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Sensitivity Analysis of a Physiochemical Interaction Model Undergoing Changes in the Initial Condition and Duration of Experiment Time

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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 single first order ordinary differential equation. In this analysis, we will study the sensitivity analysis due to a variation of the initial condition and experimental time. These results which we have not seen elsewhere are analysed and discussed quantitatively. @JASEM

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Sensitivity analysis of a model parameter over a time interval is an important mathematical technique with diverse applications (Ekuma and Idenyi, 2007; Halfon, 1977). It is a standard numerical method which is based on varying a parameter and observing its behaviour in the solution trajectory.

This paper is organized into the following sections. Section 2 is focused in defining our motivation of the sensitivity analysis and its practical application into physiochemical interaction data. Section 3 will define the mathematical formulation of the passivation process. Section 4 will illustrate the application of sensitivity analysis to two specific examples. The key results which we have achieved in this study are discussed in section 5 and analysed quantitatively.

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 parameter estimation. Although the concept of the sensitivity of model parameter 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.

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 these AI-Zn 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 Ekaka-a (2009).

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

What then is sensitivity analysis? It is simply the generic term for the change in the output of an initial value problem due to the changes in the data. How does this numerical method work? The numerical method of sensitivity or the principle of parsimony works in the following pattern:

(1) Write down some complicated interaction model
(2) Fix the values of each possible model parameter
(3) Take one parameter at a time, vary it and see how much this variation changes the solution
(4) If the variation of one parameter changes the solution a lot, then this parameter would be called a more sensitive parameter
(5) On the other hand, if the variation of another parameter produces a small change in

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solution, then this parameter would be called a least sensitive parameter.
We do not necessarily have to remove the least important parameters according to the hypothesis of the principle of parsimony. The notion of sensitivity analysis is a widely applied numerical method often being used in the study of biological, immunological and applied science problem (Alcazar and Ancheyta, 2007; Amod et al S, 1996; Astor et al 1976; Baker and Rihan, 1999).

We remark that most of these applied sensitivity analyses are considered at a particular time when a solution is reasonably constant whereas our method as proposed in this paper will consider data points over a period of time (Bart and Hill, 2005; Cariboni et al., 2007; Ekuma and Idenyi, 2006; Kleiber et al., 1998).

Sensitivity analysis is a standard method for studying mathematical models especially if a further numerical simulation is required to analyse a particular research problem. It aims to find the dependency between model predictions and the particular set of parameter values beings used Huson (1982). This knowledge can be useful in the study of other complex physiochemical interaction systems. Other related applications of sensitivity analysis in forest succession model, in orthogonolization theory, in ecosystem model development, in a distributed catchment model and in soil science have been extensively reported (Leemans, 1991; Lund and Foss, 2008; Overton, 1977; Sieber et al., 2005; Xenakis et al., 2008).

In the models of physiochemical interaction systems, a 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.

In this context, a sensitivity analysis is a general procedure which entails changing parameter values and observing the corresponding changes in the model predictions. It seems easy to describe this procedure, but conducting a detailed sensitivity analysis in any specific case is a dauting task. Problems may include

(1) How much to vary each parameter by
(2) What combinations of parameter values are acceptable
(3) What values of the explanatory variables to use
(4) Which model parameters when varied will have the biggest or smallest effect on the solutions.
(5) How to interpret the results.

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 differential equation which we have derived under some simple modifications.

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

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

Numerical Calculation of Sensitivity Analysis: Methodology and Data 1: 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 initial condition is varied. By comparing the difference of these solution trajectories and using the well established mathematical functions of 1-norm, 2-norm, and ∞-norm, we measure the cumulative percentage of varying the initial condition on the PR solution trajectory.

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

Does the initial condition 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 initial condition of this AI-Zn systems which when varied will have the biggest cumulative effect or biggest percentage change on the solution trajectory. Since the initial condition refers to the initial passivation rate, following [8] it follows that the unit of passivation rate is mg/hr.

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 initial condition.

