Scientia Africana, Vol. 12 (No.1), June 2013. Pp101-107
© College of Natural and Applied Science, University of Port Harcourt, Printed in Nigeria *ISSN 1118 - 1931*

SENSITIVITY ANALYSIS OF PHYSIOCHEMICAL INTERACTION MODEL: WHICH PAIR OF PARAMETERS IS SENSITIVE?

[1]E. N. Ekaka-a,[2]N. M. Nafo, [2]C. Isreal-Cookey and [3]E. O. CHUKWUOCHA

[1]Department of Mathematics/Statistics
University of Port Harcourt,
Port Harcourt, Nigeria.

[2]Department of Mathematics and Computer Science,
Rivers State University of Science and Technology,
Port Harcourt. Nigeria

[3]Department of Physics,
University of Port Harcourt,
Port Harcourt Nigeria

Received: 22-11-12
Accepted:05-12-12

ABSTRACT

The mathematical modelling of physiochemical interactions in the framework of industrial and environmental physics usually relies on an initial value problem which is described by a deterministic system of first order ordinary differential equations. In this paper, we considered a sensitivity analysis of studying the qualitative behaviour of a variation of two model parameters at a time on the solution trajectory of physiochemical interaction over a time interval. Our aim is to use this powerful mathematical technique to select the important pair of parameters of this physical process which is cost-effective.

Key words: Passivation Rate, Sensitivity Analysis, ODE23. ODE45.

INTRODUCTION

Following a full range of the development of a mathematical model of physiochemical interactions ([9]; [10]; [11]) and other relevant references cited therein the sensitivity analysis of the parameters of these important models remains co he an open problem and also an important scientific problem in its own right. Having developed a novel approach of conducting a systematic sensitivity analysis over a time interval ([7]), we propose to apply this numerical technique to the model equation proposed by [9].

This paper is organized into the following sections. Section 1 is focused in defining the concept of the sensitivity analysis and its practical application into physiochemical interaction data. Section 2 will discuss our results which we have obtained in section 1. Our findings are quantitatively discussed.

Sensitivity Analysis: Motivation and Application

The application of the principle of sensitivity analysis is as important as numerical concept in our study because it would be used to find those model parameters whose variation will have the biggest effect on the solution of the model equation. For physiochemical interaction problems, sensitivity analysis can indicate which parameters need to be estimated most accurately and which need only be given as rough estimates.

Hence, sensitivity analysis can guide effort in parameter estimation. Although the concept of the sensitivity of model parameters is not new, it can be recognized at as an old need within the scientific community. One of the new methods of meeting this old need is the implementation of a technique of a sensitivity analysis over a time interval which we have proposed in this paper.

Our model equation was constructed based on some important parameters namely the weight difference after exposure time *t*, the density variable, exposed specimen area and a constant whose magnitude is a function of the system of units being used ([9]).

We know that norms serve the same purpose on vector spaces that absolute value does on the real line. The concept of a norm on a vector space and that of absolute value on a real line furnish a measure of distance.

What are we looking for? We want to find those model parameters for this A1-Sn alloy systems, which when varied, have the biggest effect on the solution. Our approach in this paper is an extension of a similar numerical technique which has yielded desired results in the work of [7].

We know from our own experimental analysis that it would be misleading to judge the sensitivity of the model parameters of AI-Sn systems or physiochemical interactions without conducting a detailed methodology of achieving this.

The definition and application of the theory of sensitivity analysis has already been clearly written out in our previous analysis ([8]) Other interesting applications of sensitivity analysis can be found in the widely applied numerical method often being used in the study of biological, immunological and applied science problems ([3]. [17]. [12]. [15]. [2], [14]. [4], [18], [5]. [1], [16], [6], [19]). As far as we know, the application of sensitivity analysis can be useful in the study of other complex physiochemical interaction systems.

In the models of physiochemical interaction systems, knowledge of a sensitivity analysis can assist the modeller and the environmental scientist to decide whether the parameter estimates are sufficiently accurate for the model to give reliable results. Otherwise, a further work can be suggested in order to obtain improved estimation of those parameters which would give rise to the greatest uncertainty in model predictions.

Governing Model Equation

Following the recent formulation of [9], the rate of change of the corrosion passivation over time can be defined by the following deterministic first order differential equation which we have derived under some simple modifications

(3.1) $$\frac{d(PR)}{dt} = -\left(\frac{\rho A}{k\Delta w}\right)(PR)^2$$

where PR(0) = apha > 0. For this model development, Δw represents for the weight difference after exposure time *t* while the model parameters ρ and A represent the density and exposed specimen area. The parameter *k* is considered as a constant whose magnitude depends on the system of units being used ([9]). Following [9], the dependent variable passivation rate (PR) is defined in terms of *mm/yr* and *Δw, t. ρ*, and *A* when the experimental value of the parameter *k* is 87.6.

