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Mini Review

The Elements of the Deterministic Prediction of Physico-Chemical Phenomena

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Abstract

This paper briefly explores the roles of empiricism and determinism in science and engineering. From this analysis, I conclude that the intellectual exercise that we call "science" is best described as the transition from empiricism (i.e., from what we can observe) to determinism, which is the philosophy that the future can be predicted from the past on the basis of the natural laws that are condensations of all previous scientific knowledge. Thus, "science" is enacted by formulating theories to explain the observations and models, based on those theories, are developed to predict new phenomena. Accordingly, models are the computational arms of theories. Importantly, all models must possess a theoretical basis but not all theories need to predict. The structure of a deterministic model is that it must contain an input, a model "engine", and an output, that are all linked by a feedback loop that permits the continual updating of the model parameters and a means of assessing predictions against new observations. This latter feature, in essence, enables the application of the "scientific method" of cyclical modification/assessment that continues until the model no longer accounts for new observations. At that point, the model (and possibly the theory, as well) must be discarded and a new theory/model developed. Again, importantly, no amount of successful prediction can "prove" a theory/model to be "correct", because theories and models are merely the figments of our imagination as developed through imperfect senses and imperfect intellect. Accordingly, all theories and models are wrong at some level of detail. Contrariwise, a single failure of a model to predict an observation invalidates the theory/model unequivocally. The principal impediment to model building is complexity and it is the reason why a compromise must always be made between physical reality and mathematical tractability.

Introduction

The present paper is based upon a recent publication by the author titled "The Role of Determinism in the Prediction of Corrosion Damage" [1] in which the author uses the development of the Coupled Environment Fracture Model (CEFM) as an example of such a model. In doing so, the elements of determinism are identified and their implication for accurate prediction of crack growth rate in sensitized Type 304 stainless steel in the primary coolant circuits of Boiling Water (Nuclear Reactors (BWRs) is articulated. The current paper summarizes the concepts underpinning the deterministic prediction of new phenomena and is applicable to a wide range of physico-chemical systems. Complex industrial systems are generally unique, even when they are exactly of the same design and employ the same materials, often because of unique operating conditions and histories. Because failures of such systems (e.g., nuclear reactors) are rare events [2], it is generally impossible to develop an effective empirical database covering the range of independent variables that characterize complex, industrial systems and that might allow accurate prediction of damage. Furthermore, empirical models are commonly very expensive, because of the need for large, labor-intensive calibrating databases. Empirical models also fail to capture the mechanism of failure and they almost always fail to yield the accuracy of prediction that might render them useful for maintenance and life extension analyses. Of significant importance is that empirical models generally have limited prediction factors, PF (defined as the time of prediction/calibrating data record). Almost always, for an empirical model, 1<PF<5 whereas for deterministic models 1<PF<1000 or more. Indeed, this feature of determinism is being exploited in modeling the fate of metallic canisters for the disposal of High-Level Nuclear Waste (HLNW), where a PF of >100,000 is required to ensure that the waste can be isolated from the biosphere for sufficient time for the fission product nuclides to have decayed to harmless levels.

Why is the accurate prediction of corrosion damage so important? Corrosion damage is responsible for great economic losses in industrialized societies (3-4.5 % of GDP per year or about $630 billion to $945 billion in the US in 2020 based on a GDP of $21 trillion). The Worldwide cost is more than three to four times that figure, rendering corrosion one of the costliest of all-natural phenomena. Thus, the annual cost in the USA of earthquakes and hurricanes and are $6.1 billion and $28 billion [3,4], respectively. Furthermore, approximately 30% of the cost of corrosion could be avoided by better application of existing corrosion control technology, if only we knew in advance where and when corrosion damage will occur. Thus, if we knew the location and accumulation rate of corrosion damage in a specific location, then the system might be serviced during scheduled outages, thereby avoiding costly, unscheduled downtime. To illustrate this point, the cost of unscheduled downtime for a 980MWe nuclear power plant is $1-2 million/day [5]. As expected, the total cost is determined by the length of the outage and the cost of replacing/repairing components. Thus, a failed Low-Pressure Steam Turbine (LPST) or a Steam Generator (SG) can keep a plant offline for more than a year, resulting in a total loss of $360 million to $720 million per event. With the addition of the cost of replacing these components, the total cost approaches $1 billion. As with any business, these enormous costs are passed on to the consumers of the electricity and/or the taxpayers through increases in the retail cost of electricity. This is a particularly important issue in the present energy climate in which competition from natural gas and the so-called "renewables" (principally solar and wind), which are highly subsidized and politically favored, is intensifying. Thus, considerable incentives exists for proactively managing the development of corrosion damage, but this can only be done by employing models that can accurately predict the progression of corrosion damage in specific locations in the Reactor Coolant Circuit (RCC). This paper outlines the development one such model, the Coupled Environment Fracture Model (CEFM) that has been developed by the author and his colleagues to model the progression of Intergranular Stress Corrosion Cracking (IGSCC) damage in sensitized austenitic stainless steels (e.g., Types 304 SS and 316 SS) in the heat-transport circuits of water-cooled nuclear power reactors [1,2]. The CEFM is used here to illustrate that the development of effective, highly deterministic models for predicting the progression of IGSCC in RCCs is possible.

