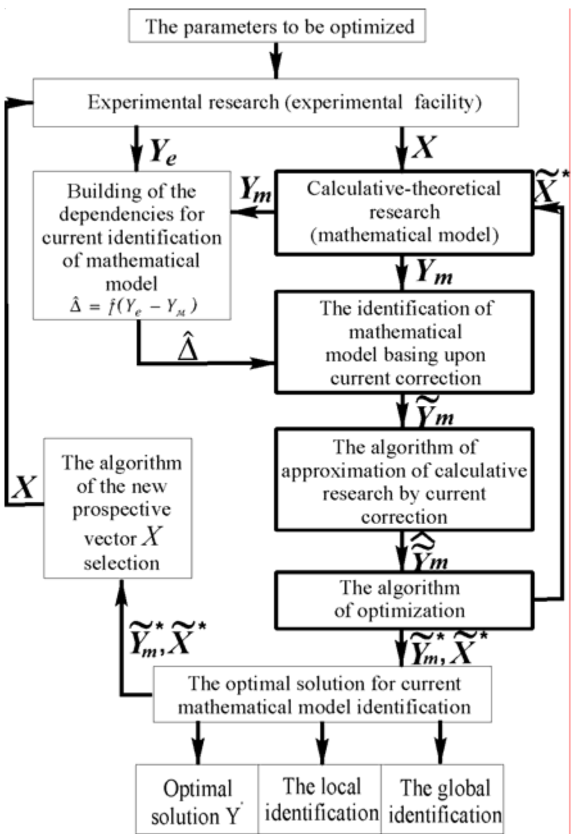
Industrial Technologies Program

Development of Semi-Stochastic Algorithm for Optimizing Alloy Composition of High-Temperature Austenitic Stainless Steels (H-Series) for Desired Mechanical and Corrosion Properties

Stochastic Optimization Algorithms Will Optimize the Composition of H-Series Steel Alloys for Optimized Mechanical and Corrosion Properties

There is an industry-wide need for improving material property performance for the applications they are currently used for and to increase their upper use temperature for applications that improve the process efficiencies, such as chemical and heat-treating processes carried out at higher than currently used temperatures. The project takes a new approach of using stochastic optimization algorithm for optimizing alloy properties with minimum number of experimental evaluations of the candidate alloys. The new approach has the potential of identifying compositions that cannot be identified without carrying out thousands of experiments. Furthermore, the approach has the potential for creating and designing alloys for each application, thereby maximizing their utilization at reduced cost.



The general scheme applied to calculation of theoretical and experimental research.

Benefits for Our Industry and Our Nation

- *The potential for energy savings from improved efficiencies of various processes in the chemicals, steel, and heat-treating industries when the alloys are commercialized is 38 TBtu/year by the year 2020.*

Applications in Our Nation's Industry

The alloys designed using the algorithms developed in this project will find applications in various industries, such as:

- Chemicals
- Forest Products
- Glass
- Petrochemical
- Petroleum
- Steel
- Supporting Industries

Project Description

The goal of this project is to adapt and use an advanced semi-stochastic algorithm for constrained multi-objective optimization and combine it with experimental testing and verification to determine optimum concentrations of alloying elements in heat-resistant and corrosion-resistant H-Series austenitic stainless steel alloys that will simultaneously maximize a number of alloy's mechanical and corrosion properties.

Barriers

- Low-fidelity analysis models are very inexpensive enabling optimization, but the validity of the obtained results can be rather low
- High-fidelity tools could be the experimental samples of the system or its components. However, the exclusive use of such high-fidelity tools in multi-objective optimization is associated with extreme time and cost expenditures
- An experimental search for optimum chemical composition of an alloy can be an unacceptably labor-intensive process

Pathways

The objectives of the project were met through the following tasks:

- Development of an initial plan of experiment (UTA)
- Analysis of the plan of experiment, identification of the objective functions, and objective constraints (UTA)
- Determining solution of M particular optimization problems for objective constraints (UTA)
- Experimental verification and identification of additional experiments needed (UTA, ORNL)
- Preparing alloys and developing tensile, creep, and corrosion data (UTA, ORNL)

Results

The major technical accomplishments from this project were the development of two new formulations for the design of superior alloy chemical compositions:

- A direct multi-objective optimization formulation that creates chemical compositions with extreme properties (maximum strength, maximum temperature, maximum time-to-rupture)
- An inverse design formulation that creates multiple new alloy concentrations, each satisfying prescribed values of desired operating stress, temperature and life expectancy

Commercialization

The tool development in this project occurred through very strong industrial interaction. For example, a large database of creep properties and detailed chemical analysis used in this project were provided by Duraloy. Based on that data, the current project identified several alternate compositions of H-series steels that could deliver improved creep strength properties. ORNL took some of the compositions identified through this analysis and further investigated them for their phase analysis and microstructural validation. Two of the compositions were produced as experimental heats and tested for their creep properties.

Further optimized H-series compositions, created using the phase stability and volume fraction, have been cast and fabricated into radiant burner tube assemblies. One of these assemblies is currently being tested at Nucore Steel.

The algorithm developed in this project has a strong commercial use potential in that it can assist in predicting the properties of the compositions that are outside the range for which the data was used. The implementation of such a capability by industry will require the development of an interactive computer-based tool with a range of property prediction options and data output that can be directly used by production, sales and design engineering staff.

Project Partners

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Bethlehem Steel Corporation
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The Timken Company
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A Strong Energy Portfolio for a Strong America

Energy efficiency and clean, renewable energy will mean a stronger economy, a cleaner environment, and greater energy independence for America. Working with a wide array of state, community, industry, and university partners, the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy invests in a diverse portfolio of energy technologies.

U.S. Department of Energy
Energy Efficiency
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