Numerical Calculation of Sensitivity Analysis: Methodology and Data.

For our present analysis, we considered two different self-written Matlab programs. The first program concerns the calculation of time PR

Scientia Africana, Vol. 12 (No.1), June 2013. Pp101-107
© College of Natural and Applied Science, University of Port Harcourt, Printed in Nigeria ISSN 1118 - 1931

solution trajectory when none of the four model parameters in the passivation phenomenon is varied while the second program concerns the calculation of the PR solution trajectory when time density parameter and the exposed specimen area *A* are varied. By comparing the difference of these solution trajectories and using time well established mathematical functions of 1-norm, 2-norm, and infinity-norm, we measure the cumulative percentage of varying the density parameter on the PR solution trajectory.

For the purpose of this sensitivity analysis, we consider the following values of data: ρ=10 g/cm^3, A=10 cm^2, k = 87.6, Δw = 0.3186 mg, t = 0 : 5 : 150 hours.

How Does the Variation of a Pair of Parameters Affect the Solution Trajectory over a Time Interval T=0:5:150?

In this section, we are interested to find the effect of varying a pair of similar model parameters on the cumulative effect or percentage change of the PR solution trajectory over a time interval.

For example, if the density parameter and the exposed specimen area take the value of 1.25, the percentage change on the solution trajectory in terms of the values of the three popular norms are 453.7, 290.2 and 77.8 for the 1-norm, 2-norm and infinity-norm. Similar calculations for other values of these two parameters and other combinations of parameters are reported next.

Here, we choose the following pairs of the model parameters of density and exposed specimen area:

(1) *p*l is a combination of these parameters when their estimated values are 1.25.

(2) *p*2 is a combination of these parameters when their estimated values are 2.50.

(3) *p*3 is a combination of these parameters when their estimated values are 5.00.

(4) *p*4 is a combination of these parameters when their estimated values are 6.00.

(5) *p*5 is a combination of these parameters when their estimated values are 7.00.

(6) *p*6 is a combination of these parameters when their estimated values arc 8.00.

(7) *p*7 is a combination of these parameters when their estimated values are 9.00.

(8) *p*8 is a combination of these parameters when their estimated values are 9.50.

(9) *p*9 is a combination of these parameters when their estimated values are 10.10.

(10) *p*10 is a combination of these parameters when their estimated values are 10.50.

(11) *p*11 is a combination of these parameters when their estimated values are 11.00.

(12) *p*12 is a combination of these parameters when their estimated values are 12.00.

(13) *p*13 is a combination of these parameters when their estimated values are 13.00.

(14) *p*14 is a combination of these parameters when their estimated values are 14.00.

Norms of solution	**ODE45 sensitivity analysis**						
Type of norm	*p1*	*p2*	*p3*	*p4*	*p5*	*p6*	*p7*
1-norm	453.7	305.30	22.70	82.70	53.20	30.80	13.60
2-norm	290.2	196.60	83.10	57.30	37.60	22,20	9.90
infinity-norm	77.8	59.90	33.20	24.90	17.70	11.00	5.20

Table 1: Sensitivity analysis: cumulative percent change for a pair of passivation parameters

Norms of solution	**ODE45 sensitivity analysis**						
Type of norm	*p8*	*p9*	*p10*	*p11*	*p12*	*p13*	*p14*
1-norm	6.40	1.20	5.70	10.90	19.70	26.90	33.00
2-norm	4.70	0.90	4.30	8.20	15.10	20.90	25.09
infinity-norm	2.50	0.50	2.40	4.70	9.10	13.10	16.70

Table 2: Sensitivity analysis: cumulative percent change for a pair of passivation parameters

Our next sensitivity analysis concerns another pair of k parameter awl the Δw parameter. Here, we will consider the combinations of these estimated values.

