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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 2005

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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.

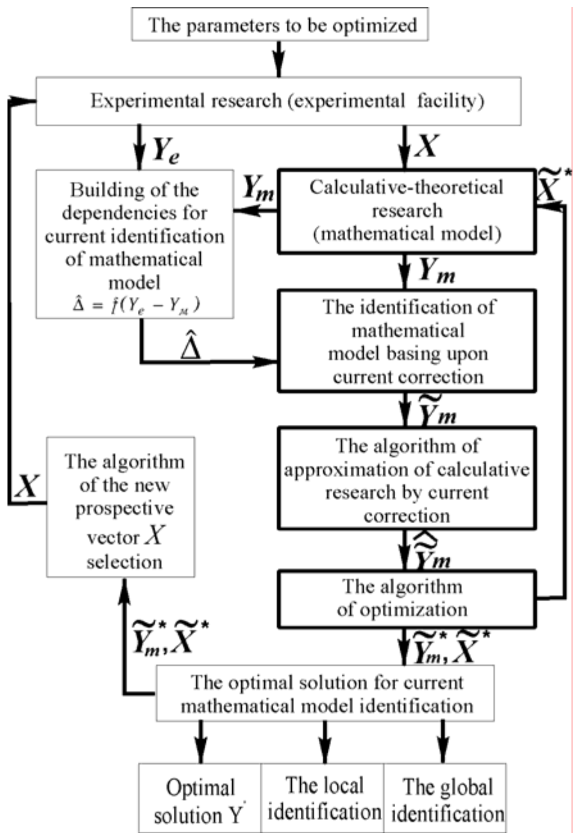

Fig. 3.1. The general scheme for optimization that verifies theoretical and experimental methods.

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

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

subject to a vector of inequality constraints

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

and a vector of equality constraints

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

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.

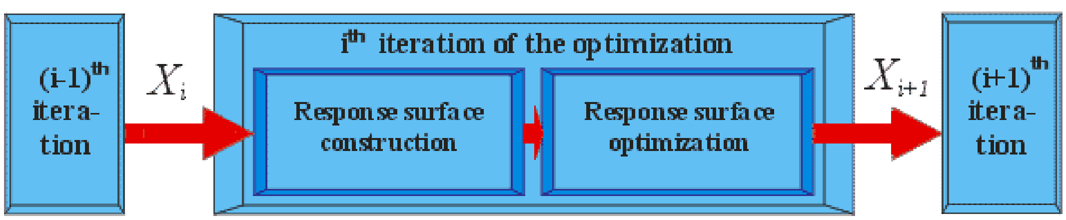

Fig. 3.2. IOSO iteration scheme.

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.

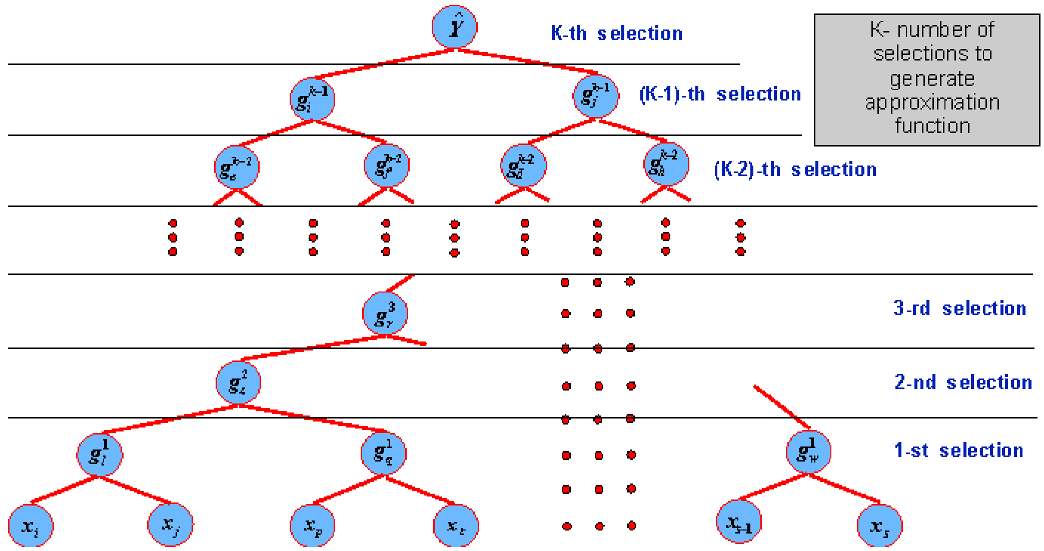

Fig. 3.3. Example of the IOSO response surface structure.

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.

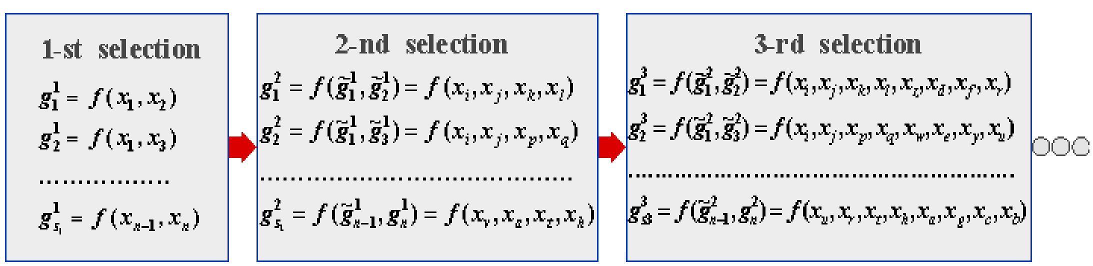

Fig. 3.4. IOSO approximation process scheme.

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.

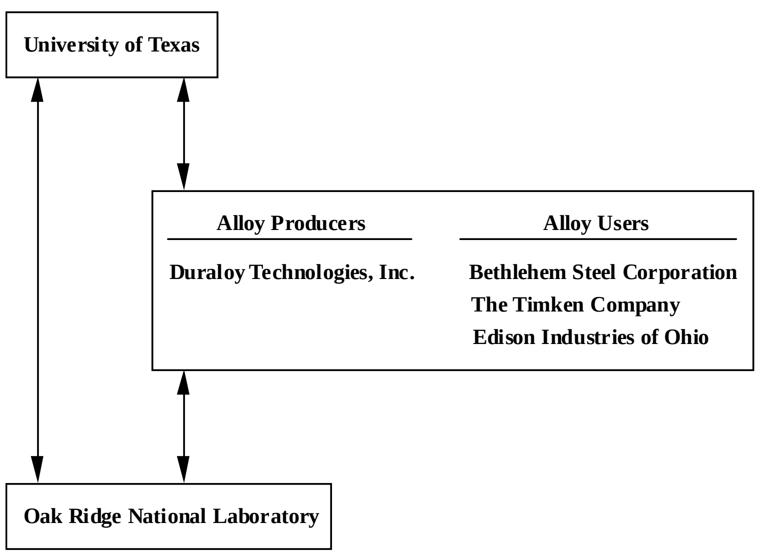

Fig. 3.5. Organization plan for the team involved in the project.

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^oF
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.

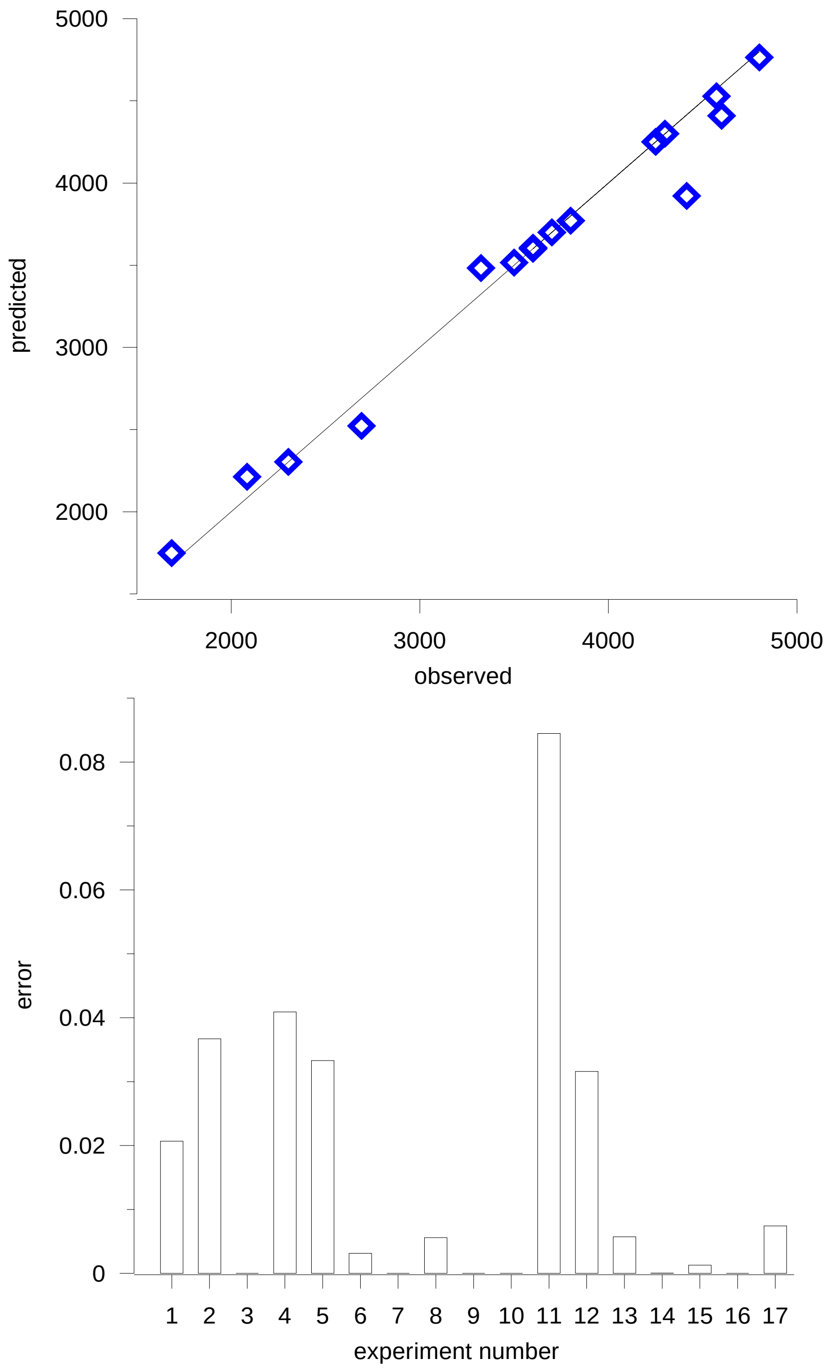

Fig. 4.1. Accuracy of ANN1.

