placed to minimize the effects of multipath signals and have the signal passing through the sample be the dominant one received. The setup, shown in Fig. 2, was calibrated with an empty sample chamber.

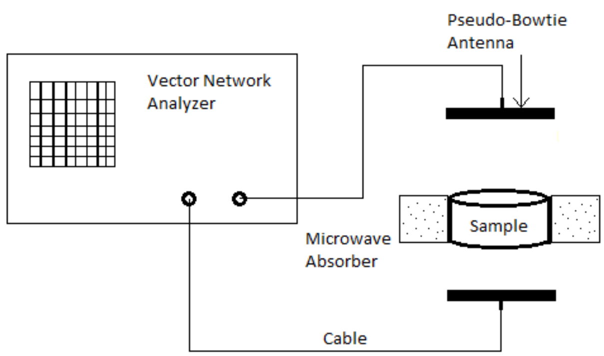

Figure 2: Measurement Setup

Three materials were chosen as test fluid constituents; water is an extremely common part of industrial fluid processes and is easily measured using microwave techniques due to its high dielectric constant; oil was chosen because of its low dielectric constant and non-polar nature which contrasts with the high dielectric polar nature of water; finally, sugar was chosen as a semi-polar constituent. These materials were mixed varying both sugar and oil between five and thirty percent of the total mass of the mixture, with water making up the remainder. This experiment was repeated while adding both starch and salt to test for system sensitivity to small amounts of additives. Matlab was used to process the data once it was taken.

IV. Signal Feature Selection

A. Data Continuity

The pseudo-bowtie antennas have a measured bandwidth of 0.75GHz to 5GHz. However, problems arose with accurately identifying the slope of the unwrapped phase received signal across the full band. Therefore, an acceptable measurement bandwidth was determined using the smoothness of the unwrapped phase as shown in Fig. 3. Only those data between the phase discontinuities were used in the analysis. The frequency band used was from 0.8GHz to 2.25GHz.

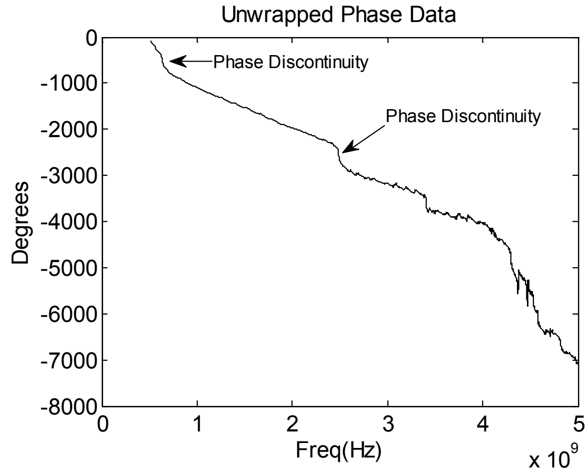

Figure 3: A plot of the unwrapped phase across the 500MHz to 5GHz band showing unwanted phase discontinuities.

B. Data Considerations

These data from the system are expected to be well behaved for small changes in the oil and sugar content of the fluid. With small enough increments of measurement, the data gathered forms a smooth curve. When both oil and sugar content is varied, this smooth curve becomes a smooth surface that can be manually inspected to identify data outliers and suspect measurements that may have been in error. An error checking procedure proved necessary since a large number of measurements were taken by several operators over an extended period of time.

While estimates of the proportions of constituents in a fluid can be made based upon phase and attenuation information alone, it was expected that a more accurate estimate would be had by including additional simply-computed signal parameters that should be predictive of or responsive to dispersion effects.

Dispersion analysis was expected to be particularly useful when any of the fluid constituents, i.e. water-based mixtures, has a strong change in permittivity over frequency. A simple calculation of signal variance was used as one dispersion parameter input for the regression machine.

The weight of the sample is also a useful input, as it can give a rough estimate of the sample's size. The estimation of the dielectric constant is dependent upon the length of the path of the signal passing through the test material. If the shape of the material is known, (in this case a cylinder of varying height), the weight will vary linearly with the length of the signal path.