In this paper, the notation of the initial condition is ic = 0.05; ic_1 stands for a 12.5% of ic*;* ic_2 stands for a 25% of ic*;* ic_3 stands for a 50% of ic; ic_4 stands for a 60% of ic; ic_5 stands for a 70% of ic; ic_6 stands for a 80% of ic; ic_7 stands for a 90% of ic

In our next series of ODE45 sensitivity calculations for a variation of the initial condition, we will consider the parameter space of (0.0475, 0.07) which corresponds to a percentage variation ranging between 95% to 140% percentage change in the initial condition parameter. Our similar results are presented in Table 2.

Table 1. Sensitivity analysis: cumulative percentage change of ic

norms of solutions	ODE45 sensitivity analysis of a variation of ic						
	ic_1	ic_2	ic_3	ic_4	ic_5	ic_6	ic_7
1-norm	60.01	43.60	24.10	18.32	13.16	8.45	4.09
2-norm	79.78	65.62	41.83	33.10	24.58	16.26	8.08
∞ - norm	87.50	75.00	50.00	40.00	30.00	20.00	10.00

Table 2. Sensitivity analysis: cumulative percentage change of ic

norms of solutions	ODE45 sensitivity analysis of a variation of ic						
	ic_8	ic_9	ic_{10}	ic_{11}	ic_{12}	ic_{13}	ic_{14}
1-norm	2.01	1.96	1.96	3.87	7.57	11.12	14.54
2-norm	4.03	0.80	4.01	8.00	15.93	23.82	31.66
∞ - norm	5.00	1.00	5.00	10.00	20.00	30.00	40.00

ic = 0.05; ic_8 stands for a 95% of *ic;* ic_9 stands for a 101% of *ic;* ic_{10} stands for a 105% of *ic*; ic_{11} stands for a 110% of *ic*; ic_{12} stands for a 120% of *ic*; ic_{13} stands for a 130% of *ic*; ic_{14} stands for a 140% of *ic*

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 duration of the experiment T in hours is varied. By comparing the difference of these solution trajectories and using the well established mathematical functions of 1-norm, 2-norm, and ∞-norm, we measure the cumulative percentage of varying the weight difference after exposure time parameter on the PR solution trajectory.

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

Does the experimental time 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 duration of the experiment of this AI-Zn systems which when varied will have the biggest cumulative effect or biggest percentage change on the solution trajectory.

Similarly, following (Ekaka-a, 2009), we shall present our results that directly relate to the notion of a cumulative percentage effect on the solution trajectories which is due to the variation of a model parameter. In this context, our calculations are presented in the next table for a variation of the duration of the passivation experiment.

In this paper, we will consider the control experimental value of 150 hours which we have assumed from the work of Ekuma et al. 2010. For example, when this model parameter is varied for 12.5 %, the new value of the experimental time in hours is 18.75. Other new values of the experimental time were similarly calculated and used to study the sensitivity analysis of the experimental time.

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

In our next series of ODE45 sensitivity calculations for a variation of the duration of experiment time in hours, we will consider the parameter space of (142.5, 210). Our results are presented next:

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

DISCUSSION

In this context, our systematic sensitivity analysis clearly shows that the duration of experiment which is defined in hours is an important model parameter than the initial condition parameter.

We observe that 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. It is our choice to implement the ODE45 numerical sensitivity calculations because this numerical scheme provides the best balance between accuracy and computational effort.

Our key achievement in this work is the fact that the duration of experiment is an important model parameter than the initial condition parameter when the 1-norm and the 2-norm sensitivity values were implemented. It is also very clear that these two model parameters can be considered as relatively equally sensitive parameters or
relatively equally important parameters for this passivation system. However, the hypothesis of a little percentage variation of a model parameter one-at-a-time to produce a biggest cumulative effect on the solution trajectories is yet to be fully tackled in this present paper.

In the context of this work, an insight of our 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. However, a further experimental work is hereby suggested in order to obtain improved estimations for the initial condition parameter and the experimental time parameter.

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