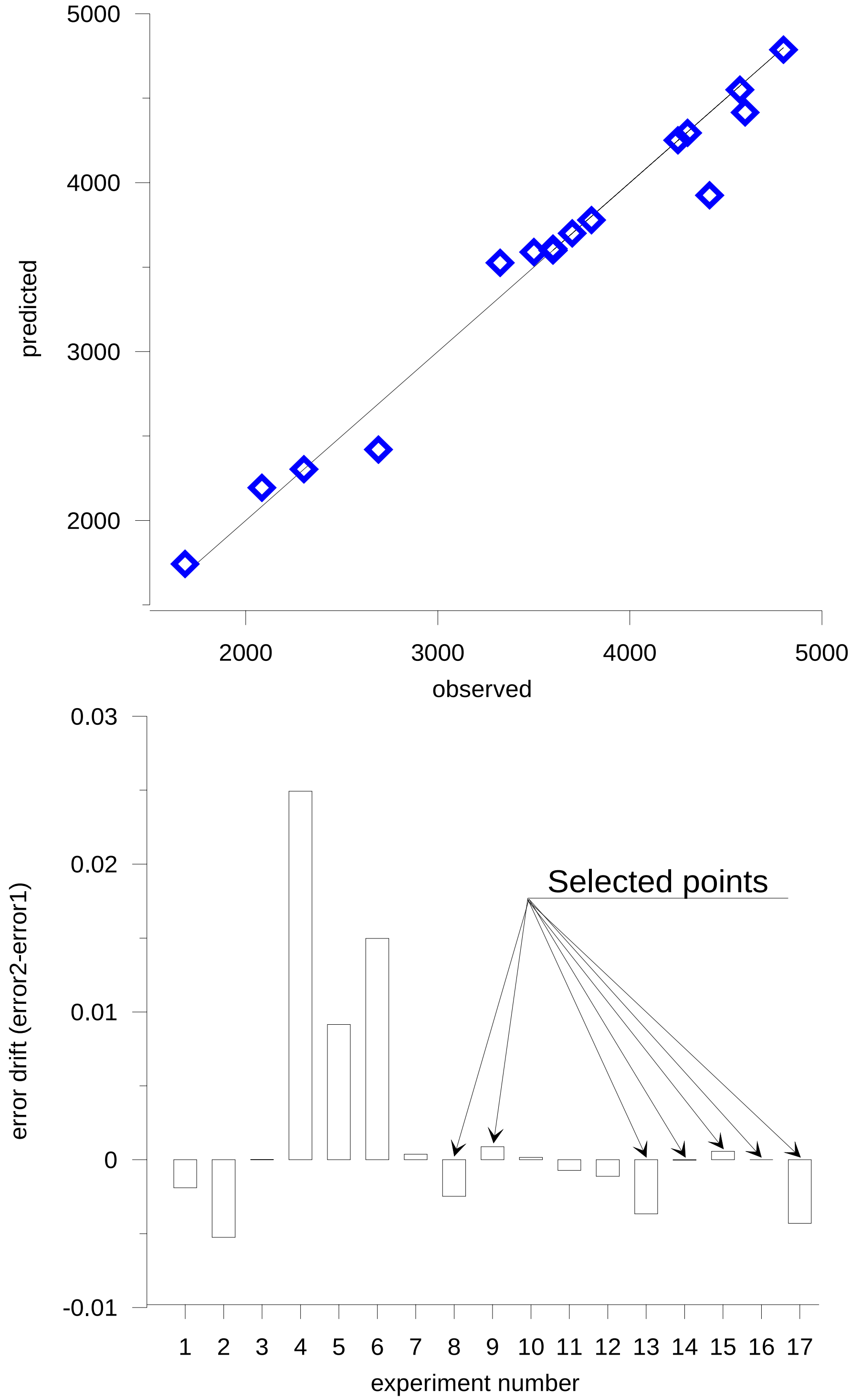

Fig. 4.2. Accuracy of ANN2.

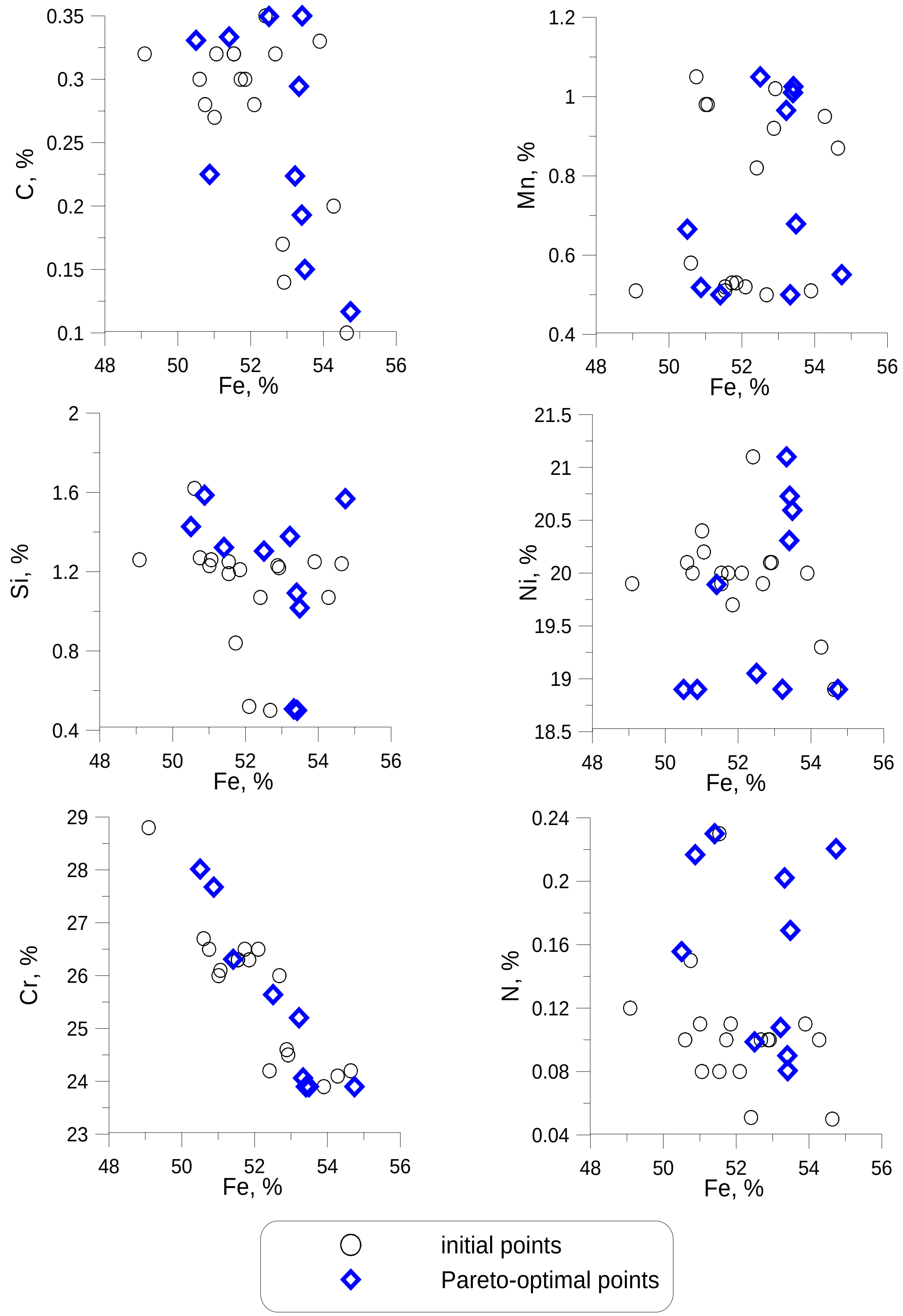

Fig. 4.3. Results of the first iteration of steel composition optimization.

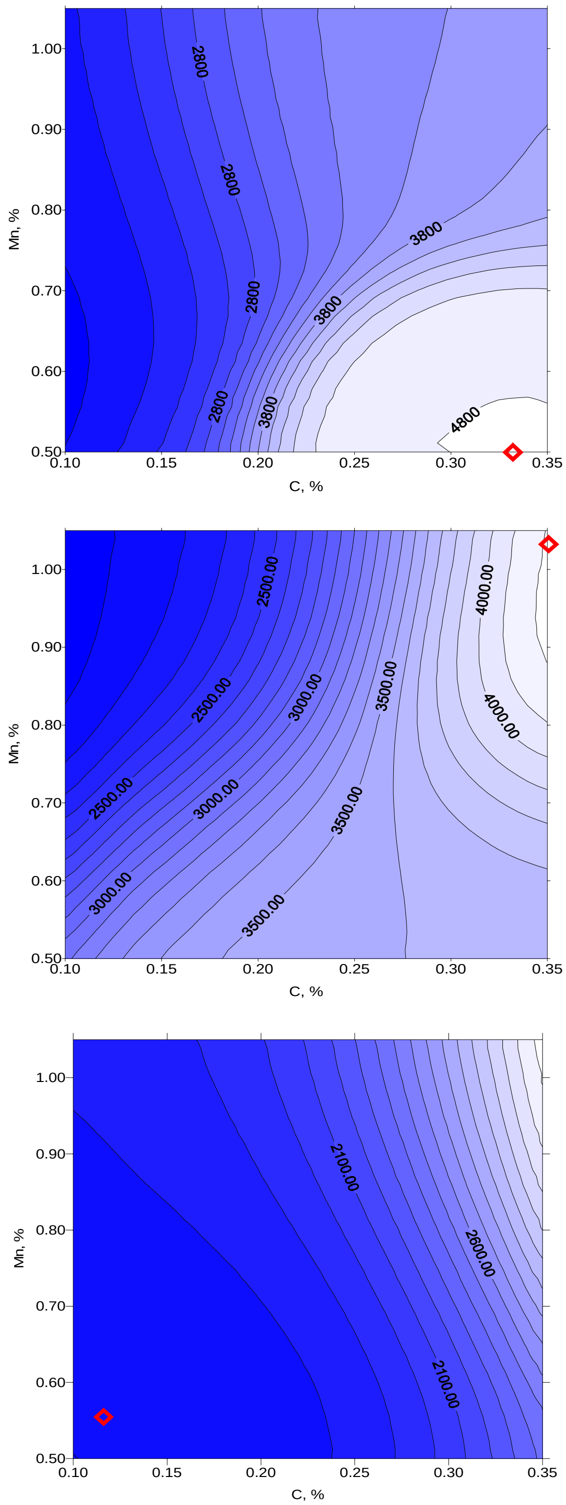

Fig. 4.4. Topology of the ANN2-based response surface in the vicinity of first, second, and tenth Pareto-optimum points for C – Mn.

