ADMINISTRATIVE INFORMATION

1. **Project Name:** Prediction of Corrosion of Advanced Materials and Fabricated Components

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5. **Date Project Initiated:** 11/17/2003

6. **Expected Completion Date:** 4/30/2007

PROJECT RATIONALE AND STRATEGY

7. **Project Objective:**

The goal of this project is to provide materials engineers, chemical engineers and plant operators with a software tool that will enable them to predict localized corrosion of process equipment including fabricated components as well as base alloys. For design and revamp purposes, the software will predict the occurrence of localized corrosion as a function of environment chemistry and assist the user in selecting the optimum alloy for a given environment. For the operation of existing plants, the software will enable the users to predict the remaining life of equipment and help in scheduling maintenance activities.

8. **Technical Barriers Being Addressed:**

Over the last two decades, many advanced metallic materials have been developed for withstanding severe corrosion and erosion that are encountered in industrial processes. However, the application of these materials by industry has fallen short of initial expectations because (i) their performance has been limited by fabrication processes, which are not considered in materials development and (ii) there has been a lack of tools to evaluate their corrosion performance in a given application prior to placing them in service. Corrosion reduces energy efficiency in chemical process industries through the consumption of energy in scheduled plant outages (for inspection and repairs), unscheduled downtime for corrosion-related failures, loss of efficiency in distillation and other separation processes, heat exchanger fouling by corrosion products, sub-optimal selection of operating temperatures to avoid corrosion risk, etc. At present, there is no technically sound basis for judging the corrosion performance of advanced metallic materials in real-world process environments without performing specific tests. Alloy designers and new process developers rely on standard laboratory tests, such as immersion tests in artificial seawater or ferric chloride to compare the performance of novel materials against previously used materials. These laboratory tests are not adequate for judging the true performance of fabricated materials in real-world environments. In some cases, pilot plant studies are conducted to select materials for the process. However, the pilot scale studies can be time-consuming and expensive. In the absence of reliable prediction techniques, industry tends to rely on conservative choices of materials or process parameters. Such conservative measures result in increased energy consumption by sub-optimal equipment design (e.g., thicker materials) or sub-optimal process conditions (lower temperature or throughput).

9. **Project Pathway:**

This project combines fundamental understanding of mechanisms of corrosion with focused experimental results to predict the corrosion of advanced, base or fabricated, alloys in real-world environments encountered in the chemical industry. The program aims to develop a software tool that will make it possible to predict the corrosion performance of base materials and fabricated components in any environment utilizing a minimum data set. At the heart of this approach is the development of correlations between local compositions in the alloy with fundamental parameters that control the occurrence of localized corrosion. The fundamental parameters that dictate the occurrence of localized corrosion are the corrosion and repassivation potentials. The program team, OLI Systems and Southwest Research Institute, has developed theoretical models for these parameters. These theoretical models are being extended to predict the occurrence of localized corrosion of base materials and heat-treated components in a variety of environments containing aggressive and non-aggressive species. The results of this project will allow process designers and operators to evaluate alloys under realistic conditions of fabrication and in-service chemical environments. Users will also be able to identify process changes, corrosion inhibition strategies, and other control options before costly shutdowns, energy waste, and environmental releases occur. These innovative corrosion mitigation measures can be tested in a virtual laboratory without risking the plant. The useful remaining life will be able to be predicted based on operating experience and projected operating conditions so that catastrophic failures can be avoided and well-planned corrosion control and maintenance actions can be proactively scheduled.

10. **Critical Metrics:**

- Demonstrate the accuracy of models for predicting both localized and general corrosion as a function of environment composition and temperature for selected base materials (baseline)
- Develop and verify methodology for predicting the effect of complex chemistry, including aggressive and inhibiting species, on the occurrence of localized corrosion of base materials (stainless steels, nickel-base alloys, copper-nickel alloys) and fabricated materials and show that it quantitatively agrees with results of standard tests; further, construct and verify methodology that quantitatively predicts the remaining life of fabricated components;
- Release this methodology to the chemical process industries in the form of an updated version of CorrosionAnalyzer, a commercial software product

PROJECT PLANS AND PROGRESS

11. **Past Accomplishments:**

- A comprehensive model has been established and extensively verified for predicting the occurrence of localized corrosion as a function of environment chemistry and temperature by calculating the corrosion and repassivation potentials.
- An experimental database has been developed to elucidate (1) the effects of various inhibiting species as well as aggressive species on localized corrosion of nickel-base alloys and stainless steels (2) the effects of heat treatment on localized corrosion and (3) the electrochemical behavior of Cu-Ni alloys.
- The models have been comprehensively parameterized for predicting general and localized corrosion for seven nickel-base alloys (22, 276, 625, 825, 600, 690, and Ni). Excellent agreement with experimental data has been obtained for alloys in various environments, including acids, bases, oxidizing species, inorganic inhibitors, etc.
- A probabilistic model has been established for predicting the long-term damage due to localized corrosion on the basis of short-term inspection results. This methodology is applicable to pitting, crevice corrosion, stress corrosion cracking and corrosion fatigue.
- A comprehensive model has been developed for predicting sensitization of Fe-Ni-Cr-Mo-W-N alloys and its effect on localized corrosion.
- CorrosionAnalyzer, a commercial software product has been developed and released to industry in an advanced preliminary version.

