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SOM Based Combined Coordinate System for N-Dimensional Data Visualization

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ABSTRACT

Modern day organizations create massive amounts of data via their daily activities. Hidden knowledge is a valuable asset to an organization which is in a competitive environment. Improved analytical techniques or tools are needed to extract the knowledge hidden in the data. Today's information will be generated from many sources and linked with many other variables, which leads to multidimensionality. Matching human perception and cognition with information visualization is getting challenging, with the increasing dimensionality in the data. Our novel concept will facilitate a scalable and less navigational 3D interactive model for the user to achieve the ultimate goal or the information of interest, and our 3D interactive visualizing technique showed increased usability on a 2D view port over 2D analytical tools. One of the main features of our novel concept is less navigation, which lead to minimizing memorization, in order to mine patterns of interest over data.

Keywords. *Interactivity, Multidimensional data, SOM, Visualization, Web base*

INTRODUCTION

In the modern world, organizations are in a competitive environment which mandates understanding hidden knowledge which is not known to competitors, to take strategic advantage over others. They will generate and collect a huge volume of data by monitoring theirown or others'business processes, or users' activities, web site tracking, sensors, finance, accounting, etc. (Khan & Khan, 2011). With the development of social networks (such as Facebook, Twitter and Web technology), internet of things (IOT)in areas such as energy, transportation, health-care, environment, manufacturing, and agriculture, internet of vehicles (IOV), Geographic Information Systems (GIS), etc.,users create records of their lives daily,based on their activities, events they attend, places visited, pictures they take, and things they enjoyed and consumed. This leads to Big Data (Assunção, Calheiros, Bianchi, Netto, & Buyya, 2015) which has five characteristics (5Vs) namely variety (several data types), velocity(processing speed), volume, veracity (trustworthiness or reliability), and value (Assunção et al., 2015; Olshannikova, Ometov, Koucheryavy, & Olsson, 2015). Because of theincreasingly popularity of Big Data, several research areas are opened up, such as improving the interaction between the user and the system by using visual queries such as direct touch (Matthias Nielsen & Kaj, 2013) with a touch screen display or respond to voice or gestures of the user, matching human perception and cognition with the information visualization techniques via virtual reality (VR), augmented reality (AR) (Grubert & Grasset, 2013), 3D

Information visualization on the traditional screens, etc., improving screen limitation (width and height of the view port) and multidimensional (N-D) data representation, and improving usability of the visualization techniques.

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Data can be categorized into several types such as one-dimensional data (e.g., time-series data), two-dimensional data (e.g., geographical maps), multidimensional data (e.g., relational tables), text and hypertext, hierarchies and graphs (e.g., telephone calls), and algorithms (Keim & Ward, 2007). Hoffman and Grinstein presented research about "Visualizations for High Dimensional Data Mining - Table Visualizations"(Hoffman & Grinstein, 1997) and explained several visualization techniques which can be used for multidimensional data, such as scatter plot matrices, multiple line graphs, survey plots, glyphs and icons, fractal foam, etc. Matthew and others described how to achieve multidimensional data visualization though mapping dimensions of data to parameters of 3D objects. They also explained how to increase the dimensions by combining 3D objects and their parameters (Pastizzo, Erbacher, & Feldman, 2002).

Tory and Moller have done research on "Human Factors in Visualization Research" (Tory & Moller, 2004). Visualizations are needed for humans to analyse data and to represent important information visually. This can be called cognitive support (a mental process involved in knowing, learning, and understanding things) and can be provided through a number of mechanisms. In their article, they explain "How Visualization Can Support Cognition" and mentioned four methods (techniques) which can be used with visualization systems to improve human cognition under this section (Card, n.d.), such as increased resources for visualization systems, reduced search, enhanced recognition, perceptual monitoring, and manipulatable medium.Allowingusers interactive explorations may improve recognition of the patterns of interest.

According to Benjamin and others, understandability of presented results will be increased, if the users can interact with the results by themselves. They suggested multiple views web architecture to address above challenge. Time varying data could be presented in a way such that the user could navigate across the time axis and analyze them (Nowke et al., 2013). Interactivity is important to navigate and explore information to mine patternsof interest, which are hidden in the data, to aid critical business decisions in an organization. Highly interactive models or systems will work incrementally and reversibly (Brodbeck, Mazza, & Lalanne, 2009; Doug A. Bowman *et al*., 2006).An unnecessary amount ofinteractions towards the data summary and detailed information may lead to the user of the application memorizing the path traveled to achieve the ultimate goal.

Bowman and others have defined this 3D interaction as "Human–computer interaction in which the user's tasks are performed directly in a 3D spatial context" (Doug A. Bowman et al., 2006). They have discussed several contexts which are using 3D interaction as desktop computing, VR, AR, large screen displays, and ubiquitous computing. They also mentioned that the implementation barriers, which live on 3D interaction interfaces such as 3D UIs, must deal with a huge amount and variety of data;standard input and display devices to use with 3D UIs may not be available; some inputs must be processed or recognized before use;3D UIs often deal with multimodal input and output;real-time responses are required; and 3D interactions may be continuous, parallel, or overlapping.They have developed a framework called CHASM (Connected Hierarchical Architecture of State Machines) to address issues with event-based programming to implement 3D interaction interfaces efficiently.

In a dataset, non-numerical data, which will be collected by interviews, documents, observation, social media, etc., also need to be analyzed and visualized(Kigongo & McAfee, n.d.). For this purpose, clustering can be used, while there is a proven result using the naïve Bayes theory

(Medhat, Hassan, & Korashy, 2014) for text categorization. In our novel concept, we are focusing on visualizing multidimensional data on a 2D view port with the aim of minimizing the memorization of the interactions conducted by the user to achieve the ultimate goal.

METHODOLOGY

Our novel concept is a self-organizing map (SOM) based N-dimensional (N-D)interactive 3D model, which was prototyped as a web based application with the implementation ofa custom communication protocol between distributed components and the data visualization component (front end),to process N-dimensional data prior to visualization. The data visualization component consistsof two models (model 1 and model 2) which will be described in detail in the later part of this section, while distributed components will assist to process and cluster N-D data prior to visualization.

The architecture shown in Fig.1 was designed to prototype our concept by considering the advantages such as distributed data processing without over-loading the visualization component, programming language independency for enhancements on either side and reusability of previous analyzed or processed data (caching results).

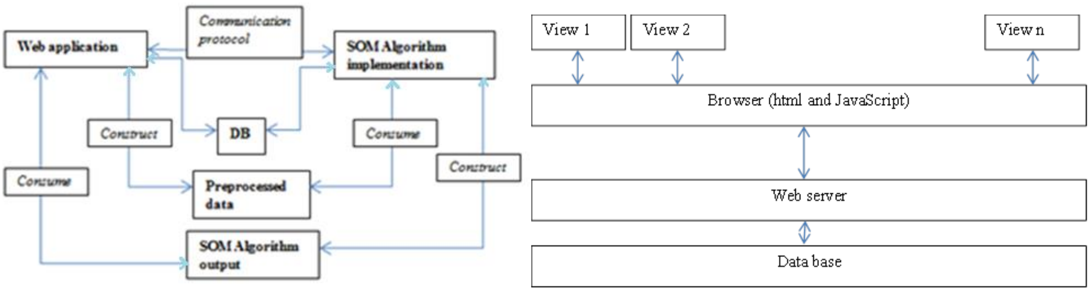

Figure 1. Analytical plugin architecture left and web based visualization architecture right

The followingsare the steps of custom communication protocol between the pluggable distributed components,which are loosely coupled, and the data visualization component (front end). The protocol facilitates enhancements to either module without destabilizing the other modules such as the "SOM algorithm implementation"ordata visualizing component.

1. *Exchange Meta data via communication protocol to construct the SOM Algorithm output. (numberOfcards, numberOfIterations, Preprocessed data location, Function like MexicanHat, FrenchHat, GaussFunction, etc.)*
2. *Construct SOM Algorithm output by SOM Algorithm implementation*
3. *Read the output by web application.*

For the explanation of our novel approach, the main topiccan be divided into two parts:"Importance of Kohonen Self-Organizing Map (SOM)" and "Importance of Combining Two Coordinate Systems."A metaphor for the novel interactive 3D model is combining two coordinate systems with an interactivity. The next two subsections will elaborate the concept in detail.

1. Importance of Kohonen Self-Organizing Map (SOM)

The self-organizing map (SOM) is a feature-extraction and data-mapping technique which was introduced by Kohonen (Grinstein, Trutschl, & Cvek, 2001; Schmuker et al., 2006). Self-organizing map (SOM) algorithm will reduce dimensionality of N-D data by projecting the clusters typically onto a 2-dimensional space.

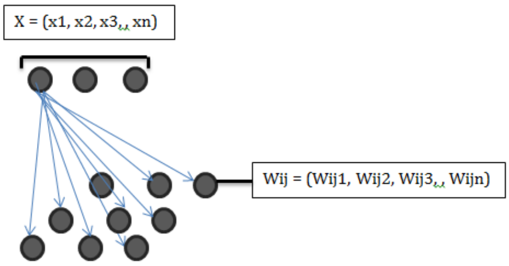

Figure 2. Diagram of a Kohonen Self-Organizing Map

The steps given below are followed when the Kohonen Self-Organizing Map is being constructed.

1. Randomize the map's nodes weight
2. Select randomly one instance
3. Find the closest node (best matching unit)

$$D_{i,j} = |X - W_{i,j}| = \sqrt{(x_1 - w_{ij1}) + .. + (x_n - w_{ijn})} \quad (1)$$

Here, i,j are output layer indexes and W is the weight vector of that position.
Winner,

$$D(k_1, k_2) = \min D_{i,j} \quad (2)$$

4. The weight of this node is updated
   Let neighborhood function
   $$h(\rho, t) = \exp\left(\frac{\rho^2}{2\sigma^2(t)}\right) \quad (3)$$
   $$\rho = \sqrt{(k_1 - i)^2 + (k_2 - j)^2} \quad (4)$$
5. The weights of the adjacent nodes are also updated
   $$W_{ij}(t+1) = W_{ij}(t) + \alpha(t)h(\rho, t)(X(t) - W_{i,j}(t)) \quad (5)$$
   Here, $\alpha(t)$ is the learning rate function
6. Reduce the intensity of the update progressively
7. Repeat 2 to 6 for n iterations

Let us assume that N-dimensional data can be represented by using symbols like Glyphs and Icons.For an example, the table given below will explain the mapping between dimensions of the N-dimensional data and parameters of the geometric objects.

Table 1. Mapping between dimensions of the data and parameters of the geometric objects

Parameters	Mapping parameter of the geometry	Remarks
Parameter one	Shape of the object	Value one: circle, Value two: square, Value three: star
Parameter two	Solidness or hollowness of the object	Value one: solid, Value two: hollow
Parameter three	Completeness of the object	Value one: complete shape, Value two: incomplete shape

The above parameters can be visualized in Fig.3 below. The left figure needed a filtering mechanism to filter unwandered patterns to understand the visualized content. That will lead to memorizing a set of actions to understand the visualized content while avoiding the ability to compare two sets of patterns at the same time. Unlike the left figure, the right figure used clustering to categorize information by avoiding the requirement of memorizing a set of actions and facilitating a comparison between two sets of patterns. The importance of the Kohonen Self-Organizing Map (SOM) for clustering is the capability to understand the similarity between two n-dimensional data instances. Unlike regression *"Fig. 4"* which has lower performance with the presence of nonlinearity, SOM facilitates analyzing and explaining the outliers present in the dataset. An outlier may not be an error; it may be an occurrence of a valid event with a time shift. In our novel concept, an SOM based approach can explain the above events with enhanced capability as the following equation explains.

Predicted Value	=	Regression Models Output	+	Effect of the time shifted event

(6)

The following explaining methods can be used to detect and differentiate outliers and errors. If an event can be detected successfully, its predicted effect can be added to the regression models output. Otherwise the effect of this parameter (predicted effect) will be ignored.Under the detection phase in our research, two novel methods have beeninvestigated, as explained below.

Method 1

Let's assume that time shifted event's occurrence can be predicted by using a set of independent variables.

Let

$X = \{x1, x2, x3, x4\}$

X is the measurements of a previously recognized event's independent parameters.

$Y = \{y1, y2, y3, y4\}$

Y is the measurements of the current event's independent parameters.

If the Euclidian distance (X, Y) < threshold

$$Y \sim X$$

Else

Ignore the effect of the event

Method 2

Let us assume that a comment or remark filed is present in the dataset. That nonnumeric field was categorized into a set of predefined categories by using naïve Bayes theory. If a new data point is received, by analyzing its nonnumeric field, it is possible to predict the behavior of that data point. In our research, it is possible to predict the behavior of the AMOUNT parameter (financial component).

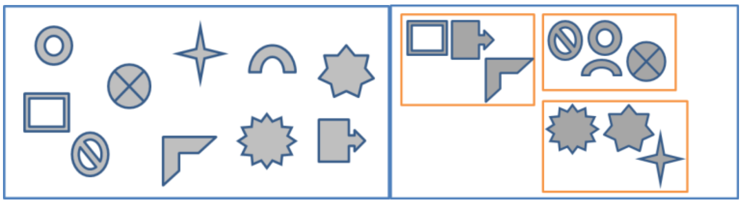

Figure 3. Left figure: N-dimensional data visualization without clustering, Right figure: N-dimensional data visualization with Self-Organizing Map (SOM) based clustering

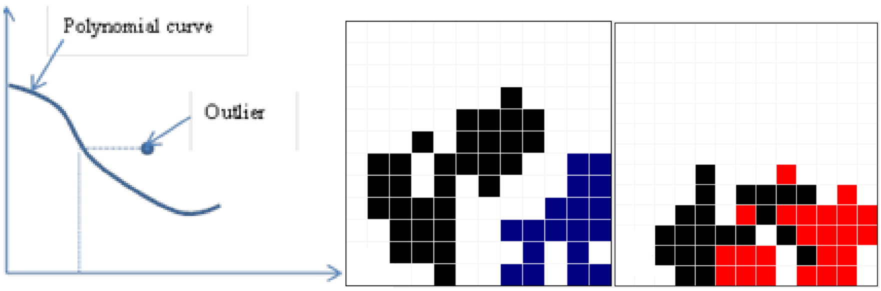

Figure 4. First figure: An outlier with polynomial curve fitting, Second figure: SOM visual representation without normalizing parameter data, Third figure: SOM visual representation with normalized parameter data.

2. Importance of Combining Two Coordinate Systems

Several coordinate systems are available to map dimensions of the multidimensional data (Janssen, n.d.) such as the Cartesian coordinate system, spherical coordinate system, etc. Volker described ellipsoidal coordinate systems which can be used for geo coordinates with increased precision over a spherical coordinate system (Janssen, n.d.). Selection of the coordinate system itself may improve the quality of the information presented.

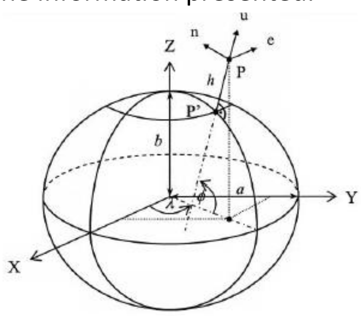

Figure 5. Ellipsoidal coordinate systems

These coordinate systems are three dimensional and it is possible to map three dimensions from a multidimensional data to these three axes. In our novel concept, we have combined two coordinate systems to increase the number of dimensions which can be represented in a way to facilitate pattern recognition to the users. For an example, it is possible to combine two Cartesian coordinate systems(*Figure 6)* or Cartesian coordinate system and a spherical coordinate system (*Figure 7.)*The advantages of this approach are the scalability for multidimensional data and less navigation for the user.

