Numerical Modeling for Corrosion

by Shinji Fujimoto

The ECS Corrosion Division was established in 1942 to organize and promote discussions associated with the behavior of materials in environments that cause corrosion, oxidation, and related surface reactions. This Division provides a forum for scientists and engineers to meet and discuss common problems in the hope of advancing research, education, and training in this important field.

Over the years, a number of the members of the Corrosion Division have served as ECS President, including H. H. Uhlig, N. Hackerman, F. L. LaQue, D. A. Vermilyea, T. R. Beck, R. C. Alkire, R. P. Frankenthal, W. H. Smyrl, B. MacDougall, and P. M. Natishan. Over the past seven decades, the Division has sponsored numerous corrosion related symposia and organized the Corrosion Monograph series of books that outline and review many areas of corrosion science and engineering. The *Corrosion Handbook*, originally edited by H. H. Uhlig in 1946 (its 3rd edition was revised by R. Winston Revie in 2011), remains one of the most popular corrosion reference books worldwide.

In this issue, we present four articles related to numerical approaches to corrosion science and engineering. Corrosion damage of equipment, production facilities, and infrastructure has severe consequences, including loss of property, interruption of production and transportation, and outage of electricity, water, and gas supplies. Such disruptions occur at a very high cost to society. While it is difficult to estimate the direct economic loss due to corrosion damage, the expense incurred to avoid/prevent corrosion damage, *i.e.*, "corrosion cost," has been estimated for several economies, including that of the U.S.,[1] Japan,[2] and the EU.[3] The corrosion cost is invariably high, at a few percentage points of GDP annually (3.1% of GDP in the U.S.[1]).

To minimize corrosion cost, a large amount of effort has been expended to facilitate prediction of corrosion damage. To accurately predict corrosion events, it is necessary to establish high-quality numerical models for a wide range of very complicated corrosion phenomena. In the decade from 1970 to 1980, numerical calculations mainly used finite element methods (FEM) and yielded deterministic models for the study of localized corrosion.[4,5] Such studies contributed to the fundamental understanding of the mechanisms of localized corrosion, but were not necessarily practical for actual corrosion prediction. Subsequently, stochastic or probabilistic models[6] were developed based on the distribution of the (corrosion-induced) failure time in the laboratory and/or in the field. These approaches introduced high-level statistics and other mathematical methods in conjunction with accumulated field data, and were successful in predicting localized corrosion phenomena, such as pitting corrosion and stress corrosion cracking experienced in process industries.[7]

To predict corrosion damage for new combinations of materials and environments, the stochastic and probabilistic approach is not necessarily effective, and deterministic models are required. Recent improvements in and development of computing technologies and calculation methods, including first principle calculations, have enabled advanced numerical modeling of corrosion phenomena as a combination of electrochemistry, solution chemistry, mass transfer, and atomistic process.

The four articles in this issue provide both an historical outline and recent developments in numerical corrosion modeling. Liu and Kelly review the fundamental numerical modeling of localized corrosion by electrochemistry and mass transfer using FEM, and introduce their recent results adopting a commercial FEM package with electrochemical modules.

The article by Amaya, Yoneya, and Onishi describes a practical corrosion prediction method for large-scale structures, such as the cathodic protection of the hull of a ship and large ocean structures using the boundary element method. The introduction of the inverse analysis method based on Bayesian estimation enables the study of large-scale structures by combining numerical calculations with in-field monitoring of parameters such as the corrosion potential.

The article by Tylor reviews the most recent *ab initio* calculations on corrosion processes at the atomistic scale and introduces approaches pertaining to molecular design of corrosion inhibitors, chemisorption of molecules and ions on metals or surface passive films that are closely related to corrosion, and characterization of the structure of the metal/oxide interface.

Finally, the article by Laycock, Krouse, Hendy, and Williams addresses both the deterministic model and the stochastic model. The authors attempt a full description of the pitting corrosion process, including initiation and propagation, on stainless steel in an attempt to develop a reliable predictive model for industrial applications.

The articles in this issue review the current validity and future possibilities pertaining to the prediction of corrosion by numerical modeling. Recently, in the area of materials science, the concept of the Materials Genome has been launched, where comprehensive approaches encompassing experimental and numerical simulation are recognized to be significant. The typical corrosion scientist is well versed in experimental work, but perhaps not so much in modeling. If this issue provides the requisite introductory guidance to numerical modeling of corrosion, the authors would be very pleased!

About the Author

Shinji Fujimoto is the Past Chair of Corrosion Division. He is currently a Professor in the Division of Materials and Manufacturing Science, Graduate School of Engineering, Osaka University, Japan. He graduated from Osaka University, and obtained Dr. Eng. degree in Metallurgical and Materials Engineering from Osaka University in March 1987. Immediately afterwards, he joined the Metallurgy and Materials Engineering Department (currently Division of Materials and Manufacturing Science), Osaka University. He was appointed to the position of Professor of Environmental Materials in 2002. He stayed at the Corrosion and Protection Centre of UMIST, Manchester, UK in 1991-1992 as a Research Associate. His research interests are corrosion science and engineering, including passivity, localized corrosion, surface modification and electrochemical characterization of metallic biomaterials. He may be reached at fujimoto@mat.eng.osaka-u.ac.jp.

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