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Industrial Materials for the Future

Final Technical Report

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

June 2006

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Disclaimer

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Abbreviations and Acronyms

ANN	artificial neural network
IMF	Industrial Materials for the Future
IOSO	indirect optimization based upon self organization
ITP	Industrial Technologies Program
ORNL	Oak Ridge National Laboratory
TMS	The Minerals, Metals, and Materials Society
UTA	University of Texas at Arlington

1. Executive Summary

An industry-wide need exists for improving material property performance for the applications that 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 the 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 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. The approach consists of the use of an advanced semi-stochastic algorithm adapted for constrained multi-objective optimization combined with selective experimental testing and verification to determine optimum concentrations of alloying elements in heat-resistant and corrosion-resistant H-Series austenitic stainless steel alloys and Ni-based superalloys.

1.1 Alloy Design Tool

The research resulted in the development of a tool for the design of high-strength H-Series steels and other types of alloys unattainable by any existing means with minimum experimental effort. Such a tool can be used to reduce or minimize the need for the addition of expensive elements such as Cr, Ni, Co, Nb, Ti, or V and still obtain the optimum properties needed to design the components. The project achieved the following objectives:

- Devised a method for the development of a new class of alloys for high-temperature strength, corrosion, and thermal fatigue resistance;
- Effectively applied combinatorial methods for rapid screening of materials for industrial applications and/or materials property optimization; and
- Acquired thermophysical property data needed for materials processing and industrial applications.

1.2 Technology Transfer

The H-Series steel producer, Duraloy, and one of the users, ISG (previously, Bethlehem Steel), were made aware of the outcome of this project through project progress presentations at the Industrial Technologies Program/Industrial Materials for the Future (ITP/IMF) annual project review meetings. This was the most direct transfer of the outcome of the project to its partners.

Technology transfer to a broader audience occurred through presentations of this work at the national meetings of The Metallurgical Society (TMS) and two topical conferences dealing with multidisciplinary analysis and optimizations. One presentation was also made at an international conference in Brazil. In addition to presentations, six technical papers were published, which further enhanced the transfer of technology.

The technology transfer from this project also benefited from the incorporation of some of the results of this project in to the Duraloy/Oak Ridge National Laboratory (ORNL) project on development of novel H-Series steels with improved strength and higher upper-use temperature.

1.3 Commercialization

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

Duraloy, the main producer of H-Series steels has not directly used the outcome of algorithm developed in this project. However, further optimized H-Series compositions that are based on ORNL work 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 Nucor steel.

The algorithm developed in this project has a strong potential for commercial use because it can assist in predicting the properties of the compositions that are within the range for which the data was used, but for which the specific composition for an application has never been produced or tested. 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 used directly by production, sales, and design-engineering staff.

1.4 Recommendations

For effective use of the outcome of the algorithm developed in this project, the development of an interactive computer-based tool with range of property-prediction options and data output that can be directly used by production, sales, and design engineering staff is recommended. After the tool is developed, selective experimental validation of certain predicted properties is highly recommended.

2. Introduction

Experts from the leading countries of the world agree that a great need exists for advancing the performance of structural materials, including strength, corrosion resistance, and upper-use temperature. The need for improved methods for manufacturing these alloys has also been identified. To meet these goals, much money is being spent to develop materials that are generally more expensive than current methods because they require special melting, processing, machining, and welding processes. This project deals with an industry-wide need for improving material property performance for the applications for which it is currently used and to increase the upper-use temperature for applications that improve process efficiencies (e.g., chemical and heat-treating processes carried out at higher than currently used temperatures). A wide range of alloys with varied components are used in high-temperature applications. These alloys are selected based upon the temperature range of operation and the desired properties as outlined below.

2.1 Alloys Studied and Project Approach

Heat-Resistant Alloy Castings: The heat-resistant casting alloys are those compositions that contain at least 12% chromium and that are capable of performing satisfactorily when used at temperatures above 1200ºF. As a group, heat-resistant compositions are higher in alloy content than the corrosion-resistant types. The heat-resistant alloys are composed principally of nickel, chromium, and iron together with small percentages of other elements. Nickel and chromium contribute to the superior heat resistance of these materials. Castings made of these alloys must meet two basic requirements:

1. Good surface film stability (oxidation and corrosion resistance) in various atmospheres and at the temperature to which they are subjected.
2. Sufficient mechanical strength and ductility to meet high-temperature service condition.

Corrosion-Resistant Alloy Castings: The corrosion-resistant castings alloys are those compositions capable of performing satisfactorily in a large variety of corrosive environments. They are composed principally of nickel, chromium, and iron, and sometimes other elements. Castings made of theses alloys offer the ease of (1) production of complex shapes at low cost and (2) securing rigidity and high strength-to-weight ratios. The selection of the proper cast alloy for a given high-temperature application requires knowledge of various factors and the related mechanical and physical properties that must be matched with them. Properties of interest include short-time tensile properties, creep strength, stress-rupture properties, hot ductility, thermal fatigue properties, oxidation resistance, carburization resistance, sulfidation resistance, and surface stability. Different properties may be appropriate for different applications, and alloys may have to be optimized for these applications.

Work to improve the creep and stress rupture properties of the heat resisting Ni-Cr-Fe alloys through the addition of small amounts of W, V, Zr, Ti, Cb, N, or combinations of them, has been pursued for several years under the Steel Founders' Society of America sponsorship and by others in the United States, Japan, and Britain. Alteration of the carbide morphology from lamellar to discrete particles seems to be the important factor. The current work takes the bold step of enhancing the performance of the steels that are currently most frequently used—H-Series steels. The project takes a new approach of using stochastic optimization algorithm for optimizing alloy properties with the minimum number of experimental evaluations of the candidate alloys. The new approach has the potential of identifying compositions that cannot otherwise be identified without carrying out thousands of experiments. Furthermore, the approach has the potential for creating and designing alloys tailored for each application, thereby maximizing

utilization and reducing cost. Such an approach is expected to minimize the time needed for successful implementation of these alloys by industry.

The goal of this project was 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. The work performed in the project is appropriate for the domestic industry because it will give it a tool to customize the properties of the alloys for customer-specified application. Such a tool can potentially reduce or minimize the need for the addition of expensive elements, such as Cr, Ni, Co, Nb, Ti, or V, and still obtain the optimum properties needed to design the components. The alloys developed using this project's algorithms will find future applications in various industries, such as chemicals, petroleum, steel, petrochemical, forest products, glass, along with supporting industries. Optimized compositions of H-Series stainless steels that could result from the use of the stochastic algorithm could result in increasing the operating temperatures by up to 50ºC. This will result in enhancing industrial efficiencies for processes such as ethylene production, secondary processing of steel, and the operation of heat-treating furnaces. The potential for energy savings from improved efficiencies of various processes in the chemical, steel, and heat-treating industry when the alloys are commercialized is shown in Table 2.1.

Table 2.1. Results of the energy benefits impact analysis by the year 2020

Vision industry	Energy savings				Total energy savings (trillion Btu)
	Electricity (billion kWh)	Gas (billion ft^3)	Oil (million barrels)	Other (trillion Btu)	
Chemical	0.56	10.4	1.6		26
Heat treating	0.15	4.7	—	—	6
Steel	—	5.8	—	—	6
Total savings	0.71	20.9	1.6	—	38

2.2 Commercialization Aspects and Path Forward

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

Duraloy, the main producer of H-Series steels has not directly used the outcome of algorithm developed in this project. However, further optimized H-series compositions based on ORNL work using the phase stability and volume fraction, have been cast and fabricated in to radiant burner tube assemblies. One of these assemblies is currently in test at Nucor 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 with in the range for which the data was used, but for which the specific composition for an application has never been produced or tested. The implementation of such a capability by industry will require the development of an interactive computer-

based tool with range of property-prediction options and data output that can be directly used by production, sales, and design-engineering staff. After the tool is developed, selective experimental validation of certain predicted properties is highly recommended.

3. Background

The primary objective of the work presented in this report was to develop a generalized methodology for the acceleration of large-scale, multi-objective, multidisciplinary, constrained-optimization problems by utilizing new approaches for multilevel analysis, parallelization, and a special treatment of the response surface. The developed methods, although of general applicability, were demonstrated by optimizing the chemical composition of H-Series stainless steels composed primarily of Fe-Cr-Ni but which contained additional alloying elements.

Development of an alloy with desirable properties (objective functions) creates a problem in identifying constraints that need to be specified on the objective functions. These constraints are absent in a more general multi-objective optimization statement. Such objective constraints should be set by the user (expert) and could be allowed to vary during the solution process. For example, the minimum acceptable value for the Young's modulus of elasticity could be specified as an inequality constraint. Or, the maximum acceptable percentage of each of the most expensive ingredients in the alloy could be specified as a cost-objective constraint. Or, the total acceptable manufacturing cost of an alloy could be specified as an equality constraint.

The typical situation when solving a real-life, multi-objective optimization problem is that a designer has several tools available for performing the evaluation of the objective functions. These evaluation tools differ according to their levels of complexity and accuracy. The low-fidelity analysis models are very inexpensive and allow us to carry out optimization, but the validity of the obtained results can be questionable. The 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 expensive and takes a long time to perform.

The problem of using an experimental search for optimum chemical composition of an alloy can be an unacceptably labor-intensive process. This experimental method requires that an extremely large number of alloy compositions be created and evaluated. This method would result in the creation of an extensive database that would include information on various properties of alloys for various combinations of a chemical structure. Such a database could then be used to solve particular problems in creating alloys with desirable properties

The key to the success of the proposed approach is the robustness, accuracy, and efficiency of the multi-objective constrained optimization algorithm. Only a few commercially available general-purpose optimization software packages exist. They all use almost exclusively a variety of standard gradient-based optimization algorithms, which are known to be unreliable because of their tendency to terminate in the nearest feasible minimum instead of finding a global optimum. Moreover, these optimizers can perform optimization only of a weighted linear combination of objective functions. This formulation does not provide a true multi-objective optimization capability, that is, each individual objective is not fully maximized. These optimizers require an extremely large number of objective function (mechanical and corrosion properties of alloys) evaluations, which makes the total number of experimental evaluations unacceptably large. The latest developments in the area of semi-stochastic, truly multi-objective constrained optimization have not been commercialized and have not been demonstrated in this field of application. The present work is based on the use and a special adaptation of a new stochastic optimization algorithm that was specifically developed for the task of optimizing properties of alloys while minimizing the number of experimental evaluations needed of the candidate alloys.

