A concise overview on optimization and modelling parameter cases in electrodeposition and composite coating technology

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Abstract
Electrodeposition technology often uses the principles of electrolysis to modify the deposition of coating material on a metal surface. Numerical modelling can be used to quickly carry out modelling and optimization of these coating and resultant corrosion study processes. This allows researchers to perform a detailed analysis of a model created to simulate, analyze, and optimize the electrodeposition process. This research provides several more efficient methods of studying and optimizing anti-corrosive coating development processes and the critical parameters involved.

Keywords: Modelling, optimization process, anticorrosion, corrosion

1 Introduction
Modeling, in simple terms, is defined as the process of developing or producing a model. A model is defined as a representation of the construction and operation of a system in view. Models are usually simplifications of the system they represent [1]. The major reason models are created is to provide a means to describe and analyze the behavior of the system before, during and after the modification of integral parameters. Models are purposed to provide as close an abstraction as possible to the system represented, incorporating most of its relevant aspects and features; while also being simple enough to allow quick comprehension of its behavior and enable rapid, iterative experimentation [1-3]. This defines a good model as one which balances simplicity and range of realistic representation. Modelling is intrinsically an iterative process, as several factors are defined and combined into one expression over successive versions of the model; a model could represent a system across several scales of operation as well [4]. There are several classifications of models intended for several different types of study. However, this review will focus on classifications of mathematical models [5].

Modelling and Simulation provide a means to carry out effective study on several physical processes, including electrodeposition, with significantly reduced time, material and energy costs [6]. Modelling is the process whereby a representation of the structure and operation of a system of interest is created. Models are used primarily for the analysis of the systems they represent, as they are complex enough to represent the interplay of the myriad properties of a system, while simple enough to allow analysis of the cause and effect relationship between various factors in physical phenomena [7-9]. Simulation using mathematical modelling is defined by [10] as a tool used in the prediction, evaluation or optimization of the performance
of a proposed or current system, or model of a system, under study over time. Simulation has the advantage of being carried out in a virtual environment, which minimizes the risk of material waste, while allowing for significantly faster iteration and analysis. Modelling and simulation is carried out with the use of specialized software designed to model physical systems as accurately as possible, allowing the simulation of a plethora of real-world phenomena. Post-simulation results can then be implemented in optimizing the corrosion inhibition process through coatings [11-13].

Research into electrodeposition and other coating methods is being limited by the amount of time and energy required to physically simulate coating and corrosion protection reactions [14-17]. Numerical modelling and simulation should provide a more efficient method of studying and optimizing anti-corrosive coating development processes and key parameters involved. Thus the review highlighted and discusses various model processes used in different coating and electrodeposition technology.

2 Mathematical Model
A mathematical model is a description of a system which utilizes mathematical concepts and language. These models are used primarily in the natural and social sciences as well as the engineering disciplines as they are suitable for describing systems which can be described with mathematical equations [1]. The following are some of the classifications of mathematical models based on their structure.

2.1. Stochastic (as opposed to Deterministic) Models:
A stochastic model is derived from a source based in randomness or probability, as it is produced from specific assumptions of the system being studied, which may or may not be accurate realistically [2].

2.2. Deterministic (as opposed to Stochastic) Models:
A deterministic model is defined by having fixed values for both the input and output variables. This implies that there is little or no probability involved and the model is based on values which do not change, which provides a greater level of accuracy.

2.3. Static (as opposed to Dynamic) Models:
A static model is that which describes a system or its operation without taking time into account. The model describes the behavior of a system at a particular specific instance of its operation, neglecting the action of time on the values of either the input or output variables of the model [3].

2.4. Dynamic (as opposed to Static) Models:
A dynamic model describes a system or its operation taking into account the effects of time on the values of either the input or output variables.

2.5. Discrete (as opposed to continuous) Models:
A discrete model describes the items being modeled as discrete from each other. Thereby limiting the effects of individual items on the behavior of each other and the system at large.

