Research Article

Determination of Principal Component for Selection of Corrosion Inhibitor using Principal Component Analysis

J. Femila Mercy Rani*[1] and D. Ramya[2]

Department of Mathematics, PSNA College of Engineering & Technology, Dindigul
Department of Mathematics, Kongunadu College of Engineering & Technology, Thottiam,Trichy

Abstract

Principal component analysis (PCA) is a unique technique for data analysis and processing, which is not based on probability model. In this study we demonstrate the application of PCA for selection of a corrosion inhibitor. A mathematical program is prepared in order to select an inhibitor, which is suitable for inhibition of an acid corrosion of mild steel at temperatures ranging from 300–330 K. At first, the necessary conditions for compiling the data were listed and then the data were subjected to the program in order to predict the principal component for selection of the inhibitor.

***Correspondence**
J. Femila Mercy Rani,
Department of Mathematics,
PSNA College of Engineering & Technology

Keywords: Principal Component Analysis, Corrosion, Inhibitor, Scilab

Introduction

It is often difficult to extract information about poorly known processes from experimental data. One of the possible approaches is to reduce the number of degrees of freedom. Principal component analysis (PCA) is a well known technique for reduction of dimension.

Application of PCA includes quasi-harmonic analysis in protein research, molecular dynamics, and to study the metabolomic data using NMR. In this study, the authors proposed to employ principal component analysis combined with a computational analysis to select suitable inhibitor for given real time problems [1-6].

Scilab is an interpreted programming language, which is associated with a rich collection of numerical algorithms. This program allows the user to develop a process in a short time. This programming tool is helpful specifically when it is used for overloaded operations. For example, in the case of corrosion inhibition process, a numerous number of inhibitors are available with different characteristics for different corrosive environments.

In order to select an efficient inhibitor for a specific circumstance, it is necessary to compile the data of the characteristically related inhibitors.

In the present study, we have made an attempt to employ the principal component analysis using the Scilab programming software for selecting a most appropriate inhibitor among the studied 6 inhibitors for different conditions. The results are discussed in the following sections.

Experimental

The knowledge about the several factors affecting the inhibition efficiency of an inhibitor is important for selection of an inhibitor. For example, generally, increase in concentration of the inhibitor increases the temperature, where as the temperature is inversely proportional to the inhibition efficiency. A program is prepared in order to select an inhibitor, which is suitable for inhibition at temperatures ranging from 300-330 K. At first, the necessary conditions for programming or compiling the data were listed as shown in the table (**Table 1**).

In this table, the inhibitors are considered as constants, where as the inhibition efficiency is the variable with respect to the varying temperatures. The program prepared for this study was executed using the Scilab software.

Table 1 Different inhibitors and their performances at different corrosion environments

Experiments/ Variables	Inhibitor	Inhibitor Concentration (ppm)	Acid Concentration (ppm)	Temperature (K)	IE%	Reference
1	2-[(E)-{(1S,2R)-1-Hydroxy-1-phenylpropan-2-ylimino}methyl]phenol	100	1	300	91	[7]
		100	4	300	43	
		100	1	330	32	
2	2,3-dihydroxyflavone	600	1	330	74	[8]
	Brugmansia suaveolens	400	1	300	93	[9]
	Cassia roxburghii	400	1	300	94	[9]
3	Brugmansia suaveolens	400	1	320	78	[9]
4	Cassia roxburghii	400	1	320	80	[9]

Results and Discussion

In this study, 3 inhibitors are taken for determination of primary component for selecting an inhibitor. And their performances at different corrosive environments are given in **Table 1**. From the listed values, a computational program was prepared and executed using Scilab software. The results are shown in **Figure 1**.

From **figure 1a**, it is obvious that experiments 2 and 3 are closer, so that we can choose either of the experimental conditions for inhibition processes. Between experiments 2 and 3, 3 is better since the IE% is higher. Experiments 1 and 4 are different and specific. Experiment 1 has the least IE% where as 4 has the highest among the experiments. Therefore, experiment 4, the inhibitor Cassia roxburghii is the most effective inhibitor at elevated temperature.

From **figure 1b**, it is understood that variables 3 and 4 are closer. It is attributed to the direct relationship between the IE% and temperature. Variables 1 and 4 are almost in 90^o angle, which is attributed to the non-linear relationship between the variables 1 and 4. Angle between variables 2 and 4 is at around 180^o, which means that increasing the acid concentration increases the corrosion rate.

(a)

