

Mechanistic Model as a Bias to Machine Learning Algorithm for Confident Prediction of Corrosion

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ABSTRACT

Bayesian network is employed to estimate a risk-based life cycle cost of corrosion for assets. It has been highly recognized that inclusion of mechanistic models to a Bayesian network can increase the confidence in estimation of corrosion rates. However, coefficients of mechanistic models are often unknown, especially when complex rate processes are involved, which discourages the usage of the model. A methodology is proposed here, to introduce a mechanistic model as a bias to a regressive machine learning (ML) algorithm. No attempts have been made to obtain phenomenological coefficients of the mechanistic model. Instead, a methodology is proposed to obtain a highly tuned parameter vector for a ML algorithm from a learning set of corrosion rate data.

Key words: corrosion modelling, machine learning algorithm, rate processes, supervised learning, non-linear regression

INTRODUCTION

A constant challenge persists among corrosion engineers to estimate and predict field corrosion rates despite the huge advancements in corrosion science. This situation has compelled the corrosion engineers to opt for the machine learning (ML) algorithms for corrosion prediction. However, the “blackbox” ML algorithms are not appreciated in high stakes decisions because they use arbitrary fitting models rather than scientific principles.¹ Learning achieved by such an algorithm is confined to itself and no useful knowledge can be acquired from it. Hence, it is necessary to include mechanistic models into machine learning algorithms for more confident prediction of corrosion rates.

According to the latest impact report by NACE, global economic loss due to corrosion was estimated to be \$2.5 trillion in 2013, of which 15 to 35% could be saved by implementing proper corrosion control and management practices.¹ Bayesian network (BN), a probabilistic learning algorithm with cause-consequence type structure, is utilized in calculation of indirect costs from the failure, especially in cases when localized failure mechanisms are expected.¹ Learning, and consequently the reliability, of BN depends on input corrosion data, which can be generated by mechanistic models, mined from expert

knowledge, or simply being available from the field.² Among these, the mechanistic models are the most preferable to generate corrosion rate data used in preparing conditional probability tables for BN.^{2,3}

However, there is an inherent inaccuracy associated with any corrosion model either due to deficient mechanistic description or unknown coefficients, which leads to poor estimation of corrosion rates. Typically, a corrosion model is constructed out of the most feasible mechanistic description derived from the experimental results. However, the models often fail to estimate accurate field corrosion rates because coefficients of the rate equations are determined from laboratory data obtained in ideal environment which may be far from the field conditions.

A hybrid approach is adopted here to use ML algorithms with input of a mechanistic model as scientific information to obtain highly tuned parameters by using corrosion data for learning. The values of these parameters may not resemble to coefficients of the rate equations. However, prediction of such a scientifically informed ML (SciML) algorithm is more reliable than the “blackbox” ML algorithms. The proposed methodology serves as a general framework to integrate a mechanistic model into a ML algorithm for more confident prediction of corrosion in high stakes decisions, which can be applied to any corrosion system after specific modifications.

CORROSION MODEL

In general, physical modelling of any corrosion system involves electrochemical reactions, chemical reactions, and mass transport of corrosive species for which rate equations are derived from the principles of electrochemistry, chemical science, and fluid mechanics. When experimental corrosion rate data evidently conforms to a particular rate law, the reaction involved is considered to be limited by that step of the overall mechanism. After confirming the “rate limiting step” for given experimental conditions, the experimental variables are further manipulated in such a way that a different step of the mechanism becomes rate limiting and so on. This procedure is repeated until all anticipated steps of the mechanism are confirmed and the master corrosion rate equation may be derived by coupling the rates of individual steps. If some of the anticipated steps of the corrosion mechanism are not feasible to conform experimentally, then they must be deduced rationally. Such mechanistic models resemble to the true nature of corrosion phenomena and thus they are highly dependable for prediction of corrosion rates if accurate values of coefficients can be determined.

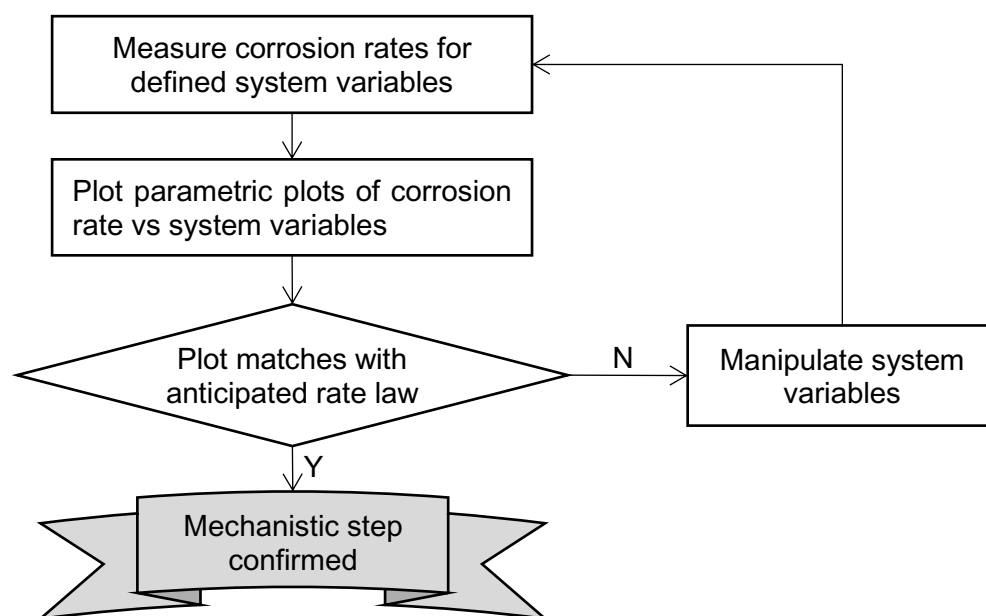


Figure 1: Steps to construct mechanistic corrosion model.