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The Role of Numerical Methods in the Sensitivity Analysis of a Density Parameter in a Passivation Rate Interaction

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ABSTRACT: The mathematical modelling of physiochemical interaction in the framework of industrial and environmental physics which relies on an initial value problem is defined by a first order ordinary differential equation. Two numerical methods of studying sensitivity analysis of physiochemical interaction data are developed. This mathematical technique is used to investigate the extent of the sensitivity of the density parameter over a time interval @JASEM.

Keywords: Passivation Rate, Sensitivity Analysis, ODE23, ODE45

Following a full range of the development of a mathematical model of physiochemical interactions (Ekuma et al. 2010, Ekuma et al. 2006, Ekuma and Idenyi, 2007) and other relevant references cited therein, the sensitivity analysis of the parameters of these important models remains to be 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 (Ekaka-a 2009, Ekaka-a and Nafo, 2011), we propose to apply this numerical technique to the model equation proposed by Ekuma et al. 2010.

This paper is organized into the following sections. Section 2 is focused in defining the concept of the sensitivity analysis and its practical application into physiochemical interaction data. Section 3 will define the model equation which is central to this present analysis while section 4 will apply the technique of sensitivity analysis over a time interval to analyse one example. Selection 5 will discuss another method of calculating sensitivity of model parameters, Section 6 will discuss our results. Our findings are quantitatively discussed in Section 7.

Sensitivity Analysis: Motivation and Application: The application of the principle of sensitivity analysis is an important numerical concept in our study because it would be used to find those model parameters whose variation will have a 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 parameters estimation. Although the concept of the sensitivity of model parameters is not new, it can be recognized 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 (Ekuma et al. 2010).

What are we looking for? We want to find how the variation of the density parameter affects the behaviour of the solution trajectory for these AI-Zn alloy systems. Our approach in this paper is an extension of a similar numerical technique which has yielded desired results in the works of (Ekaka-a 2009, Ekaka-a and Nafo, 2011).

Following from our previous study, a sensitivity analysis is a generic term which indicates the changes in the output of an initial value problem due to changes in the data. How does this numerical method work? The pattern of how the numerical method of sensitivity analysis works has already been published by us in this volume. The notion of a sensitivity analysis is a widely applied numerical method often used in the study of biological, immunological and other applied science problems (Astor et al. 1976, Overton 1977, Halfon 1977, Leemans 1991, Amod et al. 1996, Kleiber et al. 1998, Baker and Rihan 1999, Sieber and Uhlenbrook 2005, Bart and Hill 2005, Alcazar and Ancheyta 2007, Lund and Foss 2008, Cariboni et al. 2007, Xenakis et al. 2008, Ekaka-a and Nafo, 2011). Sensitivity analysis aims to find the dependency between model predictions and the particular set of parameter values one-at-a-time (Huson, 1982). This knowledge can be useful in the study of other complex physiochemical interaction systems.

For the physiochemical interaction systems, a sensitivity analysis is capable to provide the modeler and the environmental scientist the required knowledge with which to decide whether the parameter estimates are sufficiently accurate for the model to give reliable results. Hence, a sensitivity

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analysis is a general procedure which entails changing parameter values and observing the corresponding changes in the model predictions. The inherent problems which have been observed to be associated with the method of sensitivity analysis over a continuous time have been fully defined in our previous paper which has been published in this volume.

Governing Model Equation: Following the recent formulation of (Ekuma et al, 2010), the rate of change of the corrosion passivation over time can be defined by the following deterministic first order ordinary differential equation

$$\frac{d(PR)}{dt} = -\left(\frac{\rho A}{k\Delta w}\right)(PR)^2 \qquad (1)$$

where PR(0) > 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 κ is considered as a constant whose magnitude depends on the system of units (Ekuma et al, 2010). The dependent variable passivation rate (PR) is defined in terms of mm/yr, Δw, *t*, ρ, and *A*.

METHODOLOGY AND DATA

For our present analysis, we considered two different self-written Matlab programs. The first program concerns the calculation of the PR 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 the density parameter is varied. By comparing the difference of these solution trajectories and using the mathematical functions of 1-norm, 2-norm, and ∞-norm, we measure the cumulative percentage change of varying the density parameter on the PR solution trajectory.

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

Does the density parameter have the biggest effect on the *PR* solution trajectory over a time interval t = 0.5 : 150? In this section, we are interested to find if the density parameter of this AI-Zn systems which when varied will have the biggest cumulative effect or biggest percentage change on the solution trajectory.

Without a detailed explanation on how to calculate the biggest cumulative effect (Ekaka-a, 2009), we shall present our results that relate directly to the question we want to tackle. These results are presented in the following table for a variation of the density ρ parameter.