2.6. Continuous (as opposed to Discrete) Models:
A continuous model describes a system by representing the model items in a continuous form, applying effects continuously throughout the process being modeled [4].
3 Simulation
Simulation is the act of utilizing the model of a system to predict, analyze, or optimize the performance and behavior of a system being studied. Simulation is usually carried out under specific input conditions and the results generated as the output of the model are compared with the results generated from the actual system being represented. The model, during simulation, is able to utilize several configurations to study the effects of different values of several initiating variables on the results of the simulation. This ease of reconfiguration is an advantage of simulation and modelling as the act of changing parameters in the actual system represented by the model is either costly or impractical. The operation of a model can be studied and iteratively improved upon through this process of reconfiguration and analysis. The process of simulation results in data regarding the properties of the system which can be analyzed, allowing the inference of new properties regarding the behavior of the system under the specified input conditions [1].

![Simulation Example: Spur Gear Simulation](image)

In order to prevent unintended failure, simulation is often utilized before a system is altered or a new system is physically implemented. This allows the prediction of failure states before they occur, a reduction of the chances of unforeseen circumstances affecting the system, and a proper understanding of the requirements of a system, in terms of resources and time commitment, preventing the over- or implementation under-utilization of these resources [3].

3.1. Finite Element Analysis
This is a numerical method which is utilized to create solutions to problems which are common in engineering and mathematical physics, involving characteristics which are easily described by differential equations. The equations used are capable of modeling a great range of physical processes and phenomena such as those encountered within the physical sciences, including acoustic, thermal, electrical, electrochemical, as well as mechanical. Finite Element
Analysis (FEM) is based upon the principle of discretization, which involves the division of the area of interest into several element cells in which the equations governing the process being modelled can be applied and the individual results can be combined to provide a net outlook on the effects on the system. FEM itself involves reducing partial differential equations into systems of algebraic equations whose solutions describe the behavior of some system or process through a dependent variable [18].

![Figure 2. 2D Finite Element Mesh [6]](image)

3.2 Comsol Multiphysics
COMSOL Multiphysics is a predominant simulation software suite within the scientific community, due to the wide range of real-world physical devices and processes able to be visualized, modelled, and simulated within its virtual environment. COMSOL Multiphysics combines finite element analysis, a configurable solver and varieties of simulation capability within its workflow. COMSOL allows the integration of Partial Differential Equations into models in order to accurately simulate the behavior of real world processes, to the extent the of the equations applied. This provides the basis for models generated within the application suite. COMSOL also provides a unified, consistent workflow for joint simulations in normally separate branches of physics such as acoustic, electrical, thermal, mechanical, and electrochemical studies. As an aide to engineers and scientists, COMSOL provides a link to other software normally used in conjunction with simulation packages, such as MATLAB, Microsoft Excel, SOLIDWORKS, and AutoCAD amongst others. The various areas of application are represented as modules within COMSOL; these are categorized according to a specific type of physical process being studied, such as: Electrical, Mechanical, Fluid, Acoustic, as well as others. COMSOL is owned by COMSOL Inc., a private company founded in Sweden in 1986.

3.3. Numerical Modelling
Physical processes or reactions are described in science and engineering applications through the use of mathematical equations; the process of description being known as Numerical Modelling. The processes being described are intrinsically difficult to solve or compute analytically, hence the need for numerical models. When properly developed, the solutions to numerical models can provide the values of dependent variables within the equations, offering insight into the operations and properties of the system being described. Numerical
modelling has applications in several areas of science and engineering such as fluid flow, electrochemical, geological, electromagnetic, thermal, acoustic, mechanical processes amongst several others. According to [7] a numerical model should, in good principle, follow a preset workflow when describing a system. An example would be:

- **Mathematical model** – This should be a set of equations and boundary conditions describing the system in view as accurately as possible; with mathematical relations between the involved variables and constants. In practice these equations are Partial Differential Equations (PDEs), which are notably difficult to solve in a direct manner.

- **Discretization/Numerical Methods** – These are methods which transform the equations in the mathematical model into discrete forms. Discrete equations provide approximations that simplify the computation of the equation’s solution while retaining the form and description of the original equations in view. Prevalent methods of discretization include the finite element, finite difference, and finite volume method; all of which divide the item in view into smaller elements through meshing.

- **Algorithms** – These are programs written to organize and logically process problems, in this case, they are applied to solve the equations after discretization.

- **Interpretation of Results** – The results of the computation are combined and interpreted into analytical form through the use of tables, graphs, and other forms of visualization.

COMSOL Multiphysics contains interfaces capable of carrying out each of the aforementioned steps involved in a typical integrated workflow.