The technical approach uses a combination of analysis tools with different levels of sophistication in the multi-objective optimization of complex alloy systems. To reduce the computing time significantly, we planned to develop a multilevel, multi-objective constrained optimization methodology that is a modified version of a method of indirect optimization based upon self organization (IOSO) and evolutionary simulation principles [1]. This approach is intended to minimize the use of the time-consuming, complex experimental evaluations. This optimization methodology can be performed on commodity processors and is scalable; it is capable of handling hundreds and even thousands of design variables and dozens of objectives and constraints. Thus, the role of the designer is to choose the various evaluation tools and specify meaningful ranges for the design variables, the multiple objective functions, and the constraints. The generalized scheme is shown in Fig. 3.1.

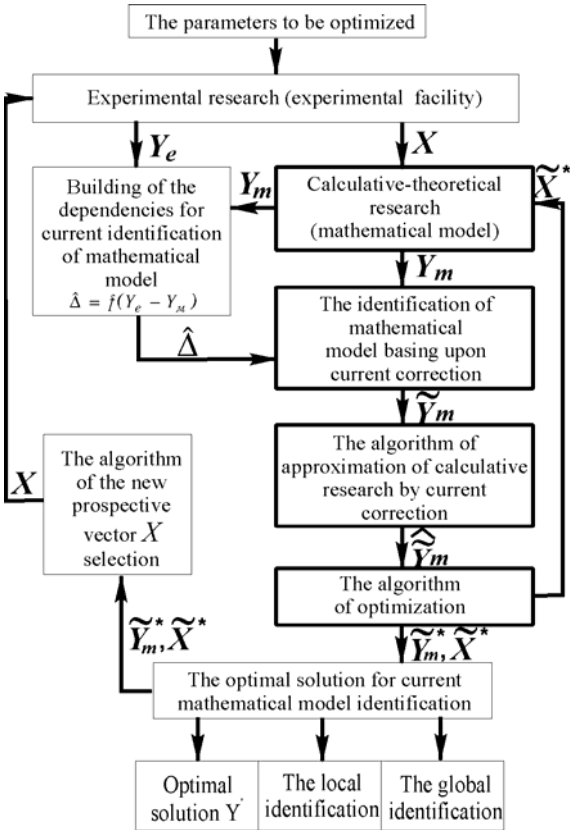

Fig. 3.1. The general scheme for optimization that verifies theoretical and experimental methods.

3.1 The Artificial Neural Network

Neural networks are methods for the quantitative recognition of patterns in data, without any a priori specification of the nature of the relationship between the input and output variables. They can model relationships of almost arbitrary complexity [2–9]. The outcome of neural network training is a set of coefficients (called weights) and determination of the functions that in combination with the weights relate the input to the output. The computer-intensive training process involves a search for the optimum nonlinear relationship between the inputs and the outputs. However, after the network is trained, estimation of the outputs for any given input is very rapid. There are methods, such as that of MacKay [6], that implement a Bayesian framework on the neural network. The error bars then depend on the specific position in input space, thus reducing the dangers of extrapolation and interpolation.

Neural network models in many ways mimic human experience and are capable of learning or being trained to recognize the correct science rather than nonsensical trends. A potential difficulty with the use of regression methods is the possibility of over-fitting data. For example, it is possible to produce a neural network model for a completely random set of data. To minimize this problem, the experimental data can be divided into two sets, a *training* dataset and a *test* dataset. The model is produced using only the training data. The test data are then used to check that the model functions properly when presented with previously unseen data [9].

In addition, artificial neural networks, once fully trained, are very efficient and accurate interpolating algorithms for any multiparameter function. Neural networks, however, are not automatically efficient and accurate search algorithms or extrapolation algorithms for venturing outside of the available database. Therefore, it is important to understand a need for mathematically sound multi-objective stochastic optimization algorithms that are capable of finding the global minimum and that can confidently search outside a given initial database.

3.2 Multi-objective Optimization

As mentioned earlier, a key part of this method is the multi-objective constrained optimization algorithm. There are only a few commercially available, general-purpose optimization software packages. Currently, the most popular commercially available, general-purpose optimization software in the United States is iSIGHT [10]. However, these software packages predominantly use a variety of standard gradient-based optimization algorithms that are known to be unreliable because of their tendency to terminate in the nearest feasible minimum instead of finding a global optimum. Moreover, these optimizers can perform only optimization of a weighted linear combination of objective functions. This formulation does not provide a true multi-objective optimization capability, that is, each individual objective is not calculated to its extreme. Furthermore, these optimizers require a large number of evaluations of objective functions (mechanical and corrosion properties of alloys), making the total number of experimental evaluations unacceptably large because no algorithms are available for confidently predicting physical properties from given alloy concentrations. The industry is probably aware of these drawbacks of the commercially available optimization software. Some industry experts are also becoming aware of the neural network approach to alloy design as practiced at Cambridge University and of the applications of genetic algorithms in materials design [11] and of its coupling with a molecular dynamics simulation approach [12]. However, for the most part, industry is not aware of the latest developments in the area of stochastic, truly multi-objective constrained optimization because these methods have not been commercialized and have not been demonstrated in this field of application.

The growing need for the multidisciplinary and multi-objective approach to design with a large number of design variables resulted in an increased interest in the use of various versions of hybrid [13], semi-stochastic [14] and stochastic [1,15–23] optimization algorithms. Including more objectives in the optimization process has similar effects as including more constraints, especially if these constraints are incorporated as penalty functions.

The *multi*-objective optimization problem maximizes a vector of n objective functions

$$max\ F_i(\overline{X}) \quad \text{for } i = 1, \ldots, n \tag{1}$$

subject to a vector of inequality constraints

$$g_j(\overline{X}) \leq 0 \quad \text{for } j = 1, \ldots, m \tag{2}$$

and a vector of equality constraints

$$h_q(\overline{X}) = 0 \quad \text{for } q = 1, \ldots, k \tag{3}$$

In general, the solution of this problem is not unique. With the introduction of the Pareto dominance concept, the possible solutions are divided into two subgroups: the *dominated* and the *nondominated*. The solutions belonging to the second group are the "efficient" solutions, that is, the ones for which it is not possible to improve any individual objective without deteriorating the values of at least some of the remaining objectives. In formal terms, in case of a maximization problem, it is possible to write that the solution $\overline{X}$ dominates the solution $\overline{Y}$ if the following relation is true.

$$\overline{X} >_P \overline{Y} \Leftrightarrow (\forall i F_i(\overline{X}) \geq F_i(\overline{Y})) \cap (\exists j : F_j(\overline{X}) > F_j(\overline{Y})) \tag{4}$$

Classical gradient-based optimization algorithms are capable, under strict continuity and derivability hypotheses, of finding the optimal value only in the case of a single objective. For these algorithms, the problem of finding the group of nondominated solutions (the Pareto front) is reduced to several single objective optimizations in which the objective becomes a weighted combination of objectives called utility function.

Multi-objective optimization algorithms that are based on a genetic algorithm have been successfully applied in a number of engineering disciplines. However, for a large number of design variables and objective functions that need to be carried to the extreme simultaneously, this approach becomes progressively too time consuming for practical applications in industry.

A new approach of using a stochastic optimization algorithm for optimizing alloy properties that requires a minimum number of experimental evaluations of the candidate alloys is used in this work. The method has the potential of identifying new compositions that cannot otherwise be identified without carrying out an unacceptably large number of experiments. Furthermore, the approach has the potential for creating and designing custom alloys for applications, thereby maximizing their utilization at reduced cost. The proposed method uses a special adaptation of a new stochastic optimization algorithm that was developed specifically for optimizing properties of alloys while minimizing the number of experimental evaluations needed for each of the candidate alloys. This multi-objective, semi-stochastic optimization algorithm incorporates aspects of a selective search on a continuously updated multi-dimensional response surface. Both the weighted linear combination of several objectives and true multi-objective formulation options creating Pareto fronts are incorporated in the algorithm. The main benefits of this algorithm are its outstanding reliability in avoiding local minimums, its computational speed, and a significantly reduced number of required experimentally evaluated alloy samples as compared to more traditional semi-stochastic optimizers such as genetic algorithms. Furthermore, the self-adapting response surface formulation used in this project allows for the incorporation of realistic nonsmooth variations of experimentally obtained data and allows for the accurate interpolation of such data.

3.3 Response Surface and Self-Organization Concepts

Our approach is based on the widespread application of the response surface technique with the adaptive use of global and middle-range multipoint approximation. One of the advantages of the proposed approach is the possibility of ensuring good approximating capabilities using minimum available information. This possibility is based on self-organization and evolutionary-modeling concepts [1]. During the approximation, the approximation function structure is being evolutionarily changed, so that it

allows successful approximation of the optimized functions and constraints, having sufficiently complicated topology.

The problem of the numerical search for Pareto-optimum solutions set in the multi-objective optimization while varying the chemical composition of an alloy would be an unacceptably labor-intensive process. An extremely large number of alloy compositions would be need and several of the properties of each of these alloys would have to be evaluated experimentally. Such problems are difficult to formalize at the initial stage because the user does not know initially the values attainable by some objectives and how the remaining objectives will vary. The number of experiments that is necessary for a true multi-objective optimization problem solution depends not only on the dimensionality of the problem (the number of ingredient species in an alloy) but also it depends to a considerable degree on the topologies of the object functions. Since the user has very little if any a priori knowledge of objective function space topology, it is very difficult to predict the number of experiments required in the optimization application proposed here.