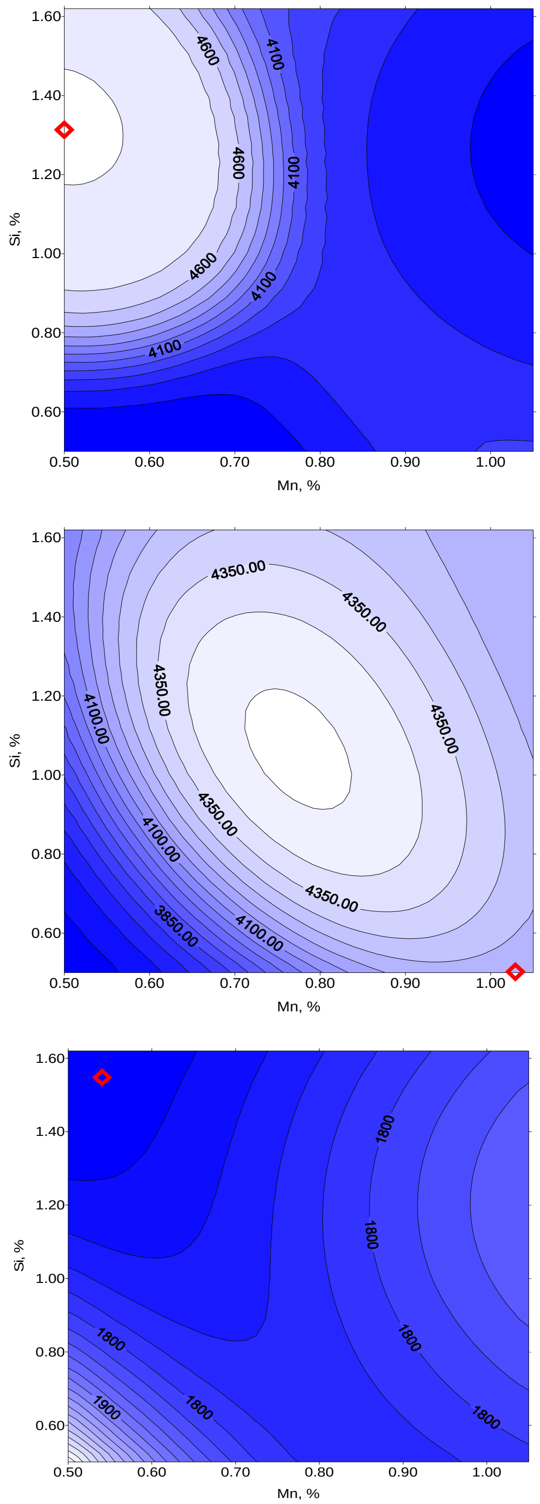

Fig. 4.5. Topology of the ANN2-based response surface in the vicinity of first, second, and tenth Pareto-optimum points for Mn – Si.

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.

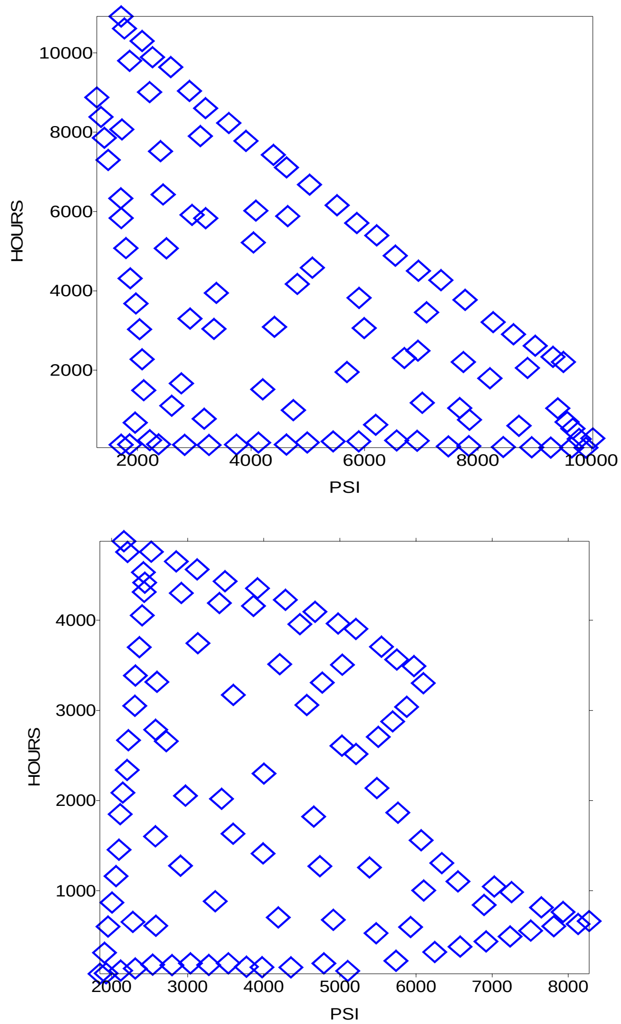

Fig. 4.6. Time-to-rupture vs strength interdependence of optimization objectives for three-objectives Pareto set with 17 chemical elements (top) and with 9 chemical elements (bottom).

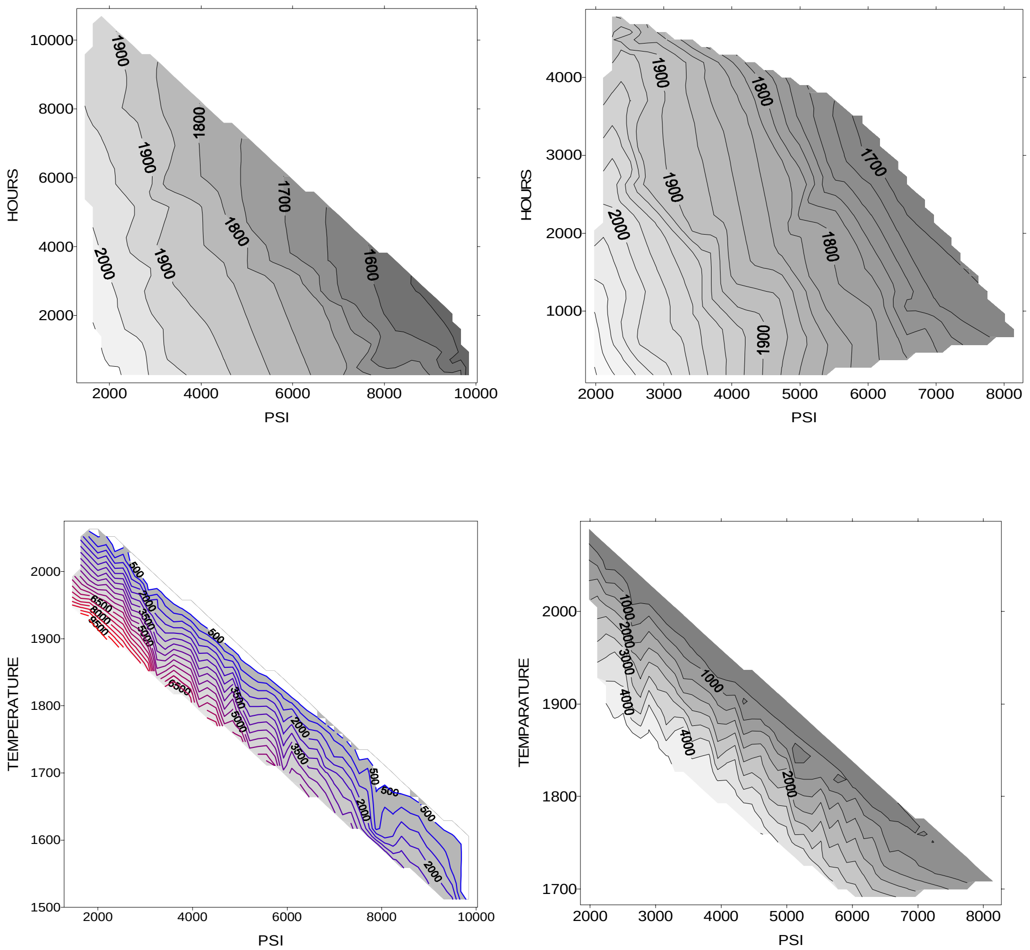

Fig. 4.7. Time-to-rupture vs strength and temperature vs strength interdependences of optimization objectives for Pareto set resulting from a three-objectives optimization with 17 chemical elements (left) and with 9 chemical elements (right).

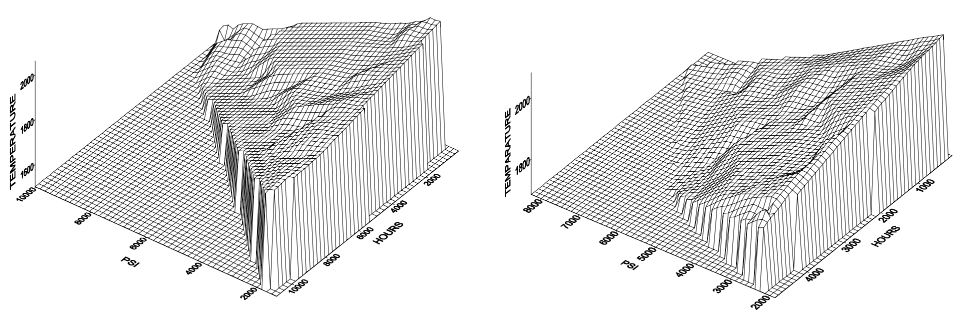

Fig. 4.8. Topography of response surfaces of three-objective optimization problems with 17 chemical elements (left) and with 9 chemical elements (right).

