

Phase IV of the CSP Consortium ended in 2010. During this phase and the 3 prior phases (I, II, III, and IV) of the CSP consortium, we have achieved the following objectives:

1. *Development of comprehensive software tools for studying the thermodynamics of corrosion*

These tools make it possible to predict under what conditions a given metal is expected to be immune to corrosion or potentially passive or undergo dissolution. Also, they predict the thermodynamically stable corrosion products. They include the following facilities:

- 1.1. *Software for generating real-solution electrochemical (Pourbaix) diagrams.* These diagrams are based on Pourbaix's concept of E-pH diagrams and are generated using our comprehensive activity coefficient models in addition to standard-state properties. Also, they offer a flexible selection of independent variables in addition to E and pH.
- 1.2. *Software for generating chemical stability diagrams.* These diagrams are useful when species concentrations and temperature are more useful as independent variables than potential.
- 1.3. *Corrosion databanks.* These databanks contain thermodynamic properties of various corrosion products.

Unlike the electrochemical models for general and localized corrosion that will be mentioned later, these facilities are available in conjunction with both the aqueous and MSE models. Details about these modules are available in the following papers:

- A. Anderko, S.J. Sanders and R.D. Young, "Real-solution stability diagrams: A thermodynamic tool for corrosion modeling" *Corrosion*, 53 (1997) 43-53
- A. Anderko and P.J. Shuler, "A computational approach to predicting the formation of iron sulfide species using stability diagrams" *Computers & Geosciences*, 23 (1997) 647-658
- N. Sridhar, D.S. Dunn, A. Anderko, M.M. Lencka and H.U. Schutt, "Effect of water and gas compositions on the internal corrosion of gas pipelines – modeling and experimental studies" *Corrosion*, 57 (2001) 221-235.
- N. Sridhar, D.S. Dunn and A. Anderko, "Prediction of Conditions Leading to Stress Corrosion Cracking of Gas Transmission Lines", in "*Environmentally Assisted Cracking: Predictive Methods for Risk Assessment and Evaluation of Materials, Equipment and Structures*", ASTM STP 1401, edited by R.D. Kane, American Society for Testing and Materials, West Conshohocken, PA (2000), p. 241.

2. *Electrochemical model of general corrosion*

This is a mixed-potential model that simulates the partial cathodic and anodic processes on a metallic surface in an aqueous environment. It represents the dissolution in the active and passive states including the active-passive transition. The model predicts the rates of general corrosion and the corrosion potential. It can be used to evaluate the effects of environment

chemistry on general corrosion for static and single-phase flowing systems. Details about this model are available in the following papers:

- A. Anderko and R.D. Young, "A model for corrosion of carbon steel in lithium bromide absorption refrigeration systems" *Corrosion*, 56 (2000) 543-555
- A. Anderko, P. McKenzie and R.D. Young, "Computation of rates of general corrosion using electrochemical and thermodynamic models" *Corrosion*, 57 (2001) 202-213
- A. Anderko and R.D. Young, "Simulation of CO₂/H₂S Corrosion Using Thermodynamic and Electrochemical Models", paper no. 31, CORROSION/99, NACE International, Houston, TX, 1999
- A. Anderko, "Simulation of FeCO₃ / FeS Scale Formation Using Thermodynamic and Electrochemical Models", paper no. 102, CORROSION/2000, NACE International, Houston, TX, 2000
- N. Sridhar and A. Anderko, "Corrosion Simulation for the Process Industry", paper no. 1348, CORROSION/2001, NACE International, Houston, TX, 2001
- N. Sridhar, C.S. Brossia, D.S. Dunn and A. Anderko, "Predicting Localized Corrosion in Seawater" *Corrosion*, 60 (2004) 915-936

3. *Electrochemical model of localized corrosion*

This model predicts the long-term occurrence of localized corrosion (i.e., pitting or crevice corrosion) by comparing the corrosion potential with the repassivation potential. The corrosion potential is calculated from the general corrosion model whereas the repassivation potential is obtained from a separate model for the repassivation of pits and crevices. In addition to providing an indicator of whether localized corrosion is likely to occur or not, it provides a maximum propagation rate for individual pits or crevices. The fundamentals and applications of this model are described in:

- A. Anderko, N. Sridhar and D.S. Dunn, "A General Model for the Repassivation Potential as a Function of Multiple Aqueous Solution Species" *Corrosion Science*, 46 (2004) 1583-1612
- N. Sridhar, C.S. Brossia, D.S. Dunn and A. Anderko, "Predicting Localized Corrosion in Seawater" *Corrosion*, 60 (2004) 915-936
- A. Anderko, N. Sridhar, L.T. Yang, S.L. Grise, B.J. Saldanha and M.H. Dorsey, "Validation of a Localized Corrosion Model Using Real-Time Corrosion Monitoring in a Chemical Plant" *Corrosion Engineering, Science and Technology*, 40 (2005) 33-42
- A. Anderko, N. Sridhar, M.A. Jakab, and G. Tormoen, "A General Model for the Repassivation Potential as a Function of Multiple Aqueous Species. 2. Effect of Oxyanions on Localized Corrosion of Fe-Ni-Cr-Mo-W-N Alloys", *Corrosion Science*, 50 (2008) 3629-3647

4. *Predicting the effects of heat treatment*

This module predicts the chromium and molybdenum depletion profiles in the vicinity of grain boundaries in stainless steels and nickel-base alloys. Based on the depletion profiles, the module predicts the effect of thermal aging on the repassivation potential and, hence localized corrosion. Also, the depletion parameter is calculated to indicate the susceptibility to intergranular attack and intergranular stress corrosion cracking.

- A. Anderko, N. Sridhar, and G. Tormoen, "Localized Corrosion of Heat-Treated Alloys. II. Predicting Grain Boundary Microchemistry and Its Effect on Repassivation Potential", *Corrosion Eng. Sci. Tech.*, in press
- N. Sridhar, G. Tormoen, S. Hackney, and A. Anderko, "Effect of Aging Treatments on the Repassivation Potential of Duplex Stainless Steel S32205", *Corrosion*, in press

5. *Deterministic extreme value statistics*

This module predicts the evolution of corrosion on the basis of short- and medium-term exposure data. It is based on damage function analysis combined with probabilistic treatment of corrosion. It can be applied to various forms of corrosion and predicts not only the probability of failure as a function of exposure area (which is the domain of classical extreme value statistics) but also extrapolates the corrosion damage with respect to exposure time. The details are given in:

- G. Engelhardt and D. D. Macdonald, "Unification of the Deterministic and Statistical Approaches for Predicting Localized Corrosion Damage. I. Theoretical Foundation", *Corrosion Science*, 46 (2004) 2755
- D.D. Macdonald and G.R. Engelhardt, "Unification of the Deterministic and Statistical Approaches for Predicting Localized Corrosion Damage in Aircraft Aluminum Alloys", 9th Joint FAA/DoD/NACE Conference on Aging Aircraft, Atlanta, GA (2006)

6. *Databank of parameters*

In conjunction with the models described above, parameters have been developed to represent the electrochemical behavior of the following alloys in common aqueous environments:

Carbon steel
Stainless steels: 304, 316, 13Cr, 254SMO
Nickel-base alloys: 600, 690, 825, 625, 276, 22
Aluminum