These results are presented in Table 1. The meaning of each notation of the density parameter ρ is as follows: ρ_1 stands for a 12.5 % of ρ; ρ_2 stands for a 25 % of ρ; ρ_3 stands for a 50 % of ρ; ρ_4 stands for a 60 % of ρ; ρ_5 stands for a 70 % of ρ; ρ_6 stands for a 80 % of ρ; ρ_7 stands for a 90 % of ρ; ρ_8 stands for a 95 %of ρ; of ; ρ_9 stands for a 101 % of ρ;ρ_{10} stands for a 105 % of ρ; ρ_{11} stands for a 110 % of ρ; ρ_{12} stands for a 120 % of ρ; ρ_{13} stands for a 130 % of ρ; ρ_{14} stands for a 140 % of ρ.
TABLE 1. Sensitivity analysis: cumulative percent change of a density parameter ρ = 10; ρ_1 stands for a 12.5% of ρ; ρ_2 stands for a 25% of ρ; ρ_2 stands for a 50% of ρ;ρ_4 stands for a 60% of ρ; ρ_5 stands for a 70% of ρ;ρ_6 stands for a 80% of ρ;ρ_7 stands for a 90% of ρ

Our next ODE45 sensitivity calculations for a variation of the density parameter will consider the parameter space (9.5, 14) which corresponds to a percentage variation ranging between 95% to 140% percentage change in the density parameter. Our similar results are presented below:

Table 1: Sensitivity Analysis of a Density Parameter ρ = 10 Using a Solution Trajectory Method

Variations of the density parameter ρ	Sensitivity Values Using Mathematical Norms		
	1-norm	2-norm	Infinity-norm
ρ_1	219.90	137.51	47.71
ρ_2	125.60	81.65	33.21
ρ_3	51.80	35.45	16.94
ρ_4	36.13	25.10	12.38
ρ_5	24.06	16.93	8.71
ρ_6	14.44	10.28	5.52
ρ_7	6.57	4.72	2.62
ρ_8	3.14	2.27	1.28
ρ_9	0.60	0.43	0.25
ρ_{10}	2.90	2.11	1.22
ρ_{11}	5.57	4.07	2.40
ρ_{12}	10.36	7.61	4.56
ρ_{13}	14.53	10.74	6.55
ρ_{14}	18.20	13.52	8.38

Table 2: Sensitivity Analysis of a Density Parameter ρ = 10 Using a Steady-State Method

Variations of the density parameter ρ	Sensitivity Values Using Each Type of Numerical Scheme	
	ODE 45	ODE 23
ρ_1	539.17	539.70
ρ_2	261.08	261.21
ρ_3	93.06	93.10
ρ_4	62.77	62.78
ρ_5	40.69	40.70
ρ_6	23.90	23.90
ρ_7	10.67	10.67
ρ_8	5.06	5.07
ρ_9	0.95	0.96
ρ_{10}	4.60	4.60
ρ_{11}	8.80	8.80
ρ_{12}	16.17	16.17
ρ_{13}	22.44	22.44
ρ_{14}	27.83	27.83

Table 2. Sensitivity analysis: cumulative percent change of a density parameter ρ = 10; ρ_8 stands for a 95% of ρ; ρ_9 stands for a 101% of ρ; ρ_{10} stands for a 105% of ρ;ρ_{11} stands for a 110% of ρ; ρ_{12} stands for a 120% of ρ;ρ_{13} stands for a 130% of ρ;ρ_{14} stands for a 140% of ρ.

METHOD OF STEADY-STATE

In the absence of a closed-form solution for most nonlinear equations, a steady-state can in most instances be found when the rate of change of interacting populations over time is equated to zero. As a parameter of a model equation is slightly varied, the steady-state value or the limiting value in response to this change will also vary. In this context, the percentage change of the difference between the steady-state when the parameter is varied and the steady-state when the parameter is not varied will be used to measure the sensitivity or parameter ranking for each model parameter in the model equation.

For example, when the new value of ρ is 1.25, the steady-state value due to this variation over a time interval T = 0 : 5 : 150 in hours is 0.0115 whereas the steady-state value without a variation over the same time interval is 0.0018. In this scenario, the estimated percentage change of the difference between these two steady-states is 539.17 when the ODE45 numerical computation is implemented whereas the estimated percentage change of the difference between these two steady-states is 539.70 when the ODE23 numerical computation is similarly implemented. The same numerical technique was applied for each variation of the density parameter of this model equation. Since the value of the percentage change is the same for the density parameter ρ and the exposed specimen area *A*, we will only present the calculations for the density parameter in this present study for the ODE45 and the ODE23 numerical computations for the purpose of computational robustness over a time interval. Our results are fully presented in the Tables 3 and 4 below.