3.4 Summary of Indirect Optimization Based upon the Self-Organization (IOSO) Algorithm

Every iteration of IOSO consists of two stages. The first stage is the creation of an approximation of the objective function(s) (Fig. 3.2). Each iteration in this stage represents a decomposition of the initial approximation function into a set of simple approximation functions so that the final response function is a multilevel graph. That is, the evolutionary self-organizing algorithms are based on the modified version of the method of accounting for the groups of arguments. Such algorithms employ the evolutionary procedure of constructing approximation functions in the form of multilevel graphs (Fig. 3.3) and solving the structure-parametric approximation problem in the process.

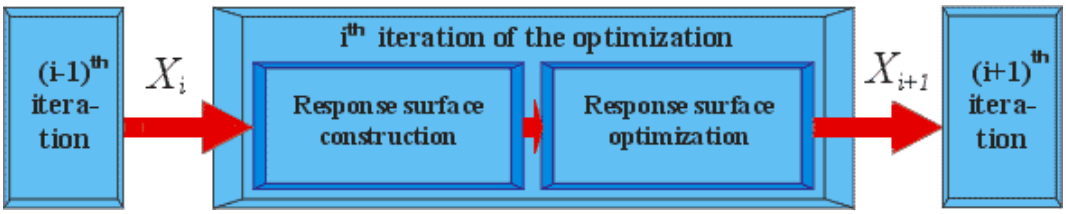

Fig. 3.2. IOSO iteration scheme.

The second stage is the optimization of this approximation function. This approach allows for corrective updates of the structure and the parameters of the response surface approximation. The distinctive feature of this approach is an extremely low number of trial points to initialize the algorithm. During each iteration of IOSO, the optimization of the response function is performed only within the current search area. This step is followed by an actual experimental evaluation for the obtained point. During the IOSO operation, the information concerning the behavior of the objective function in the vicinity of the extremum is stored, and the response function is made more accurate only for this search area. Thus, during each iteration, a series of approximation functions (Fig. 3.4) for a particular objective is built. These functions differ from each other according to both structure and definition range.

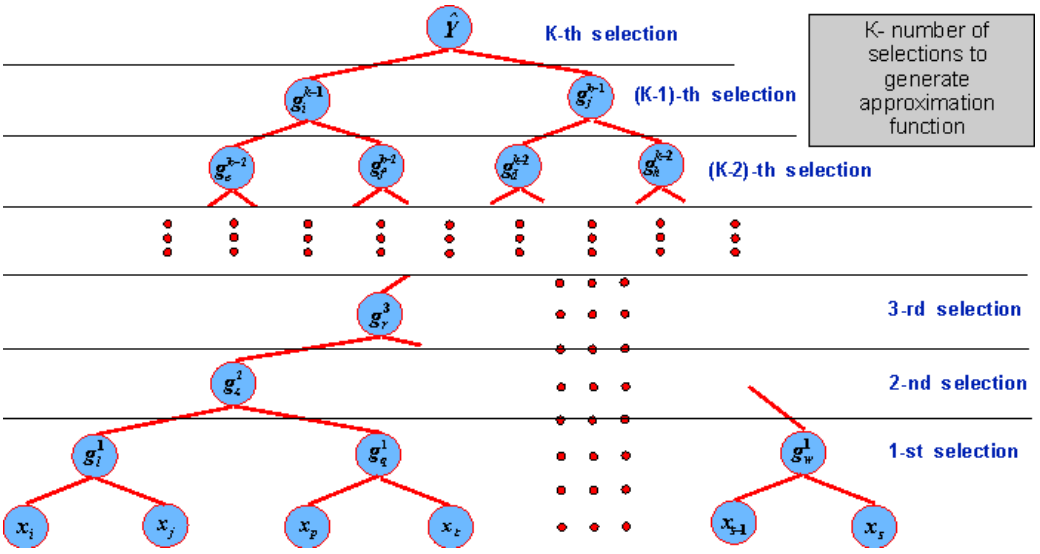

Fig. 3.3. Example of the IOSO response surface structure.

The subsequent optimization of these approximation functions allows us to determine a set of vectors of optimized variables. IOSO using Sobol's algorithm [24] was used for redistribution of the initial points in the multidimensional function space. IOSO also includes algorithms of artificial neural networks (ANN) that utilize appropriately modified radial-basis functions in order to enrich the original data set and build the response surfaces. The modifications consisted in the selection of ANN parameters at the stage of their training that are based on two criteria: minimal curvature of response surface and provision of the best predictive properties for a given subset of test points, $W_{best} \in W_{ini}$. Each iteration of alloy composition multi-objective optimization technique involves the following steps.

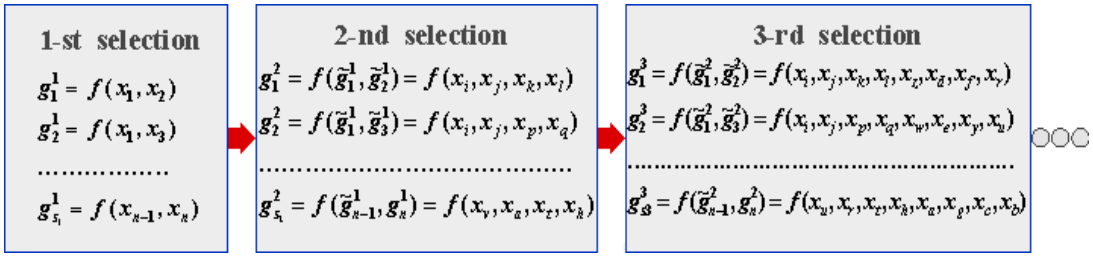

Fig. 3.4. IOSO approximation process scheme.

1. Building and training ANN1 for a given set of test points proceeding from the requirement $W_{best} = W_{ini}$.
2. Conducting multi-objective optimization with the use of ANN1 and obtaining a specified number of Pareto optimal solutions P_1.
3. Determining a subset of test points W_{best} that are maximally close to points P_1 in the space of variable parameters.
4. Training ANN2 proceeding from the requirement to provide the best predictive properties for obtained subset of test points $W_{best} \in W_{ini}$.

5. Conducting multi-objective optimization with the use of ANN2 and obtaining a set of Pareto-optimal solutions P_2.

In general, the database contains information on experimentally obtained alloy properties compiled from different sources and obtained under different experimental conditions. As a result, for alloys with the same chemical compositions, there can be considerable differences of measured properties. These differences can be explained as errors due to the particular conditions existing during the experiments (measurement errors) and by the effect of certain operating conditions (e.g., thermal condition of alloy making). Unless operating conditions are quantified numerically, their influence is regarded as an additional chance factor. In its simplified form, the methodology can be presented as the following set of actions.

1. *Formulation of optimization task.* These tasks include selection of variable parameters, definition of optimization objectives and constraints, and setting initial (preliminary) ranges of variable parameters variations.
2. *Preliminary reduction of the experimental database.* At this stage, the points meeting the optimization task statement are picked up from the database so that alloys having chemical composition outside the chosen set of variable parameters are rejected. Alloys for which there is no data for at least one optimization objective are rejected. In addition, alloys with chemical compositions outside the set range of variable parameters are rejected.
3. *Final reduction of the experimental database.* Since accuracy of the building of response surfaces substantially depends on uniformity of distribution of variable parameters in the surveyed area, rejection of experimental data points falling outside of the universal set is performed. At the end of this stage, a final range of variable parameters for optimization is set.
4. *Execution of multi-objective optimization.* This results in a specified number of Pareto optimal solutions.
5. *Analysis of optimization results.*
6. *Carrying out an experiment.* The experiment will obtain a set of Pareto optimal alloy compositions (or a certain subset) and analysis of the results obtained.
7. *Change of optimization problem statement and returning to Step 2.* The problem statement includes the number of simultaneous objectives and constraints and the set and range of variable parameters,
8. *Modification of database and returning to Step 4.*
9. *Stop.*

The objective of this project was to demonstrate the use of the computational tool to predict the effect of varying composition on properties of H-Series and other alloys. Alloy properties of interest to be optimized include strength (tensile and creep properties) and corrosion (high-temperature oxidation, carburization, sulfidation and low-temperature corrison in various solutions).

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

Task 1: Development of initial plan of experiment (University of Texas at Arlington [UTA])

1.1 Generate alloy compositions with only 6 elements

1.2 Generate alloy compositions with 7 to 16 elements

Task 2: Analysis of the plan of experiment, identification of the objective functions and objective constraints (UTA)

2.1 Objectives to identify will include tensile, creep, and corrosion data

2.2 Objective constraints will include the acceptable number of alloying elements and use temperature and time

Task 3: Determine solution of M particular optimization problems for objective constraints defined in Task 2 (UTA)

3.1 Determine solutions for tensile properties
3.2 Determine solutions for tensile and creep properties
3.3 Determine solutions for tensile, creep, and corrosion properties

Task 4: Experimental verification and identification of additional experiments needed (UTA, Oak Ridge National Laboratory [ORNL])

4.1 Complete experimental verification of tensile solution
4.2 Complete experimental verification of tensile and creep solutions
4.3 Complete experimental verification of tensile, creep, and corrosion properties

Task 5: Prepare alloys and develop tensile, creep, and corrosion data (UTA, ORNL)

5.1 Test alloys for tensile properties
5.2 Test alloys for creep properties
5.3 Test alloys for corrosion properties

Task 6: Meetings and technical reports

6.1 Hold one technical meeting each year
6.2 Complete final report

This work was performed by a team consisting of the University of Texas, Oak Ridge National Laboratory, and industries as outlined in Fig. 2.1.

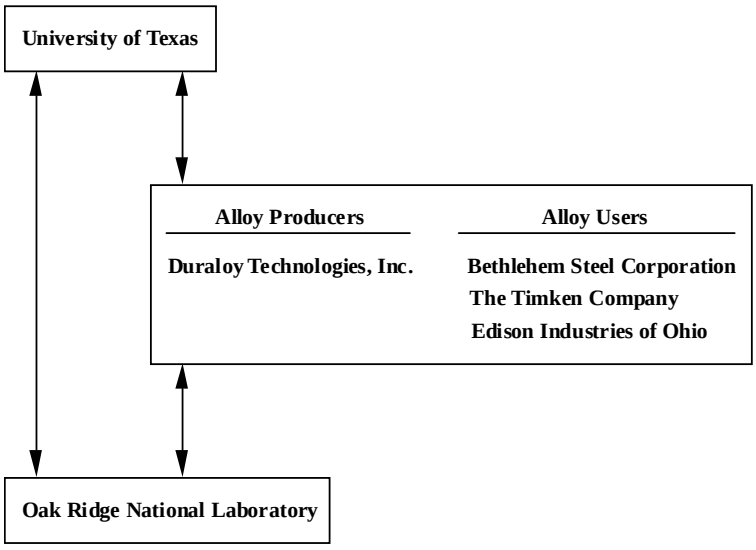

Fig. 3.5. Organization plan for the team involved in the project.