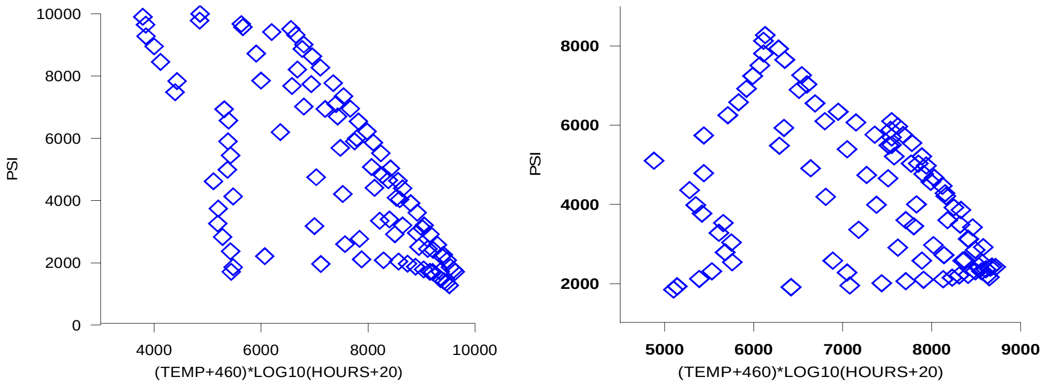

Fig. 4.9. Larsen-Miller diagram for Pareto sets resulting from a three-objective optimization with 17 chemical elements (left) and with 9 chemical elements (right).

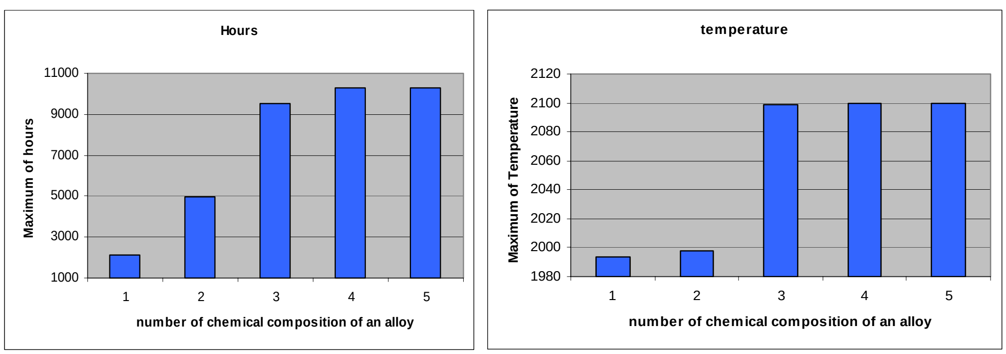

Fig. 4.10. Influence of the number of optimized alloying elements on the properties of the optimized superalloy; 1 – eight element, 2 – nine elements, 3 – eleven elements, 4 – fourteen elements, 5 – seventeen elements. A similar trend was observed with the maximum strength.

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.

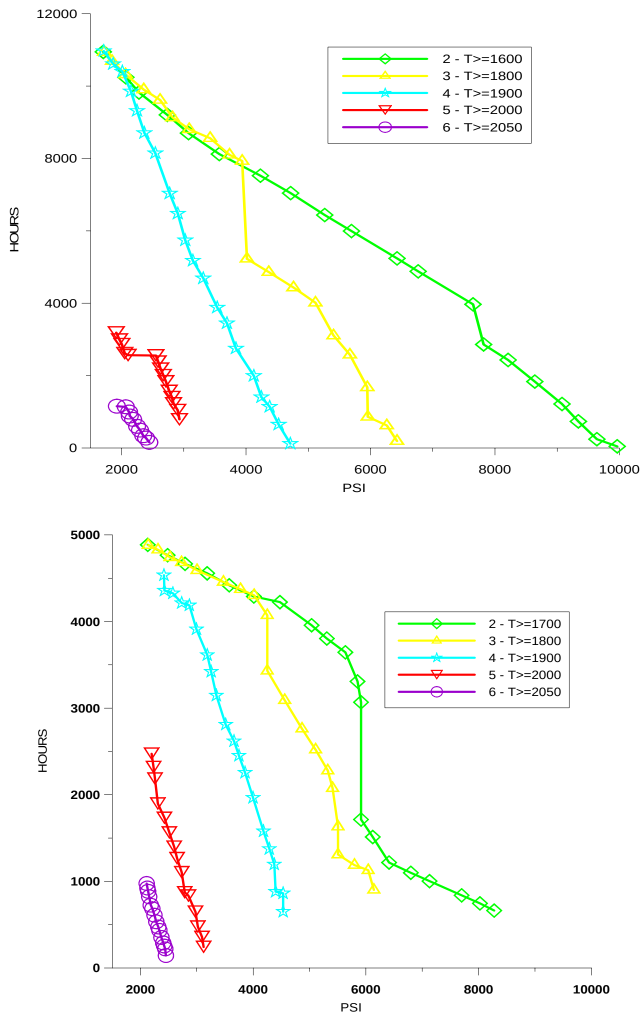

Fig. 4.11. Sets of Pareto optimal solutions of five two-objective optimization problems with 17 chemical elements (top) and with 9 chemical elements (bottom).

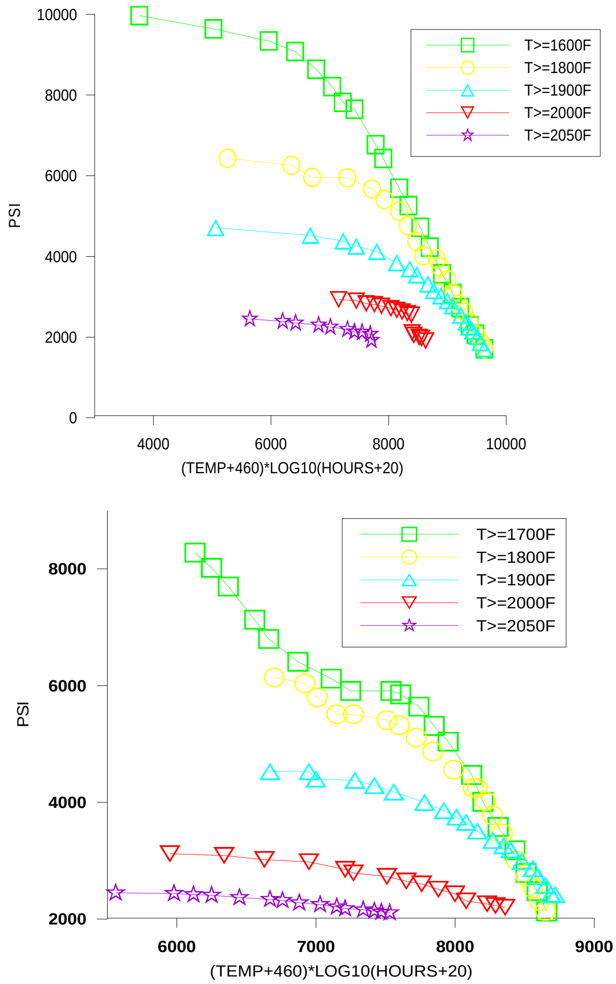

Fig. 4.12. Larsen-Miller diagrams for Pareto sets resulting from five two-objective optimization problems with 17 chemical elements (top) and with 9 chemical elements (bottom).

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.

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Appendix: Publications

1. Optimization of Alloy Chemistry for Maximum Stress and Time-to-Rupture at High Temperature

2. Semi-Stochastic Multi-Objective Optimization of Chemical Composition of High-Temperature Austenitic Steels for Desired Mechanical Properties

3. Inverse Design of Alloys for Specified Stress, Temperature, and Time-to-Rupture by Using Stochastic Optimization

4. Robust Optimization of Concentrations of Alloying Elements in Steel for Maximum Temperature, Strength, Time-to-Rupture, and Minimum Cost and Weight

10th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference, AIAA paper 2004-4348,
Albany, NY, Aug. 30 – Sept. 1, 2004.

Optimization of Alloy Chemistry for Maximum Stress and Time-to-Rupture at High Temperature

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Indirect Optimization based upon Self-Organization (IOSO) algorithm was used in conjunction with experimental evaluations of maximum strength and time-to-rupture at high temperature to maximize these two properties in nickel based steel alloys. This research provides the first realistic demonstration of the entire alloy design optimization procedure and simultaneous experimental verification of this procedure. We started by using 120 experimentally tested nickel based alloys and optimized six alloying elements in order to predict 20 new alloy compositions with potentially better properties. After experimentally testing these 20 new alloys, it was found that 7 of them indeed had superior strength and time-to-rupture at high temperature as compared to the original 120 alloys. The IOSO optimization procedure was repeated a total of four times whereby 20 new alloys were predicted and experimentally tested during each of the four design iteration cycles. The properties of the newly found alloys consistently continued improving from one iteration to the next. This was confirmed by experimentally evaluating these new alloys. This alloy design methodology is applicable to arbitrary alloys. It does not require any mathematical modeling of the physical properties since they are determined experimentally. This assures the reliability of this approach to alloy design and makes it affordable since it requires a relatively small number of new alloys to be manufactured and experimentally tested.

I. Introduction

There is a continuous industry-wide need for improving properties of high-temperature steel alloys. Since very small variations of concentrations of alloying elements can result in significant variations of the physical properties of the alloys, it is of utmost importance to find the most appropriate concentrations of each of the alloying elements so that the desired alloy properties are extremized. Probably the most prominent center for research activity in certain aspects of predictive modeling and regression analysis in super-alloys is at Cambridge University in the U.K.[1-3]. Their approach is to use artificial neural network logic for a non-linear regression analysis and a *de facto* data mining. 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 avoid this difficulty, 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 behaves itself when presented with previously unseen data.

In addition, artificial neural networks, once fully trained, are very efficient and accurate interpolating algorithms for any multi-parameter function. However, this does not mean that the neural networks are automatically efficient and accurate search algorithms or extrapolation algorithms. These, they are not. Therefore, it is important to understand a need for a mathematically sound multi-objective stochastic optimization algorithms that are capable of finding the global minimum and confidently search outside a given initial data base.

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This is a novel approach to alloy design that does not utilize the wealth of knowledge accumulated in the field of metallurgy and crystallography.

This approach has the potential[4] of predicting superior alloy compositions while requiring a reasonable number of new alloys to be manufactured and tested instead of performing a classical parametric analysis that would require orders of magnitude more alloys to be manufactured and tested. Furthermore, this approach has the potential for creating and designing alloys for each application, thereby maximizing their utilization at reduced cost.