The most damaging forms of corrosion are localized corrosion processes, such as Pitting Corrosion (PC), Stress Corrosion Cracking (SCC), Corrosion Fatigue (CF), Hydrogen Embrittlement (HE), Flow-Assisted Corrosion (FAC), and Crevice

Corrosion (CC), because they often lead failures with little warning. To date, predictions have been made largely based on empirical statistical models, such as, Extreme Value Statistics (EVS), which generally have failed to provide sufficiently accurate predictions to be useful from an engineering perspective, although they often bring allow the effective ordering of observations. The principal difficulty is that the damage depth (e.g., pit depth or crack length) within a large population is determined by two parameters in the Gumbel distribution function: the location parameter and the shape parameter [2]. In the empirical form of EVS, both of these parameters must be determined by calibration, which requires a large database of crack depth (for example) at various times in the past. This is so, because in the original EVS model, no method was available for predicting deterministically the time dependencies of the two parameters or their values. Thus, the predicted result had to be known in advance of the prediction being made. This limitation was addressed by the development of Deterministic Extreme Value Statistics (DEVS) and Deterministic Monte Carlo Simulation (DMCS) [2], but to the author's knowledge, these models have only been applied to the SCC failure of LPST blades and natural gas pipelines [2].

Philosophical Basis of Determinism vs Empiricism

The philosophical basis of science has been discussed extensively, extending all the way back 2870 years when Aristotle (384-322 BC) published his treatise, Physiks [6] in 350 BC. Aristotle is often credited with defining the concept of causality, upon which modern science is based. Although he did discuss at some length the relationship of "cause" and "effect", he did not do so in terms of modern, quantifiable physical concepts, such as "force" or "displacement", respectively. Nevertheless, Aristotle, for his time, displayed great insight into the philosophical basis of the natural World and his views have been propagated through the ages. Indeed, it is possible to detect in his writings, the foundation of Newton's Laws of Motion, which are generally regarded as being the basis of modern physics. Presumably, Newton was aware of the writings of Aristotle, as were most natural philosophers of the time. However, a comprehensive discussion of the philosophy of science is well beyond the scope of this paper and this important subject will not be discussed further in this paper. The views expressed here on "science" are strictly those of the author, and no pretense is made that the views represent those of mainstream scientists or scientific philosophers.

The author's Extensive inquiry into the nature of science and the role of determinism in the scientific process, has led him to the view that "science" is the transition from empiricism (observations) to determinism resulting in the formulation the natural laws, which are condensations of all scientific knowledge. The process involves the formulation of postulates that are empirically based, from which are developed theories and models with the latter being the calculational arm of the former. The natural laws of relevance in of the development of the CEFM are the laws of the Conservation of Mass, the Law of the Conservation of Charge, and the Faraday's Law of Mass-Charge Equivalency. A particularly important feature of the natural laws is that they are time- and space-invariant. Note that a theory and the resulting model may be based upon one or more (often multiple) natural laws, and it is important to emphasize that all laws must be compatible in that any given law cannot violate other laws that may be only peripherally related to the subject at hand. If such a conflict exists, one or both are not "natural laws", and the conflict must be resolved before proceeding further. The transition from empiricism to determinism, and hence "science", involves the development of theories and models that are compatible with all natural laws, with the "scientific method" being used to nudge the models toward reality, recognizing that "reality" is a figment of the observer's imagination. These concepts are discussed in greater detail below.