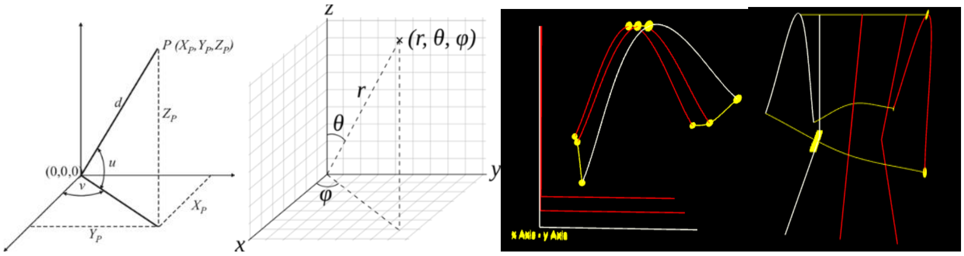

Figure 6. From left 1. Cartesian coordinate system,2. spherical coordinate system right, 3. Front view of the Self-organizing map (SOM) based 3D user interaction model 1, 4. Side view of the Self-organizing map (SOM) based 3D user interaction model1

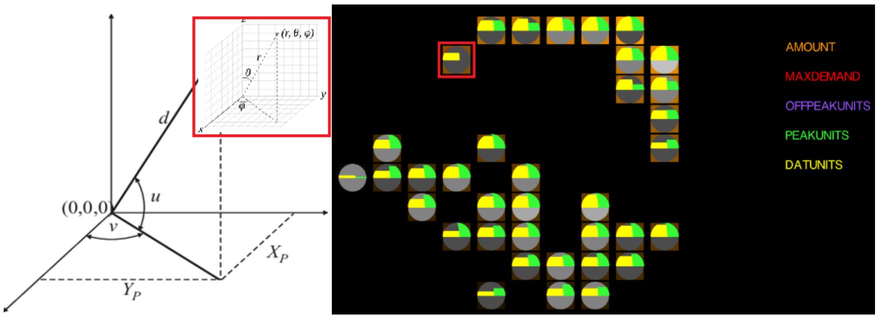

Figure 7. Left: Combining cartesian coordinate system with spherical coordinate system, Right:Output of the Self-organizing map (SOM) based 3D user interaction model 2

As the following paragraph explains, our metaphor for filtering is rotation of the sub coordinate system around its axis. As Figure 6. describes (3rd and 4th), the user can experience the behavior of the parameters by looking at different angles such as front and side views. As per the side view, the user can examine the shape of the curve (yellow color), which goes through the points of the N-dimensional instances' parameters' values of a single instance. That shows the trend among the parameters' values for a single instance. Comparison of such curves will give the trend among the trends of the N-dimensional data instances.

In data visualization there are interaction techniques such as filtering, zooming, distortion, linking, brushing, etc. In our novel concept, we have facilitated the filtering requirement via the rotation operation as described below. This method will avoid memorizing filtering operations which were performed by the data analyzer, leading to improved usability. By using rotation action upon a singleN-D data instance (sphere), viewer can analyze one dimension at a time as shown in the figurebelow (MAXDEMAND, DATUNITS, PEAKUNITS, and OFFPEAKUNITS).

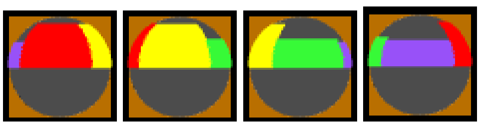

Figure 8. Five dimentions of the spherical coordinate system

As described above in *Figure 6* (3rd and 4th), as another advantage of the novel concept (metaphor),it will creata curve (yellow color) per each set of N-dimensional data instances. The above curves can be uniquely classified by using six statistical parameters namely Peak, RMS, Crest Factor, Kurtosis, Impulse Factor, and Shape Factor (Fengfeng Xi, Qiao Sun, & Krishnappa, 2000). By using thesesix statistical parameters, we have converted trend curves into a new domain,plotted them in a 3D space and observed the patterns. It clusters N-dimensional data instances in a similar manner to the output of model 2. That was considered as a cross verification for our novel concept self-organizing map (SOM) based 3D user interaction model for multidimensional data exploration.

RESULT AND DISCUSSION

Our novel concept's prototype was evaluated by using the workflowshown below and an electricity consumption dataset. Statistical analysis (mean, standard deviation) showed that MAXDEMAND parameter has a higher variation over DATUNITS, PEAKUNITS, and OFFPEAKUNITS parameters. The same was implied by our 3D visualization models. The model showed a significant different between high AMOUNT value cluster and low AMOUNT value cluster,Figure. 11. The results (Table 2, standard deviation and correlation with AMOUNT (financial) parameter) implied that MAXDEMAND parameter has contributed significantly to the cost of electricity consumption over other parameters. Users were asked to identify the same with the novel 3D visualization model. They observed the above information successfully (MAXDEMAND parameter as the most significant parameter to reduce or increase cost).

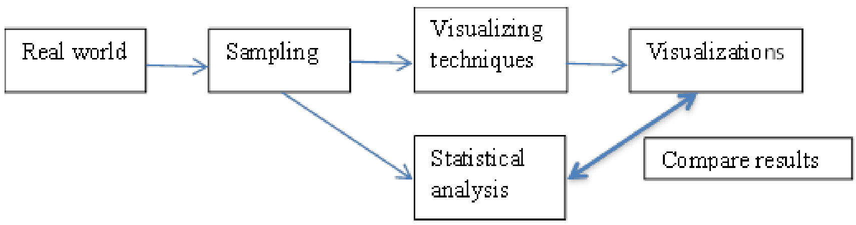

Figure 9. Workflow for validation and evaluation of visualization technique

Table 2. Statistical analysis of the dataset

	DATUNITS	PEAKUNITS	OFFPEAKUNITS	MAXDEMAND	AMOUNT
Mean (normalized parameters)	0.516	0.640	0.680	0.373	*0.435*
Standard deviation (normalized parameters)	0.196	0.248	0.237	0.254	*0.259*
Correlation with AMOUNT parameter	0.801	0.040	-0.057	0.804	*1.000*

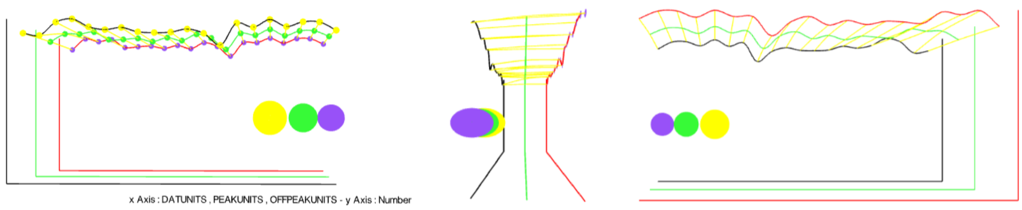

Figure 10. From left 1. Front view of the Self-organizing map (SOM) based 3D user interaction model 1, 2. Side view of the Self-organizing map (SOM) based 3D user interaction model 1, 3. Rear view of the Self-organizing map (SOM) based 3D user interaction model 1

Figure 10. aboveexplained the front view of the model 1 and can depict the trend of the three parameters (DATUNITS, PEAKUNITS, and OFFPEAKUNITS) over a time period. This graph shows four dimensions as DATUNITS, PEAKUNITS, OFFPEAKUNITS, Date (period), and normalized values of the above mentioned three parameters. The summary of relationships among the three parameters over a time period are shown as three spheres at the bottom of the line. The radii of these three spheres represent the correlation between the three parameters. By looking at the sizes of the spheres, we can directly decide whether there are any interesting patterns to mine.

Fig. 10 aboveexplained the trends among the three parameters (DATUNITS, PEAKUNITS, and OFFPEAKUNITS) over a time period. If the shapes of the curves are similar, we can assume that the trend among the trends of the three parameters is similar. For an example DATUNITS and PEAKUNITS parameters are increasing over a period while OFFPEAKUNITS parameter is remaining same. If OFFPEAKUNITS parameter's cost is lesser than PEAKUNITS parameter's cost, the organization canmove peak load to off peak by the means of shifting PEAKUNITS parameter's increase to the OFFPEAKUNITS, to reduce the consumption cost.

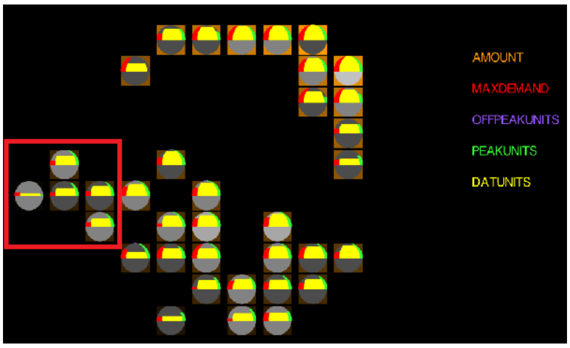

Figure 11. Multidimentional data visualization of the electricity consumptions by using model 2

Multidimensional data can be clustered by using SOM algorithm. As per the above figure, Fig. 11, data points in the marked areas are related and similar. An outlier plotted in that area can be described by using knowledge of the neighborhood node. It clearly showed that outliers are not present in the analyzed dataset, because all the multidimensional data points were clustered into two clusters. A user of the application can mark an area which can be considered similar. Then that area will be considered as the boundary for that cluster to analyze outliers and detect whether they are time shifted events or truly errors. The top right corner representsN-D data points with high AMOUNT value, while the bottom area represents N-D data points with low AMOUNT value. If high amount is observed in a node which is placed in the low amount cluster by the SOM algorithm, it follows that one or more parameters were managed incorrectly. Correctly managing those parameters will lead to reducing the cost of electricity consumption.

CONCLUSION

Our novel approach SOM Based Combined Coordinate System for N-Dimensional Data Visualization was evaluated by designing a usability experimental setup with an appropriate number of subjects. It showed improved usability and information related to pattern recognition over 2D analytical tools. Understanding of the visualized contents and taking the maximum benefit of the approach depends on the user's creativeness, level of intelligence, and past experience about the domain and the dataset. Our SOM based 3D interactive visualizing technique showed an increased usability on a 2D view port over 2D analytical tools.

With increased usage of an analytical system or approach, anexcessive amount of knowledge will be generated. Collecting, storing, and retrieving that knowledge will be the future work of this research project. N-dimensional data instances with the same features (same SOM location output) will be placed in an overlapped manner. Density information of the location will be visualized by opacity of the sphere placed on the location.Detaileddecomposition of the location information will be part of the future work for this research.

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Effect of replacement of wheat flour with sweet potato flour on quality characteristics of muffins

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ABSTRACT

This research was conducted to develop a low gluten muffin, supplemented with sweet potato flour and to evaluate its nutritional and sensory qualities. The fresh roots of sweet potato (var. *Wariyapola Red*) were peeled, washed and cut into thin slices. The slices were washed, dried in the dehumidifier drier, ground into flour using an electric grinder, sieved through 710 nm sieve, and packed in air tight glass containers. Different composite blends of wheat and sweet potato flour were mixed in the ratios of 100:00, 80:20, 70:30, 60:40, and 50:50 to prepare muffins. These muffins were analysed for physicochemical and mineral parameters, antioxidant capacity, and sensory attributes using standard protocols. The results revealed that the moisture, ash, fibre, vitamin A, and calcium content increased while fat, protein, iron, and phosphorus content decreased with increasing content of the sweet potato flour from 0 to 50%. However, the total antioxidant capacity was increased from 542.2 to 786.4 mg AA/100g with increasing sweet potato flour from 0 to 50%. The volume of a muffin decreased from 105.3 cm^3 to 91.9 cm^3, while its weight increased from 87.12 g to 96.36 g with increasing sweet potato flour substitution. The sensory assessment showed that there were significant differences ($p<0.05$) among the treatments in terms of colour, texture, taste, aroma, and overall acceptability. The mean sensory scores showed that consumers preferred the muffins made from 100% wheat flour. However, muffins from the composite flours with 30% sweet potato flour substitution were highly accepted by the panellists. The muffins made from 30% sweet flour and 70% wheat flour had nutritional, physical, and sensory attributes comparable to the muffins produced with 100% wheat flour.

Keywords: *Anti-oxidant capacity, composite flour, muffins, quality, sweet potato flour.*

INTRODUCTION

Muffins are a type of semi-sweet cake and are similar to cupcakes which are largely consumed by children as well as elders. They are normally made with wheat flour. According to Kim *et al*. (2012), all bakery products made from refined wheat flour are nutritionally poor, lackingin dietary fibre, phyto-nutrients, and bioactive compounds. However, recently findings have shown, in new product development, that composite flour can be used to improve nutritional value and sensory quality of the products (Ammar *et al*., 2009). An increased consumption of dietary fibre is recommended by nutritionists to improve health. A high dietary fibre content of food is one of the most important factors to reduce the cardiovascular diseases, diabetes and obesity (Brennan, 2005).

Sweet baked products in general, and muffins in particular, are highly appreciated by consumers because of their soft texture and characteristic taste. The principal ingredients of muffins—flour, sugar, fat, and egg—play an important role in the structure, appearance, and eating quality of the

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final product (Martínez-Cervera *et al*., 2012).Muffins are also characterized by a porous structure and a spongy texture. These attributes are measured, among others, by global density, crust/crumb ratio, moisture content of crumb and crust, crumb porosity and density, and textural properties, which can all be influenced by operative conditions (Baik *et al*., 2000).

Sweet potatoes are commonly used in traditional dishes. In order to increase the usage sweet potatoes, it can be transformed into flour and partially replace wheat flour in making bakery products.The development of processed products from sweet potatoes play a major role in raising awareness on the potential use of the crop around the world. Depending on varieties, sweet potatoes are low in protein but rich in dietary fibre and carbohydrate content, so a successful combination of a sweet potato variety with high nutritive value with wheat flour for muffin production could be nutritionally beneficial. Fibre is an important nutritional contributor of sweet potatoes in the human diet. Thus, a combination of wheat flour and sweet potato flour enhances the fibre content of muffins and may have a significant effect on human health (Bovell-Benjamin, 2007).

The incorporation of functional ingredients into bakery products has attracted increased attention from the food industry due to their positive effects on chronic diseases (Martins *et al*., 2017). Addition of various proportions of sweet potato flour in wheat flour can increase the nutritive value in terms of fibre and carotenoids. This also helps in lowering the gluten level and providing nutrition for celiac patients (Tilman *et al*., 2003).However, the complete replacement of gluten from bakery products is still a technological challenge (Bourekoua *et al*., 2016).

The present study was aimed at replacing the wheat flour in muffins by sweet potato flour (gluten-free flours) in order to increase the fibre and other nutrients, to develop muffins with good taste, texture and appearance, which resemble as closely as possible, the wheat flour-based products, and also to investigate the nutritional value and impact on sensory properties and physical parameters of muffins supplemented with sweet potato flour.

MATERIALS AND METHODS

Preparation of Sweet Potato Flour

The red skinned sweet potato (Variety: *Wariyapola red)* purchased from the commercial cultivators (low country wet zone) was used. The fresh roots were peeled, washed, and cut into thin slices. The slices were soaked in water for 90 min and dried in the dehumidifier at 60 °C for 10 hrs. The chips were then ground into flour using an electric grinder, sieved through a 710nm sieve, packed in air tight glass containers, and stored in cool, dry place until further use.

Ingredients and Preparation of Composite Flour for Muffins

Composite flour - 100g; Sugar - 70g; Margarine - 25g, Baking Powder - 1tsp; Salt - ½tsp; Whole Milk - 1cup; Vanilla Extract - 1tsp; Egg – 2.
The following five different composite flour blends, including the control were prepared.