The key to the success of the proposed research is the robustness, accuracy, and efficiency of the proposed multi-objective constrained optimization algorithm. There are only a few commercially available general-purpose optimization software packages. However, semi-stochastic truly multi-objective constrained optimization algorithms have not been commercialized yet and have not been demonstrated in this field of application. This research is based on the use and a special adaptation of a new stochastic optimization algorithm specifically for the task of optimizing properties of alloys while minimizing the number of experimental evaluations of the candidate alloys. Indirect Optimization based upon Self-Organization (IOSO)[5-10] multi-objective optimization algorithm is of a semi-stochastic type incorporating certain aspects of a selective search on a continuously updated multi-dimensional response surface. Both 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 like genetic algorithms[11-13]. Furthermore, the self-adapting response surface formulation used in this project allows for incorporation of realistic non-smooth variations of experimentally obtained data and allows for accurate interpolation of such data.

1.1 Summary of IOSO Algorithm

Each iteration of IOSO consists of two steps. The first step is the creation of an approximation of the objective function(s). Each iteration in this step represents a decomposition of the initial approximation function into a set of simple approximation functions so that the final response function is a multi-level graph.

The second step 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 the process of each iteration of IOSO, the optimization of the response function is performed only within the current search area.

This step is followed by a direct call to the 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 saved, and the response function is made more accurate only for this search area. While proceeding from one iteration to the next, the following steps are carried out: modification of the experiment plan; adaptive selection of current extremum search area; choice of the response function type (global or middle-range); transformation of the response function; modification of both parameters and structure of the optimization algorithms; and, if necessary, selection of new promising points within the researched area. Thus, during each iteration, a series of approximation functions for a particular objective of optimization is built. These functions differ from each other according to both structure and definition range. The subsequent optimization of these approximation functions allows us to determine a set of vectors of optimized variables.

During this work[5] algorithms of artificial neural networks (ANN) were used that utilized radial-basis functions modified in order to 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 given subset of test points $W_{best} \in W_{ini}$. Each iteration of alloy composition multi-objective optimization technique involves the following steps:

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 (for example, 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 actions:

1. Formulation of optimization task, that is, 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 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 also 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 resulting in a specified number of Pareto optimal solutions.
5. Analysis of optimization results.
6. Carrying out experimental evaluations of the newly found alloys to obtain a set of Pareto optimal alloy compositions (or a certain subset) and analysis of the results obtained.
7. Change of optimization problem statement (number of simultaneous objectives and constraints, the set and range of variable parameters), and returning to step 2.
8. Modification of database and returning to step 4.
9. Stop

II. Problem Statement

This work was aimed at optimizing nickel based heat-resistant alloy castings containing ***Ni, C, Cr, Co, W, Mo, Al, Ti***, ***B, Nb, Ce, Zr, Y***, and trace amounts of ***S, P, Fe, Mn, Si, Pb, Bi***. Thermal treatment of the samples involved heating them to 1210 C, holding for 4 hours, and air cooling. During the tests the stress at room temperature (sigma) and the time to survive until rupture at temperature of 975 C and stress of 230 N/mm^2 were measured. The technology used in the casting allowed us to alter the chemical composition by varying concentrations of the following elements: ***Ni, C, Cr, Co, W, Mo, Al, Ti***. The concentrations of ***Nb, B, Ce, Zr, Y*** in all test samples were 1.1%, 0.025%, 0.015%, 0.04%, and 0.01%, respectively.

Average concentrations of trace alloying elements were: S (0.0037%), P (0.006%), Fe (0.085%), Mn (0.013%), Si (0.067%), Pb (0.0005%), Bi (0.0005%).

In this task the concentrations of seven elements: ***C, Cr, Co, W, Mo, Al, Ti*** were used as variable parameters.

The percent of nickel represented the remaining amount of the alloying mixture. User-specified minimum and maximum allowable values of the seven alloying elements are presented in Table 1.

Table 1. Prescribed ranges of optimization variables

Element	Minimum %	Maximum %
C	0.13	0.20
Cr	8.0	9.5
Co	9.0	10.5
W	9.5	11.0
Mo	1.2	2.4
Al	5.1	6.0
Ti	2.0	2.9

The optimization was conducted by simultaneously maximizing stress (SIGMA) and time-to rupture (HOURS). At each optimization iteration, a two-criterion optimization task with a specified number of Pareto optimal points was solved. The user-specified number of Pareto points was 20.

III. Optimization Results

The total number of experimentally evaluated alloy samples during the solution of this particular optimization problem was specified by the user to be 200. At the start, the initial experiment plan including 120 points was developed by distributing their chemical compositions via Sobol's algorithm[14]. This information was used for building an approximation function (a multi-dimensional response surface (Fig. 1)) for the first iteration. This approximation function was optimized using a variant of IOSO. The result was a set of chemical compositions of 20 new alloys which could be a part of the current Pareto set (Fig. 2).

Next step was manufacturing and experimental evaluation of the two properties (maximum stress and time-to-rupture at 975 C) for each of these 20 newly found alloys.

Then, we defined a Pareto set using all (120 + 20 = 140) experimental points. This research shows that only seven out of 20 newly found alloys belong to the current Pareto set after the first iteration. This means that all triangles in Fig. 2 are real-life materials with new chemical compositions, but only 7 of them belong to the current Pareto set because these chemical compositions can improve both optimization objectives for real-life materials. The remaining 13 newly found alloys are not the best as revealed by the experimental research, because these alloys do not belong to the current Pareto set after the first iteration for real-life material. This is why we named these 13 alloys as "points with bad predictive properties" (Fig. 2). But, these 13 new alloys bring some new information about topology of the objectives. That is why we can now build a new approximation function (response surface) with a higher level of accuracy.

Second iteration followed the same procedure, but now we used all 140 experimentally evaluated alloys (7 of them were in the current Pareto set after the first iteration).

So, each iteration includes:

1. building approximation function where
   for 1st iteration we used 120 experimental points, for 2nd iteration we used 140 experimental points, for 3rd iteration we used 160 experimental points, for 4th iteration we used 180 experimental points);
2. optimization of this approximation function with the objective of determining 20 alloys with new chemical compositions which can improve current Pareto set.
3. experimental evaluation of the 20 new alloys;
4. defining current Pareto set for the current number of the experimentally evaluated points (after 1st iteration we used 140 experimental points, after 2nd iteration we used 160 experimental points, after 3rd iteration we used 180 experimental points, after 4th iteration we used 200 experimental points).

As a result of this procedure, we obtained 7 current Pareto set after 1st iteration, 11 after 2nd iteration, 8 after 3rd iteration, 7 after 4th iteration (Figs. 3, 4 and 5).

During optimization, the average error in prediction capabilities of the response surfaces formed during each of the four optimization iterations were constantly improving (Figs. 6-9) and the average error in the representation of the responses surfaces was monotonically decreasing (Fig. 1).

It should be pointed out that the presented work represents an automatic search for concentrations of alloying elements that will simultaneously provide extreme values of several objectives. This is a different concept from an inverse determination of chemical concentrations of alloying elements that will create alloys which satisfy prescribed values of multiple physical properties[15].

IV. Conclusions

The novel approach to optimizing physical properties of alloys by utilizing experimental data and a stochastic evolutionary optimization algorithm has proven that it is possible to find Pareto fronts of optimal solutions that are significantly "out-of-the-initial-box". The obtained results have demonstrated efficiency of the proposed technique of multi-criteria optimization of alloy chemical compositions. The proposed approach made it possible to obtain six Pareto optimal alloy compositions that ensured the strength of up to approximately 1300 N/mm^2 at room temperature and the survival time of up to 100 hours at high temperature (975 C). As can be seen from Fig.5, a tradeoff between the stress at room temperature and the time-to-rupture at high temperature was reached. After fourth iteration, seven Pareto optimal solutions were obtained.

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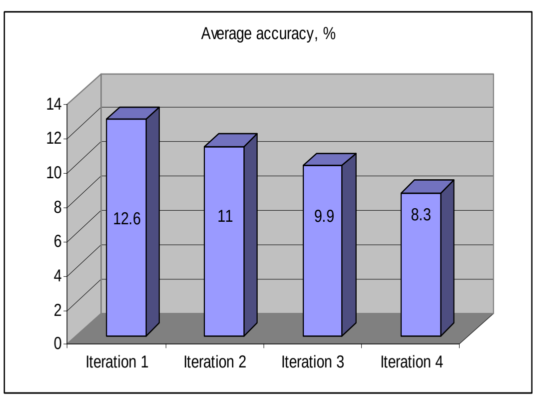

Figure 1. Average error of response surfaces representing experimental data.

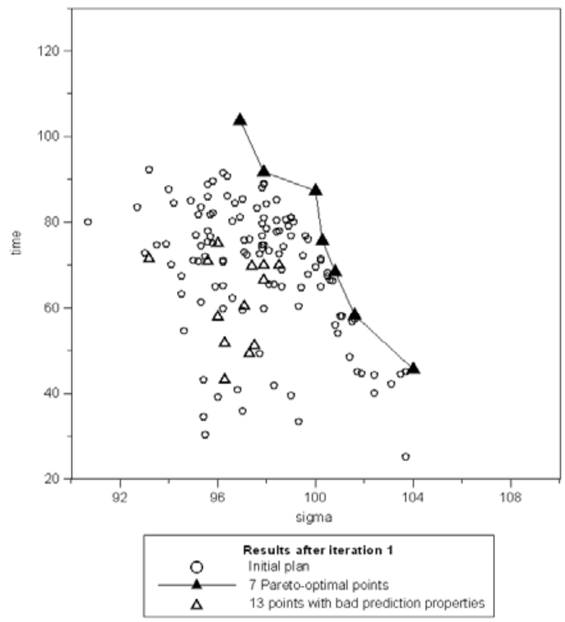

Figure 2. Initial 120 nickel based alloys and 20 alloys predicted by the 1st iteration with IOSO optimizer and consequently experimentally tested for maximum strength and time-to-rupture at 975 degrees Celsius.