### 3.4. Review of Modelling and Simulation on Electrodeposition

A study, by [8] was carried out, detailing the effect of the modification of parameters in the electrodeposition of Silicon-Carbide particles, with respect to the effect of particle concentration, as well as the heat treatment, on the hardness, wear resistance and molecular structure of the deposited coatings. The substrate used in this study was AISI 1018 steel electrode; the electrodeposition process proceeded with the deposition of the aforementioned particle on the substrate, followed by the heat treatment within a certain temperature range. The properties of import to the study were the friction coefficient, hardness, and wear resistance and the results showed that the particular distribution of the Silicon-Carbide particles within the metallic matrix provided improved values for several coating properties, such as the hardness and wear resistance, while reducing the value of the friction coefficient. The substrate alloy was amorphous in nature pre-deposit, however, it underwent a phase transformation into an amalgam of amorphous and crystalline phases during the thermal treatment, specifically at temperature values between 400°C and 500°C. The authors associated the phase transformation with the precipitation of an intermediary compound (Ni₃P) and Nickel (Ni) Crystals. The peak value for the hardness property was noted at a coating temperature of 500°C.

[11, 12] carried out the development of composite coatings with the use of in-situ electrodeposition in order to bring about the improvement of several mechanical and anti-corrosive properties in the mild steel substrate. The study utilized a composite-based coating derived from varying proportions of Zinc, Aluminium, Tin IV Oxide, and Titanium IV Oxide. The properties of import in this study were the hardness, wear resistance, as well as anti-corrosion. The author analyzed the anti-corrosive properties using the linear polarization method, carried out with the substrate immersed in 3.65% Sodium Chloride medium. The
coatings were characterized using a plethora of techniques including scanning electron microscopy, x-ray diffraction, energy dispersive spectroscopy, atomic force microscopy and optical microscopy analyses. The thermal treatment was carried out for a period of 2 hours, at temperatures of 200-, 400, and 600°C. The results generated showed that the coatings were stable within the deposited interface, with homogenous placement of the internal grain structure of the coating interface. The author attributes the overall improvement of characteristics to the unified distribution as well as the refinement of the crystals, the conjoined precipitation of the composites located at the metal lattice, and the adherent nature of the additives, all in relation to the electrodeposition process conditions.

A study carried out in 2015 by [11] in which hydroxyapatite layers were deposited onto a CoCrMo (Cobalt-Chromium-Molybdenum) substrate, normally used in dental applications as bio-metallic implants. The deposition parameters of note in this study were the pH of the electrolyte, which was examined in varying incremental values in order to correlate the values on the structural and biological performance characteristics of the electrodeposited coatings. The results were then modelled with the use of Zview modelling software in conjunction with COMSOL Multiphysics to model the electrochemical impedance spectroscopy (EIS), as well as the potentiodynamic polarization within the simulated body. The results showed a good correlation between the model generated by both the Zview and COMSOL applications and the experimental results obtained. The values obtained from the Zview model implied the barrier characteristics of the coatings were improved as a result of the increasing pH of the deposition process. The results show the overall improvement of corrosion resistance concurrent with an increase in the electrolyte pH during the deposition. A peak density and minimal coating size were obtained with pH values of 6.

[2] developed a mathematical model in tandem with the simulation of an electrodeposition process, in order to ascertain the effect of the electrolyte current density and conductivity on the resultant thickness of the deposited layer. The simulation was carried out simultaneous with a physical electrodeposition process, in order to correlate and validate the model and simulation results. Copper and a Cobalt-Chrome alloy were chosen as the electrodes with copper sulphate as the working electrolyte. A Finite Element Solver, namely COMSOL Multiphysics, was utilized in simulating the coating process and the resultant thickness under a range of process state parameter values; a 2D representation of the process was utilized in the simulation in order to simplify the model and minimize unnecessary complexity in the FE solver’s computation. The physical deposition utilized various conductivity levels and current density values in successive plating samples after which characterization was carried out in the form of thickness analysis as well as SEM (Scanning Electron Microscope) images. The simulation results showed agreement with the experimental thickness values, with a slight variance in regions with an increased effect of the generated electrochemical double layer occurring during the deposition process, which was not represented in the model.