T_1 - 100:0 wheat : sweet potato flour (control)
T_2 - 80:20 wheat : sweet potato flour
T_3 - 70:30 wheat : sweet potato flour
T_4 - 60:40 wheat : sweet potato flour

T_5 - 50:50 wheat : sweet potato flour

Preparation of Wheat and Sweet Potato Incorporated Muffins

The composite flour, baking powder and salt were sieved together. Sugar and margarine were creamed together for 1 min using a hand mixer. Eggs were whipped separately for 5 min. Whipped egg was added to the cream and mixed together with the addition of vanilla extract for 3 min. Finally, the composite flour was added and mixed well for 2 min with the addition of milk. The muffin batter (60g) was added to each cup and baked at 180°C for 30 min using a baking oven. After baking, muffins were cooled and stored at room temperature.

Nutritional and Sensory Analysis of Wheat and Sweet Potato Blended Muffins

The freshly prepared muffins from wheat - sweet potato flour blends were analyzed for moisture, ash, protein, crude fibre and fat using standard AOAC (2000) methods. The mineral content of the muffin was determined by using the method described by AOAC (2005).Vitamin A was determined by using the method of Kumar and Rajput (2011). Antioxidant activity was determined using the method described by Khaled *et al.* (2015). Mineral elements such as, iron and calcium were determined by atomic absorbance spectrophotometry. The phosphorus content was determined using a colorimetric method (Saha and Gilbreath, 1991). Acceptability of samples were judged by 20 semi-trained panelists and the samples were subjected to a nine-point hedonic test to determine the consumers' degree of liking. The sensory characters such as, colour, taste, texture, flavour and overall acceptability of the wheat-sweet potato blended muffins were judged by this method.

Statistical Analysis

The data of the nutritional parameters were analyzed by Analysis of Variance (ANOVA) (α =0.05) and the differences between means was compared using Duncan's Multiple Range Test (DMRT). Data related to sensory evaluation were analyzed using the Tukey's Studentized Range test. Both nutritional and organoleptic analysis was done through Statistical Analysis System (SAS) software statistical package.

RESULTS AND DISCUSSION

Nutritional Composition of the Freshly Prepared Sweet Potato Flour

Freshly made sweet potato flour contained 7.0% moisture, 9.4% fibre, 1.93% ash, 0.5% fat, 2.3% protein and 1.04% total sugar. The nutritional composition of sweet potato flour were in accordance with the results obtained by Endrias *et al*. (2016). Sweet potato flour compared to wheat flour contains a lower level of crude protein, crude fat, moisture, phosphorus, and iron, and a higher levels of total ash, crude fibre, vitamin A, and calcium.Therefore, addition of sweet potato flour to wheat flour may help increase nutrients in muffins.

Nutritional Qualities of Wheat and Sweet Potato blended Muffins

The nutritional qualities of muffins made from wheat flour and sweet potato flour blends are shown in Table 1. As demonstrated in Table 1, moisture and ash content of the muffins, which were prepared with different ratios of wheat and sweet potato flour, increased with increasing ratios of sweet potato flour, while fat content decreased. The moisture content of muffins gradually increased from 8.73 to 11.95% with the addition of sweet potato flour from 0 to 50% (Table: 1). This increment could be attributed to the water binding capacity of sweet potato flour. The results are in agreement with those of Endrias *et al*. (2016).

Table 1: Nutrient Composition of the Sweet Potato–Wheat Composite Flour Muffins

Treatments	Moisture %	Ash %	Fat %	Fibre %	Protein %
T_1	8.73±0.18^{cd}	0.52±0.02^{cd}	2.89±0.05^{a}	6.51±0.15^{bc}	8.63±0.04^{a}
T_2	9.61±0.15^{c}	1.03±0.02^{c}	2.25±0.03^{b}	8.87±0.09^{c}	8.33±0.06^{a}
T_3	9.89±0.14^{c}	1.12±0.03^{c}	2.21±0.04^{b}	11.99±0.16^{b}	8.25±0.09^{a}
T_4	10.83±0.19^{b}	1.24±0.02^{b}	1.79±0.05^{c}	12.06±0.12^{b}	7.75±0.06^{b}
T_5	11.95±0.18^{a}	1.28±0.04^{a}	1.68±0.03^{c}	12.16±0.05^{a}	7.63±0.12^{ab}

The values are means of triplicates ± standard error.

$^{a\text{-}d}$ The means with the same letters within the same column are not significantly different at 5% level

(T_1: 100% wheat flour; T_2: 80% wheat flour 20% sweet potato flour; T_3: 70% wheat flour 30% sweet potato flour; T_4: 60% wheat flour 40% sweet potato flour; T_5: 50% wheat flour 50% sweet potato flour)

The ash content of muffins gradually increased from 0.52 to 1.28% with the increment of the sweet potato flour from 0 to 50% as shown in Table 1. This may be attributed to the presence of sweet potato flour because it contains a higher ash content compared to wheat flour. These results are in agreement with results reported by Aniedu and Agugo, (2010). As shown in Table 1, the fat content of muffins decreased from 2.89 to 1.68% with increment of the sweet potato flour from 0 to 50%. These reductions in fat content of muffin due to sweet potato flour contain low fat when compared to wheat flours. These results were well agreed with the findings of Endrias *et al*. (2016).

The fibre content of muffins increased with increment of the sweet potato flour from 0 to 50% as shown in Table 1. Muffins consisting of 100% wheat flour have the least mean fibre content while muffins consisting of 50% sweet potato flour have the highest value. This increment in fibre content could be due to the high quantity of fibre in sweet potato flour compared to wheat flour. Thesefindings are in agreement with the results of Ifie (2011). The protein content of muffins decreased as substitution levels of sweet potato flour increased from 0 to 50% as shown in Table 1. This could be as a result of the lower protein content in sweet potato flour compared to wheat flour. The present finding was consistent with the reports of Endrias *et al*. (2016).

The minerals and vitamin A content of the composite muffin is presented in Table 2.The vitamin A and calcium of the muffin increased from 11.15 to 358.5 µg/100g and 24 to 29.5 mg/100g, respectively, with the increase of the sweet potato flour from 0 to 50%.The work reported on sweet potato showed that this crop is rich in nutrients (Simonne, 1993). Calcium is necessary for supporting bone formation and growth, whilevitamin A is an essential nutrient required for maintaining immune function (Stephensen, 2001). It also helps in the maintenance of healthy teeth, skeletal and soft tissue, mucous membranes and skin. It is often known as retinol because it produces the pigment in the retina of the eye. Iron and phosphorus content decreased from 3.18 to 1.98 mg/100g and 278.9 to 167.5 mg/100g, respectively, with the increase of the sweet potato flour from 0 to 50%.This could be due to the high amount of iron and phosphorus present in the when compared with the sweet potato. Phosphorus works closely with calcium to build strong bones and teeth. It is stored in the bone as calcium phosphate (Vallet-Regi and González-Calbet, 2004).

Table 2: Mineral and Vitamin Content of Sweet Potato-Wheat Composite Flour Muffins
The values are means of triplicates ± standard error.

Treatments	Vitamin A (µg/100g)	Calcium (mg/100g)	Phosphorus (mg/100g)	Iron (mg/100g)
T_1	11.15 ± 0.03^{d}	24.0 ± 0.1^{cd}	278.9 ± 0.2^{a}	3.18 ± 0.04^{a}
T_2	58.42 ± 0.09^{c}	25.2 ± 0.1^{d}	235.8 ± 0.2^{a}	2.75 ± 0.02^{a}
T_3	118.4 ± 0.1^{ab}	26.8 ± 0.2^{c}	212.3 ± 0.1^{b}	2.56 ± 0.05^{a}
T_4	258.3 ± 0.2^{b}	28.2 ± 0.1^{b}	198.4 ± 0.1^{b}	2.25 ± 0.08^{b}
T_5	358.5 ± 0.1^{a}	29.5 ± 0.1^{a}	167.5 ± 0.1^{bc}	1.98 ± 0.02^{c}

The values are means of triplicates ± standard error.
The means with the same letters are not significantly different at 5% level

(T_1: 100% wheat flour; T_2: 80% wheat flour 20% sweet potato flour; T_3: 70% wheat flour 30% sweet potato flour; T_4: 60% wheat flour 40% sweet potato flour; T_5: 50% wheat flour 50% sweet potato flour)

The total antioxidant activity (Figure 1) increased from 542.2 to 786.4 mg AA/100g with the increasing of the sweet potato flour from 0 to 50%. This could be due to the high amount of antioxidants present in the sweet potato. Sweet potato is specifically known to contain significant amounts of vitamins and minerals, and is reported to possess rich antioxidant contents especially in the form of phenolics (Kunyanga *et al*., 2012).

Physical properties of sweet potato-wheat composite flour muffins

The weight of wheat-sweet potato blended muffins increased (Table: 3) with the increment of sweet potato flour from 0 to 50%. The lowest weight of 87.12 g was observed in 100% wheat flour containing muffins while the highest value of 96.36 g was recorded in 50% sweet potato flour blended muffins ($p < 0.05$). The same trend was observed by Onuegbu e*t al*. (2013) using different composite flours.This might be due to the higher water absorption capacity of sweet potato flour than the wheat flour.

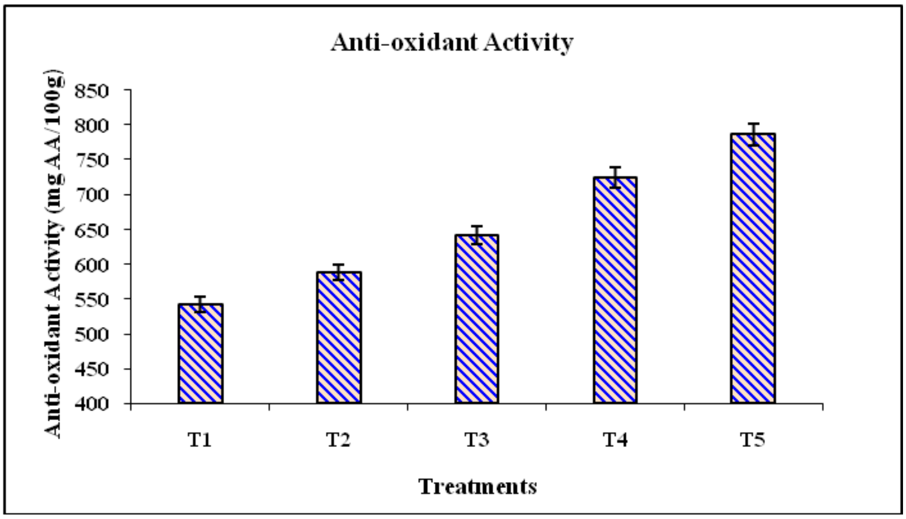

Figure 1: Anti-oxidant Activity of Wheat and Sweet Potato Composite Flour Muffins
The values are means of triplicates
The vertical bars indicate the standard errors
(T_1: 100% wheat flour; T_2: 80% wheat flour 20% sweet potato flour; T_3: 70% wheat flour 30% sweet potato flour; T_4: 60% wheat flour 40% sweet potato flour; T_5: 50% wheat flour 50% sweet potato flour).

Table 3: Physical Properties of Sweet Potato-Wheat Composite Flour Muffins

Treatments	**Weight (g)**	**Volume (cm^3)**
T_1	87.12±0.12^d	105.25±0.14^e
T_2	89.18±0.09^c	103.24±0.11^d
T_3	91.28±0.14b^c	101.39±0.09^c
T_4	95.36±0.08^b	96.09±0.07^b
T_5	96.36±0.07^a	91.85±0.02^a

The values are means of triplicates ± standard error.
The means with the same letters are not significantly different at 5% level

(T_1: 100% wheat flour; T_2: 80% wheat flour 20% sweet potato flour; T_3: 70% wheat flour 30% sweet potato flour; T_4: 60% wheat flour 40% sweet potato flour; T_5: 50% wheat flour 50% sweet potato flour)

The volume of the muffins decreased with the increment of sweet potato flour from 0 to 50%. Muffins with 100% wheat flour had the highest volume (105.25 cm^3) and muffins with 50% sweet potato flour had the lowest (91.85 cm^3) volume ($p<0.05$). This reduction might be due to the lower gluten level presence during dough formulation while increasing the sweet potato flour.This findings were in accordance with EI- Zainy *et al*. (2010).

Sensory Analysis of Muffin Supplemented with Sweet Potato Flour

The sensory analysis of muffins supplemented with sweet potato flour was shown in Figure 2. The quality of food, aside from microbial aspects, is generally based on colour, flavour, texture and nutritive value.

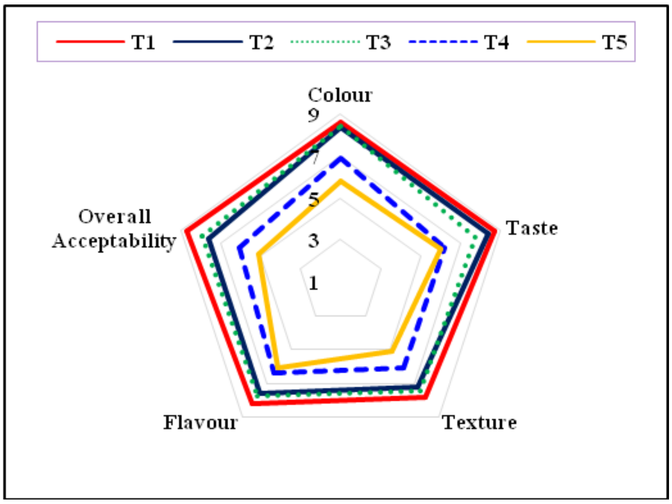

Figure 2: Sensory Analysis of Muffins supplemented with Sweet Potato Flour (T_1: 100% wheat flour; T_2: 80% wheat flour 20% sweet potato flour; T_3: 70% wheat flour 30% sweet potato flour; T_4: 60% wheat flour 40% sweet potato flour; T_5: 50% wheat flour 50% sweet potato flour)

Overall acceptability is a concept of the overall performance of the final product. Therefore, the sensory analysis is very important. According Tukey's Studentized Range Test, as shown in the Figure 3, there were no significant differences ($p>0.05$) among the muffins supplemented with 30% of sweet potato flour (T_3) and 100% wheat flour muffins (T_1). Muffins supplemented with 50% of sweet potato flour had the least score in overall acceptability. The results in this study agreed with the findings of Endrias *et al*. (2016).

CONCLUSIONS

This study was carried out to evaluate the effect of replacement of wheat flour with sweet potato flour on quality characteristics of muffins. Mixture of wheat flour and sweet potato flour could make a good baking product, which should increase the economic value. This decreases the import of wheat flour, reduce the use of sugar, and increase the value of sweet potato. The outcome of the present study can be used as valuable information for the development of high fibre low gluten muffins. However, muffins made using 30% sweet potato flour substitution (Treatment 3) was acceptable by consumers.This leads to the conclusion that nutritionally improved and consumer-acceptable muffins can be prepared by substituting up to 30% sweet potato flour in wheat flour.

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Fabrication of a Zn / natural graphite rechargeable cell with an ionic liquid based polymer electrolyte

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ABSTRACT

Rechargeablecells have received considerable attention for the purpose of serving for various energy requirements. As many of them are made with lithium and other expensive, hazardous materials and liquid electrolytes, different approaches are being considered to replace those materials with low cost and safe materials substitutes. In addition, there is much interest now on ionic liquids (ILs) as they are reliable substitutes for many of the toxic solvents used in preparing polymer electrolytes. The present study is based on the preparation and characterization of an IL based polymer electrolyte and evaluation of its performance in a Zn/natural graphite rechargeable cell. An electrolyte with polyvinylidene fluoride co hexafluoropropylene as the polymer, zinc chloride as the salt, and 1-ethyl-3-methylimidazolium chloride as the IL has a conductivity of 8.90 x 10^{-3} Scm^{-1}. The conductivity mechanism follows Arrhenius behavior. It is purely an ionic conductor having an electrochemical stability window of 0.6 V. The cell in the configuration, Zn / polymer electrolyte / natural graphite has an open circuit potential of 1.0 V. Cyclic voltammetry and galvanostatic charge discharge tests prove the compatibility of the electrolyte / electrodes for continuous operation. Higher scan rates are not suitable for operation as the time durations are not sufficient for the reactions to take place and hence, performance values are low. It can be stated that presence of Zn, natural graphite with IL based electrolytes are not undergoing parasitic reactions as occurs in liquid electrolyte based lithium rechargeable cells.