Finally, pure "determinism" in any model is an idealized, unachievable state since all models contain data and concepts that are empirically based, and the CEFM is no exception. Thus, the temperature dependence of the Crack Growth Rate (CGR) can be calculated, by first calibrating the CEFM on two CGR data at different temperatures for specified values of the other independent values. With this minimal calibration, the CEFM accurately predicts the response of the CGR on the various independent variables within the range of experimental observation. Importantly, the CEFM predicted the previously unreported dependence of the CGR on the Electrochemical Crack Length (ECL). Elsewhere [1], the author describes a deterministic model for predicting the rate of propagation of an Intergranular Stress Corrosion Crack (IGSCC) in sensitized Type 34 SS in the Primary Coolant Circuits (PCC) of Boiling Water (Nuclear) Reactors (BWRs) operating at any power level and with a specified water chemistry [7-20]. The theoretical basis of the CEFM is the Differential Aeration Hypothesis (DAH), which has been the mainstay of localized corrosion studies for about a century. The important aspect of the CEFM that was not captured by previously in the study of Stress Corrosion Cracking (SCC) is flow of the current from the crack tip resulting from metal dissolution, which is annihilated on the external surface by oxygen reduction or hydrogen evolution (Figure 1). The model solves for the current and potential distributions using the Nernst-Planck equations in both the crack internal and external environments and then finds, iteratively, the potential at the crack mouth at which the current exiting from the crack is quantitatively annihilated on the external surface as indicated in Figure 1.

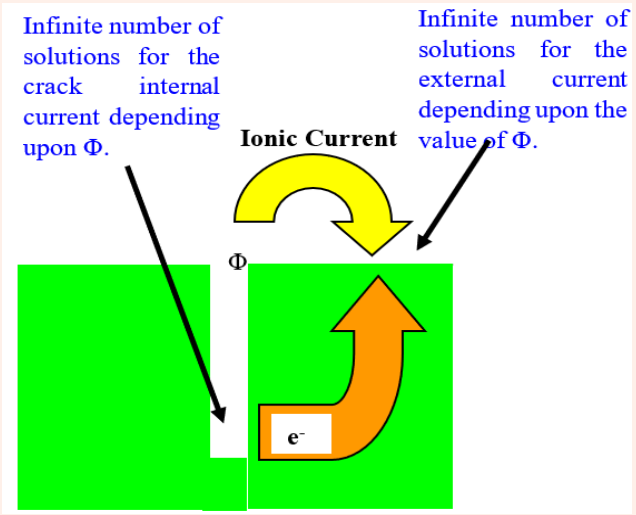

Figure 1: Schematic of the origin of the coupling current in stress corrosion cracking, according to the CEFM. The coupling current is required by the differential aeration hypothesis for localized corrosion, and the conservation of charge requires that the electron current flowing from the crack to the external surface must be equal to the positive ionic current flowing through the solution from the crack to the external surface.

The calculated potential distribution within the crack is then used to calculate the metal dissolution current density at the crack tip from which the CGR is estimated from Faraday's law. The model "engine" is based upon the natural laws referred to above and the constraints are the conservation laws including the conservation of mass, charge, and the equivalency of mass-charge as expressed through Faraday's law. Ideally, before any model building occurs, the literature should be searched for all information that is available for the system. This was done retroactively in the present case, as is done for most models, by searching the scientific, engineering, and anecdotal databases for Crack Growth Rate (CGR) data as a function of the selected independent variables; namely, in this case, Temperature (T), Electrochemical Potential (ECP), Degree of Sensitization (DoS), Stress Intensity Factor (K_I), Conductivity (κ), Yield Strength (YS), and solution composition, principally, the pH. As expected, the matrix of the dependent variable vs the independent variables was found to be sparse, because not all independent variables were reported by the authors. For example, the ECP was seldom reported, except for the more modern, laboratory studies after effective reference electrodes that could operate at 288 °C had been developed. However, knowing the temperature and the composition and hydrodynamics of the system, the ECP can be predicted with acceptable precision using the Mixed Potential Model (MPM) [1,2]. Likewise, if the solution composition is reported, the calculation of the conductivity can be performed. In this manner, the matrix was "filled out" so that a complete CGR vs T, ECP, DoS, K_I, κ, and YS database could be developed.