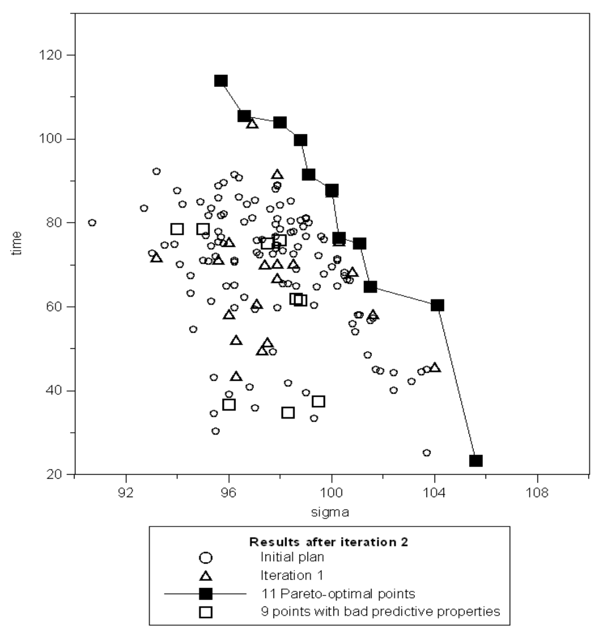

Figure 3. Initial 120 alloys plus 20 alloys from first iteration and 20 alloys predicted by the 2nd iteration with IOSO optimizer. All were then experimentally tested for maximum strength and time-to-rupture at 975 degrees Celsius.

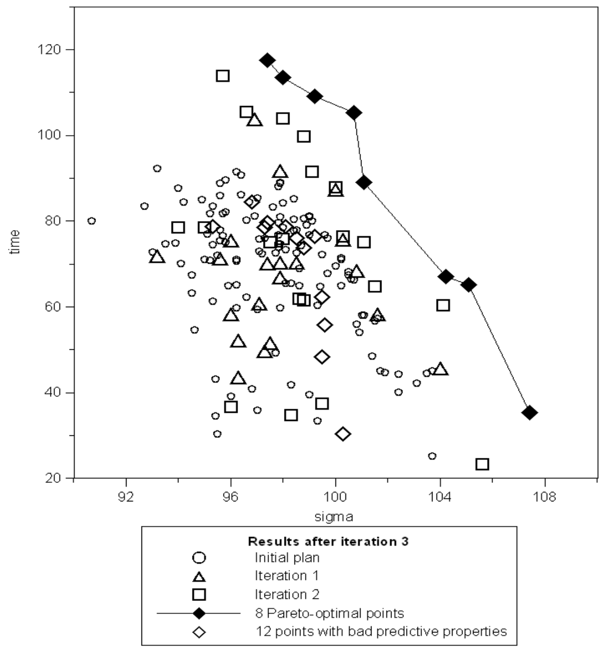

Figure 4. Initial 120 alloys plus 20 alloys from 1st iteration, plus 20 alloys from 2nd iteration, plus 20 alloys predicted by the 3rd iteration with IOSO optimizer. All were then experimentally tested for maximum strength and time-to-rupture at 975 degrees Celsius.

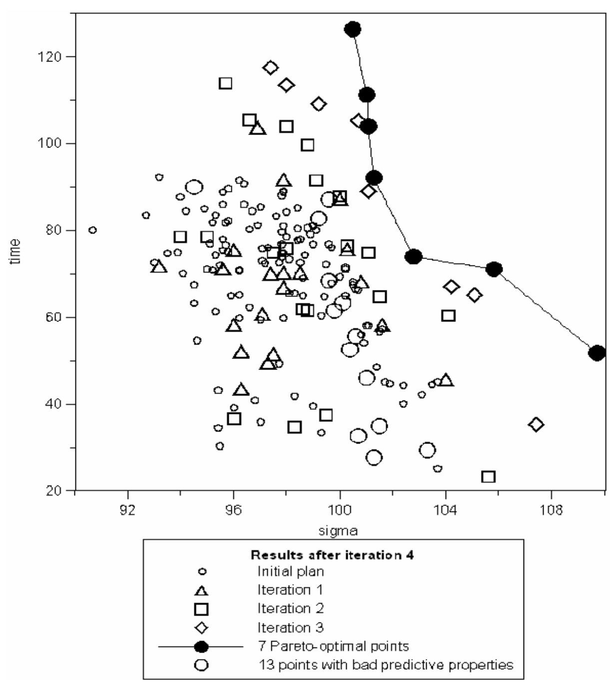

Figure 5. Initial 120 alloys plus 20 alloys from 1st iteration, plus 20 alloys from 2nd iteration, plus 20 alloys from 3rd iteration, plus 20 alloys predicted by the 4th iteration with IOSO optimizer. All were then experimentally tested for maximum strength and time-to-rupture at 975 degrees Celsius.

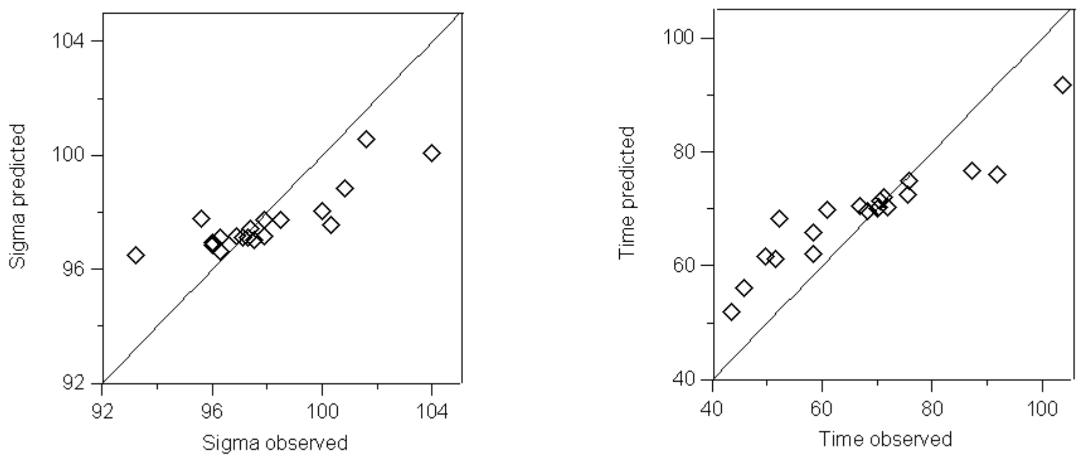

Figure 6. Predicted and observed values of two optimization criteria after first iteration.

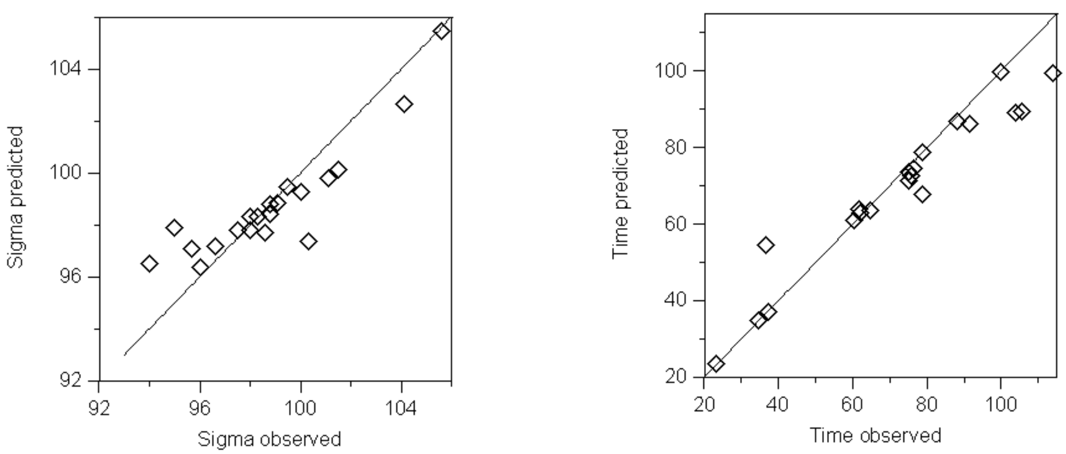

Figure 7. Predicted and observed values of two optimization criteria after second iteration.

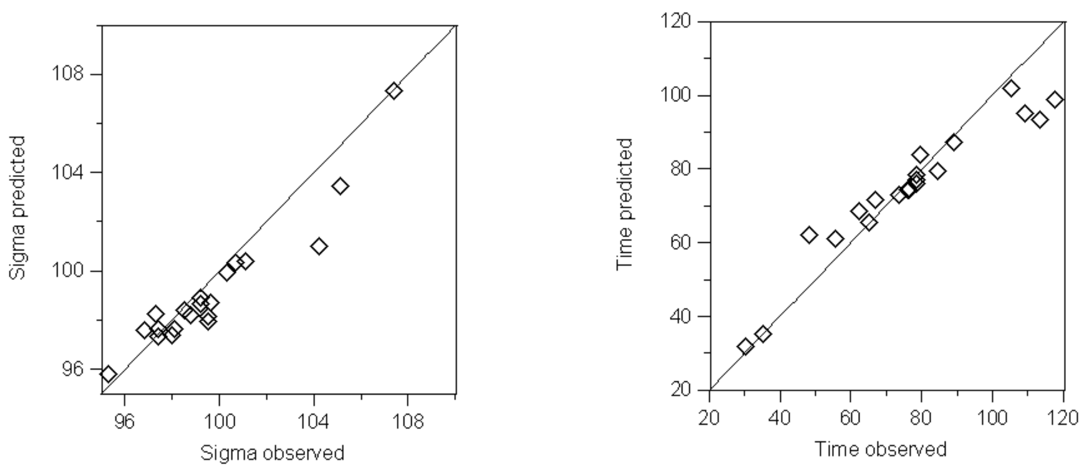

Figure 8. Predicted and observed values of two optimization criteria after third iteration.

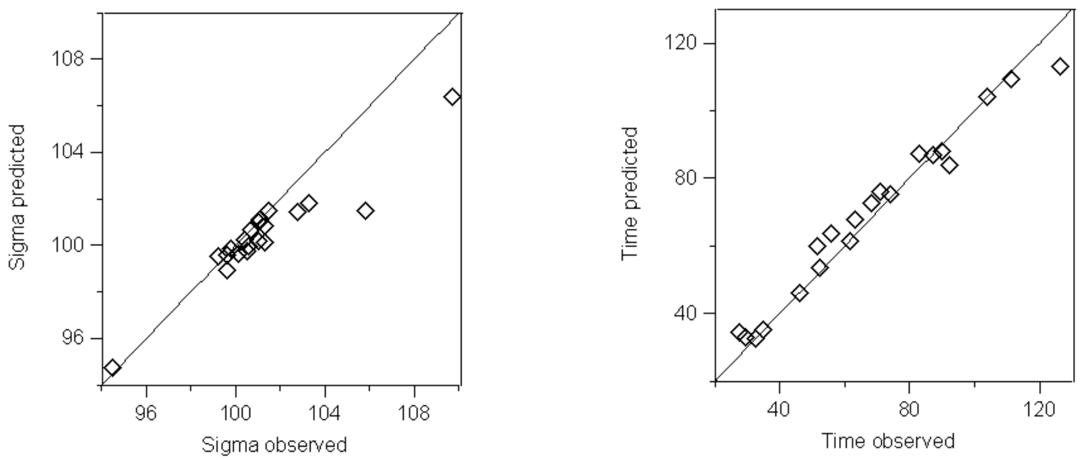

Figure 9. Predicted and observed values of two optimization criteria after fourth iteration.