Keywords : *cyclic voltammetry, ionic liquids, natural graphite, Zn rechargeable cells*

INTRODUCTION

Rechargeable cells have played an exceptionally important role in modern technology-based society in fulfilling the thirst for energy. Much attention has been focused on lithium based rechargeable cells due to the remarkable performance of lithium as an anode (Armand and Tarascon, 2008; Brandt, 1994). Many of them have liquid electrolytes and expensive cathodes. However, due to rising concerns over green environmental concepts and economic factors, as well as crucial drawbacks of lithium rechargeable cells such as problems of handling and disposing of lithium, leaking of liquid electrolytes, high cost etc., nowadays attention has been diverted to developing rechargeable cells with safer as well as lower cost materials. This has spotlighted the importance of exploring and investigating non-lithium based low cost cells with non-liquid electrolytes. In place of lithium, many research activities are being done on materials like Zn, Mg and Al (Tian *et al*., 2017; Prasadini *et al*., 2018). Graphite, which is available in many countries as a valuable natural resource, has also received tremendous attention to be used for rechargeable cells. Up to now, many of the research activities have been carried out using commercially

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available graphite. Specially in Sri Lanka, no proper attention has been given to natural graphite (NG) to be used for scientific applications though there are several mines in the island. Since several decades ago, polymer electrolytes have been receiving noticeable attention among the scientific community as a viable substituent for liquid electrolytes and it has been possible to develop a large number of polymer electrolytes incorporating various polymers, salts and solvents [Kumar and Sampath, 2004; Priya and Suthanthiraraj, 2013; Rajendran, 2004]. However, the presence of solvents in polymer electrolytes has later been identified as a demerit, and as such, attempts have been launched to discover substitutes for them. Recently, ionic liquids (ILs), which are room temperature molten salts having bulky, asymmetric organic cations and inorganic anions, have been found to be a better replacement for solvents (Sapri *et al*., 2017). These ILs have been incorporated in preparing polymer electrolytes in many ways and they have been employed for various applications too.

The present investigation is based on the preparation of an IL based polymer electrolyte and fabricating a rechargeable cell with Zn and NG.

METHODOLOGY

Preparation of IL based polymer electrolyte

Polyvinylidene fluoride co hexafluoropropylene (PVdF co HFP) (ALDRICH), zinc chloride ($ZnCl_2$) (ALDRICH) and 1-ethyl-3-methylimidazolium chloride (1E3MICl) (ALDRICH) were selected as the polymer, the salt, and the ionic liquid (IL) respectively. The required amount of PVdF co HFP was dissolved in acetone by magnetic stirring. Then, IL and $ZnCl_2$ were added and stirring was continued further until a homogeneous solution was obtained. The composition of the electrolyte was 1 PVdF co HFP: 3 $ZnCl_2$: 1 IL (by weight basis). The resulting solution was poured into a glass Petri dish and kept in a vacuum oven to allow solvent evaporation. A thin electrolyte film free from pin holes could be obtained after 24 hours.

Preparation of electrodes

NG received from Bogala Graphite Lanka Limited was used without further treatment. Polyvinylidene fluoride (PVdF) (ALDRICH) was used as the binder in NG electrode. First, PVdF was dissolved in acetone using magnetic stirring and after it dissolved properly, NG was added. The resulting slurry was cast on a stainless steel (SS) die of a brass cell holder. Upon drying, it was used to assemble the cell. A circular shape Zn pellet was used as the other electrode.

Characterization of the polymer electrolyte

A circular shape electrolyte film was loaded inside a brass sample holder in between two well-cleaned SS dice. Impedance data were gathered from room temperature to 50 °C using a Metrohm Impedance Analyser. The thickness of the film was measured using a micrometer screw gauge to calculate the conductivity. A DC potential of 1 V was applied across an electrolyte film sandwiched in between two SS dice and the variation of current with time was monitored. To identify the electrochemical stability window of the electrolyte, linear sweep voltammetry test was performed for a cell of the configuration, SS / polymer electrolyte / Zn within the potential window 0.1 V and 0.9 V at the scan rate 10 mVs^{-1} using a two electrode setup of the Metrohm potentiostat. SS was used as the working electrode whereas Zn served as the reference and the counter electrodes (Prasanna and Suthanthiraraj, 2016).

Fabrication and evaluation of the cell

Cell of the configuration, Zn / polymer electrolyte / NG : PVdF was assembled inside a brass holder which is sealed by means of an O ring. Cyclic voltammetry (CV) test was performed first by varying the scan rate in the potential window 0.2 V to 0.8 V. Then, continuous CV test was done in the same potential window at the scan rate 10 mVs^{-1}. Potential variation with time during charging and discharging at a constant current was observed under the galvanostatic charge discharge test. The constant current was 6 x 10^{-5} A.

RESULTS AND DISCUSSION

Characterization of the polymer electrolyte

Figure.1 illustrates the variation of the conductivity of the polymer electrolyte with temperature

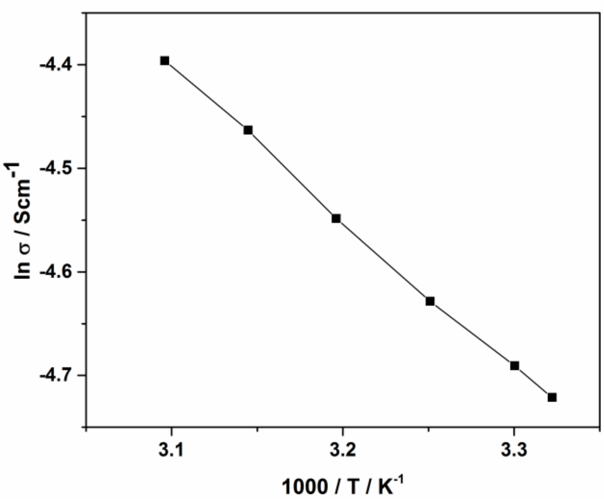

Figure 1. Variation of the conductivity of the polymer electrolyte with temperature

Conductivity (σ) values were calculated using the equation$\sigma = (1/R_b)(t/A)$, where R_b is the bulk electrolyte resistance, t is the thickness and A is the area of the electrolyte film (Khanmirzaei and Ramesh, 2014). R_b was determined from the Nyquist plot drawn between the real and the imaginary parts of the complex impedance obtained from impedance data. The room temperature conductivity was found to be 8.90 x 10^{-3} Scm^{-1}. It is a very suitable value for using this electrolyte for ambient temperature applications. According to the results, conductivity has increased with temperature. This proves that conductivity is a thermally agitated phenomenon. With increasing temperature, the salt can dissociate to a greater extent, resulting in more charge carriers, which would raise the conductivity. Also, if there are ion aggregates in the system, they also get dissociated. As a whole, the number of charge carriers in the electrolyte increases. Furthermore, upon temperature increase, charge carriers get energized and become more mobile. This too causes the conductivity to rise noticeably. The variation of the conductivity with temperature follows a linear behavior which implies that conductivity mechanism of the electrolyte takes place via Arrhenius behavior, given by the equation,$\sigma = A\exp(-E_a/k_BT)$ where$\sigma$is the conductivity, A is the pre-exponential factor, E_a is the activation energy, k_B is the Boltzman factor and T is the absolute temperature. This behavior correlated to the ion migration takes place via a hopping mechanism. Existence of the linear behavior throughout the temperature range suggests that the same ion conducting mechanism is retained in the system.

Fig. 2 shows the current variation through the electrolyte with respect to time under the effect of a DC voltage of 1 V.

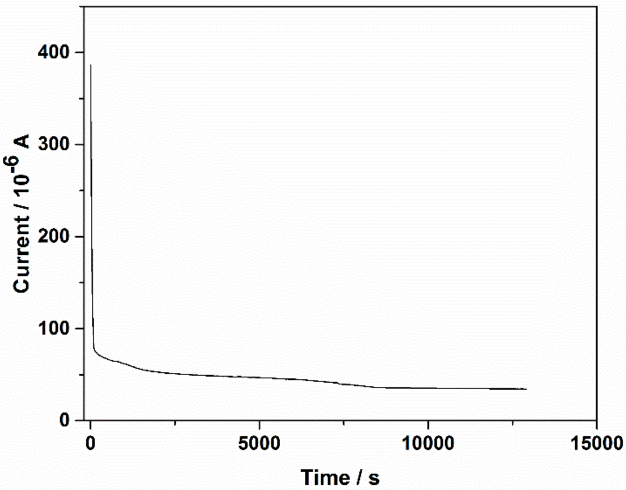

Figure 2. DC polarization curve of current variation with time of the cell configuration, SS / polymer electrolyte / SS (SS : stainless steel)

An abrupt current decrease is seen initially, followed by a stable variation with time. The initial drop is due to the polarization of ions due the blocking effect of stainless steel electrodes. The stable state arrives due to the movement of electrons. As the drop is very high, it can be concluded that ions are more dominant in the electrolyte than the electrons. In other words, it confirms that the electrolyte is a good ionic conductor. This fact can be further proved with the value of ionic transference number (t_i) which is calculated using the equation, $t_i = (I_i - I_s) / I_i$ (Kumar *et al.,* 2011). Here, I_i is the initial current and I_s is the stable current. The calculated t_i is 0.91. This is a good indication to show that electrolyte is predominantly an ionic conductor.

Figure 3 illustrates the linear sweep voltammogramme (LSV) of the polymer electrolyte. It is a powerful technique to determine the electrochemical stability window within which the electrolyte is electrically stable. From the results, it is found out that the electrochemical stability window of the electrolyte is from 0.2 V to 0.8 V.

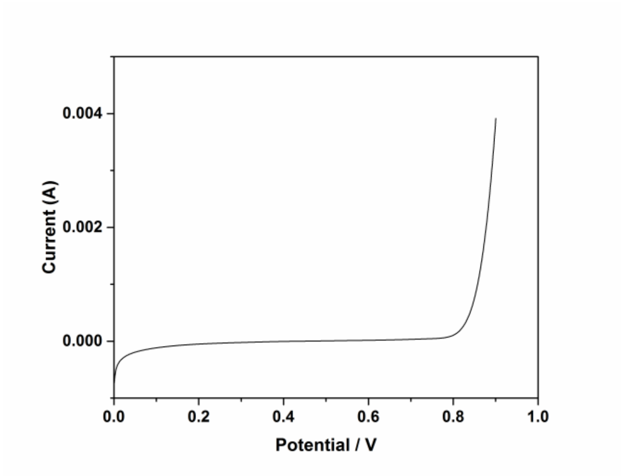

Figure 3. Linear sweep voltammogramme of the cell with the configuration, SS / polymer electrolyte / Zn at the scan rate of 10 mVs^{-1}.

Evaluation of the cell

The open circuit potential of the cell was 1.0 V. This is an accepted value for low power requirements. Also, by coupling several similar cells, it is possible to utilize this for high power applications.

Fig. 4 depicts the cyclic voltammogrammes obtained by varying the scan rate within the potential window, 0.2 V to 0.8 V. The reason for selecting the particular window is it is the electrochemical stability window found from LSV test. Peaks in the cyclic voltammogrammes are relevant to the reactions take place in the cell. It is noted that while increasing the scan rate, the peaks tend to disappear.

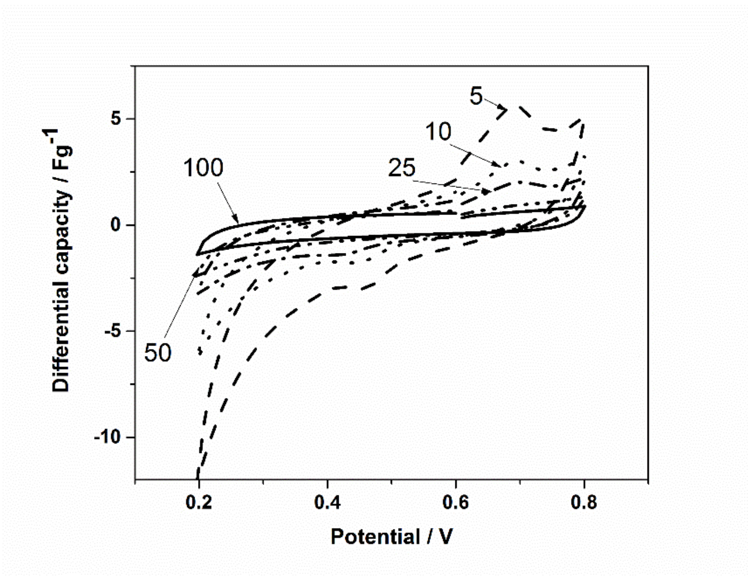

Figure.4 Cyclic voltammogrammes for different scan rates within the potential window, 0.2 V – 0.8 V

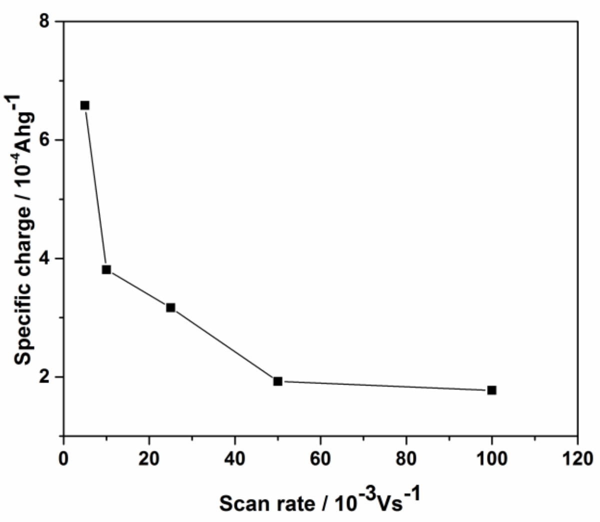

Figure 5. Variation of specific charge with the scan rate

Fig. 6 shows the variation of specific charge with cycle number. It is clear from the results that reduction of specific charge upon continuous cycling is not very fast. This is a positive feature to employ this cell for applications. The slow decrease of specific charge is an indication of the absence of parasitic reactions that are possible among electrolyte and electrodes. At the presence of lithium as well as toxic solvents in polymer electrolytes, many have reported about such reactions (Tarascon and Armand, 2001). Hence, it is possible to showcase the suitability of using Zn, natural graphite electrodes as well as polymer electrolytes with ILs.

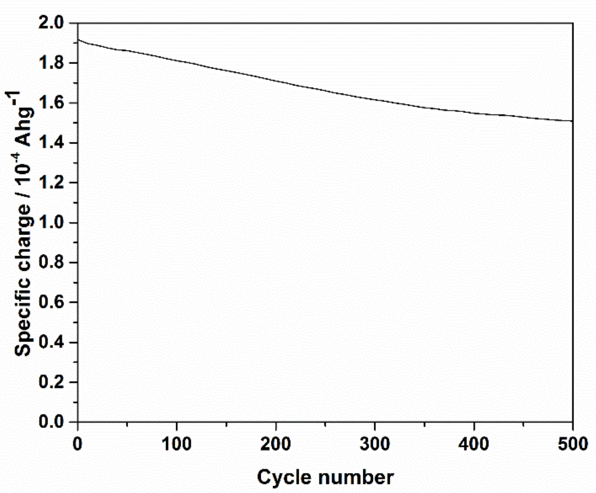

Figure 6. Variation of specific charge with cycle number obtained from cyclic voltammetry test at the scan rate of 5 mVs^{-1}

Figure 7. illustrates the variation of specific discharge capacity with cycle number obtained from galvanostatic charge discharge test.