4. Results and Discussion

The initial data were the results of experimental testing of 17 samples of H-Series steels with different percentages of alloying components. The experimental data for creep rupture strength after 100 h at 1800ºF (982ºC) is presented in Table 4.1. Note that the poor set of available experimental data (only 17 points for 6 independent variables) and nonuniformity of their distribution in the space of design variables do not allow accuracy of the results in the first iteration of this multi-objective optimization methodology. However, the main goal of this research is to create a plan for future experiments, which will allow us to improve the accuracy of the optimized steel composition for the next iterations.

Table 4.1. Initial data set

Nominal composition (wt %)							1800°F
Fe	C	Mn	Si	Ni	Cr	N	10^2h (Psi)
54.64	0.1	0.87	1.24	18.9	24.2	0.05	1684
52.92	0.14	1.02	1.22	20.1	24.5	0.1	2084
52.88	0.17	0.92	1.23	20.1	24.6	0.1	2303
54.28	0.2	0.95	1.07	19.3	24.1	0.1	2691
51.01	0.27	0.98	1.23	20.4	26	0.11	3324
50.75	0.28	1.05	1.27	20	26.5	0.15	3500
52.1	0.28	0.52	0.52	20	26.5	0.08	3600
51.73	0.3	0.53	0.84	20	26.5	0.1	3800
50.6	0.3	0.58	1.62	20.1	26.7	0.1	4300
51.85	0.3	0.53	1.21	19.7	26.3	0.11	4250
51.06	0.32	0.98	1.26	20.2	26.1	0.08	4415
51.54	0.32	0.51	1.25	20	26.3	0.08	4600
51.54	0.32	0.52	1.19	19.9	26.3	0.23	4800
52.68	0.32	0.5	0.5	19.9	26	0.1	3600
49.09	0.32	0.51	1.26	19.9	28.8	0.12	3600
53.9	0.33	0.51	1.25	20	23.9	0.11	3700
52.409	0.35	0.82	1.07	21.1	24.2	0.051	4573

4.1 Design Variables and Multiple Optimization Objectives

As the independent design variables for this problem, we considered the percentages of the following components: C, Mn, Si, Ni, Cr, and N. Ranges of their variation were set according to lower and upper bounds of the available set of experimental data. The bounds are presented in Table 4.2.

Table 4.2. Specified ranges of design variables

	C	Mn	Si	Ni	Cr	N
Min	0.1	0.5	0.5	18.9	23.9	0.05
Max	0.35	1.05	1.62	21.1	28.8	0.23

As the main optimization objective, we considered the creep rupture strength of the H-type steel for a 100 h rupture life under 1800ºF (982ºC). Other objectives have been chosen to reduce the cost of the steel. In this work, three additional objectives simultaneously minimize the percentages of Mn, Ni, Cr. Thus, the multi-objective optimization problem had six independent design variables and four simultaneous objectives. We defined the desirable number of Pareto optimal solutions as ten points.

4.2 Numerical Results

Fig. 4.1 demonstrates the results characterizing the accuracy of the obtained response surface based on ANN1. For most of the available experimental points, the mean error of the prediction created by ANN1 does not exceed 4%. The exception is observed for the experimental point No. 11, where mean error is 8.4%. As a result of this four-objective constrained optimization problem solution, a subset of experimental points $W_{best} \in W_{ini}$, which contained points No. 8, 9, 13, … , 17, was obtained. The training of ANN2 allowed us to improve the accuracy of approximation for these points of the experimental data set (Fig. 4.2). Then, the four-objective optimization task was actually solved by using ANN2, resulting in a Pareto-optimal set of ten new alloy compositions. This set is presented in Table 4.3.

Table 4.3. Set of ten Pareto-optimal solutions

Pareto-optimal composition (wt %)							1800ºF
Fe	**C**	**Mn**	**Si**	**Ni**	**Cr**	**N**	**Psi (predicted values)**
51.41	0.33	0.50	1.32	19.89	26.31	0.23	4804
53.42	0.35	1.03	0.50	20.73	23.90	0.08	4214
52.51	0.35	1.05	1.30	19.05	25.64	0.10	4031
50.50	0.33	0.67	1.43	18.90	28.02	0.16	3828
53.33	0.29	0.50	0.51	21.10	24.06	0.20	3607
53.41	0.19	1.01	1.09	20.31	23.90	0.09	2350
53.22	0.22	0.97	1.38	18.90	25.20	0.11	2338
50.88	0.22	0.52	1.59	18.90	27.68	0.22	2257
53.49	0.15	0.68	1.02	20.60	23.90	0.17	2235
54.74	0.12	0.55	1.57	18.90	23.90	0.22	1706

Fig. 4.3 shows the ten new (optimized) chemical compositions that should be used to create the next generation of physical alloy samples that will need to be experimentally tested. One can see that carrying out the experimental research for the predicted alloy compositions will make the distribution of the experimental points more uniform, and thus it will improve the quality of the response surfaces. Figures 4.4 and 4.5 show the examples of ANN2 response surface topology in the vicinity of the first, second, and the tenth point from the obtained Pareto set.

A second database containing 201 experimentally tested alloys was also used for the study. A preliminary analysis of data showed that for certain alloys no complete information exists on alloy chemical composition. Such alloys were excluded from further analysis. Besides, some chemical elements (V, Bi, Se, Zr, Sb, Cd) were present in a very small number of alloys, which made it impossible to assess their effect from information in this database. Such alloys were also excluded from further analysis. The remaining database had 176 alloys. At the next stage, an evaluation was made of uniformity of distribution of the percentage values of different elements in the existing range. Certain alloying elements had concentrations differing very strongly from the universal set (e.g., the percentage of sulfur in one of the alloys exceeded the average value by some ten times). Such alloys were excluded from further analysis. The remaining database had 158 alloys.

The following parameters were then used as optimization objectives:

1. Stress (PSI – maximize),
2. Operating temperature (T – maximize), and
3. Time to "survive" until rupture (HOURS – maximize).

During this research, the solution of a simultaneous three-objective optimization problem and a series of two-objective problems were accomplished using cases in which one of the considered parameters was constrained.

4.3 Influence of the Number of Alloying Elements

In this problem the percentages of the following 17 alloying elements were taken as independent variables: *C, S, P, Cr, Ni, Mn, Si, Cu, Mo, Pb, Co, Cb, W, Sn, Al, Zn, Ti*. The ranges of these elements were set as follows. First, minimum and maximum values for the existing set of experimental data ($Exp\_min_i, Exp\_max_i,\ i = \overline{1,17}$) were defined. Then, new minimum and maximum values for each of the 17 elements were obtained according to the following simple dependencies: ($Min_i = 0.9 \cdot Exp\_min_i, Max_i = 1.1 \cdot Exp\_max_i,\ i = \overline{1,17}$). The allowable ranges are given in Table 4.4. While the lower range for Cr and Ni content almost corresponds to AISI 310 scale-resistant stainless steel, the upper range of Cr and Ni content correspond to super alloys [25]. It should be pointed out that the chemistry of the two types of alloys is entirely different.

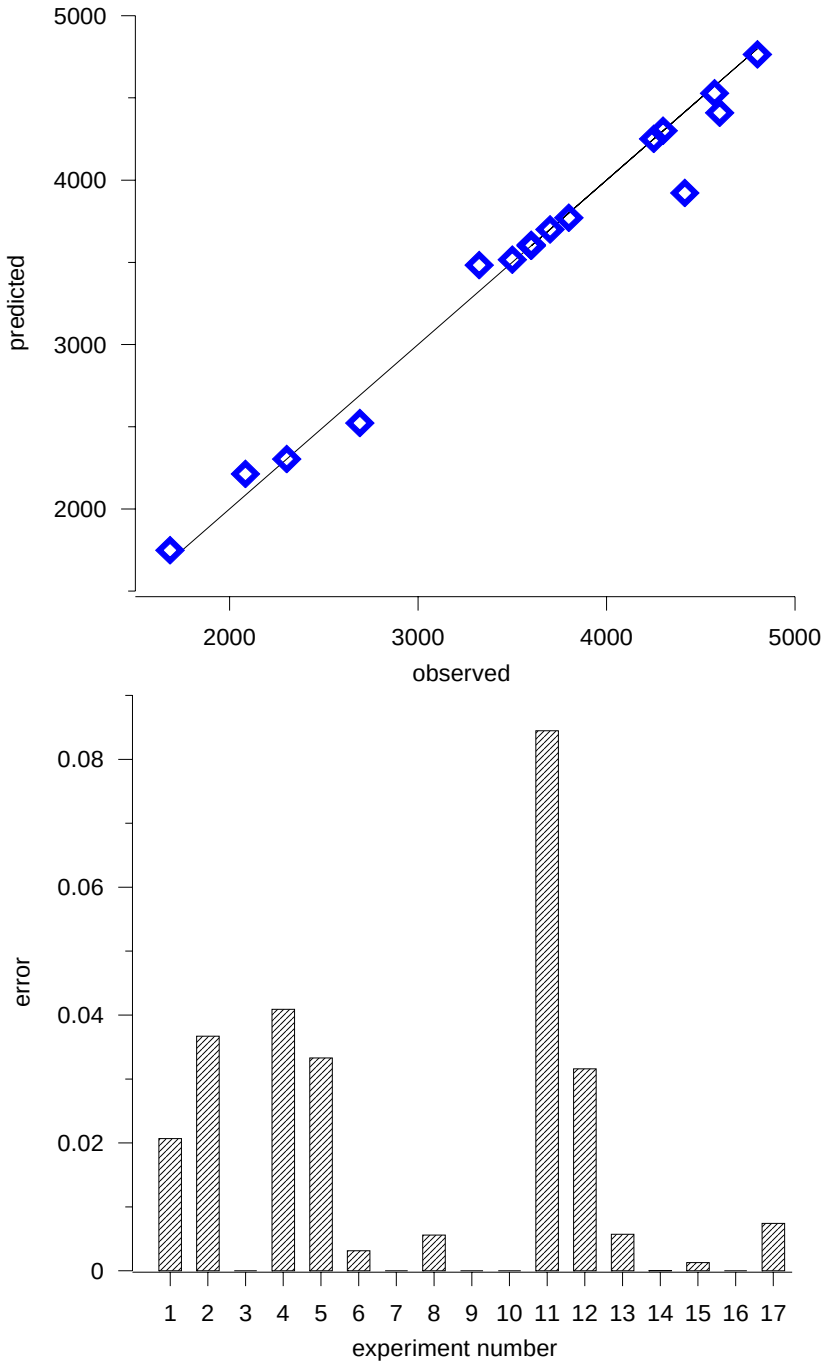

Fig. 4.1. Accuracy of ANN1.