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San Diego, CA, March 2-6, 2003.

SEMI-STOCHASTIC MULTI-OBJECTIVE OPTIMIZATION OF CHEMICAL COMPOSITION OF HIGH TEMPERATURE AUSTENITIC STEELS FOR DESIRED MECHANICAL PROPERTIES

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Abstract

An advanced semi-stochastic algorithm for constrained multi-objective optimization has been adapted and combined with experimental testing and verification to determine optimum concentrations of alloying elements in heat-resistant and corrosion-resistant H-Series austenitic stainless steel alloys. The objective was to simultaneously maximize a number of alloy's mechanical properties. This research will result in a rigorous tool for the design of high-strength H-Series steels and other types of alloys unattainable by any means existing at the present time. Such a material-by-design tool will also be able to reduce or minimize the need for the addition of expensive elements such as Cr, Ni, Co, Nb, Ti, V, etc. and still obtain the optimum properties of an alloy.

Introduction

There is an industry-wide need 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. Instead of using still relatively unreliable and computationally highly complex thermodynamic models for the prediction of physical properties of alloys with given chemical compositions, we have adopted a new approach of using a stochastic optimization algorithm and actual experimental evaluations of the candidate alloys. This approach has the potential of identifying new compositions that have superior properties, while requiring only dozens rather than thousands of different alloy samples to be created and experimentally tested. Furthermore, this approach has the potential for creating and designing alloys for each application, thereby maximizing their utilization at reduced cost. . This work on designing a new class of alloys for high-temperature strength, corrosion, and thermal fatigue resistance falls into a category of "combinatorial methods" for rapid screening of materials for industrial applications and/or materials property optimization. It also stimulates acquisition of thermo-physical property data needed for materials processing and industrial application, a clear path to solution of major problems in modeling, process simulation, and control.

The key to the success of this entire approach is the robustness, accuracy, and efficiency of the multi-objective constrained optimization algorithm. There are only a few commercially available general-purpose optimization software packages. 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 [2,3,4]. Moreover, these algorithms 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 fully maximized. Furthermore, 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.

We have adapted an advanced semi-stochastic algorithm for constrained multi-objective optimization [1] and have combined 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 properties Semi-stochastic, truly multi-objective constrained optimization algorithms have not been commercialized yet and have not been demonstrated in this field of application. This work is based on a special adaptation and use of such an algorithm specifically for the task of optimizing properties of alloys while minimizing the number of experimental evaluations of the candidate alloys. This multi-objective optimization algorithm is of a semi-stochastic type incorporating certain aspects of a selective search on a continuously updated multi-dimensional response surface. Both 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 like genetic algorithms. Furthermore, the self-adapting response surface formulation used in this research allows for incorporation of realistic non-smooth variations of experimentally obtained data and allows for accurate interpolation of such data. This optimization algorithm also allows for a finite number of chemically non-reacting ingredients in the alloy, for a finite number of physical properties of the alloy to be either minimized or maximized, and for a finite number of equality and inequality constraints.

Multi-Objective Optimization Concepts

With the continuing growth of computing resources available, the attention of design engineers has been rapidly shifting from the use of repetitive computational analysis, personal experience, and intuition, towards reliable and economical mathematically based optimization algorithms. This trend has exposed the practical limitations of traditional gradient-based optimization approaches [2] that easily terminate in a local minimum, can usually produce only single-objective optimized solutions, and require that the objective function satisfies continuity and derivability conditions. These facts, together with the growing need for the multi-disciplinary 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 [3,4], semi-stochastic [5,6,7,8] and especially stochastic [9,10] constrained optimization algorithms. It should be pointed out that including more objectives in the optimization process often has similar effects on the overall optimization effort required 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

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

subject to a vector of inequality constraints

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

and a vector of equality constraints

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

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 *non-dominated*. 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 non-dominated solutions (the Pareto front) is reduced to several single objective optimizations where 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 [5]. However, for a large number of design variables and objective functions that need to be extremized simultaneously, this approach becomes progressively too time consuming for practical applications in industry.

Our approach is based on the widespread application of response surface methodology, based upon the original approximation concept, within the frameworks of which we adaptively use global and middle-range multi-point approximations. One of the advantages of this approach is the possibility of ensuring good approximating capabilities using a minimum amount of available information. This possibility is based on self-organization and evolutionary modeling concepts [1,7]. During the approximation, the approximation function structure is being evolutionarily changed, so that it allows us to approximate successfully the optimized functions and constraints having sufficiently complicated topology. The obtained approximation functions can be used by multi-level procedures [7] with the adaptive change of simulation level within both a single and multiple disciplines of object analysis, and also for the solution of their interaction problems.

Multi-objective optimization problem solution [7,8] is based on the use of approximation functions for individual objectives and constraints. The current search area of adaptive changing makes it possible to search numerically the Pareto-optimal set without the use of any versions of composite objective functions (convolution approach). To reduce the computing time significantly, we have developed a multi-level multi-objective constrained optimization methodology that is a modified version of a method of Indirect Optimization based upon Self-

Organization (IOSO) [1] and evolutionary simulation principles. Each iteration of IOSO algorithm consists of two steps. The first step is the creation of an analytical approximation of the objective function(s). Each iteration in this step represents a decomposition of the initial approximation function into a set of simple analytical approximation functions so that the final response function is a multi-level graph. The second step 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 (typically 30 to 50 values of the objective function for the optimization problems with nearly 100 design variables). 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. While proceeding from one iteration to the next, the following steps are carried out: modification of the experiment plan; adaptive selection of current extremum search area; choice of the response function type (global or middle-range); transformation of the response function; modification of both parameters and structure of the optimization algorithms; and, if necessary, selection of new promising points within the researched area. Thus, during each iteration, a series of approximation functions for a particular objective of optimization is constructed. These functions differ from each other according to both structure and definition range. The subsequent optimization of these approximation functions allows us to determine a set of vectors of optimized variables.

It should be pointed out that the IOSO approach is different than the artificial neural network approach that performs fast interpolation of the existing experimental data sets [11,12]. Our approach combines a multi-level graph theory, a special version of radial basis function formulations [13], and neural networks into a self-adaptive response surface optimization algorithm capable of exploring and optimizing data that is outside of the original data set.

Technical Feasibility and Objectives

The problem of search for Pareto-optimum solutions set while varying chemical composition of an alloy would be an unacceptably labor-intensive process. This is because of an extremely large number of alloy compositions that would need to be created and because several of the properties of each of these alloys would have to be evaluated experimentally. In this case, we can speak only about the creation of some rather extensive database including the information on various properties of alloys for various combinations of a chemical structure.

With reference to a particular problem of creation of an alloy with desirable properties, there will inevitably arise a problem of constraints that need to be specified on the objective functions. Such objective constraints should be set by the user (expert) and could be allowed to vary during the solution process. For example, minimum acceptable value for the Young's modulus of elasticity could be specified as an inequality constraint. Or, 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.

Thus, we can consider the possibilities of using the means and methods of optimization (and, in particular, IOSO) for the solution of particular problems of alloy's properties optimization. Unfortunately, such problems, as a rule, are difficult to formalize at the initial stage, since the user does not know initially what values certain objectives could attain and how the remaining objectives will vary. For example, for the optimization of a problem in the car industry with six variables we needed approximately 60 experiments when using the basic IOSO algorithm. However, for optimization of the classical Rosenbrock test function, having only two variables, it was necessary to perform almost 300 objective function evaluations. Thus, it is very difficult to predict the number of experiments required in the optimization application utilized here. Therefore, it seems that such problems of optimization can be solved only in an interactive mode, when the user during the solution can change both objective constraints and objective functions. In this case, one can speak about optimally controlled experiments. Let us consider several different scenarios for the solution of optimization problems for these conditions.

The first approach is to perform a general multi-objective optimization of the material properties. Within the framework of this strategy we are to solve the multi-objective optimization problem (to find the Pareto set) using the general IOSO algorithm. This strategy is the most accurate, but it requires a very large number of experiments.

The second approach is an interactive step-by-step optimization of the material properties. The first step of this strategy is to create an initial plan of experiments. This involves the formulation of a single (hybrid) optimization objective by the user (this objective may be the convolution of particular objectives with different weight coefficients assigned to each of them) and one optimization step to minimize this objective. The result of this strategy is the single (not Pareto-set) solution. However, during such relatively efficient quasi multi-objective optimization process we can accumulate the information about the particular objectives and construct progressively more accurate response surface models.

In order to develop and realize the most effective optimization strategies (both of the first and the second kind) we have to perform a thorough preliminary search for the classes of base functions that will be able to construct the most accurate response surface models.

Brief Description of Methodology

The methodology for steel optimization is subject to several simultaneous objectives in the organization and conduct of an iterative optimized experiment. The result of these studies is the Pareto-optimal set of steel compositions that simultaneously optimizes the chosen objectives. The multi-objective optimization algorithm is based upon the use of a response surface technology developed within the frameworks of the IOSO concept. Here, response surfaces are created that are based on the available experimental data. During the conduct of research the information is being stored concerning the properties of steel in the vicinity of the Pareto set. This allows us to improve the accuracy of the results. Every iteration of this optimization methodology results in the formulation of a new set of alloy compositions, which are promised to be Pareto optimal and need experimental studies to obtain the true values of the objectives. While conducting this work we used the algorithms of artificial neural networks (ANN) for creating the response surfaces. We also used radial-basis functions that were modified for the specifics of this optimization research. The essence of modification is the selection of ANN parameters during the network training stage. They are determined from the minimum curvature of the response surface and provide the best predictive properties for the given set of experimental points $W_{best} \in W_{ini}$. In engineering terms, every iteration of multi-objective optimization methodology for H-series steel composition consists of following steps:

1. Constructing and training the ANN1 for a given set of experimental points based on the condition $W_{best} = W_{ini}$.
2. Carrying out multi-objective optimization using ANN1 and obtaining the pre-defined number of Pareto-optimal solutions P_1.
3. Determination of a subset of experimental points W_{best}, which are the closest to P_1 points in the space of design variables.