A numerical method was generated by [5] which tracked the interface between metal particles undergoing deposition and the electrolyte utilized during the aforementioned deposition process. Several tools such as COMSOL, PHYSICA and PHOENICS were utilized in this study to properly represent the several physical phenomena then-in-view. A multi-scale design process was utilized in the description of the deposition of holes in printed circuit boards, allowing for interaction between participating elements at both the macro- and micro- level, followed by numerical simulation verifying the specific transport process occurring in the deposition cell. Thus, allowing the specific process parameters and condition
to become evident for future study. Megasonic agitators, in the form of megasonic transducers, were placed in the plating cell in order to effect an improvement of the electrolyte convection through an effect known as acoustic streaming. The model was successfully validated able to accurately predict the distributions of pressure, ion concentration and velocity within any section of the cell in view; methods were also developed to derive the velocity distribution of the acoustic streaming.

3.5. Review of Numerical Simulation on Corrosion

[12] performed a numerical simulation of flow-induced corrosion damages utilizing the ANSYS software to model, simulate and analyze the flow assisted corrosion of pipelines. The study utilized the description of chemical kinetics taken from published literature and specific conditions and assumptions were chosen to define the system, such as: an infinite mixing rate for the overall reaction kinetics, an adiabatic wall enclosing the pipeline, with a Reynolds number of $5.67 \times 10^4$ describing the flow, and a compressed liquid as the active fluid. The simulation was carried out at an inlet temperature of 280°C and a pressure of 80 Mpa. It was discovered that the inclusion of the adiabatic wall parameter affected the overall average kinetics, providing a better simulation result than that provided by the simulation without the effect of the adiabatic wall.

[13] carried out a study utilizing a Finite element method (FEM) model established by the authors to simulate the micro-galvanic corrosion induced by the action of a single cathodic intermediary particle in an Aluminum matrix. The hindrance effected by the spatial arrangement of Al(OH)$_3$ on the electrode surface and in the liquid phase, was contended by taking into account the reduction in surface activity and mass transport rates in the conductive solution utilized in the process. The results show that density of the corrosion product precipitates affected the blocking effect of the electrode surface, as well as the mass transport of the species, amongst others. It was noted that the most severe acidification appeared with the precipitate density level at the intermediate point of the densities investigated, as a result of the competitive interaction between ions released from the anodic dissolution reaction and the dilution of the anolyte within the volume which had been separated from the bulk solution, highlighting the significance of porosity values of the corrosion product on the progress of localized corrosion within the system.

[14] performed a study on the corrosion process of steel bars in concrete within a chloride environment. A numerical model was developed to investigate the time-dependent process of non-uniform corrosion of steel bars at different locations within concrete, also taking into account the effects of longitudinal cracking on the diffusion properties of chloride and oxygen. The corrosion process is noted to be activated around the circumference of steel bars when the chloride level of the bar reaches the threshold at that specific point, determined through measuring the chloride penetration. The corrosion rate around the surface of a steel bar at that point can then be derived using electrochemical theory, allowing a description of the cross-section of the steel bar visualizing the timeline of damage from corrosion. It was noted from the results of the study that the distribution of the rust layer calculated by the model was similar to that obtained through physical experimentation carried out on concrete with conditions analogous to those found in the natural environment. This served as validation for the model developed.

[16] carried out a study in which the process of corrosion degradation was modelled serially utilizing cellular automata in order to articulate the contained component of corrosion, factoring in the mechanical component arising from the concentration of stress caused by the
defect. This mechanical component of the model was created with the use of Finite Element Analysis techniques. This simultaneous utilization of Cellular Automata and Finite Element Analysis, as well as cross-analysis of their respective results provided an effective model which described the development of stress-assisted corrosion pitting. The experimental results, when tallied with the results from the simulation carried out with the model created showed a general concurrence, thereby validating the model. The model developed showed that the rate of propagation of localized corrosion is significantly increased by the presence of mechanical effects, such as plastic strain.

**Conclusions**

From the overview study, electrodeposition products, in the forms of coatings have widespread applicability within manufacturing and engineering industries, due to the desire for the general improvement of mechanical, chemical and electrochemical properties in materials utilized in these industries. However, electrodeposition and other coating methods are been limited by the amount of time and energy required to physically simulate coating and corrosion protection reactions. Thus, numerical modelling and simulation from this overview has provided a more efficient method of studying and optimizing anti-corrosive coating in a bit to limit time constrains and situate proper bath framework.

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