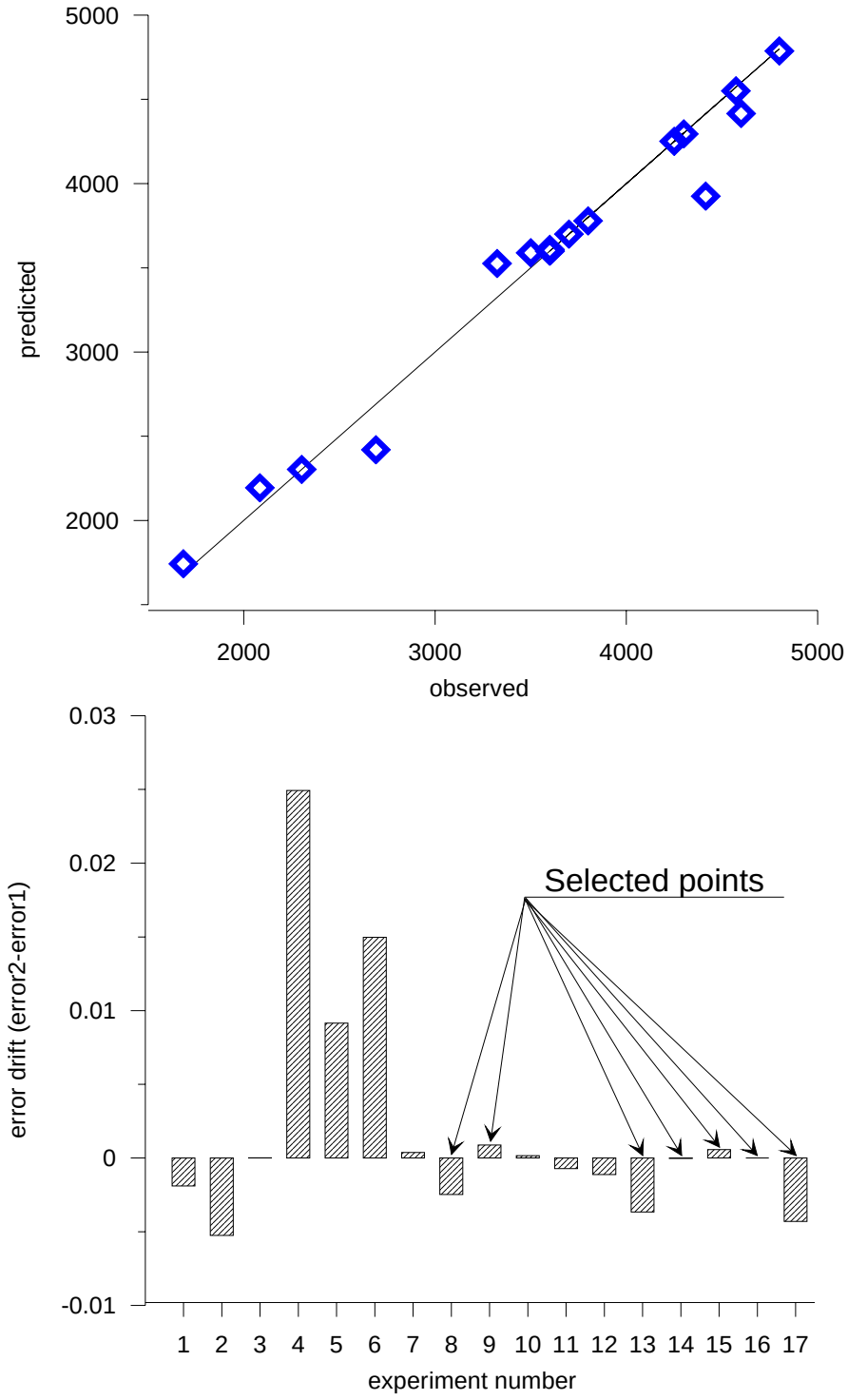

Fig. 4.2. Accuracy of ANN2.

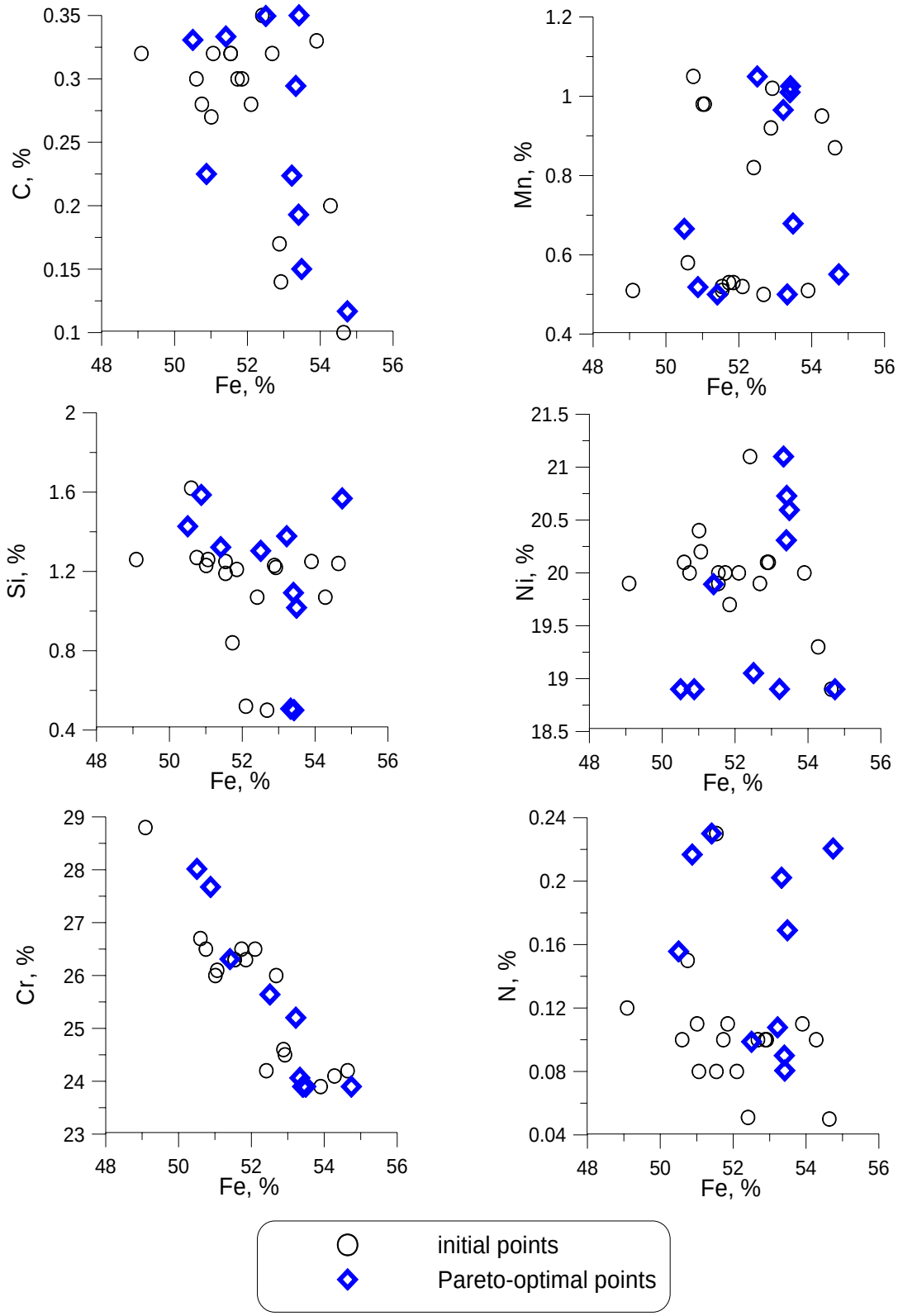

Fig. 4.3. Results of the first iteration of steel composition optimization.