(1) *kd*1 is a combination of these parameters when k = 10.9-5 and Δw = 0.0477.
(2) *kd*2 is a combination of these parameters when k = 21.90 and Δw = 0.0954.
(3) *kd*3 is a combination of these parameters when k = 43.80 and Δw = 0.19084.
(4) *kd*4 is a combination of these parameters when k = 52.56 and Δw = 0.1912.
(5) *kd*5 is a combination of these parameters when k = 61.32 and Δw = 0.223.
(6) *kd*6 is a combination of these parameters when k = 70.08 and Δw = 0. 2519.
(7) *kd*7 is a combination of these parameters when k = 78.84 and Δw = 0.2867.
(8) *kd*8 is a combination of these parameters when k = 83.22 and Δw = 0.3626.
(9) *kd*9 is a combination of these parameters when k = 88.476 and Δw = 0.3855.
(10) *kd*10 is a combination of these parameters when k = 91.98 and Δw = 0.4008.
(11) *kd*11 is a combination of these parameters when k = 96.36 and Δw = 0.4198.
(12) *kd*12 is a combination of these parameters when k = 105.12 and Δw = 0.458.
(13) *kd*13 is a combination of these parameters when k = 113.S and Δw = 0.4962.
(14) *kd*14 is a combination of these parameters when k = 122.64 and Δw = 0.5344.

Norms of solution	**ODE45 sensitivity analysis**						
Type of norm	*kd*1	*kd*2	*kd*3	*kd*4	*kd*5	*kd*6	*kd*7
1-norm	77.50	72.40	54.40	49.93	40.92	31.20	20.99
2-norm	66.90	61.70	44.40	40.37	32.50	24.36	16.12
infinity -norm	55.20	49.50	32.20	28.56	21.88	15.55	9.75

Table 3: Sensitivity analysis: cumulative percent change for a pair of passivation parameters

Norms of solution	**ODE45 sensitivity analysis**						
Type of norm	*kd*8	*kd*9	*kd*10	*kd*11	*kd*12	*kd*13	*kd*14
1-norm	6.02	1.21	6.08	12.20	24.60	37.08	49.60
2-norm	4.52	0.90	4.51	8.96	17.83	26.58	35.17
infinity -norm	2.53	0.49	2.37	4.65	8.98	12.98	16.66

Table 4: Sensitivity analysis: cumulative percent change for a pair of passivation parameters

Scientia Africana, Vol. 12 (No.1), June 2013. Pp101-107
© College of Natural and Applied Science, University of Port Harcourt, Printed in Nigeria ISSN 1118 - 1931

Our final level of sensitivity analysis concerns another pair of initial value parameter and the experimental time changes in hours. In this scenario, we will consider the combinations of these estimated values. In this level of analysis, we will consider the parameter space when the initial value parameter is varied between the range of 12.5 percent to 140 percent and the experimental time changes range from 14 hours to 238 hours.

In this scenario, the notation *ict*1 stands for the case when the initial condition is 0.0063 and the experimental time is 11 hours, the notation *ict*2 stands for the case when the initial condition is 0.0125 arid the experimental time is 28 hours, the notation *ict*3 stands for the case when the initial condition is 0.025 and the experimental time is 56 hours uptil *ict*l4 which stands for the case when the initial condition is 0.07 and the experimental time is 238 hours. The corresponding magnitudes of the sensitivity values when the initial value parameter and the experimental time are varied are presented below.

Norms of solution	**ODE45 sensitivity analysis**						
Type of norm	*ict1*	*ict2*	*ict3*	*ict4*	*ict5*	*ict6*	*ict7*
1-norm	56.06	61.36	50.26	28.57	20.41	12.92	6.13
2-norm	71.73	60.32	41.17	26.79	19.16	12.20	5.83
infinity-norm	87.40	75.00	50.00	40.00	30.00	20.00	10.00

Table 5: Sensitivity analysis: cumulative percent change for a pair of passivation parameters

Norms of solution	**ODE45 sensitivity analysis**						
Type of norm	*ict*8	*ict*9	*ict*10	*ict*11	*ict*12	*ict*13	*ict*14
1-norm	7.85	11.68	15.82	19.56	22.72	25.90	28.90
2-norm	7.06	9.36	12.54	15.50	18.25	21.36	24.54
infinity-norm	5.00	4.34	5.65	10.00	20.00	30.00	40.00

Table 6: Sensitivity analysis: cumulative percent change for a pair of passivation parameters

DISCUSSION OF RESULTS

What have we learnt?

Our systematic sensitivity analysis shows that the biggest effect on the passivation solution trajectory due to a small variation of these pairs of model parameters can be observed for the pair of density parameter and the exposed specimen area parameter. In this context, the density and the exposed specimen area parameters are important parameters whereas the other pairs of model parameters which we have considered in this paper can be seen as equally important. In terms of cost-effectiveness and model parameter estimation formalisms, the density and the exposed specimen area parameters can be selected first while other combinations of parameters are fixed.