Data surface plots are useful in determining which signal features contain the most information about the test material. Several different calculations were made on the measurement signals and of these, seven were deemed good candidates to be used as inputs to the neural network.

The signal mean (Fig. 4), and peak values (Fig. 5), are used as attenuation estimates. The location in time of the signal peak (Fig. 6), and the slope of a linear regression of phase (Fig. 7), are used as estimates of delay through the test material. The variance (Fig. 8) and the half amplitude pulse width (Fig. 9 were used as estimators for the signal dispersion. The first centroid of the signal (Fig. 10) is related to both the signal dispersion and the delay of the signal through the test material. The weight and temperature of the sample were also fed into the neural network to help the prediction.

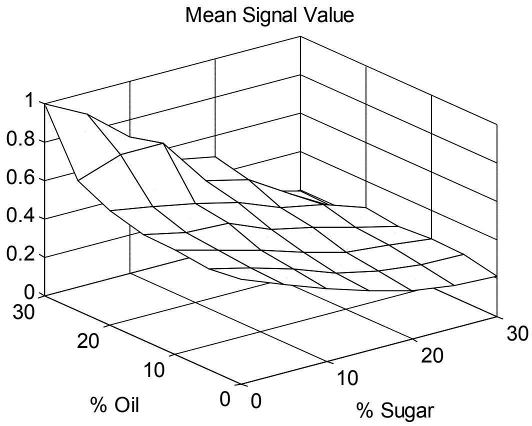

Figure 4: Normalized signal mean value. Data originally in amplitude units with a minimum of 0.597 and a maximum of 2.527.

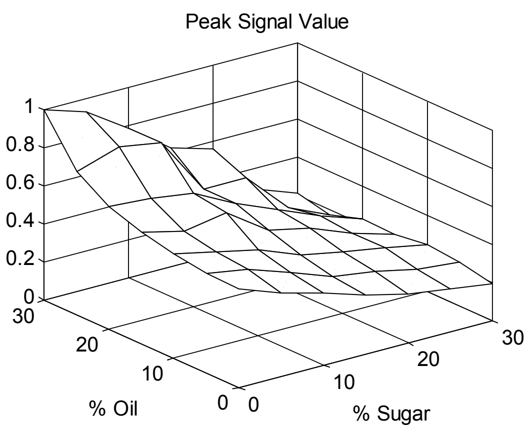

Figure 5: Normalized peak signal value. Data originally in amplitude units with a minimum of 162.4 and a maximum of 913.2.

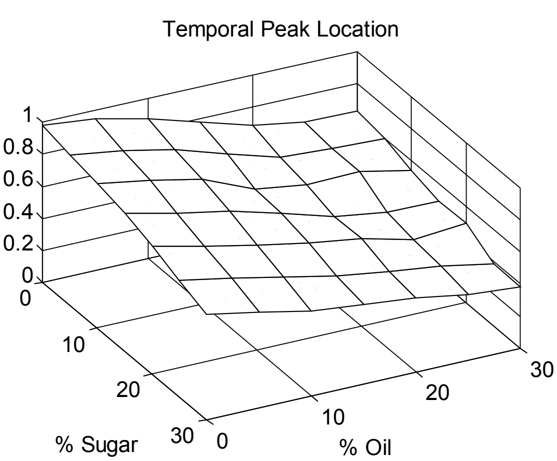

Figure 6: Normalized temporal peak location. Data originally in nanoseconds with a minimum of 235.50 and a maximum of 236.32.