Table 3. Sensitivity analysis: cumulative percentage change of the duration of experiment time T

norms of solutions	ODE45 sensitivity analysis of a variation of T						
	18.75	37.5	75	90	105	120	135
1-norm	219.90	125.60	51.80	36.13	24.06	14.44	6.52
2-norm	137.51	81.65	35.45	25.10	16.93	10.28	4.72
∞ - norm	47.71	33.21	16.94	12.38	8.71	5.52	2.62

Table 4. Sensitivity analysis: cumulative percentage change of the duration of experiment time T

norms of solutions	ODE45 sensitivity analysis of a variation of T						
	142.5	151.5	157.5	165	180	195	210
1-norm	3.14	0.60	2.90	5.57	10.36	14.53	18.20
2-norm	2.27	0.43	2.11	4.07	7.61	10.74	13.52
∞ - norm	1.28	0.25	1.22	2.40	4.56	6.55	8.38

Table 3. Sensitivity analysis: percent change of a density parameter ρ = 10 due a changing steady-state value using ODE45 and ODE23 numerical computations; ρ_1 stands for a 12.5% of ρ ; ρ_2 stands for a 25% of ρ ; ρ_3 stands for a 50% of ρ ; ρ_4 stands for a 60% of ρ ; ρ_5 stands for a 70% of ρ ; ρ_6 stands for a 80% of ρ ; ρ_7 stands for a 90% of ρ.

The next series of sensitivity calculations for a variation of the density parameter will consider the parameter space of (9.5, 14) which corresponds to a percentage variation ranging between 95% to 140% percentage change in the density parameter. These results are presented in the table below.

TABLE 4. Sensitivity analysis: percentage change of a density parameter $\rho = 10$ for a changing steady-state value using ODE45 and ODE23 numerical computations; ρ_8 stands for a 95% of ρ; ρ_{11} stands for a 110% of ρ;ρ_{12} stands for a 120% of ρ; ρ_{13} stands for a 130% of ρ; ρ_{14} stands for a 140% of ρ

Our systematic sensitivity analysis of the density parameter clearly shows how the cumulative percentage change behaves due to a variation of this model parameter. Despite the numerical scheme being implemented, the cumulative percentage change obtained by using any of these popular mathematical norms to measure the size of the parameter modification on the solution behaves monotonically. A critical value of $\rho = 10.1$ shows a change from a decreasing value of the cumulative percentage change due to a change in the value of the density parameter to a slight increase in the value of the cumulative percentage change. Both methods of calculating the sensitivity of the density parameter in this passivation problem agree with this observation.

Since our ODE45 sensitivity calculations show similar behaviour on the solution trajectory with the ODE23 sensitivity calculations, we have only presented our results for the ODE45 in this paper for the first method of calculating the sensitivity of the density parameter. In this scenario, it is our choice to implement the ODE45 numerical sensitivity calculations because this numerical scheme provides the best balance between accuracy and computational effort.

In the second method of calculating the sensitivity of the density parameter, we have implemented the calculations for the ODE45 and the ODE23 numerical schemes in order to illustrate the robustness of their application in terms of the quantitative results which we have obtained in this present study.

We also observe that the cumulative percentage change on the solution trajectory do not differ so much when implementing either the ODE23 or the ODE45 sensitivity scheme. Therefore, our results clearly show that the application of these ODE numerical schemes is a robust numerical method for calculating the changes that we would expect to see in the solution due to a variation of this density parameter. It is important to mention in this context that the density parameter ρ and the exposed specimen area A can be classified as equally important parameters in the passivation phenomenon because they produce the same biggest effect on the PR solution trajectories when either of these parameters is varied. This is why we have only presented our sensitivity calculations for the density parameter in this study.

Conclusion: In this important numerical analysis application of a sensitivity analysis of the density parameter of our AI-Zn physiochemical interactions, if we vary this model parameter a little, we have observed a biggest effect on the solution trajectory. It is our expectation that these contributions which we have not seen elsewhere would contribute better insights about the application of sensitivity analysis of physiochemical interactions data in terms of a parameter estimation theory especially in the overall interest of the scientific community in Nigeria and the other scientific communities in the world where sophisticated mathematical modelling and computational capacity building and model development are lacking.

The key results which we have achieved in this study can be used to explain issues such as the effect of varying the density parameter over a time interval on the passivation rate. This contribution is an attempt to discuss the importance of a further parameter estimation of this parameter. Our present result compliments the current findings of Ekuma et al. 2010. For the purpose of comparison with the standard sensitivity analysis method, two types of numerical methods have been utilized to calculate the sensitivity of the density parameter.

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