12. **Future Plans**:

Date	Milestone/Deliverable	Partner Activities
9/06	Finalizing the experimental database for Cu-Ni alloys and the effect of heat treatment on localized corrosion of Fe-Ni-Cr-Mo-W-N alloys	SwRI: Augmenting database OLI: Updating model parameters
9/06	Finalizing the model for predicting the effect of heat treatment on localized corrosion	OLI: Model implementation
3/07	Release a final commercial version of the CorrosionAnalyzer that includes prediction of the effect of heat treatment on localized corrosion and probabilistic prediction of propagation of localized corrosion	OLI: Software development Industrial Steering Group: Testing the software and feedback to OLI

13. **Project Changes:**

Measurements of the microstructure of heat-treated duplex stainless steel samples have been subcontracted to the Michigan Technological University rather than the Oak Ridge National Laboratory, as previously planned. This subcontract has contributed to elucidating the relationship between microstructure and the degradation of localized corrosion resistance of heat-treated duplex steels. Other technical activities are proceeding as planned. A six-month, no-cost extension of the project has been requested because of the anticipated delay in obligating the remaining funds. This will result in some delay in the final tasks of the project.

14. **Commercialization Potential, Plans, and Activities:**

The primary vehicle for the commercialization of this technology will be OLI Systems' CorrosionAnalyzer, a software tool that is currently used, in a more limited version, by many companies in the chemical process industry. The capabilities of the CorrosionAnalyzer are being dramatically enhanced as a result of this project. In process design, the results of this project (encapsulated in the CorrosionAnalyzer) will provide the industry with (1) reliable prediction of the tendency of base alloys for localized corrosion as a function of environmental conditions, (2) a quantification of the effect of heat treatment on corrosion resistance of fabricated elements, and (3) understanding of how to select alloys for corrosive environments. In process operations, the software will help to predict the remaining useful life of equipment based on limited input data. As industrial and infrastructure systems age (chemical process plants, pipelines, refineries, power plants, etc.), this will address the considerable economic incentive to avoid unscheduled outages and to extend operation beyond the design lifetime. Commercialization of the technology involves:

1. *Establishing an effective channel to the market.* OLI is utilizing its existing network of worldwide agents, strong, established client relationships, and marketing partners. One of OLI's principal strengths is its extensive penetration of the major companies comprising the CPI, currently exceeding 75 major CPI companies. The existing client relationships are an immediate pathway to commercialization of the proposed products.
2. *Technology transfer through industry groups, technical papers, professional association meetings.* OLI regularly publishes in peer-reviewed journals and presents at NACE meetings. Also, OLI provides periodic free regional seminars to inform and educate the industry.
3. *Establishment of software training courses and dedicated customer technical support.* This is a normal business practice for OLI. OLI has an excellent reputation in these areas.
4. *Application-specific projects, consulting and technical service.* Based on the software, technical services are offered to the industry on a project basis. Several successful projects have already been completed.

15. **Patents, Publications, Presentations:**

1. 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.
2. C.S. Brossia, A. Anderko and N. Sridhar, "Predicting the Long-Term Localized Corrosion of Alloys in Complex Industrial Environments", paper no. 172, EUROCORR 2004, Nice, France.
3. A. Anderko, N. Sridhar and C.S. Brossia, "Prediction of Corrosion of Nickel-Base Alloys and Stainless Steels in Oxidizing Environments Using Thermodynamic and Electrochemical Models", paper no. 05053, CORROSION/2005, Houston, TX.
4. N. Sridhar, C.S. Brossia, G. Tormoen and A. Anderko, "Life Prediction of Systems Subject to Localized Corrosion from a Limited Experimental Data Set", CORROSION/2005, Houston, TX.
5. N. Sridhar, "Continuum and Mesoscale Modeling of Localized Corrosion – Status and Future", Advanced Modeling of Corrosion Damage Evolution, ONR Workshop, Warrenton, VA, 6/14/2005.
6. A. Anderko, "Thermodynamic and Electrochemical Models for Predicting General and Localized Corrosion", Advanced Modeling of Corrosion Damage Evolution, ONR Workshop, Warrenton, VA, 6/14-15/2005.
7. A. Anderko, N. Sridhar, G. Tormoen and C.S. Brossia, "Modeling Localized Corrosion in Complex Process Environments in the Presence of Inhibitors", paper no. 06215, CORROSION/2006, San Diego, CA, March 12-16, 2006.
8. G. Engelhardt and D. Macdonald. "Monte Carlo Simulation of Localized Corrosion Damage", submitted to Corrosion Science.
9. G. Engelhardt et al., "Use of Channel Electrode for Electrochemical Kinetic Studies", submitted to Electrochimica Acta.