Modeling of Corrosion of Corrosion Resistant Alloys:

A Mechanistic Approach to Predict Corrosion in Chemical Processes Environments including Mixed Acids and Salts

Conversations with OLI Experts on Science of Electrolyte Chemistry
Issue 4.0

OLI Expert: Dr. Ali Eslamimanesh

Key Questions for the OLI Expert:

- **Why is corrosion important in chemical industry?**

The chemical processes environments often contain corrosive multicomponent systems including mixed acids as well as their mixtures with or without salts usually accompanied by various types of gases. These components potentially lead to significant corrosion issues in chemical processes brining about equipment failure and the regular shutdowns and overhauls of the chemical plants. For instance, high corrosion rates can be seen on piping, pumps, boilers, and reactors depending on the operational conditions. By the way, a comprehensive study by National Association of Corrosion Engineers (NACE) in 2016 showed that the direct cost of corrosion in industry is B$276 / year which is equivalent to 3.1% of US GDP.

- **How about corrosion in oil and gas industry? What are the main issues?**

Corrosion phenomena in the petroleum industry are one of the major issues that affect the integrity of production, process, and transportation facilities. In the recent decades, the main concern has been the production of oil, gas, or gas condensates from deep wells where temperature, pressure, and pH can exceed the resistance thresholds of materials that are typically used in the operations. In practice, presence of aggressive species such as chlorides, carbon dioxide, and hydrogen sulfide at high concentrations can result in substantial general and localized corrosion, particularly when large amounts of formation and/or injection water are produced. Localized corrosion is of particular interest, because it that can be a precursor to stress corrosion cracking (SCC) which is a common problem in the aforementioned systems.

- **If corrosion problem is so severe, what types of materials are used in construction of the corresponding processes equipment?**

Typically, corrosion resistant alloys (CRAs) are applied in such environments. The usage of these materials has been soaring due to the need for improving equipment reliability and safety in operations in which considerable amounts of corrosive fluids are present.

- **How resistant are the corrosion resistant alloys to corrosion?**

Although CRAs are much more resistant to general (or uniform) corrosion compared to carbon steel or low alloy steels, depending on their elemental structures, they can be susceptible to localized corrosion as well as environmentally assisted cracking (EAC) in harsh sour environments in the forms of sulfide stress cracking (SSC) and stress corrosion cracking.

- **We know that there are widely-used standards for material selection for these processes. Then, why do we study the corrosion theoretically?**

That is true. In practice, determination of the applicability domain of CRAs are done pursuing one or several of these steps: 1. Standards and guidance documents such as NACE, ASME, or ASTM standards; 2. Direct laboratory tests like weight loss or electrochemical measurements; 3. Empirical correlations as a function of specified alloy components and/or ranges of corrosive components.

However, these solutions suffer from the lack of a common and general methodology. For instance, inconsistent test results and interpretations may be obtained from different test laboratories, which might lead to inappropriate qualification of CRAs. Plus, in order to provide reliable qualifying results, laboratory tests need to be performed under proper definition of corrosion test requirements and wide range of desired operational conditions.

As a consequence, there is a need to establish predictive models that could quantify and simulate the behavior of CRAs in complex process environments. Development of such models require in depth theoretical study of corrosion through a mechanistic approach.

- **What are the key elements of the OLI Systems general corrosion model?**

Our corrosion modeling framework consists of a thermophysical and an electrochemical module. The thermophysical module describes the phase and chemical equilibrium in the aqueous system and consequently computes the speciation, activities and transport properties of solution species that participate in interfacial reactions. These quantities are then plugged in the electrochemical module, which is based on the mixed-potential theory, in order to simulate the kinetics of electrochemical reactions. The electrochemical module considers various partial cathodic and anodic reactions that may occur on the surface of the metal or alloy and also the transport processes for the electrochemically active species. The key feature here is that the model accounts for the active-passive transition and dissolution in the passive state.

- **What are the challenges in corrosion modeling of CRAs used in the chemical environments where we have acid mixtures along with salts?**

As a matter of fact, there are plenty of data for bare metals or alloys in various single-component chemicals (e.g. pure acids) exists in the literature that are being used for material selection. However, the chemical process fluids that we encounter in chemical industry are rarely single-component acids and are often found to contain various salts from catalysts, impurities from mixing water, or corrosion products.

The corrosion rate in many mixtures is a complex function of solution and alloy composition, which limits interpolation or extrapolation of data from a small number of experimental measurements. For example, fluoride acts as an aggressive species in dilute sulfuric acid, but it is considered as a corrosion inhibitor in concentrated sulfuric acid. Having said that, with appropriate parametrization, a mechanistic model can provide insightful solutions to these challenges and eventually bring about reliable prediction of corrosion behavior of CRAs in such systems.

- **Is OLI Systems corrosion model able to determine the susceptibility of CRAs to sulfide stress cracking in oilfield operations? If yes, how?**

The answer is yes but to a reasonable extent. I will tell you how. In the OLI's corrosion model, the repassivation potential (or protection potential) is calculated by solving the expression for the current density in an occluded localized corrosion environment, in the limit of repassivation. This parameter is then compared with the corrosion potential calculated from the general corrosion module to evaluate the general corrosion and the maximum localized corrosion propagation rates.

Considering the fact that the sulfide stress cracking (SSC) tendency correlates with the maximum propagation rate for localized corrosion, the results of the corrosion model can be compared directly with the applicability domain of a particular alloy under stress as a function of operational conditions like temperature, pH, chloride concentrations, and partial pressure of H_2S. It is, however, worthwhile to point out that this method considers only the electrochemical phenomena in the system and does not treat the effects of stress and mechanical properties.

- **What materials/tools are available for our viewers to learn more about prediction of corrosion of CRAs?**

The OLI Systems corrosion model is incorporated in OLI Corrosion Analyzer V10 and OLI Studio V10.

For more details on OLI Systems corrosion model, its components and applicability, the viewers are encouraged to consult the following publications of ours:

Eslamimanesh, A., Anderko, A. and Lencka, M.M., 2019, May. Prediction of general and localized corrosion of corrosion-resistant alloys in aggressive environments. In CORROSION 2019. NACE International.

Anderko, A. and Sridhar, N., 2015, May. Corrosion of Ni-based alloys and stainless steels in mixed acids and salts–experimental and modeling results. In CORROSION 2015. NACE International.

Anderko, A., Engelhardt, G.R., Cao, L., Gui, F. and Sridhar, N., 2016. Localized Corrosion of Corrosion-Resistant Alloys in Oil and Gas Production Environments: II. Corrosion Potential. In NACE International Corrosion Conference Proceedings. NACE International.

Anderko, A., Gui, F., Cao, L., Sridhar, N. and Engelhardt, G.R., 2015. Modeling localized corrosion of corrosion-resistant alloys in oil and gas production environments: part I. repassivation potential. Corrosion, 71(10), pp.1197-1212.

Sridhar, N., Thodla, R., Gui, F., Cao, L. and Anderko, A., 2018. Corrosion-resistant alloy testing and selection for oil and gas production. Corrosion Engineering, Science and Technology, 53, S1, pp.75-89.

Anderko, A., Cao, L., Gui, F., Sridhar, N. and Engelhardt, G.R., 2017. Modeling Localized Corrosion of Corrosion-Resistant Alloys in Oil and Gas Production Environments: Part II. Corrosion Potential. Corrosion, 73(6), pp.634-647.

July 2020