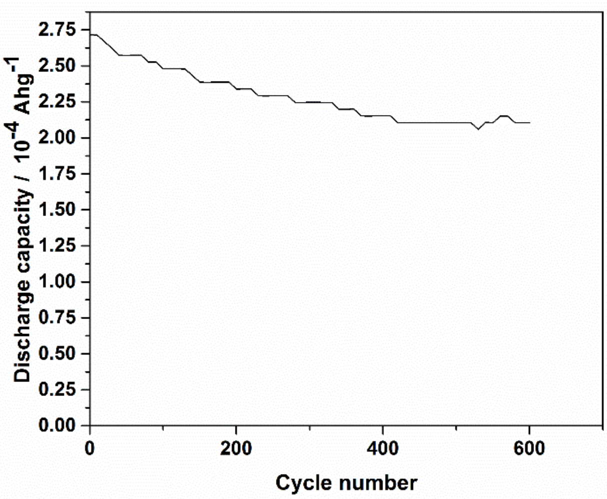

Figure7. Variation of specific discharge capacity with cycle number under a constant current of 6 x 10^{-5} A

Similar to the observation from continuous cycling under the cyclic voltammetry test, reduction of specific discharge capacity is not very significant. This well proves the suitability of the cell for continuous operations.

CONCLUSIONS

The polymer electrolyte prepared using an IL shows a room temperature conductivity of 8.90 x 10^{-3} Scm^{-1}. The electrolyte is predominantly an ionic conductor, which makes it more suitable for serving as a passage for ion movement. A considerable stability window is available with the electrolyte. The Zn / NG based cell has a satisfactory open circuit potential. Results of the cyclic voltammetry test as well as the galvanostatic charge discharge test prove the compatibility of the electrolyte / electrodes combination in order to sustain good stable performance even over long term operations.

ACKNOWLEDGEMENT

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The commercial viability of producing urea by utilizing natural gas discovered in the marginal reservoir Dorado

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ABSTRACT

The island nation of Sri Lanka became a plantation economy back in the 19th and 20th centuries,and a significant number of farmers' livelihoods still depend on agriculture itself. With the low cost of transportation and high solubility, urea fertilizer is leading the industry of agriculture. The current local urea demand is completely met by importations. A constant supply of Natural Gas (NG) is essential to manufacture urea locally. This study mainly focuses on introducing a viable solution for completely importing urea using indigenous gas in place. Amongst the discoveries made around the country, the Dorado reservoir exhibits high quality with a clean, thick deposition. In order to assess the feasibility, the reservoir potential was reviewed and production and supply profiles of NG were analysed by acquiring data regarding local demand quantities. A cost benefit analysis of establishing a urea plant was prepared with the involvement of a German organization. Previously identified economical quantity and price was applied to the Fiscal Regime for the Dorado reservoir with the assistance of PRDS and three case scenarios were proposed. The cases involve developing NG by the investing company with the most economical gas rate identified,*i.e.*, 70 MMScf/d, where around 20 MMScf/d of it will be utilized to manufacture urea. The excess production of NG will either be sold to the government or integrated to a power plant, which is preferred as it introduces additional benefits to the economy. Further analysis can be made depending on different modes and methods of transporting NG and locations of the plants which can manipulate the costs with better focus on achieving higher yield.

Keywords: Urea, Reservoir Potential, Viability, Natural Gas, Dorado Reservoir

INTRODUCTION

Exploration history

The history of oil/ gas exploration in Sri Lanka runs back in time to the 1960s. Since then, several attempts have been made to discover reservoir rocks in the sedimentary basins identified by exploration work. During 1972-1975 the first three exploration wells,Pesalai-1, Pesalai-2, and Pesalai-3,were drilled in the Cauvery Basin of Sri Lanka. Later, Palk Bay-1 and Delft- in 1976 and Pedro-1 and Pearl -1 in 1981 were drilled but there have not been any significant hydrocarbon discoveries except a small discovery in Pesalai-1. Seismic surveys have been carried out to acquire vital data in 2001, 2005, 2009, and 2012. Most recently starting from 2011 four new wells Dorado, Dorado-north, Barracuda and Wallago have been drilled and natural gas discovered from Dorado and Barracuda wells (Figure 1) (Ratnayake *et al*., 2017; Gamage *et al*., 2018).

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The Petroleum Resources Development Secretariat (PRDS) was established in 2003 with the vision of ensuring all Sri Lankans benefit from the petroleum resources of the country by managing the industry in an equitable, safe and environmentally sustainable manner. The mandate of the Secretariat includes discharging of some functions which are to be assigned from time to time by the Cabinet of Ministers. The Secretariat also acts for and on behalf of the State for all purposes related to Petroleum Resources Agreements entered into, with the State.

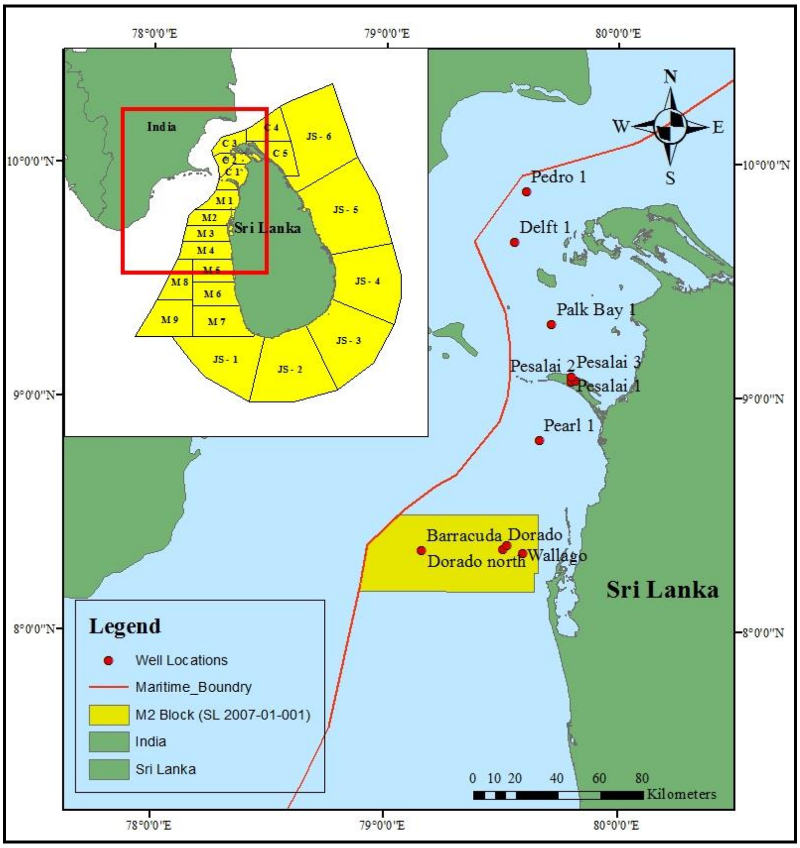

Figure 1. Mannar Basin and the wells drilled in the block SL 2007-01-001 (Block M2)

The Cauvery Basin, Mannar Basin and Lanka Basin are the main prospective offshore sedimentary basins recognized around Sri Lanka. The Mannar basin covers an area of approximately 42,000km^2 with a possible sediment accumulation ofup to 10km in the deep water areas. The very first hydrocarbon discovery in the Mannar basin was made in 2011 in the block SL2001-01-001 popularly known as the block M2. The M2 block covers an area of approximately 2912 km^2. Following the bidding round carried out in 2008, in which several investing companies participated, the block was awarded to Cairn Lanka (Pvt) Ltd. After acquiring, processing and interpreting new geotechnical data, Cairn Lanka (Pvt) Ltdproceeded to drill four wells in the block. Two of those wells showed a significant net gas pay thickness of hydrocarbons and these two reservoir discoveries were named as Dorado and Barracuda (Figure 1) (Ratnayake *et al.*, 2017). Dorado reservoir exhibits high quality, with a clean, thick deposition and straightforward for development. The main objective was set as the Dorado reservoir due to the above reason.

Urea

Sri Lanka is a plantation economy famous for its production and exportation of agricultural crops and a significant number of farmers' livelihoods still depend on agriculture itself. Fertilizers being a crucial factor for agriculture, nitrogenous fertilizers have become the most preferred category among farmers.

With high solubility and high nitrogen content, urea is leading the nitrogenous fertilizer industry. Urea is popularly known as Carbamide in the chemical industry with the molecular formula of NH_2CONH_2. As a country rich with farmers who still earn their living through agriculture, yet categorized as a developing island nation, Sri Lanka is highly in need of urea to establish its economical sustainability.

Sri Lanka completely meets its current urea market demand by importations. In fact, a hundred percent of the urea usage in Sri Lanka is imported from countries such as India, United States, Brazil, Thailand, and Australia. Considering the process of industrial urea production, the following steps can be identified as the major steps. Ammonia and carbon dioxide are initially reacted to form ammonium carbamate and then dehydrated to urea. With this our attention is drawn towards the production of ammonia. Ammonia production process incorporates two main stages.

1. Manufacture of H_2 (Steam Reforming)
2. Synthesis of Ammonia (Haber Process)

A natural gas feedstock needs to be subjected to the process of steam reforming in order to deliver hydrogen. Then hydrogen is combined with atmospheric nitrogen to produce ammonia via the process of Haber-Bosch.

These natural gases are sedimented inside the pores of sedimentary rocks and are trapped under the trap rocks. Natural gas and oil are generated from source rocks only after heating and compacting. The identification of these sedimentary rocks is crucial in the process of oil/gas exploration. Geophysical techniques such as seismic, gravity, magnetic, and electrical surveys are used in prospecting for natural gas resources (Silva *et al.*, 2018).

According to above details, it can be identified that a constant hydrocarbon generation is essential to discover a solution for the national dependence on complete importation of urea. At the same time, the fact that Sri Lanka has discovered a rich hydrocarbon net gas pay thickness has fostered anopportunity. Therefore it is high time to give some serious attention to the matter with a wide focus.

The main objectives of the research study are to identify the feasibility of producing urea using natural gas in the Dorado Reservoir and to introduce a viable solution forcompletely importing urea using indigenous gas in place. Determining numerous commercial options of using the reservoir potential of Dorado Reservoir in Mannar Basin in support of producing urea locally, carrying out a cost-benefit analysis on establishing a urea production plant and the process of producing urea in Sri Lanka and to grab international attention towards the potential of hydrocarbons in Sri Lanka were few other objectives of carrying out the research.

METHODOLOGY

Reservoir Potential and Production Profile

The maximum economical gas plateau rate was anticipated from the production profile of the Dorado reservoir. The most likely economical production profile has been previously anticipated by PRDS for a possible power off-take of close to 630MW (50% PF).Using the same production profile and fiscal regime for this research study was advised by the PRDS. The production profile of a reservoir involves the daily gas rates anticipated throughout the expected economic life time. After reviewing the Reservoir Potential, the value was then used to further analyze the production profile. The daily rate is depreciated over a depleting rate according to the reservoir characteristics and the Reservoir Potential.

The PRDS has come up with the daily rates according to which the Dorado reservoir is expected to be developed over its economic life time. The data regarding the supply rates or the expected developing rates were acquired from PRDS and analyzed with graphs to identify the economically viable indigenous gas solution for urea production.

The maximum economical gas plateau rate was obtained while identifying the economic limit. The variation of the expected daily production gas rate was used to identify the gap between the expected natural gas supply and the daily production of the Dorado reservoir.

Statistical data

The data obtained from the Sri Lanka Customs regarding urea importation was used to forecast demand for the year in which the plant is expected to initiate its operations. Extrapolation techniques were followed in this forecasting and the software “Minitab” used to arrive at more accurate figures. The daily gas rate required to fulfill the forecast future demand was calculated using a rule of thumb delivered by Ferrostaal Topsoe GmbH.

The capital and operational costs of establishing a urea production plant was estimated with the involvement of the German organization; Ferrostaal Topsoe GmbH. Using the cost factors and urea production quantities, a descriptive cost benefit analysis was carried out in the form of a Fiscal Model for the urea plant to arrive at the most economical quantity and price.

Applying the Fiscal Regime for Dorado

Two main options were primarily assumed when testing different values on the model. These options were based on the anticipated daily natural gas rate with the assumptions of developing the Dorado reservoir primarily for the sole purpose of urea production at 20MMScf/d or as an integrated project at 70MMScf/d with other possible uses. Under each option, two different case scenarios were considered assuming minimum and substantial benefits to the host government based on the various biddable fiscal terms of the 2013 MPRA (Figure 2).

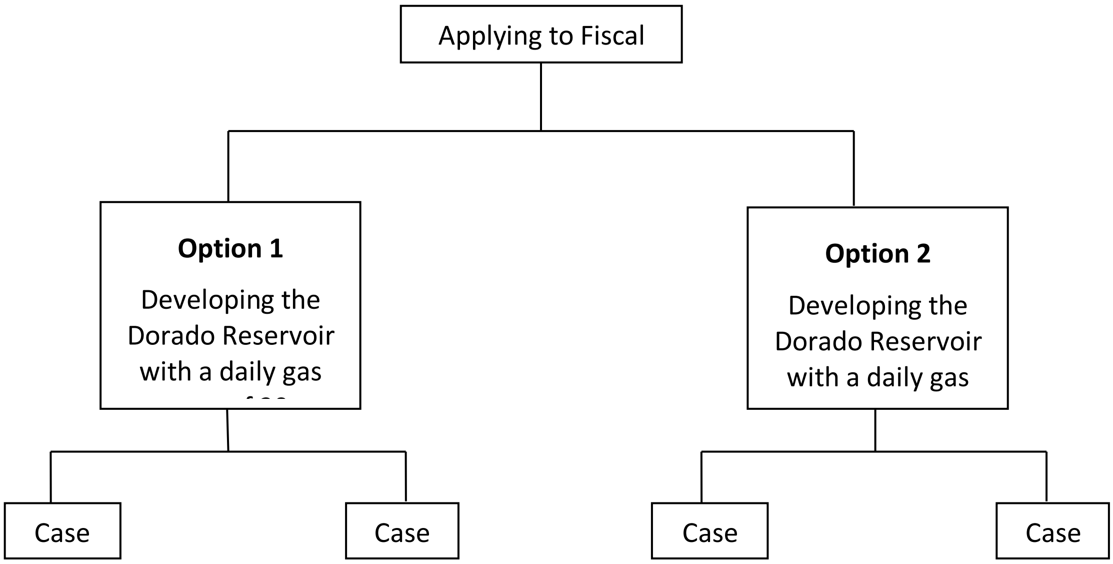

Figure 2. Diagram showing the basis of assumptions made

The Fiscal Regime for the Dorado reservoir is based on several mandatory fiscal terms.

1. Signature Bonus
2. Production Bonus
3. Royalty
4. Cost Recovery
5. Profit Share
6. Tax
7. State Participation interest through an NOC – 15% of the contractor participating interest
8. Other contributions including Local Content Development Provisions

Different case scenarios were proposed based on a suitable commercial approach to launch urea production using Natural Gas resources of Sri Lanka. These were identified based on the output results obtained from the Fiscal Regime for Dorado reservoir.

RESULTS AND DISCUSSION

Results

The production curve for the Dorado Reservoir was further analyzed with the data obtained from PRDS which has been developed anticipating optimum economic benefits (Figure 3). With an identified Reservoir Potential of 334 BCF, the highest gas plateau rate was determined as 67.12 MMScf/d (close to 70 MMScf/d), as possible for a contract rate of sale gas to obtain the most economical field development scenario for the Dorado field considering the fiscal terms mentioned in Appendix (IV) with worst possible assumptions to the host government at a gas price varying from 8 – 12.5 $/MMbtu. This economic gas rate close to 70 MMScf/d proceeds for a span of 8 years and depletes until the economic limit.