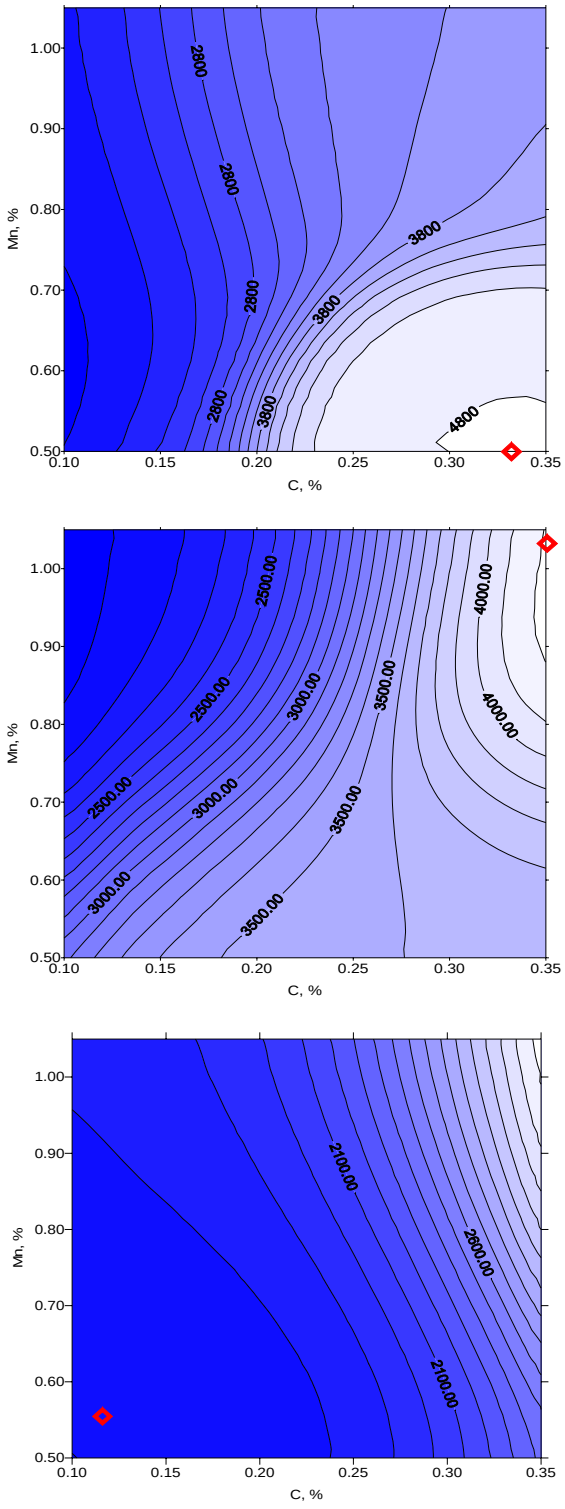

Fig. 4.4. Topology of the ANN2-based response surface in the vicinity of first, second, and tenth Pareto-optimum points for C – Mn.

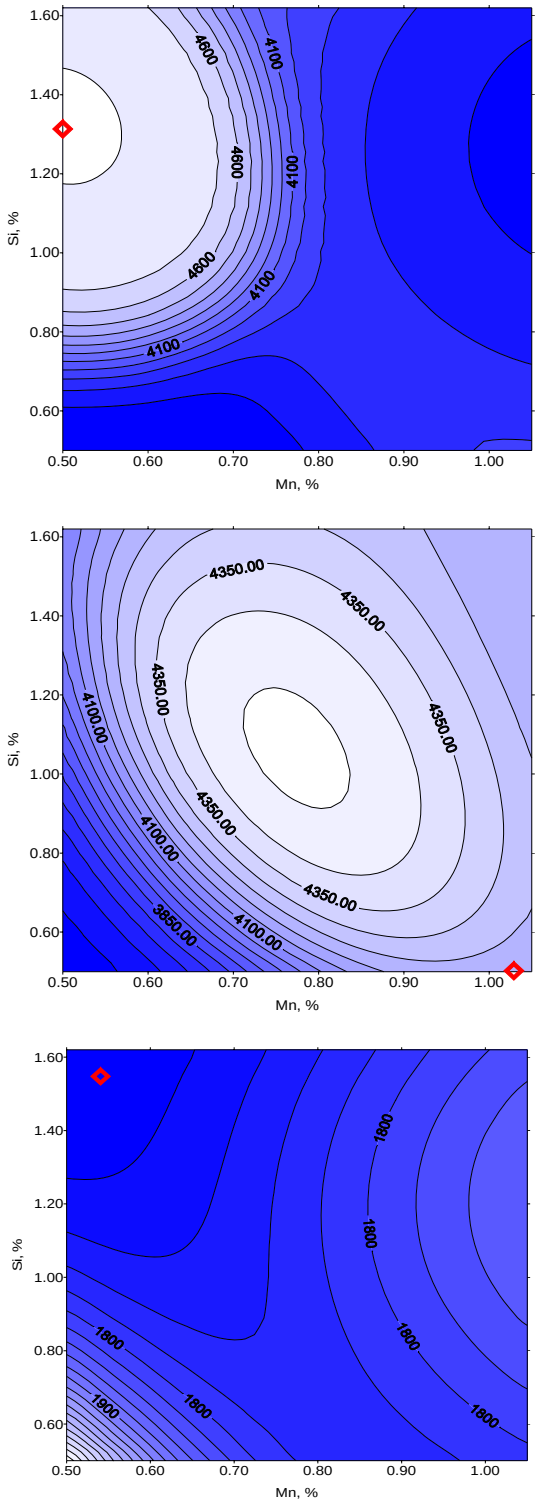

Fig. 4.5. Topology of the ANN2-based response surface in the vicinity of first, second, and tenth Pareto-optimum points for Mn – Si.

Table 4.4. Ranges of variation of 17 independent variables (chemical elements in the steel alloy)

	Elements (wt %)								
	C	**S**	**P**	**Cr**	**Ni**	**Mn**	**Si**	**Al**	
Min	0.063	0.001	0.009	17.50	19.30	0.585	0.074	0.001	
Max	0.539	0.014	0.031	39.80	51.60	1.670	2.150	0.075	
	Elements (wt %)								
	Mo	**Co**	**Cb**	**W**	**Sn**	**Zn**	**Ti**	**Cu**	**Pb**
Min	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.016	0.001
Max	0.132	0.319	1.390	0.484	0.007	0.015	0.198	0.165	0.006

The three-objectives optimization run was then repeated with only the following nine chemical elements as independent variables: *C, Cr, Ni, Mn, Si, Mo, Cb, W,* and *Ti*. We followed the same steps during the optimization as were used when solving the problem with 17 variables. But, in this case, there were noticeable differences due to accuracy deterioration of the response-surface representation. Thus, when using fewer alloying elements while decreasing the number of variables for the same experimental dataset, additional noise was introduced into this data set.

4.4 Simultaneous Optimization of Three Objectives for Alloys Having 17 Chemical Elements

During the first stage, the problem of simultaneously optimizing three objectives was solved with 100 points of Pareto optimal solutions. Figure 4.6 presents the obtained Pareto optimal solutions in objectives' space (PSI – HOURS). Analysis of this figure allows us to extract an area of admissible combinations of different optimization objectives. It can be seen that results are distributed in the admissible part of the objectives' space quite uniformly. Such a distribution offers a possibility for a significant improvement of accuracy of response surfaces on the condition that the experiments will be carried out at the obtained Pareto optimal points. In principle, the first iteration of the process of alloy chemical composition optimization by several objectives could be regarded as complete. Then, in accordance with the elaborated technique, it is necessary to conduct experiments at the obtained Pareto optimal points, evaluate the accuracy of the predicted values of partial optimization criteria, and either complete the process or perform another iteration. However, such a strategy is more time consuming than necessary for a researcher who knows the tasks more accurately. It can be seen that the ranges of variation of optimization objectives for the obtained Pareto set are very wide. At the same time, if a researcher can formulate the problem more specifically (for example, by setting constraints on the objectives) the volume of experimental work can be substantially reduced.

Figure 4.7 presents interdependence of the chosen optimization objectives built on the obtained set of Pareto optimal solutions. Figure 4.8 demonstrates the difference in topology of the multi-objective function space when using different numbers of alloying elements. The Larsen-Miller diagram (Fig. 4.9) shows PSI on the vertical axis and *Temp. log (HOURS + 20) on the horizontal axis (temperature in Rankine degrees). Here, logarithm is with the basis 10, while temperature is in Rankine = temperature in Fahrenheit + 460. Figure 4.10 illustrates the general trend in the capability of the optimizer to create alloys with superior performance as a function of the number of alloying elements chosen for optimization.

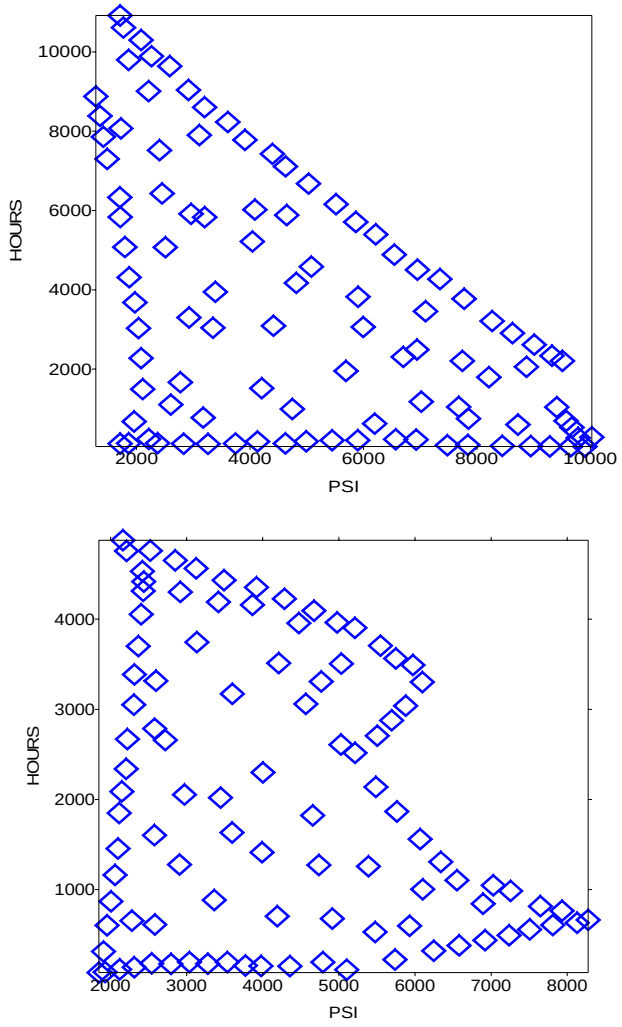

Fig. 4.6. Time-to-rupture vs strength interdependence of optimization objectives for three-objectives Pareto set with 17 chemical elements (top) and with 9 chemical elements (bottom).