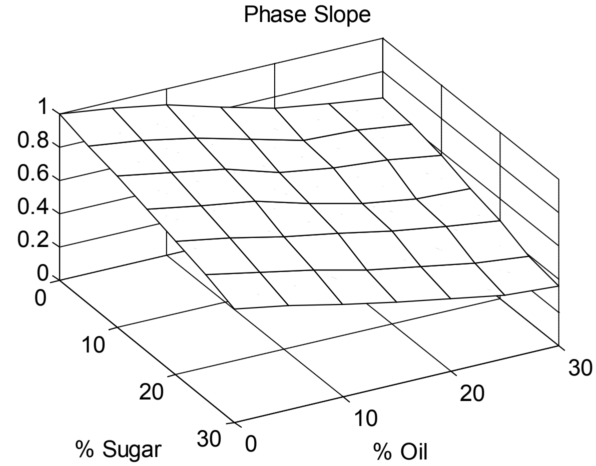

Figure 7: Normalized frequency domain phase slope. Data originally in degrees per hertz with a minimum of 1.841e-9 and a maximum of 10.585e-9.

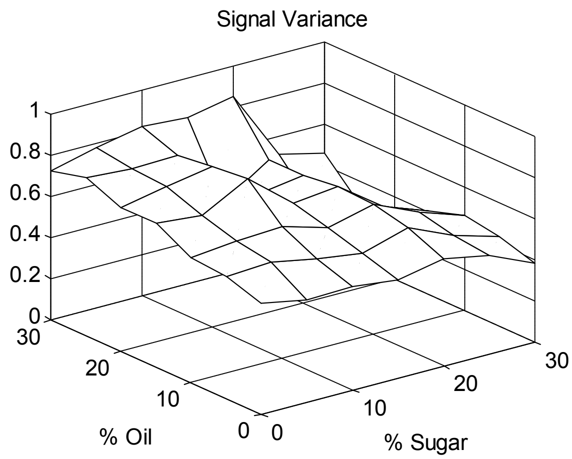

Figure 8: Normalized signal variance. Data originally in square nanoseconds with a minimum of 20.8 and a maximum of 47.7.

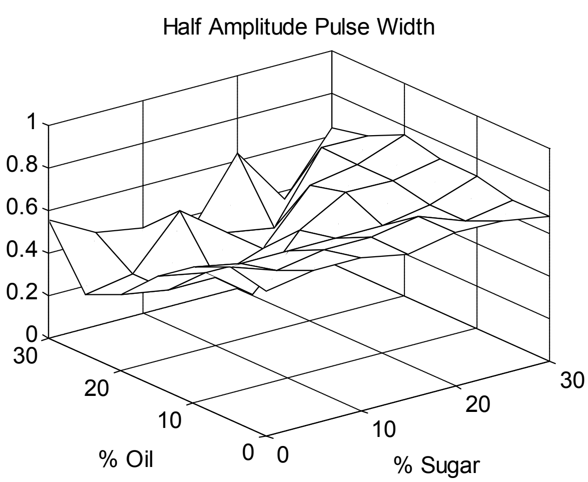

Figure 9: Normalized received half amplitude pulse width. Data originally in nanoseconds with a minimum of 0.316 and a maximum of 0.496.

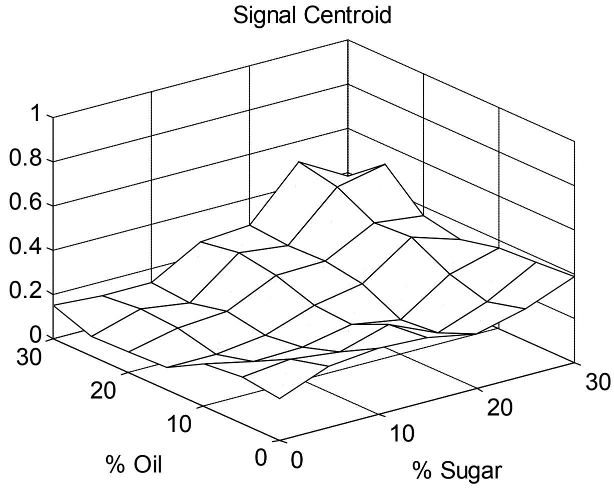

Figure 10: Normalized signal centroid. Data originally in nanoseconds with a minimum of 238.5 and a maximum of 242.9.