Considering depletion of the gas production over the years, the need for an additional natural gas source was identified. If not for an additional source, the excess supply rate will have to be depreciated over the time period. It was identified that the addition has to be incremental starting from the year 2030. The anticipated supply rate to the Urea plant which was calculated based on the Urea plant statistics, was also displayed in the same graph for the convenience of the user to identify the production and supply gap. (Figure 3)

The quantities and prices of urea imported over the years of 2000 - 2017 were obtained from the Sri Lanka Customs. Using trend analysis, the data were extrapolated by the software "Minitab" to arrive at the forecast quantities for the years from 2023 – 2050 considering the estimated economic limit of the Dorado reservoir and future Barracuda/other gas development prospects (Figure 4). The above years were considered because the research focuses on a project over 27 years, to initiate construction by 2023 with a construction period of 2 years. The life span of the urea plant was decided to be 25 years. The following equation was obtained with respect to the trend line by analyzing data with the use of MINITABsoftware.

$$y = 312977 + 1892 \times t$$

The trend line is given by the line with red color dots in the Figure 3 and can therefore be extended further while maintaining the same gradient to obtain the future demand quantities. This method of obtaining forecast values for a given data set is called extrapolation.

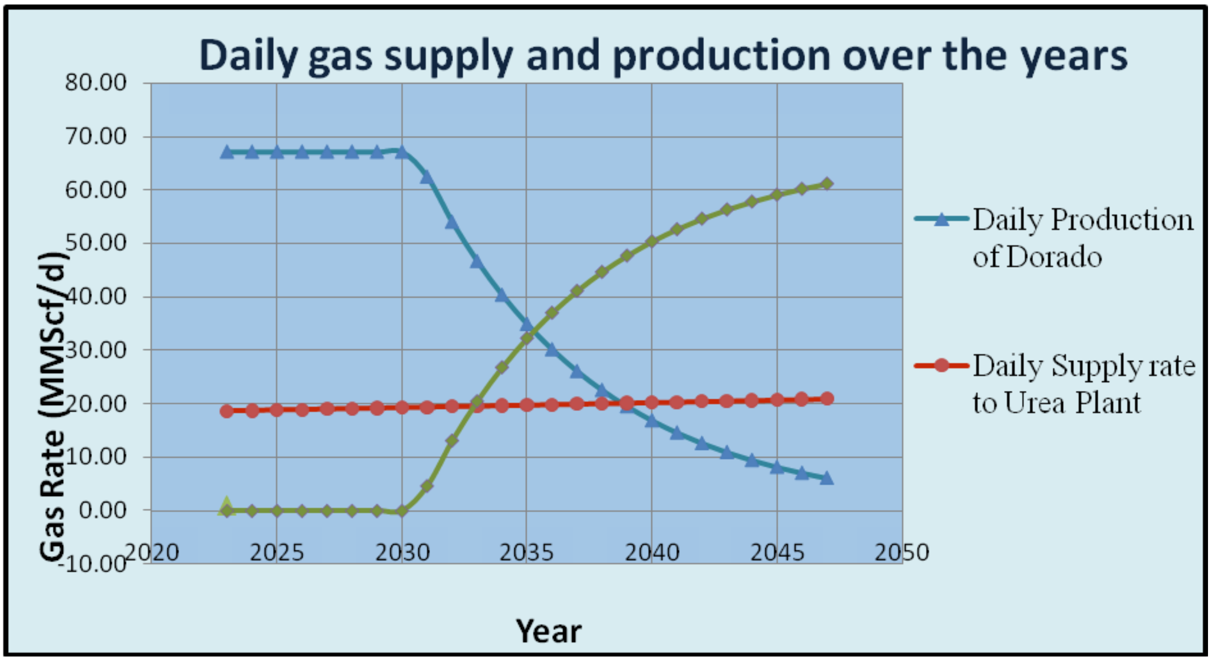

Figure 3. The graph showing the production profile and daily gas supply rate for Dorado reservoir along with the assumed integration of Barracuda reservoir/ other NG source

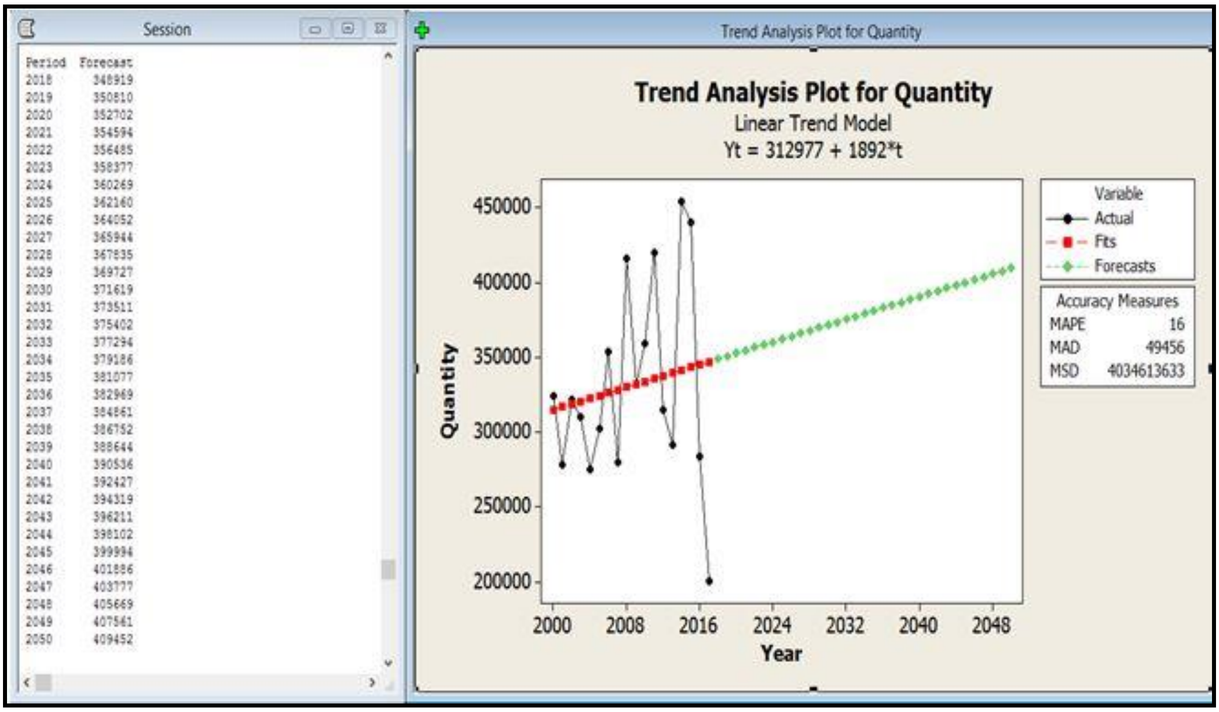

Figure 4: Forecast demand quantities

The quantity of gas needed to meet the forecast demand was then calculated with the information obtained from FerrostaalTopsoe GmbH. A descriptive fiscal model for the ureaplant was prepared with the use of cost factors obtained from the German company and the demand identified to arrive at the optimum quantity and gas price. The optimum quantity was determined to be 18.8 MMScf/d and the optimum price to be 10$/MMbtu.

These values were tested with the Fiscal Regime of the PRDS based on 2013 Model Petroleum Resources Agreement(MPRA)

The gas supply needed for the respective years was determined using the data obtained from FerrostaalTopsoe GmbH. It is also assumed that there could be a possibility to integrate the Barracuda discovery or any other imported gas/in-house gas prospectsby 2030 maintaining daily gas requirementto operate this urea production plant for 25 years. The assumed incremental proportion that is to be integrated with the Dorado reservoir is also shown in the Figure 2.

Discussion

Considering the results identified above, the following cases are discussed.

Case 1: Investment considering development of gas fields and establishment of a urea plant as an integrated project by a third party investor

Development of the Dorado reservoir for the sole production of urea with a daily natural gas rate close to 20 MMScf/d was considered, as it is the identified daily gas rate required to meet the forecast demand. The plant life was considered to be 25 years in carrying out the calculations. A NPV close to $200 million and an IRR of 20% (at a discount rate of 10%) was obtained from the Fiscal Model prepared for the urea plant for in-house use. Although this scenario is economical for the urea plant, this is not economically viable with regards to the Dorado reservoir. This is due to the resulting negative NPV to the fiscal dynamics of the Dorado for a maximum supply close 20MMScf/d.

Therefore the following optional cases were proposed to utilize the excess of economically viable daily rate close to 70 MMScf/d of gas produced from this reservoir together with urea production.

Case 2: Investment considering development of gas fields and establishment of a urea plant supplying excess gas to existing power plants readily convertible by 2025 as an integrated project.

Establishment of a urea plant by an investing company to produce the forecast demand while supplying the excess Natural Gas quantity close to 50 MMScf/d to an existing readily convertible power plant located at Kerawalapitiya in the Western Province for a period of 25 years or more. Additionally to the costs of the Urea Plant, it is proposed that the cost to transport the excess Natural gas to the power plant via a subsea/onshore will be borne by the investing company or government. Depending on the option, the additional costs will be added to the gas price and gas will be made available at the delivery point to CEB according to an agreed formula indexed to oil or gas as mutually agreed by both parties.

Case 3: Investment considering development of gas fields and establishment of a urea plant supplying the excess to the government for other possible applications

Development of the Dorado reservoir by the investing company with a daily gas rate close to 70 MMScf/d is considered where around 20 MMScf/d of it will be utilized to manufacture urea for in-house usage. The excess natural gas production will be sold to the government. According to the calculations carried out, the Sri Lankan government is currently spending around 16 $/MMbtu for natural gas when importing urea. With this case scenario, government can buy NG at a lower rate, around 10 $/MMbtu and utilize the excess as an energy source or a feedstock in all the other possible sectors: power, transport, industry, household and commerce.

CONCLUSIONS

Sri Lanka is able to meet the forecast local urea demand by utilizing a daily natural gas production rate close to 20MMScf/d discovered in the Dorado Reservoir. But the most economical daily gas rate for the Dorado Reservoir is close to 70MMScf/d. The excess quantity can either be supplied to existing power plants or sold directly to the government.

It is economical to the Sri Lankan government to buy NG as currently they are spending around 16 $/MMbtu of Natural Gas when importing. But under this scenario NG can be bought at a rate around 10$/MMbtu without transportation cost. However, the scenario is highly dependent on the agreement of government and their rules and regulations.

Supplying the excess quantity to a power plant is preferred as the forecast urea demand of Sri Lanka can be undoubtedly achieved while also supplying a 500MW power plant. Three readily convertible CGGT power plants exist in Kerawalapitiya and Kalanitissa. Depending on the option of transporting NG to the power plant, additional costs will be added to the gas price according to an agreed formula indexed to oil or gas on mutually agreed terms.

The project can only proceed for around 17 years if executes solely with the Dorado Reservoir. This is due to the reservoir depleting beyond 2030, resulting in an economical cut off and an investor cut-off. Therefore the addition of an incremental amount to the production is essential. Other means of natural gas are considered to be integrated so that the same rate is maintained throughout the project life span. Integration of the Barracuda reservoir is preferred in order to maintain a constant supply rate. But this depends greatly on the success of the extensive studies which are needed to be carried out. Additionally, the world trend of petroleum is moving towards natural gas,and even Sri Lanka is currently considering importing LNG. Therefore in another 17 years' time, options will be available to afford the necessary gas integration.

The commercialization of urea production confronts a number of challenges, by overcoming which the project can be optimized. Flexibility of Fiscal Regime policies are expected by the contractors, which will attract more investors towards the project. Extensive studies can be carried out by varying the modes and methods of transporting NG to the relevant plants.

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'E-Nose'- Design and testing of an electronic device for aroma detection

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ABSTRACT

In the recent past aroma detection has become a significant component in industrial instrumentation and automation field. Electronic noses are developed using a gas sensor array to detect the aroma compounds. These devices are working with the help of pattern recognition software and algorithms. This study describes the design and development of the portable electronic nose device for the detection of the aroma compounds, experimental testing and a mathematical model for the identification of the chemical compounds. The chemical compounds tested are ethanol, acetone and water. The response of sensors raw values were recorded, baseline corrected and averaged. The principal component analysis for these sensor responses are 99.95% of information given with two principal components in the dimensionality reduction. Furthermore, this E-Nose can detect and discriminate among the given substances with 100% accuracy using the 3Nearest Neighbors classification technique.

Key words— aroma detection system; electronic nose; e-nose; gas sensors; MOS sensors.

INTRODUCTION

Electronic Nose (E-Nose) is an artificial olfaction system which can detect different aroma compounds. Electronic noses are used in different types of application such as agriculture and food quality control (Ghasemi-Varnamkhasti, Mohtasebi, Siadat, & Balasubramanian, 2009;Wilson, 2013; Zhou & Wang, 2011;Bhattacharyya *et al.*, 2008; Tozlu & Okumuş, 2018), biomedical applications (Wilson & Baietto, 2011), industrial security purpose (López, Triviño, Calderón, Arcentales, & Guamán, 2017) and environment quality (Bourgeois, Burgess, & Stuetz, 2001; Bourgeois, Romain, Nicolas, & Stuetz, 2003; Capelli, Sironi, & Del Rosso, 2014). E-nose systems consist of sensors which response to different classes of chemical compounds present in a given aroma sample. Accordingly there are sensors which can detect levels of alcohol, hydrocarbons, carbon monoxide, ammonia, hydrogen sulfide, natural gas, etc. (hek, (n.d)). These gas sensors could be either optical (absorption, fluorescence), thermal (pellistor), electrochemical (chemiresistive, potentiometric, amperometric) or gravimetric (James, Scott, Ali, & O'Hare, 2005). The selection of gas sensors for a particular application depends on the aroma profile (Ghasemi-Varnamkhasti et al., 2009; Schaller, Bosset, & Escher, 1999; Wilson & Baietto, 2011). When developing e-nose systems the design of sensors chamber, flow rates, sensor response are important (Schaller et al., 1999). The sensor chamber often consists of a series of gas sensors and the response is recorded as varation of resistance or conductance in aroma sample (Haddi *et al.*, 2011; Sharma, Ghosh, & Bhattacharya, 2013). The system parameters show variations in terms of

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sensor warm up time, purging time and flow rate, sampling time number data recording cycles (sniffing cyles) *(Haddi et al*., 2011; He *et al.*, 2012; Sharma *et al*., 2013; Tian, Cai, & Zhang, 2012). The commonly used statistical methods for e-nose data analysis are principal component analysis (PCA), variance analysis (ANOVA) and clustering methods (Scott, James, & Ali, 2006). In addition artificial intelligence methods are also used for the data analysis (Scott *et al.*, 2006). The e-nose systems currently in market are custom designed (Electronic Nose, (n.d.); Portable elctronic nose, (n.d.)), often preprogrammed to detect a limited number of volatile organic compounds, and offer no flexibility to upgrade through custom programming.

The main objective of this study is to develop a low cost “e-Nose” system and test it in a controlled environment. The unique design of the e-nose system utilizes four metal oxide sensors (MOS) in the sensor chamber and records aroma level as the sensor raw values. In this project alcohol, acetone, and water have been used in order to validate and evaluate the discrimination capacity of the sensor arrays. This device is developed to be used in measuring aroma levels in food related industries where aroma levels can be recorded and compared as a quality controlling device.