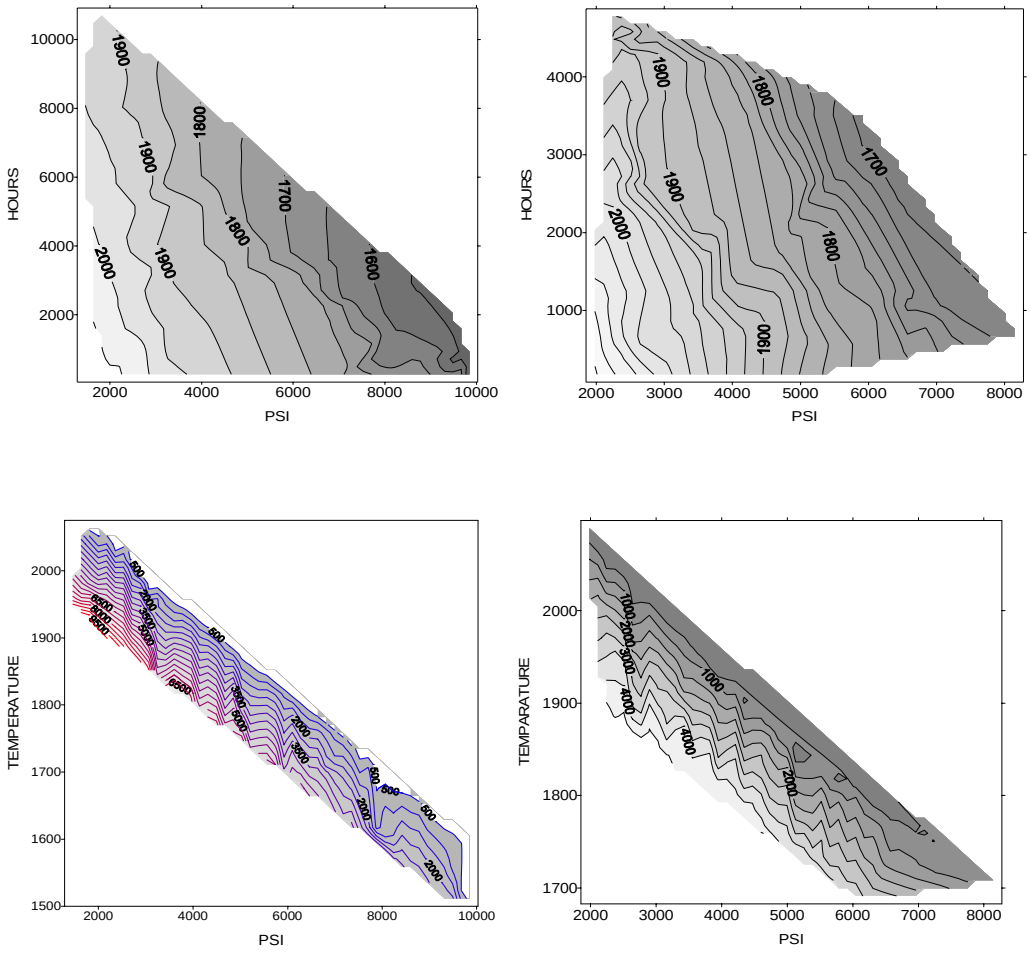

Fig. 4.7. Time-to-rupture vs strength and temperature vs strength interdependences of optimization objectives for Pareto set resulting from a three-objectives optimization with 17 chemical elements (left) and with 9 chemical elements (right).

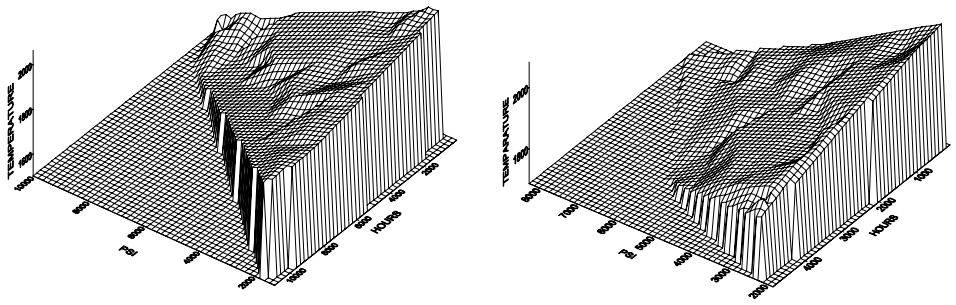

Fig. 4.8. Topography of response surfaces of three-objective optimization problems with 17 chemical elements (left) and with 9 chemical elements (right).

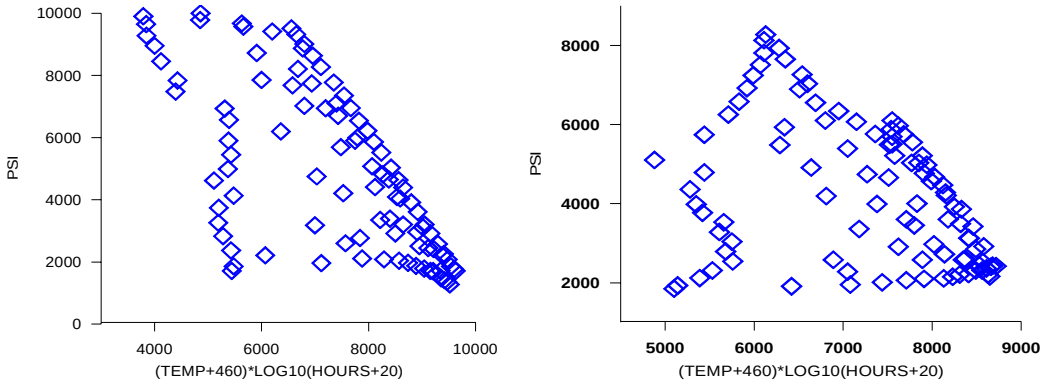

Fig. 4.9. Larsen-Miller diagram for Pareto sets resulting from a three-objective optimization with 17 chemical elements (left) and with 9 chemical elements (right).

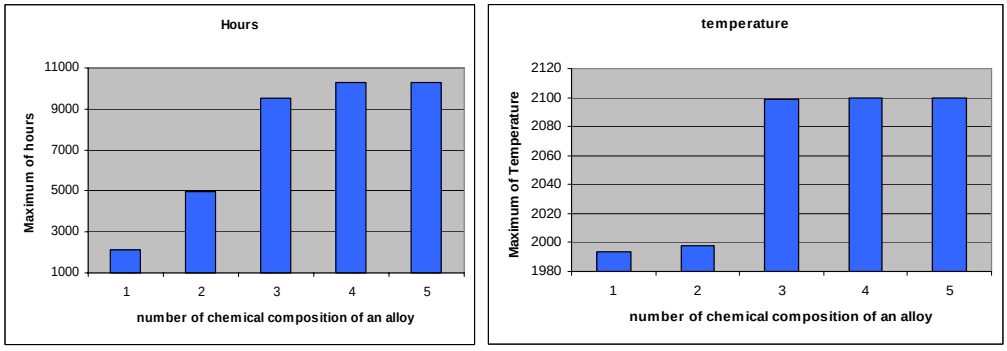

Fig. 4.10. Influence of the number of optimized alloying elements on the properties of the optimized superalloy; 1 – eight element, 2 – nine elements, 3 – eleven elements, 4 – fourteen elements, 5 – seventeen elements. A similar trend was observed with the maximum strength.

Analysis of these figures shows that the increase of temperature, for instance, leads to a decrease of compromise possibilities between PSI and HOURS. Hence, if a researcher knows exactly in what temperature range the alloy being designed will be used, it would be more economical to solve a sequence of two-objective optimization with an additional constraint for the third objective. Thus, a more efficient approach to optimizing alloy compositions could be to solve a sequence of two-objective optimization problems in which PSI and HOURS are regarded as simultaneous objectives, while imposing the following constraints on temperature:

- Problem 2. - $T \geq 780\,\mathrm{C}$ (1600ºF), number of Pareto optimal solutions is 20.
- Problem 3. - $T \geq 982\,\mathrm{C}$ (1800ºF), number of Pareto optimal solutions is 20.
- Problem 4. - $T \geq 1038\,\mathrm{C}$ (1900ºF), number of Pareto optimal solutions is 20.
- Problem 5. - $T \geq 1093\,\mathrm{C}$ (2000ºF), number of Pareto optimal solutions is 15.
- Problem 6. - $T \geq 1121\,\mathrm{C}$ (2050ºF), number of Pareto optimal solutions is 10.

The decrease of the number of simultaneous optimization objectives (transition from three- to two-objectives problem with constraints on temperature) leads to a decrease of the number of additional

experiments needed, at the expense of both decreasing the number of Pareto optimal points and decreasing the ranges of chemical compositions. Figure 4.11 presents sets of obtained Pareto optimal solutions in objectives space. It can be seen that maximum achievable values of HOURS and PSI and the possibilities of compromise between these parameters largely depend on temperature. For instance, the increase of minimum temperature from 870ºC to 1038ºC leads to a decrease of attainable PSI by more than 50%. At the same time, limiting the value of HOURS will not alter with the change of temperature. Larsen-Miller diagrams for this set of cases (two-objective optimization for five temperatures) are shown in Fig. 4.12.

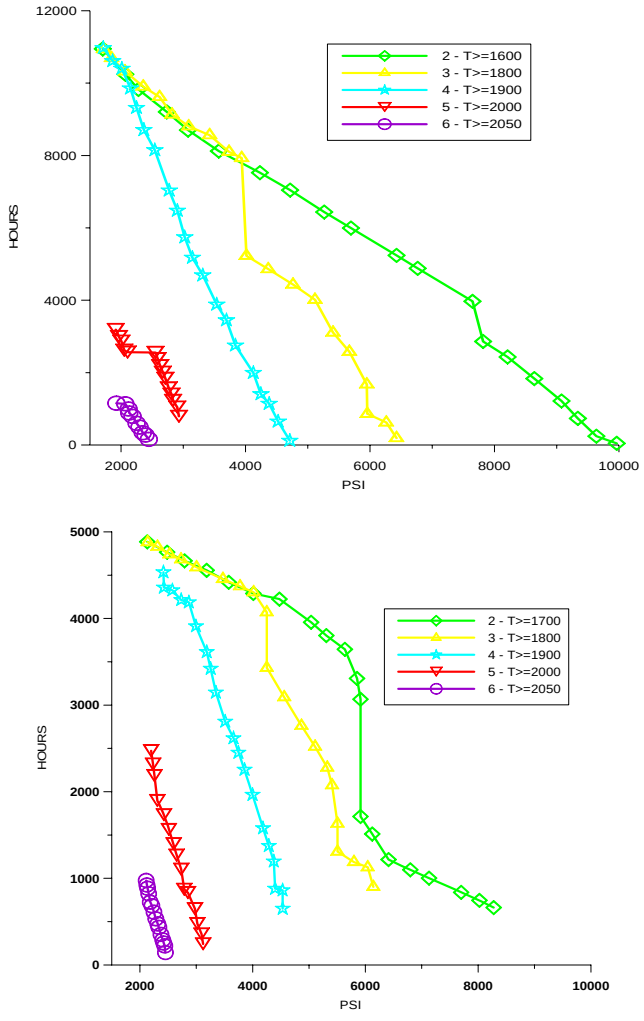

Fig. 4.11. Sets of Pareto optimal solutions of five two-objective optimization problems with 17 chemical elements (top) and with 9 chemical elements (bottom).