The collected data were analyzed using an Artificial Neural Network (ANN) comprising an input layer of the independent variables, an output layer of the dependent variable (CGR), and three hidden layers all of which were linked to the neurons in the preceding and following layers by connections of specific weights [21,22]. The data were divided into three groups; 70% were employed in training the net, 15% were employed to evaluate the net, and the remaining 15% were used to predict the CGR in the case were there were no reliable measures of that quantity. The data for each group were chosen randomly. The net was trained by in a supervised learning, back propagation manner until the square root of the sum of the squares of the differences between the predicted and observed CGRs was at a minimum via optimization of the weights between each neuron in the preceding and following layers. A plot was then made of the ANN predicted CGR vs the observed CGR as displayed in Figure 2. If the net predicted the observed CGR with infinitely high fidelity, the plot would be a straight line of 45° slope, as indicated by the solid line in Figure 2. Instead, as expected, the data are scattered about this line with the 95th percentiles being indicated within the two broken lines. The scatter suggests that

the ANN can predict the CGR to the 95th percentile to within ± 0.4 of a log unit; a level of precision that is much greater than that indicated by plotting the CGR against a single independent variable (e.g., K_I) as had been done in the past. From the weights between the various neurons in the ANN, it is possible to calculate the relative contributions of the various independent variables to the dependent variable (CGR); that is, the weights define the "character" of the crack growth process in the alloy [21,22]. These contributions are given in Table 1. The first column lists the independent variables and the second states the range over which each independent variable varies in the database. The third column presents the contributions for IGSCC in sensitized Type 304 SS [21] while Columns 4 and 5 present the corresponding data for Alloy 600 [22].

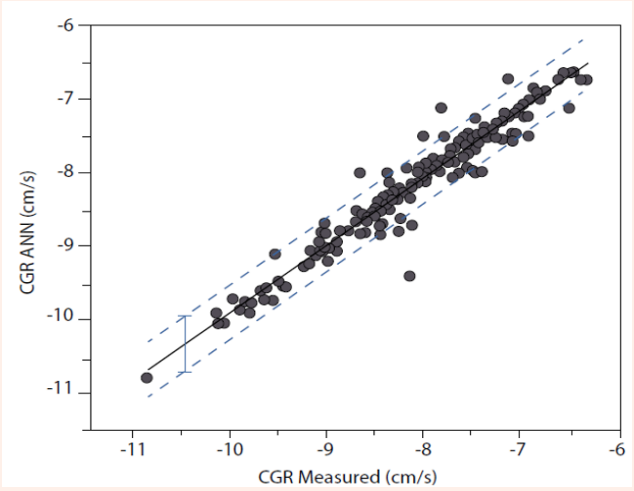

Figure 2: Logarithmic plot of ANN predicted CGR against measured CGR in the training and validation subsets of the database for sensitized Type 304 SS in BWR primary coolant (pure water at 288 °C). The broken lines define the 95th percentiles of ± 0.4log (CGR CEFM). After Shi et.al. [21]. The axes are the logarithms to the base 10.

Table 1: Contributions of various independent variables to IGSCC in sensitized Type 304 SS and Alloy 600 in simulated BWR primary coolant and simulated PWR coolant, respectively [22,23].

Independent Variable	Range	Type 304 SS in BWR Primary Coolant	Range	Alloy 600 in PWR Primary Coolant
Temperature (°C)	25 - 292	17.8	290 - 360	18.6
ECP (V_{she})	-0.575 – 0.496	43.6	-1.096 to -0.610	14.1
Stress Intensity Factor (MPa·√m)	10.4 – 67.78	10.8	4.6 - 101	15.2
Conductivity (μS/cm)	0.52 – 5.72	14.0	1.7 -11.6	14.1
Degree of Sensitization (DoS) (C/cm^2)	0 – 33.79	13.8	-	-
Yield Strength (MPa)	N/I	-	211 - 500	12.0
[LiOH] ppm	N/A	-	0 - 10	4.0
[H_3BO_3] ppm	N/A	-	0 - 1800	7.6
pH	N/A	-	5.52 – 9.19	14.5

For sensitized Type 304 SS in simulated BWR primary coolant, the most important contributions are from environmental variables (ECP>temperature>conductivity) followed by the metallurgical variable (DoS), and finally from the mechanical variable (stress intensity factor) [21]. Insufficient data were reported for the carbon content, heat treatment protocols and parameters, yield strength, hardness, extent of cold work, etc, to include those variables in the analysis, even though their impact on IGSCC in sensitized Type 304 SS is well-known. Furthermore, the pH for pure water is determined by the dissociation constant for water assuming the absence of acidic or basic impurities and, therefore, is not an independent variable. The contributions to the character demonstrate that IGSCC in sensitized Type 304 SS in simulated BWR primary coolant is primarily an electrochemical process augmented by metallurgy and mechanics.