METHODS AND MATERIALS

E-Nose Design

The E-Nose system developed here contains three main parts, (i) Data acquisition system hardware, (ii) Gas sensor chamber, and (iii)Vacuum pumps. A schematic diagram of the developed E-Nose system is shown in Figure 1 and the e-nose system constructed is given in Figure 2. Data acquisition system was developed with ARDUINO Mega. Arduino and related hardware are used to design the data acquisition system to record the sensor data when testing a sample. Acquired data from sensors were saved in an SD card. Inlet 1 and Inlet 2 are used to insert the reference air and aroma of sample to the sensor chamber alternatively. The sensor chamber contained four MOS sensor array placed in a closed air tight box. Vacuum pump (12V) was used to draw the reference air and sample air to be analyzed at the inlet and another pump (12V) at the outlet for sensor chamber cleaning. Environment air was used as the reference air in this study and to clean the sensor chamber between two sample measurements.

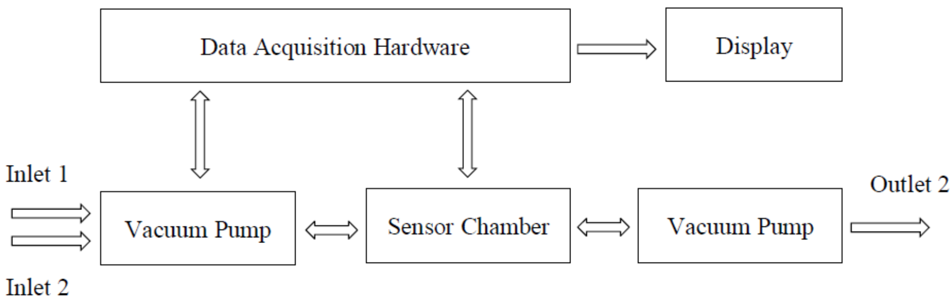

Figure 1: Schematic Diagram of Electronic Nose System

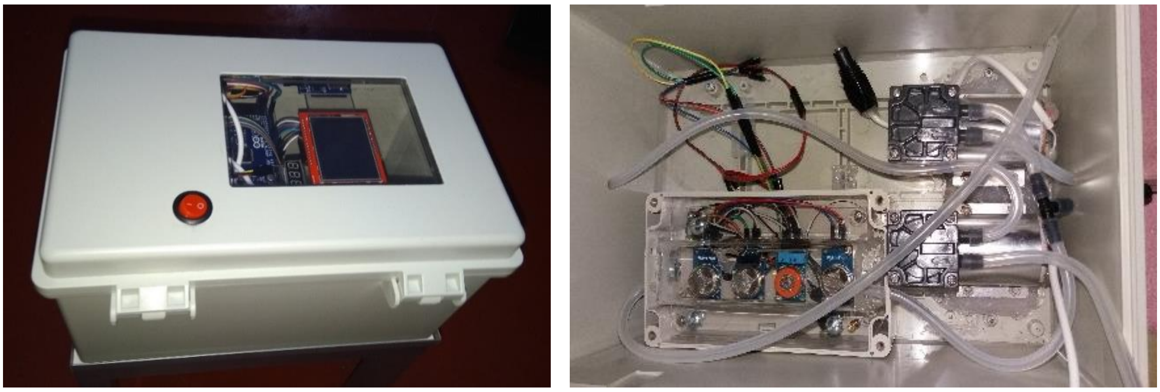

Figure 2. (a) E-nose system developed in this study (b) the sensor chamber

One sniffing cycle of sample contains the following events: sensor cleaning, sniffing process, odor lock, and sensor cleaning. A sample sniffing cycle of E-Nose system is shown in **Figure 3**. At the end of each sniffing cycle, one minute cleaning time is given for the clearing of any residual chemical in the sensor chamber. The next cycle begins soon after the cleaning and the instrument continue to collect data until the process is terminated by the user.

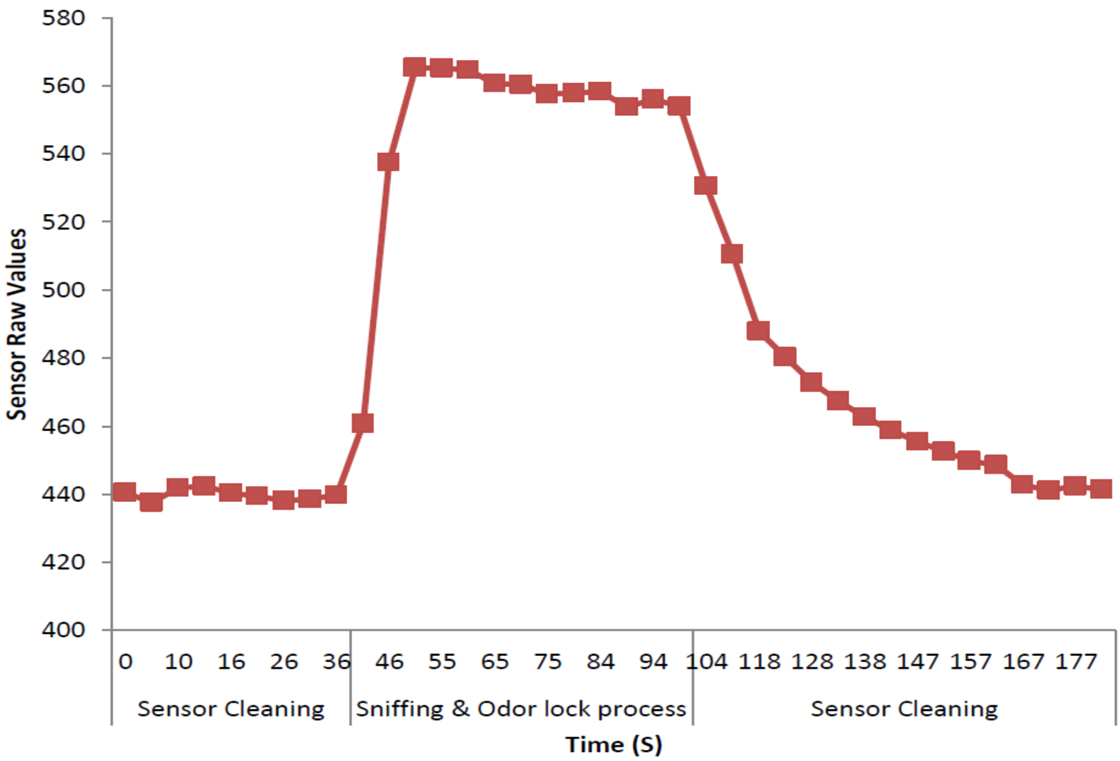

Figure 3. Samplesingle sniffing cycle of E-nose system

The sensor chamber was built using a sensor array encapsulated in an air tight water proof case with dimensions 3.5 cm x 14 cm x 3 cm. MOS gas sensors (MQx (x=2, 3, 4, 5)) were arranged in a linear direction to develop the sensor array in this study.The sensitivity of MOS gas sensors is given in the **Table 1** (HANWEI ELETRONICS CO., 2015; “MQ-2 Semiconductor Sensor for Combustible Gas,” 2016; “Mq-4,” n.d.; “MQ-5 Gas Sensor Technical Data,” n.d.). The sensor chamber and vacuum pumps were connected using transparent tubes.

Table 1: Sensors used in sensor chamber

Sensors	Sensitivity to chemicals
MQ 2	Hydrogen, LPG, Methane, CO, Alcohol, Propane
MQ 3	Alcohol, Benzene, Hexane, LPG, CO, Methane
MQ 4	LPG, CH4, Hydrogen, CO, Alcohol, Smoke
MQ 5	LPG, Hydrogen, Methane, Alcohol, CO

Experimental Set-up

Alcohol, Acetone and Water were used to validate the E-Nose system in this study as pure substances. Small glass bottles (40 mL) were used for the alcohol (9 mL, reagent grade), acetone (9 mL, reagent grade) and water at room temperature. The sensor responses were recorded for three samples of each substance. The time of one sniffing cycle was limited to 3 minutes (1 minute for cleaning, 1 minute for sniffing and odor lock process and I minute for cleaning). The data collection was done for each sample for period of three successive sniffing cycles. Environment air was used to clean the sensor chamber and sample air inlet was closed while sensor chamber was cleaning. A continuous gas flow was maintained in the sensor chamber except during odor lock process. Then same experimental procedure was done for the mixture of those chemicals to evaluate the sensor array. Data obtained from the sensor array were stored in the micro Secure Digital (SD) card to conduct the data analysis.

Discrimination Model

Data obtained from the experiment were preprocessed initially in order to produce the optimal data model. Baseline of sensor response signal and peak alignment correction were done during the preprocessing step (López et al., 2017). In the baseline correction process, sensor response of environment air condition was subtracted from the sensor response of sample. An assumption was made as all experiments started at same time when correcting the peak alignment. In order to avoid the misalignment, all the sensor response of each test was linked together (4 sensors x 50 time points = 200 experimental data points). Finally, 33 experiments were used to build the discrimination model.

After the data preprocessing step, Principal Component Analysis (PCA) (Bartholomew, 2010; Lazaro, Ballado, Bautista, So, & Villegas, 2018; Liu et al., n.d.) was done to build the model to discriminate among the different classes. In the first step, preprocessed data were high (33 experiments X 200 data points). Then these preprocessed data were reduced to 33 experiments X number of principal components. After the dimensionality reduction process, the 3Nearest Neighbors (k-NN, k=3) (Cunningham & Delany, 2007; Moise et al., n.d.) algorithm was used for the classification process. The cross validation technique (Iii, 2009; Jung & Hu, 2015) was used to obtain the classification rate of the model.

RESULTS AND DISCUSSION

Figure 4, Figure 5 and Figure 6 show that the raw signal response values of the sensor array when the E-Nose was exposed to ethanol, acetone, and water, respectively. According to these figures, during the first 36 seconds, the sensor chamber was exposed to the environment air. Then the sensor response was changed when sample air was sniffed to the sensor chamber. This sniffing and odor lock process was done for 50 seconds. An elevated sensor raw value is obtained for each sensor MQx during odor lock period, which ultimately decreased during 70 seconds of cleaning process

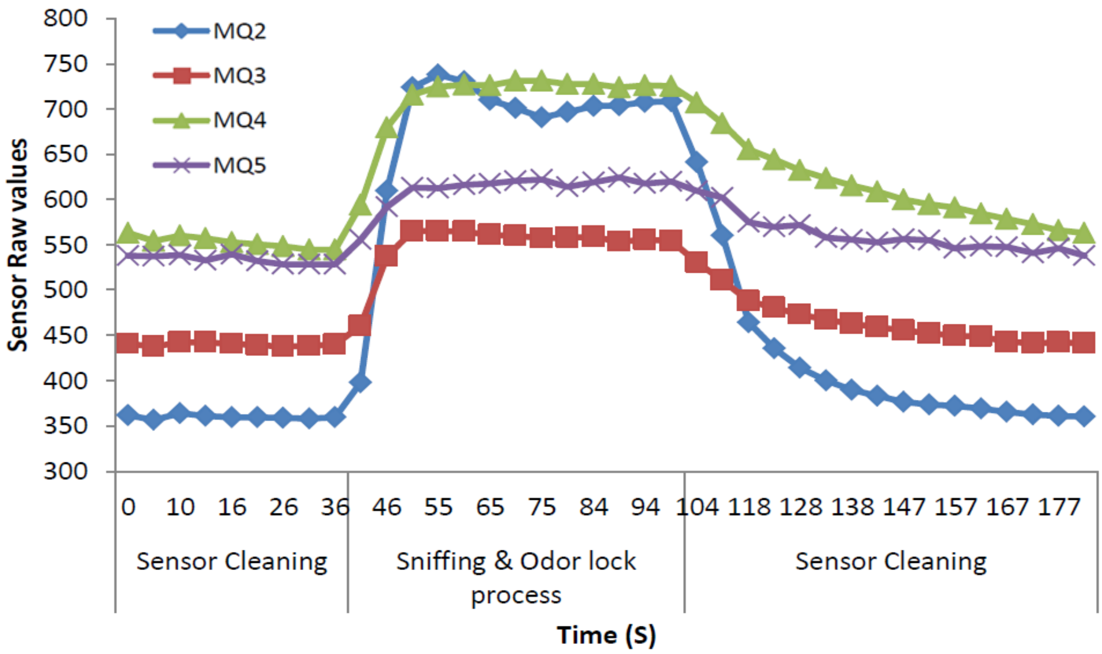

Figure 4. Response values of sensor array when exposed to ethanol

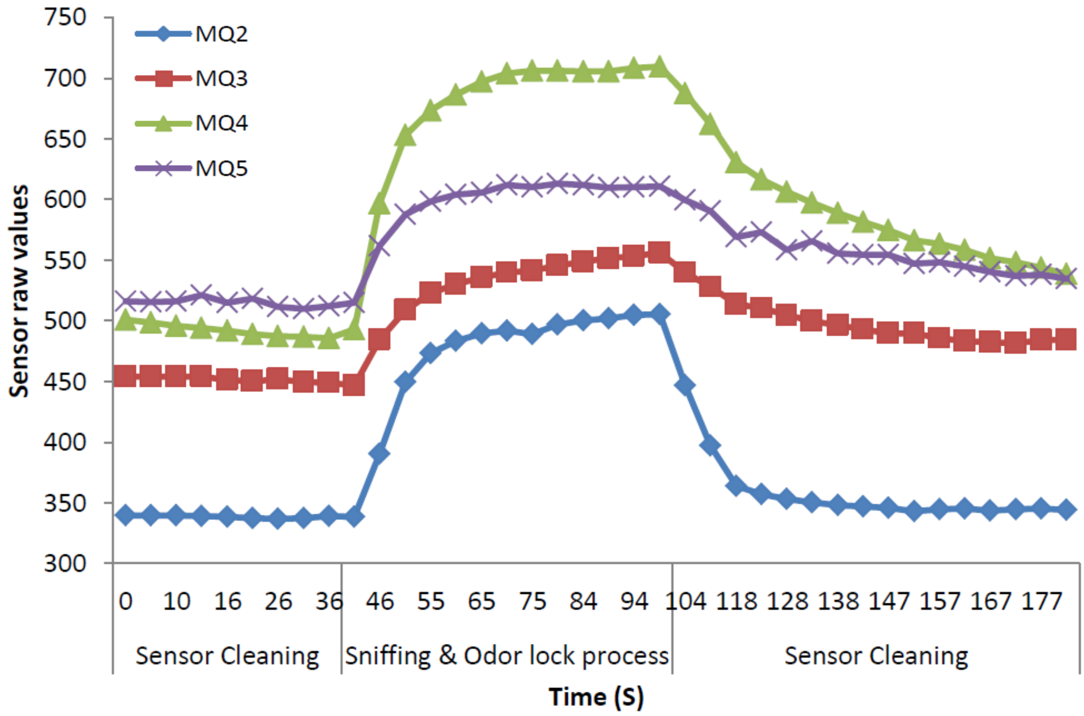

Figure 5: Response values of sensor array when exposed to acetone

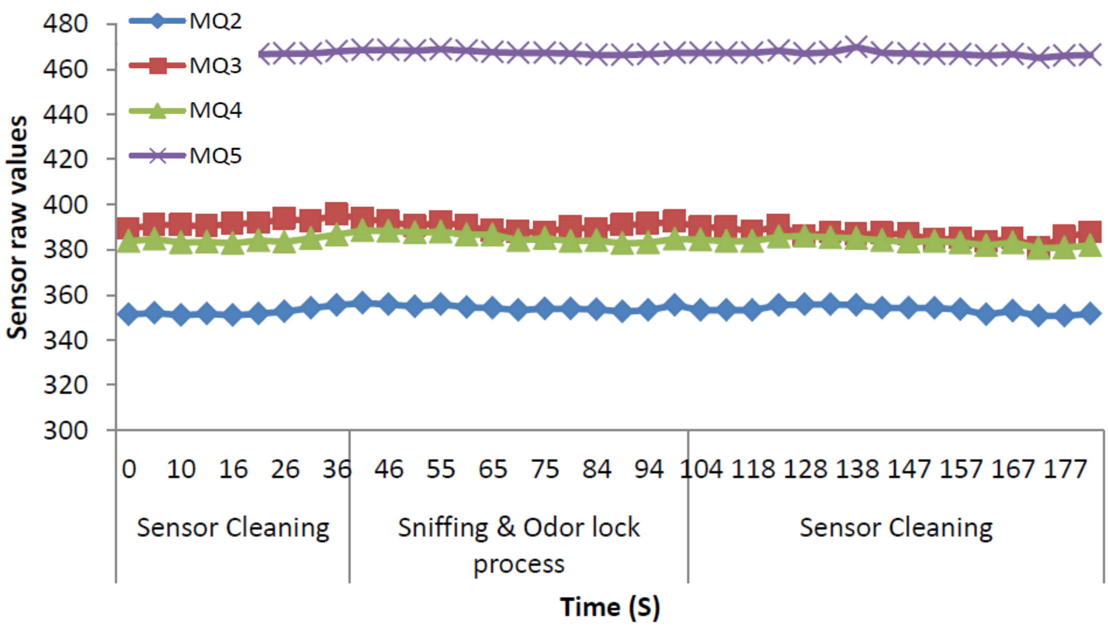

Figure 6. Response values of sensor array when exposed to water

However, the sensor raw values for baseline corresponding to the time period prior to the odor lock and after the odor lock are different for each sensor. Therefore, baseline correction is necessary to compare sensor raw values obtained for each MQx sensor. Figure 7 and Figure 8 show that the baseline corrected sensor raw signal response values when exposed to ethanol and acetone.