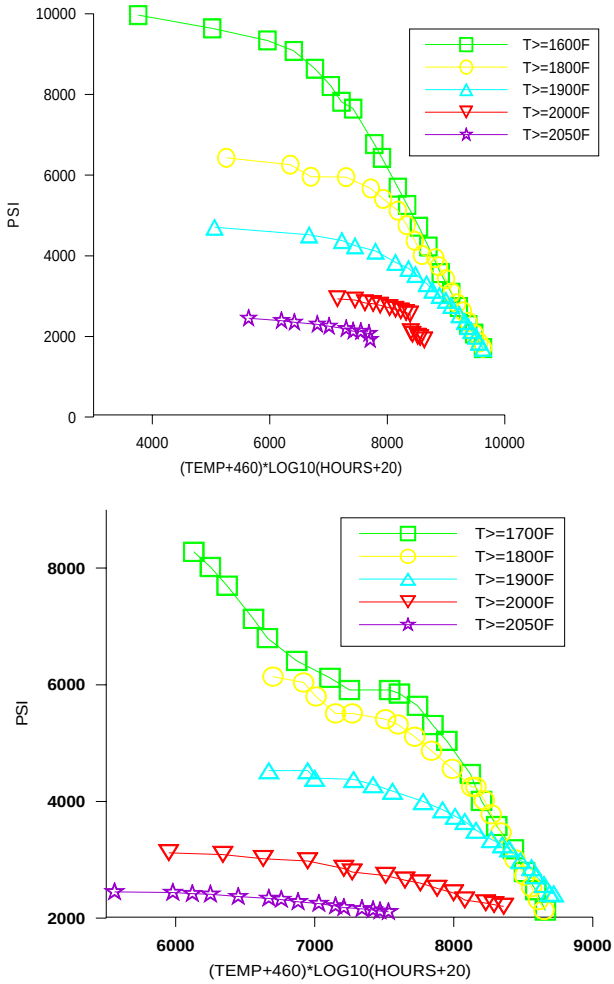

Fig. 4.12. Larsen-Miller diagrams for Pareto sets resulting from five two-objective optimization problems with 17 chemical elements (top) and with 9 chemical elements (bottom).

5. Accomplishments

The tool developed 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 was provided by Duraloy. Based on Duraloy supplied 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 phase analysis and microstructural validation. Two of the compositions were produced and tested for their creep properties.

Duraloy, the main producer of H-Series steels has not directly used the outcome of algorithm developed in this project. However, further optimized H-Series compositions based on ORNL work using the phase stability and volume fraction have been cast and fabricated into radiant burner tube assemblies. One of these assemblies is currently in test at Nucor 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 within the range of the data used, but the specific composition for an application has not yet been produced or tested. The implementation of such a capability by industry will require the development of an interactive computer-based tool with range of property prediction options and data output that can be used directly by production, sales and design engineers.

For convenience, a web site containing pertinent papers, reports, and other information on this project has been established at http://www.ms.ornl.gov/mpg/sikka.html.

5.1 Technical Accomplishments

The major technical accomplishment from this project was the development of two new formulations for the design of superior alloy chemical compositions: (1) a direct multi-objective optimization formulation that creates chemical compositions with extreme properties (maximum strength, temperature, and time-to-rupture) and (2) an inverse design formulation that creates multiple new alloy concentration, each satisfying prescribed values of desired operating stress, temperature and life expectancy.

Both alloy design methods used an evolutionary optimization algorithm that utilizes neural networks, radial basis functions, Sobol's algorithm, and self-adapting multidimensional response surface concepts. Since physical/mechanical properties of all alloys used in this study were performed using standard experimental techniques, the predicted properties of the optimized alloys are considered to be automatically validated.

The alloy design methods developed in this project are applicable to the design of any type of alloy and can easily accommodate desired features of new alloys such as low cost, low weight, availability, and processability. Conceptually, these alloy design methods could also incorporate uncertainty in the alloy manufacturing and testing procedures and in thermal and mechanical posttreatment of the new alloys.

Results from this project were reported in six technical papers (see Sect. 5.3 for details).

5.2 Technology Transfer

The H-Series steel producer, Duraloy, and one of the users, ISG Plate (previously Bethlehem Steel), were made aware of the outcome of this project through project progress presentations at the ITP/IMF annual project review meetings. This was the most direct transfer of the outcome of the project to its partners. Technology transfer to a broader audience occurred through presentations of this work at the national meetings of TMS and two topical conferences dealing with multidisciplinary analysis and optimizations. One presentation was also made at an international conference in Brazil. In addition to presentations, six technical papers were published, which further enhanced the transfer of technology. Also, some of the results of this project were incorporated into the Duraloy/ORNL project on development of novel H-Series steels with improved strength and higher upper use temperature.

5.3 Publications

Journal Articles

I. N. Yegorov-Egorov and G. S. Dulikravich, "Chemical Composition Design of Superalloys for Maximum Stress, Temperature, and Time-to-Rupture using Self-Adapting Response Surface Optimization," *Materials and Manufacturing Processes*, **20,** no. 3 (May 2005).

I. N. Yegorov-Egorov and G. S. Dulikravich, "Inverse Design of Alloys for Specified Stress, Temperature, and Time-to-Rupture by Using Stochastic Optimization," *Inverse Problems in Science and Engineering*, **13,** no. 6 (December 2005).

Papers in Conference Proceedings

G. S. Dulikravich, I. N. Egorov, V. K. Sikka, and G. Muralidharan, "Semi-Stochastic Multi-Objective Optimization of Chemical Composition of High-Temperature Austenitic Steels for Desired Mechanical Properties," pp. 801–814 in *Metallurgical and Materials Processing Principles and Technologies (Yazawa International Symposium), Vol. 1: Materials Processing Fundamentals and New Technologies*, ed. F. Kongoli, K. Itakagi, C. Yamaguchi, and H-Y Sohn, TMS Publication, San Diego, Calif., March 2–6, 2003.

N. Yegorov-Egorov and G. S. Dulikravich, "Inverse Design of Alloys for Specified Stress, Temperature, and Time-to-Rupture by Using Stochastic Optimization," *Proceedings of International Symposium on Inverse Problems, Design, and Optimization — IPDO*, ed. M. J. Colaco, G. S. Dulikravich, and H. R. B. Orlande, Rio de Janeiro, Brazil, March 17–19, 2004.

G. S. Dulikravich, I. N. Yegorov-Egorov, V. K. Sikka, and G. Muralidharan, "Optimization of Alloy Chemistry for Maximum Stress and Time-to-Rupture at High Temperature," 10th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference, Albany, N.Y., Aug. 30–Sept. 1, 2004.

G. S. Dulikravich and I. N. Yegorov-Egorov, "Robust Optimization of Concentrations of Alloying Elements in Steel for Maximum Temperature, Strength, Time-to-Rupture, and Minimum Cost and Weight," invited lecture, *ECCOMAS 2005: Computational Methods for Coupled Problems in Science and Engineering*, ed. M. Papadrakakis, E. Onate, and B. Schrefler, Fira, Santorini Island, Greece, May 25–27, 2005.

Presentation Only (Abstract)

G. S. Dulikravich, I. N. Yegorov-Egorov, V. K. Sikka, and G. Muralidharan, "Semi-Direct and Inverse Design of High-Temperature Alloys Using Multi-Objective Stochastic Optimizaiton," invited lecture, Symposium on Materials by Design: Atoms to Applications, 2004 Annual Meeting of TMS, Charlotte, N.C., March 14–18, 2004.

6. Conclusions

Two new formulation methods for the design of superior alloy chemical compositions have been developed.

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

Both alloy design methods use an evolutionary optimization algorithm that utilizes neural networks, radial basis functions, Sobol's algorithm, and self-adapting multidimensional response surface concepts.

Evaluations of physical properties of all alloys were performed using classical experimental techniques, thus automatically confirming the validity of the predictions of properties of the optimized alloys. These alloy design methods are applicable to design of any type of alloys and can easily account for additional desired features of new alloys such as low cost, low weight, availability, and processability. Conceptually, these alloy design methods could also incorporate uncertainty of the alloy manufacturing and testing procedures and thermal and mechanical posttreatment of the new alloys.

7. Recommendations

For effective use of the outcome of the algorithm developed in this project, the development of an interactive computer-based tool with range of property prediction options and data output that can be directly used by production, sales and design engineering staff is recommended. After the tool is developed, selective experimental validation of certain predicted properties is highly recommended.

Analytical tools such as those developed in this project need very large well-characterized databases. Within the databases, the algorithm can lead a variety of alternate compositions or properties for a specified composition. The extrapolation of predicting capability outside the range of data requires experimental validation. For the use of the project outcome, results need to be converted into an interactive computer-based tool that can produce data output in the forms that the industrial engineers are used to seeing. This development needs further support.

The major barrier to developments of this approach is the need for large well-characterized property databases with detailed chemical analysis. Although, a good database existed for creep properties, similar database corrosion properties is not easy because of the large number of variables involved and many different test methods used. Thus, an effort is needed to find a way to normalize the corrosion database.

8. References

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