These features were chosen because of their physical meanings as well as their smoothness. Several signal properties, such as skewness and kurtosis (shown in Fig. 11) were not used because they either had a very rough surface plot or had no simple connection to the properties of the test material. All of the surface plot figures are normalized using the minimum and maximum values across the whole dataset. The figures show only the first forty-nine datapoints of this set.

V. Regression Machine Training

A. Neural Network Implementation

Most of the measurements only estimate various parameters of the test material. As such, supervised training of a layered perceptron regression machine [11][12] can be used to aggregate these measurements and better estimate the fluid constituent proportions. A feedforward neural network [13][14] with a single hidden layer was chosen to compress these nine inputs down to two outputs of water and oil content by percent mass. The sugar content is the remainder of the sample. The squashing function for the hidden layer of the neural network is a sigmoid and on the output layer it is linear. A total of three hundred forty-two data points were used in the training of the neural network. Seventy percent of the data was used for the actual training, fifteen percent was used as validation for a stop criterion and the last fifteen percent was used as test data to see how the network would perform on unseen data.

B. Neural Network Performance Measures

The performance of neural networks is difficult to measure when given a low number of test and training points; however, creative use of standard training methods can give a good measure of the performance of a given neural network topology [12].

Given a set of data, a standard practice is to use a portion of the data for training, another portion for validation, and a third portion for testing. The neural network training ends when the validation data achieves a certain amount of accuracy, but the test data is never used in the training loop. Because of this, the test data is a true measure of how the neural network performs when given data it has not seen before.

Randomly selecting the training, validation and test data over many repeated training processes and saving the performance of the test data each time will give a good approximation of the performance of the neural network on that set of data. This method can be used to measure the performance of a neural network of a certain topology on a set of data. Once this is done, standard statistical methods can be used to measure error.

Networks with several different topologies were trained. The efficacy of these configurations was compared based on the root mean square (RMS) error of the network outputs for the test data over hundreds of trials.

The number of nodes in the hidden layer was varied from five to thirty. Based on the RMS errors from the networks of various sizes, it was determined that a network with from eighteen to twenty nodes in the hidden layer could learn the dataset better than networks with either larger or smaller hidden layers. A single layer is always sufficient, though not necessarily optimal in terms of minimal hidden neuron count, to effectively capture neural network mappings [15][16]. Validation optimization was observed to gracefully degrade with hidden neuron count around the best configuration.

A single network that produced two outputs, oil and water percentages, was compared with two independent networks that each produced a single output. When each of the networks had too few hidden nodes, the two independent networks could learn to match the dataset better than a single network. However, when the number of hidden nodes in each network was increased, the single network performed just as well as the two independent networks.

Because there were few data points where the sample was over eighty-five percent water or less than fifty-five percent water, the training sample was artificially increased by duplicating these data points. This action is necessitated by the need to give each representative mixture level equal representation in the training data set [17]. Since this allowed the same data point to be in both the training set and the test set, it drastically decreased the RMS error in the regions where data was duplicated. Because this operation weighted the data set more towards the ends of the spectrum, it was expected that the RMS error for the middle, where data was not duplicated, would increase. However, this duplication of data actually decreased the RMS error slightly for the middle of the spectrum, indicating that the network was able to learn the entire function better.

The results from training one hundred networks with nineteen hidden nodes using the artificially expanded data set are shown in Figures 11 to 14. Fig. 11 and Fig. 12 show the network output for the test sets. Fig. 13 and Fig. 14 show the means and ninety-five percent confidence intervals computed from the test set data. The ninety-five percent confidence intervals average ± 6.9 percentage points from the mean value for both water and oil.