A similar analysis of IGSCC in mill-annealed Alloy 600 in simulated PWR primary coolant (H_3BO_3/LiOH) was also reported by Shi et.al. [22], in which the independent variables gleaned from the database are T, ECP, KI, conductivity, yield strength, [LiOH], [H_3BO_3], and pH. The concentrations of boric acid and lithium hydroxide typically vary from 2000 ppm to 0 ppm and 0 ppm to 4 ppm, respectively, from the beginning to the end of a fuel cycle during normal power operation. Since the pH is determined by [LiOH] and [H_3BO_3], strictly pH, is, again, not an independent variable. However, it was included in the analysis because pH does have a discernible effect on the CGR. As shown in Table 1, the character of IGSCC in Alloy 600 is markedly different from that in Type 304 SS, being equally environmental (T, ECP, conductivity, pH), metallurgical (yield strength), and mechanical (KI) in character. In both cases, electrochemistry (ECP, conductivity, pH) plays an important role in determining CGR, but electrochemistry was ignored for many years because such studies tended to be carried out in Mechanical Engineering and Nuclear Engineering departments in universities and in research institutes/national laboratories where electrochemical expertise was minimal. In the author's opinion, this reflected the fact that electrochemistry is seldom included in the teaching curricula in those disciplines. Regardless of the tortured path taken to include electrochemistry in such studies, any viable theory and resulting model must account for the characters identified above including the electrochemical character.

A comprehensive way in which to assess the predictions of a CGR model, such as the CEFM, is to use the model to calculate the CGR for the set of independent variables for each datum in the observed CGR database and then to plot the CEFM-predicted CGR against the observed values. Such a plot is displayed in Figure 3. The plot shows that the CEFM and the ANN agree within a 95th percentile of ± 0.4 Log units (± a factor of 2.5) over wide ranges in the independent variables. This is about the accuracy with which CGR can be measured under optimal conditions and this has led to the opinion that the CEFM can calculate the CGR about as accurately as it can measured for the ranges of the independent variables considered in this study. Finally, the application of the CEFM to predicting the evolution of IGSCC damage in an operating BWR is illustrated in Figure 4, which shows a comparison of predicted crack length in the heat-affected zone of the H3 weld in a BWR core shroud as a function of time after Outage 11. The software package employed in this prediction (ALERT) included a subprogram for describing the thermal hydrodynamics of the primary coolant circuit, another subprogram for predicting the concentrations of the radiolysis products (O_2, H_2, H_2O_2, e-, OH, H, HO_2, etc., and the CEFM that calculated the ECP and the CGR for the inputs that it receives from the prior subprograms. The CGR was then integrated over the prior operating history of the reactor to yield the integrated damage (the crack length) at any specified time after startup of the reactor. Because the initiation time of the crack was unknown, the trajectory of the calculated damage (ALERT in Figure 4) was made to pass through the datum for the start of the operating period after Outage 11 by adjusting the crack initiation time. Accordingly, only the comparison between the predicted crack length and the observed value for 20 months after the 11th outage has probative value. The close agreement between the predicted and the observed crack length attests to the practicality of modeling the progression of IGSCC damage in the components within the PCCs of operating BWRs. Extrapolating the crack length back to zero crack length theoretically should yield the crack initiation time but this was not done because of the paucity of the data recognizing that the initiation time is a statistically distributed quantity.