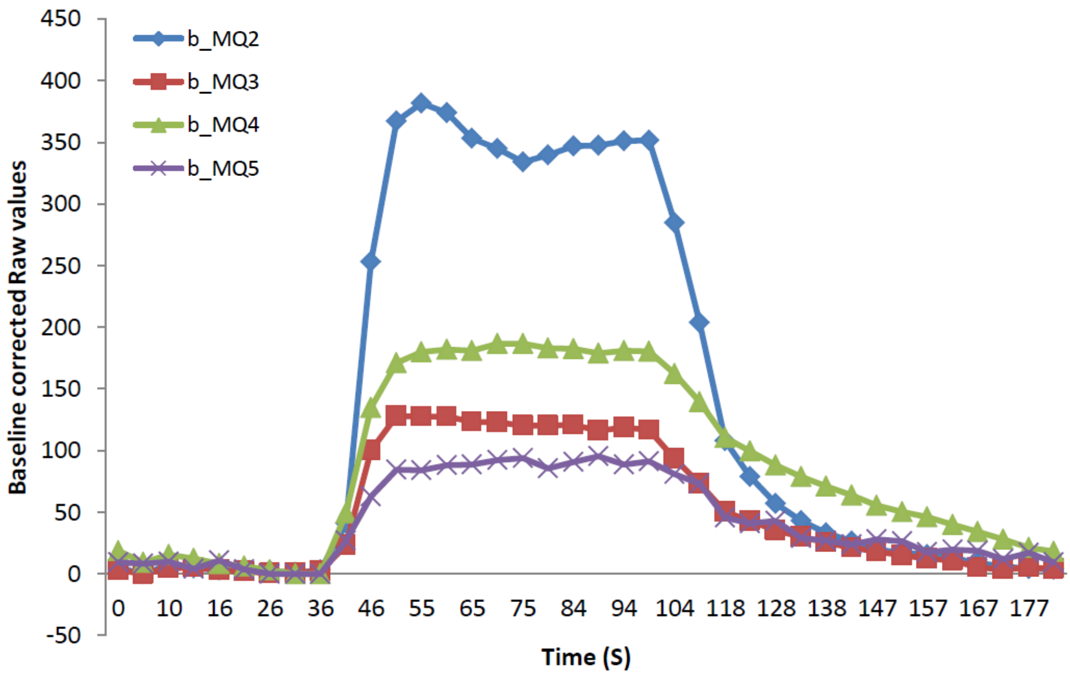

Figure 7. Base line correctedsensor response values when exposed to ethanol

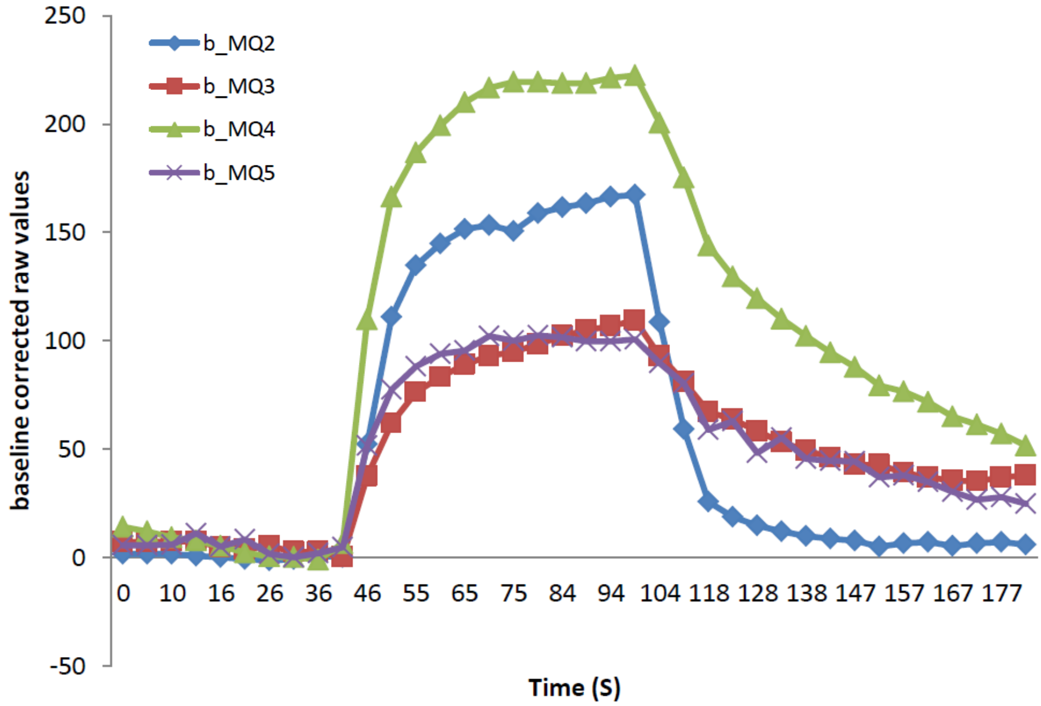

Figure 8. Base line correctedsensor response values when exposed to Acetone

According to the Figure 7, MQ2 sensor is most sensitive to the ethanol and MQ5 is least sensitive to the ethanol. It can be seen in Figure 8 that MQ4 and MQ2 are more sensitive to the acetone than others. Then peak alignment was done to the base line corrected odor locked sensor response signal values.

After the preprocessing step, three experiments of each substance are shown in Figure 9.Intensity of water is nearly zero while acetone and ethanol give high response to the sensor array. The intensity of ethanol is higher than acetone and water. MQ2 and MQ5 have nearly same response to the ethanol and acetone. MQ3 has some sensitivity compared to other sensors when the sensor array is exposed to water. Sensitivity of sensors MQ3 for ethanol is higher than acetone and water as expected according to Table 1 above.

After the preprocessing step, dimensionality reduction was done using principal component analysis. There may be variance loss, when converting the dimensional space to two dimensional space during PCA process. Therefore, variance ratio explained should be identified to find how much variance can be attributed to each of the principal components when performing dimensionality reduction. In this PCA model, first principal component contains 93.67% of the variance and the second principal component contains 6.28% of the variance. Together two components contain 99.95% of the information. Therefore, the raw matrix is reduced to 2 principal components.Eleven samples of each class are projected in the PCA model. Dimensionality reduced PCA model results are shown in Figure 10. It can be seen that acetone, water, and ethanol are completely separated when projecting the PCA model (blue- acetone, red- ethanol, yellow- water) in Figure 10. It is because of the variation in the sensor responses in the presence of different organic compounds. It can be stated that E-Nose system can discriminate among the different substances. Therefore the preprocessing step is important for the model evaluation.

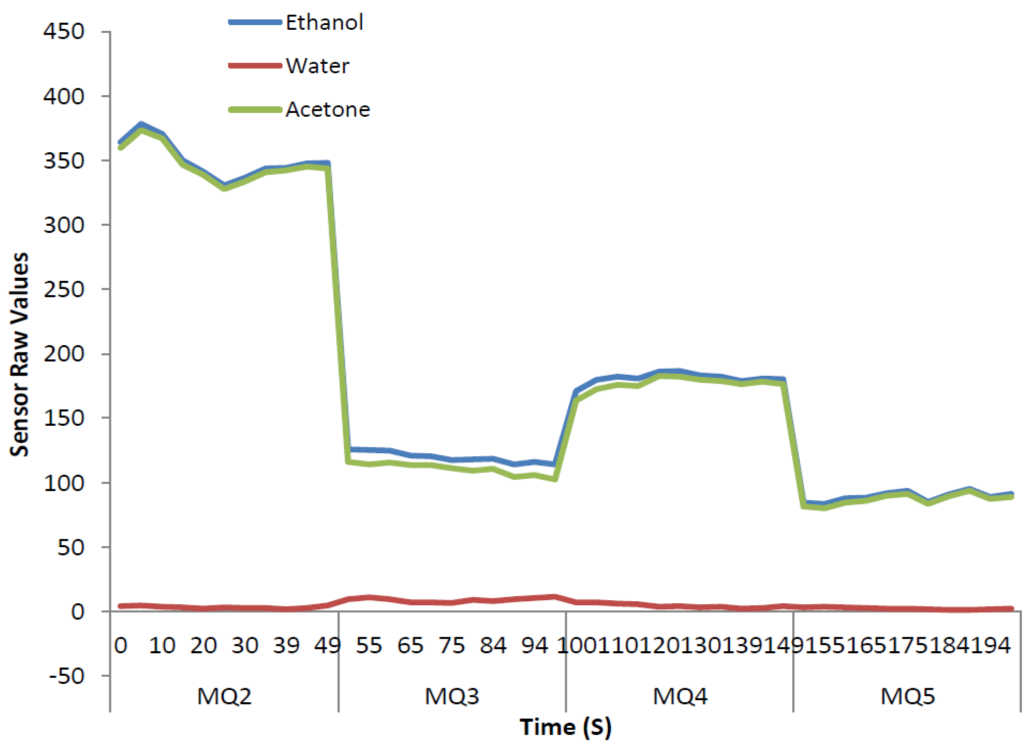

Figure 9. preprocessed sensor array values of ethanol, acetone, and water

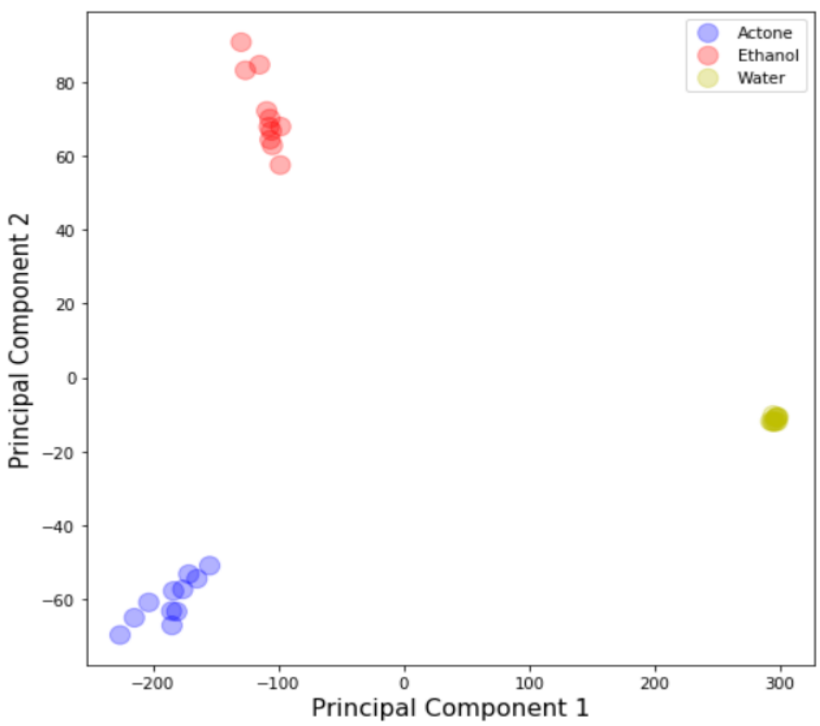

Figure 10. Two dimensional representation of the classification problem

A k-fold cross-validation method was used to assess the performance of classification in a practical way. Classification results were estimated using 10-fold cross validation technique and performed using k-NN (k=3) classification process. Classification rate was obtained as 100% with k=3. Confusion matrix of this classification process is given in Table 2.

Table 2: Confusion matrix obtained from 3-NN classification process

Confusion Matrix		**Predicted class**			**Total**
		Acetone	Ethanol	Water	
Real Class	Acetone	2	0	0	2
	Ethanol	0	4	0	4
	Water	0	0	3	3
Total		2	4	3	9

According to the Table 02, it can be said that samples are predicted 100% correctly as real samples. The sensor array was exposed to mixture of those chemicals. The response of sensor array when exposed to mixture of chemicals is represented in Figure 11.

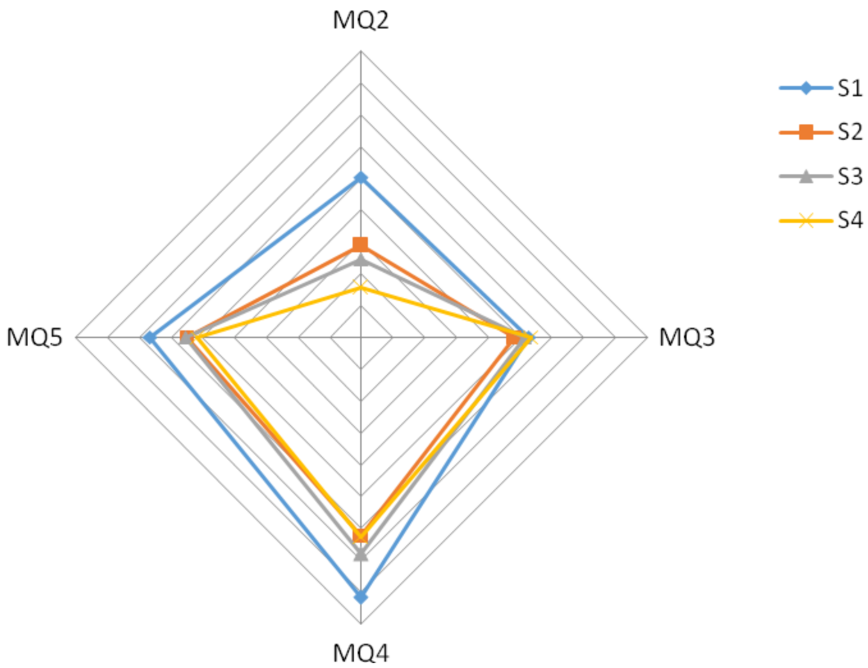

Figure 11. Sensor response when exposed to a mixture of chemicals
(S1: Acetone/water mixture 1:1, S2: Ethanol/water mixture 1:1, S3: Acetone/ethanol mixture 1:1, S4: Acetone/ethanol/water mixture 1:1:1)

When considering the outset of the spider, it can be clearly found out each mixture has a unique response for each of four sensors.

CONCLUSIONS

An effective aroma detection system developed using an array of gas sensors is presented in this paper. Three different organic substances were analyzed using the developed system and 100%

accuracy obtained by a k-nearest neighbor classification process. The 2 component PCA model indicates clear discrimination among three substance with 99.95% information. Validation of the system using more organic solvents and real world products is ongoing at present.

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