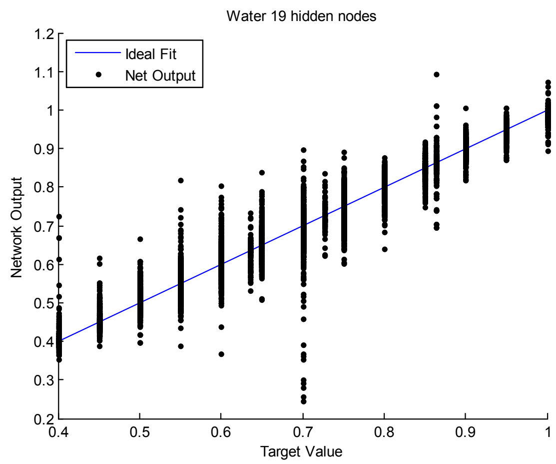

Figure 11: Network water output for test sets.

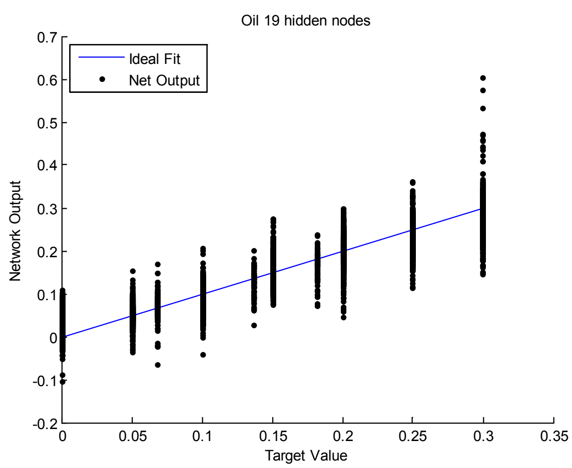

Figure 12: Network oil output for test sets.

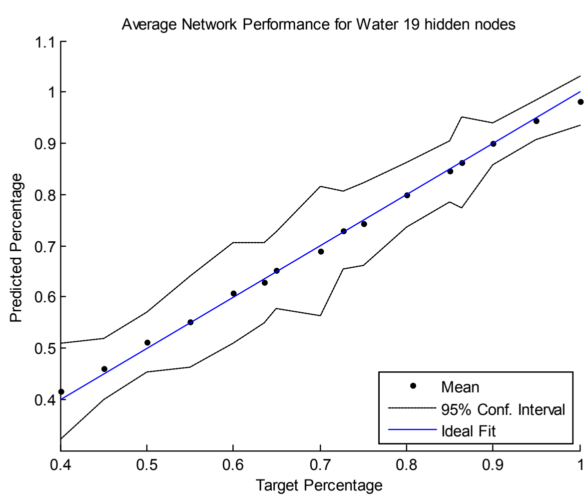

Figure 13: Neural network ninety-five percent confidence interval for water

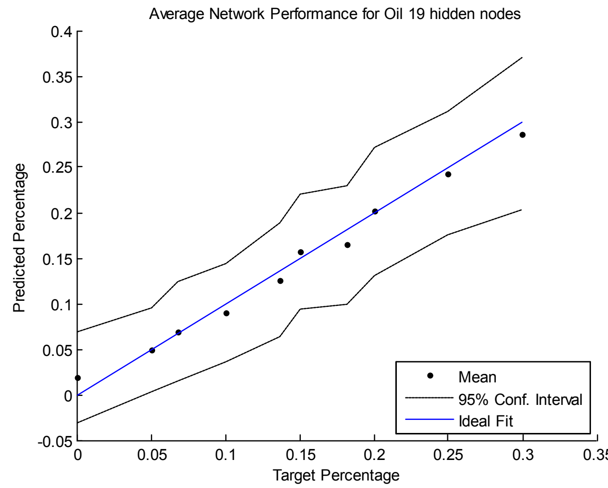

Figure 14: Neural network ninety-five percent confidence interval for oil.

VI. Conclusions

The proportions of constituents in a ternary mixture of water, oil and sugar can be estimated based upon the effects of their complex permittivities on a microwave signal. This method has been shown to work in a semi-open system. A neural network has been shown to be able to perform this estimation and a test for the performance of neural network topologies on this data was developed.

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