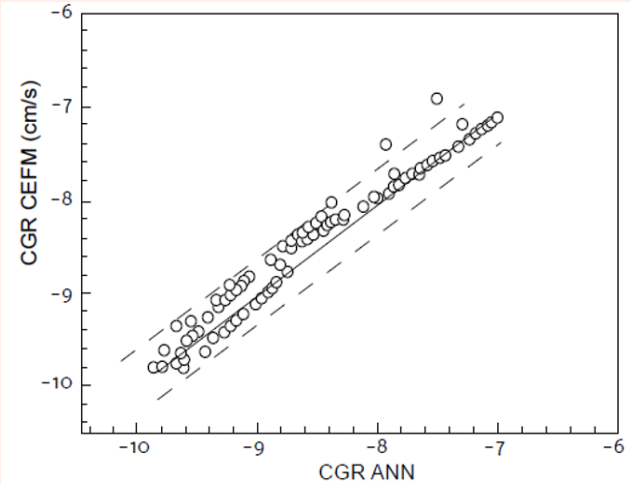

Figure 3: Comparison between CGR for IGSCC in sensitized Type 304 SS in simulated BWR primary coolant (pure water at 288 °C, calculated via the trained ANN and that calculated using the CEFM for identical sets of independent variables. The broken lines define the 95th percentile of ±0.4Log units. Adapted from [21].

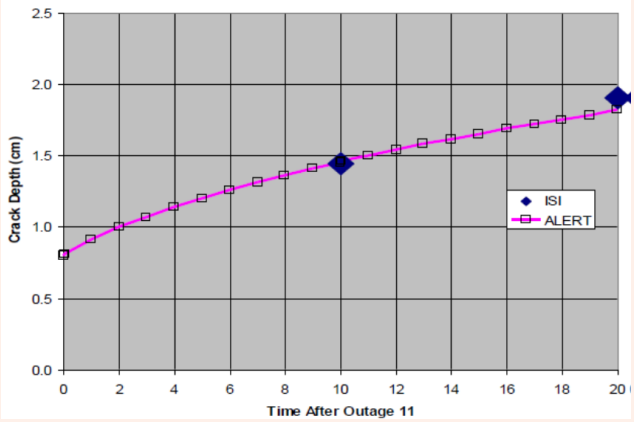

Figure 4: Comparison of predicted crack length in the heat-affected zone of the H3 weld in a BWR core shroud as a function of time after Outage 11. ♦ Tang et al. [23].

Summary and Conclusions

"Science" is portrayed as the evolution of empiricism (observation) to determinism, where the future can be predicted from the past upon the basis of the natural laws, which are the condensation of all previous scientific knowledge. However, this view must be tempered with the caveat in that the system evolutionary path must be defined in terms of those independent variables that have a significant impact on the dependent variable. This is commonly the most unpredictable problem in predicting future behavior. Nevertheless, predictions are made by using deterministic models, which are the calculational arms of theories. The salient issues in this process are summarized as follows.

a. All theories and models are incorrect because they are conceived via imperfect senses and intellect, so that they can never describe "reality". However, they are nudged toward that ideal goal by the "scientific method" of cyclical prediction and evaluation.

b. The theories themselves must be based upon observation using postulates that are consistent with observation and assumption that, while not necessarily being demonstratably true, are reasonable expectations of current knowledge.

c. In the "scientific method", the model must not be evaluated against the same data and postulates that were used in formulating the theory and calibrating of the model.

d. The theory itself should be "global", in that it accounts for all known observations about the system and "local" theories are discouraged, because they are based upon incomplete information, often being only based upon observations made by a single researcher.

e. Importantly, all deterministic models must possess a theoretical basis but not all theories need to calculate.

f. All deterministic models must contain a feedback loop that facilitates the enactment of the "scientific method", in which the model is continually tested against new observations. If discrepancies are observed, the model is modified within the bounds of observation and the prediction is repeated.

g. A deterministic model generally comprises constitutive equations that describe the operation of the model and constraints, the latter commonly being the natural conservation laws. The number of constitutive equations and the number of constraints must be at least equal to the number of unknown parameters in the model.

h. If no amount of change within the bounds of observation can resolve differences between the predicted and observed dependent variable, the model and the theory must be discarded. It is important to note that no amount of successful prediction can "prove" a model and its underlying theory to be correct but only one instance of disagreement is necessary to prove the model and theory incorrect.

Model building is illustrated by describing the development of the Coupled Environment Fracture Model (CEFM) that was developed by the author and his colleagues for predicting crack growth rate due to Stress Corrosion Cracking (SCC) in structural alloys in the primary coolant circuits of water-cooled nuclear power reactors, particularly Boiling Water Reactors. The theoretical basis of the CEFM is the Differential Aeration Hypothesis (DAH) that has stood the test of time in describing localized corrosion processes, such as SCC, pitting corrosion, and crevice corrosion.

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