CONCLUDING REMARKS AND FURTHER RESEARCH

Our key achievement in this paper is the fact that the density and the exposed specimen area parameters can be considered as an important pair of model parameters of this passivation system over a time interval. As far as we know, this is a cost-effective result which we have not seen elsewhere. It can be attractive to environmental scientists and numerical analysts alike who are actively researching how to solve a major component of the passivation system by using the technique of sensitivity analysis over a time interval. We hope that the insight which this study has produced can be used to tackle some concerns among experimental scientists.

A further extension to analyse other parameter combinations which we did not consider in this paper is suggested.

REFERENCES

Akasar L.A, Ancheyta J. (2007). Sensitivity analysis based methodology to estimate the best set of parameters for heterogeneous kinetic models, *Chemical Engineering Journal* 128(2-3), 85-93.

Amod S. Battaglio M., and Bllomo N (1996). Nonlinear models in soils consolidation theory parameter sensitivity analysis, Mathematical and Computer Modelling 24(3), 11-20.

Astor P.H, Pattern B.C, and Estbcrg G.N (1976). The Sensitivity Substructure of Ecosystems, In B.C. Pattern (Editor), Systems Analysis and simulation in Ecology, Vol. IV, Academic Press, (New York), 390-429

Baker C.T.H and Rihan F.A (1999). Sensitivity Analysis of Parameter in Modelling With Delay Differential Equations, MCCM Numerical Analysis Report, No. 349, Manchester University.

Ban U. and Hill M.C (2005). Numerical methods for improving sensitivity analysis and parameter estimation of virus transport simulated using sorptive-reactive processes, *Journal of Contaminant Hydrology* 76(3-4), 251-277.

Cariboni J. Gatelli D., Liska R., and Saltelli A (2007). The role of sensitivity analysis in ecological modelling, Ecological Modelling 203, 167-182.

Ekaka-a E.N (2009). Computational and Mathematical Modelling of Plant Species Interactions in a Harsh Climate, PhD Thesis, Department of Mathematics, The University of Liverpool and The University of Chester, United Kingdom, 2009.

Ekaka-a, E.N. and Nafo, N.E. Parameter Ranking of Stock Market Dynamics: A Comparative Study of the Mathematical Models of Competition and Mutualistic Interactions, *Scientia Africana*, Vol. II (No. 1), June 2012, pp. 36-43.

Ekuma C.E, Idenyi N.E. and Owate I.O (2010), Application of statistical technique to the analysis of passivation of Al-Sn alloy systems in brine, *Journal of Chemical Engineering of Material Science* 1(1), 1-7.

Ekuma C.E and Idenyi N.E (2006). The Inhibition Characteristics of Brine on the Corrosion Susceptibility of Al-Sn Alloy Systems, *Journal of Applied Sciences* 6(8), 1751-1755.

Ekuma C.E. and Idenyi N.E (2007). Statistical Analyses of the Influence of Environment on Prediction of Corrosion from its Parameters, *Res. J. Phys*. USA 1(1), 27-34.

Halfon E. (1977). Analytical Solution of the System Sensitivity Equation Associated with A Linear Model, Ecological Modelling 3, 301-307.

Huson L.W. (1982). A graphical aid to multivariate sensitivity analysis, Ecological Modelling 16, 91-98.

Kleiber S.I, Antuney H, and Hlen T.D, Kowalczck P (1998). Parameter sensitivity in nonlinear mechanics,

Scientia Africana, Vol. 12 (No.1), June 2013. Pp101-107
© College of Natural and Applied Science, University of Port Harcourt, Printed in Nigeria *ISSN 1118 - 1931*

European *Journal of Mechanics-A/Solids* 17(4), 702-703.

Leenians R. (1991). Sensitivity analysis of a forest succession model, Ecological Modelling 53, 247-262.

Lund B.F and Foss B.A (2008). Parameter ranking by orthogonalization-Applied to nonlinear mechanistic models, Automatica 44(1), 278-281.

Overton W.S (1977). A Strategy of Model Construction, In C.A.S. Hall and J.W. Day (Editors), Ecosystem Modelling in Theory and Practice, Wiley, (New York), 1977.

Sieber A. and Uhlenbrook S. (2005). Sensitivity analysis of a distributed catchment model to verify the model structure, *Journal of Hydrology* 310(1-4), 216-235.

Xenakis U, Ray D, and Mcncuccini M. (2008). Sensitivity and uncertainty analysis from a coupled 3-PG and soil organic matter decomposition model, Ecological Modelling 219, 1-16.