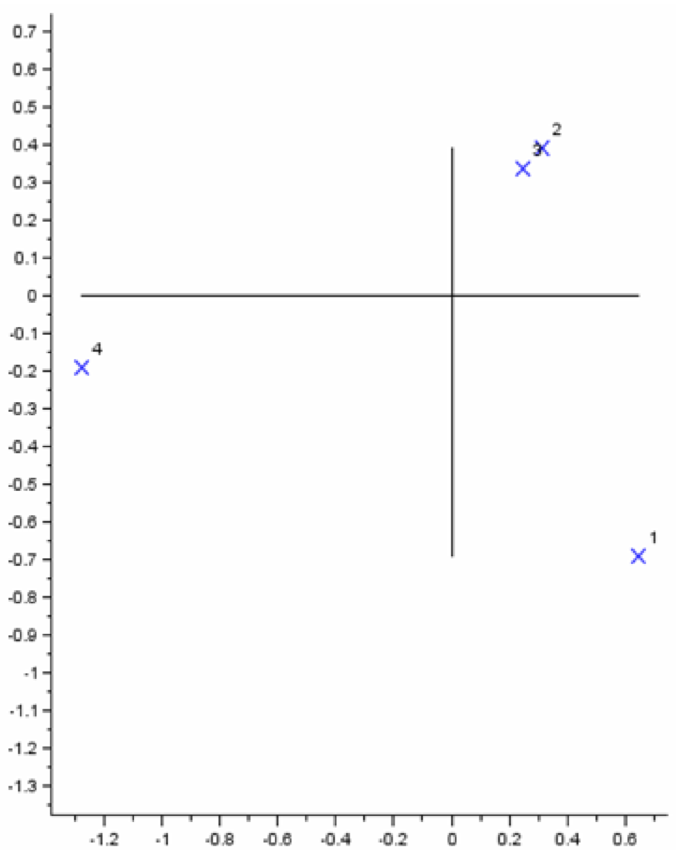

Figure 1a Principal component analysis using Scilab

(b)

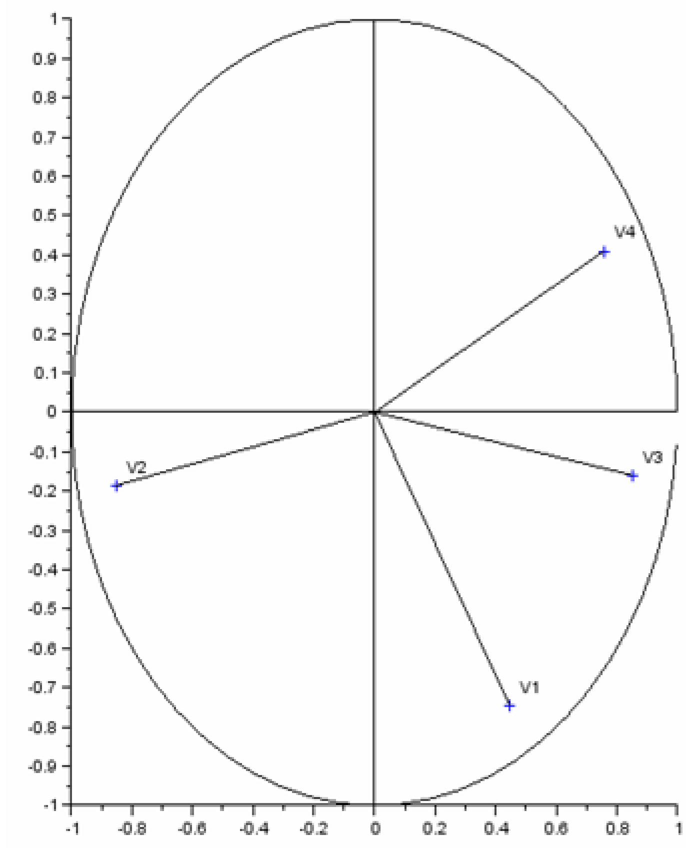

Figure 1b Principal component analysis using Scilab

Conclusion

PCA is a versatile technique for reducing the dimensionality in order to determine the principal component. In the present study, it is proposed that principal component analysis combined with computational analysis could be useful for determining and selecting a suitable inhibitor. Similarly, several inhibitors can be considered and included in the table for creating a data base from which the researchers can choose the efficient inhibitor for selected processes.

References

[1] Jolliffe IT (1986) Principal Component Analysis, New York, SpringerVerlag

[2] S. Vaidyanathan, W.B. Dunn, G.G. Harrigan and D.B. Kell, Metabolomics by numbers: acquiring and understanding global metabolite data, *Trends in Biotechnology* 22 (2004), pp. 245–252.

[3] J.K. Nicholson, J.C. Lindon and E. Holmes, “Metabonomics”: understanding the metabolic responses of living systems to pathophysiological stimuli via multivariate statistical analysis of biological NMR spectroscopic data, *Xenobiotica* 29 (1999), pp. 1181–1189.

[4] R. Stoyanova and T.R. Brown, NMR spectral quantitation by principal component analysis, *NMR in Biomedicine* 14 (2001), pp. 271–277.

[5] J.C. Lindon, E. Holmes and J.K. Nicholson, Pattern recognition methods and applications in biomedical magnetic resonance, *Progress in Nuclear Magnetic Resonance Spectroscopy* 39 (2001), pp. 1–40.

[6] D. Kesavan, M. Muthu Tamizh, N. Sulochana, R. Karvembu, J Surfact Deterg (212) 15:751-756.

[7] M. Gopiraman, C. Sathya, S. Vivekananthan, D. Kesavan, and N. Sulochana, JMEPEG (2012) 16:240-246.

[8] M. Gopiraman, P. Sakntha la, D. Kesavan, V. Alexramani, I. S. Kim, N. Sulochana, J Coat Technol Res 9 (1) 15-26, 2012.

Publication History

Received	03rd Feb 2014
Revised	17th Feb 2014
Accepted	25th Feb 2014
Online	04th Mar 2014