4. Training the ANN2-based on the insurance of the best predictive properties applying to the obtained subset of experimental points $W_{best} \in W_{ini}$.
5. Carrying out multi-objective optimization using ANN2 and obtaining the pre-defined number of Pareto-optimal solutions, P_2.

Initial Data Set

The initial data were the results of experimental testing of 17 samples of H-series steels with different percentage of alloying components. The experimental data for creep rupture strength after 100 hours at temperature of 1800 F is presented in Table I. Note that the poor set of available experimental data (only 17 points for 6 independent variables) and non-uniformity of their distribution in the space of design variables do not allow us to hope to obtain good accuracy of the results in the first iteration of this multi-objective optimization methodology. However, the main goal of this research is the creation of a plan of future experiment, which will allow us to improve the accuracy of the optimized steel composition for the next iterations.

Table I. The 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

Design Variables and Multiple Optimization Objectives

As the independent design variables for this problem we considered the percentage of the following components: C, Mn, Si, Ni, Cr, 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 II.

Table II. The 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 after 100 hours under the temperature of 1800 F. Other objectives have been chosen issuing from the necessity to reduce the cost of the steel. In this work, the additional three objectives were to simultaneously minimize the percentages of Mn, Ni, Cr. Thus, the multi-objective optimization problem had 6 independent design variables and 4 simultaneous objectives. We defined the desirable number of Pareto optimal solutions as 10 points.

Numerical Results

Figure 1 demonstrates the results characterizing the accuracy of the obtained response surface based on ANN1. One can see that for most of the available experimental points mean error of the prediction created by the 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 (Figure 2). Then, the four-objective optimization task was actually solved by using ANN2 resulting in a Pareto-optimal set of 10 new alloy compositions. This set is presented in Table III.

Table III. The Set of Ten Pareto-Optimal Solutions

Pareto-optimal Composition (Wt. %)							1800F
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

Figure 3 shows the 10 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 and 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.

Summary

A conceptually new method has been developed for determining proper chemical compositions of high-temperature steels that will have simultaneously optimized multiple physical properties. The method is based on a novel semi-stochastic multi-objective optimization algorithm that can utilize experimentally evaluated physical properties of a relatively small number of different alloy samples. The final outcome of the development of this type of multi-objective semi-stochastic optimization could be the ability of H-series stainless steel producers and users to predict either the alloy compositions for desired properties or to predict properties of given alloy compositions. Furthermore, this methodology is quite general and could be applied to multi-objective optimization of compositions of other types of metal alloys and even polymers.

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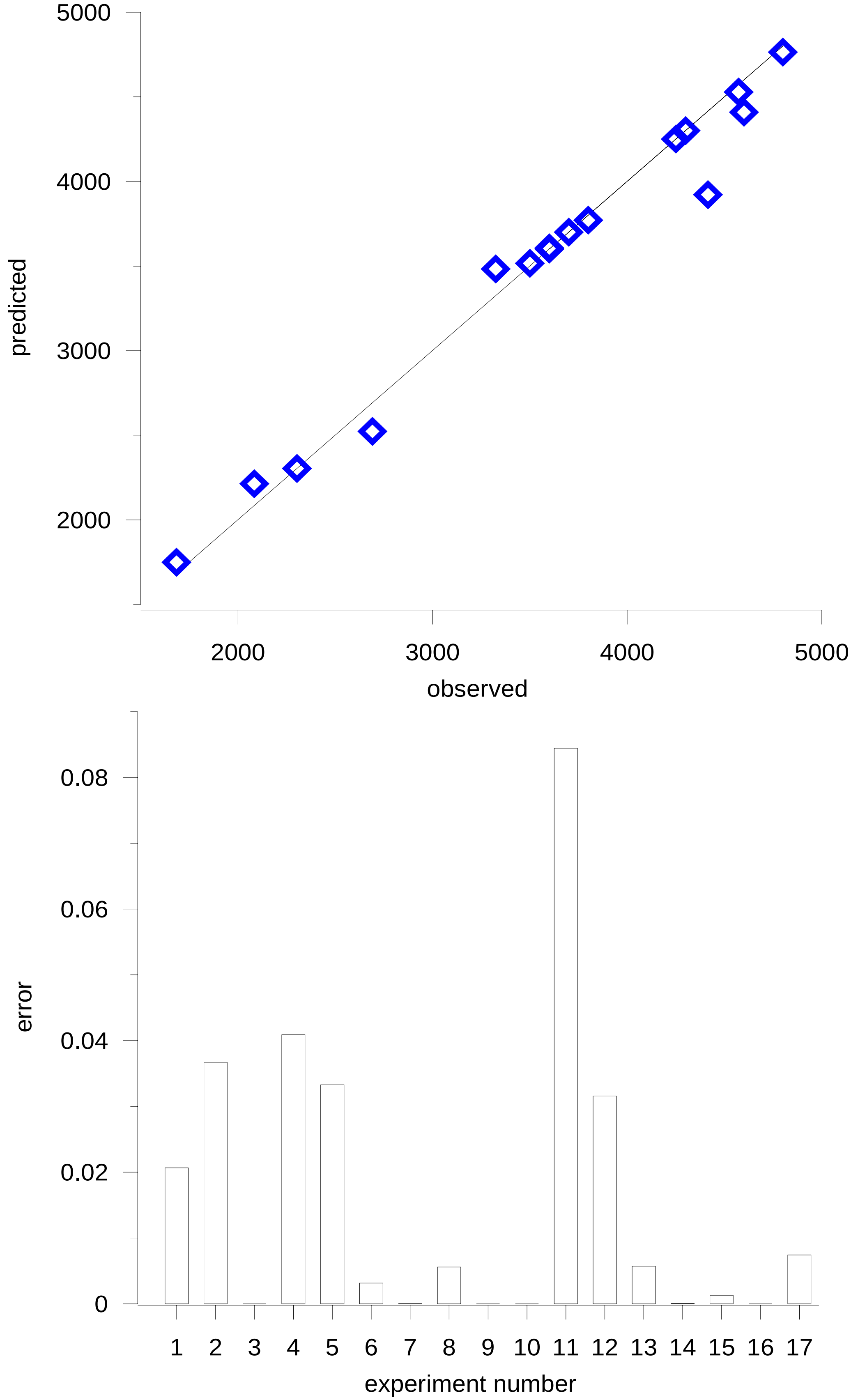

Figure 1: Accuracy of the ANN1.

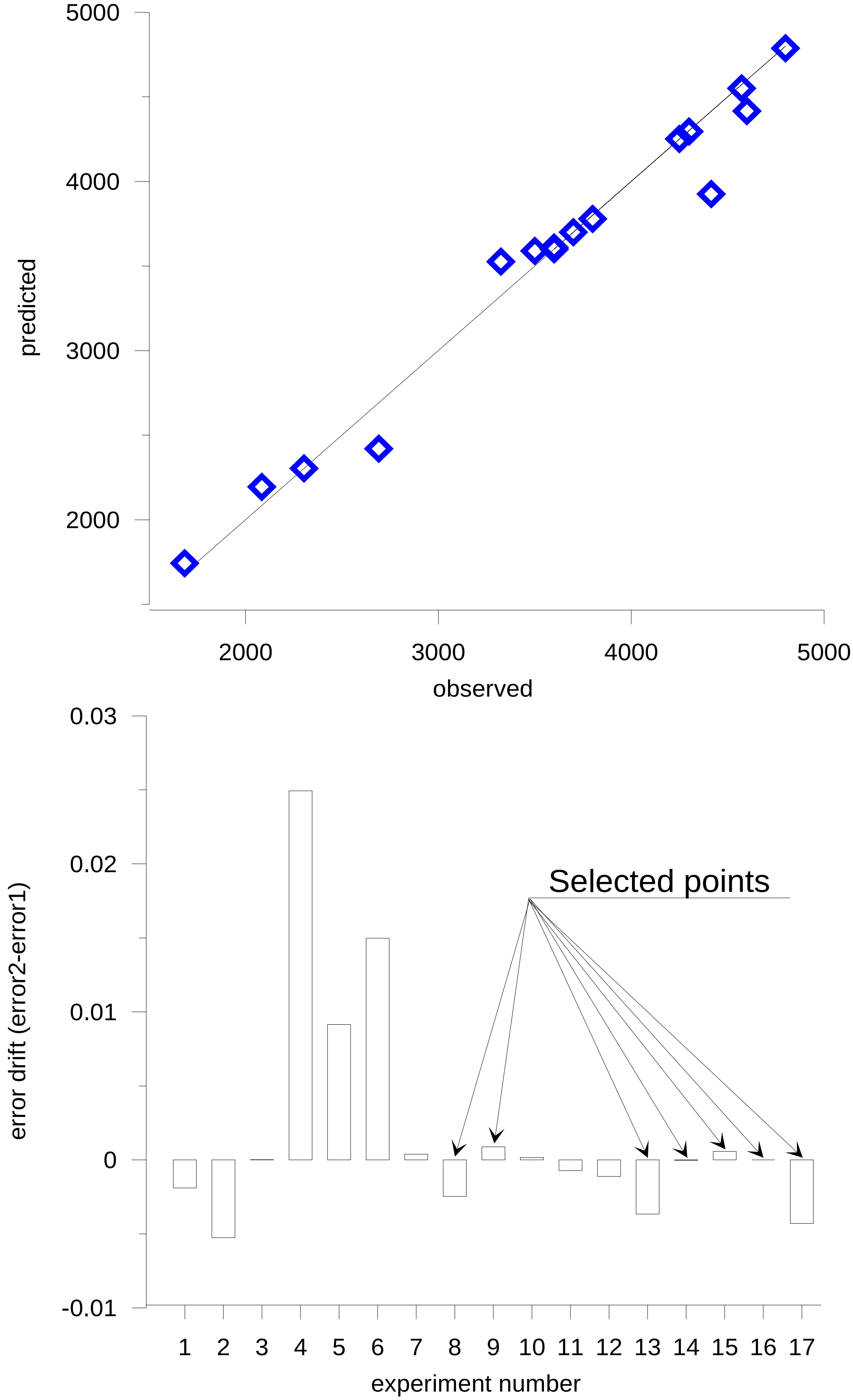

Figure 2: Accuracy of the ANN2.

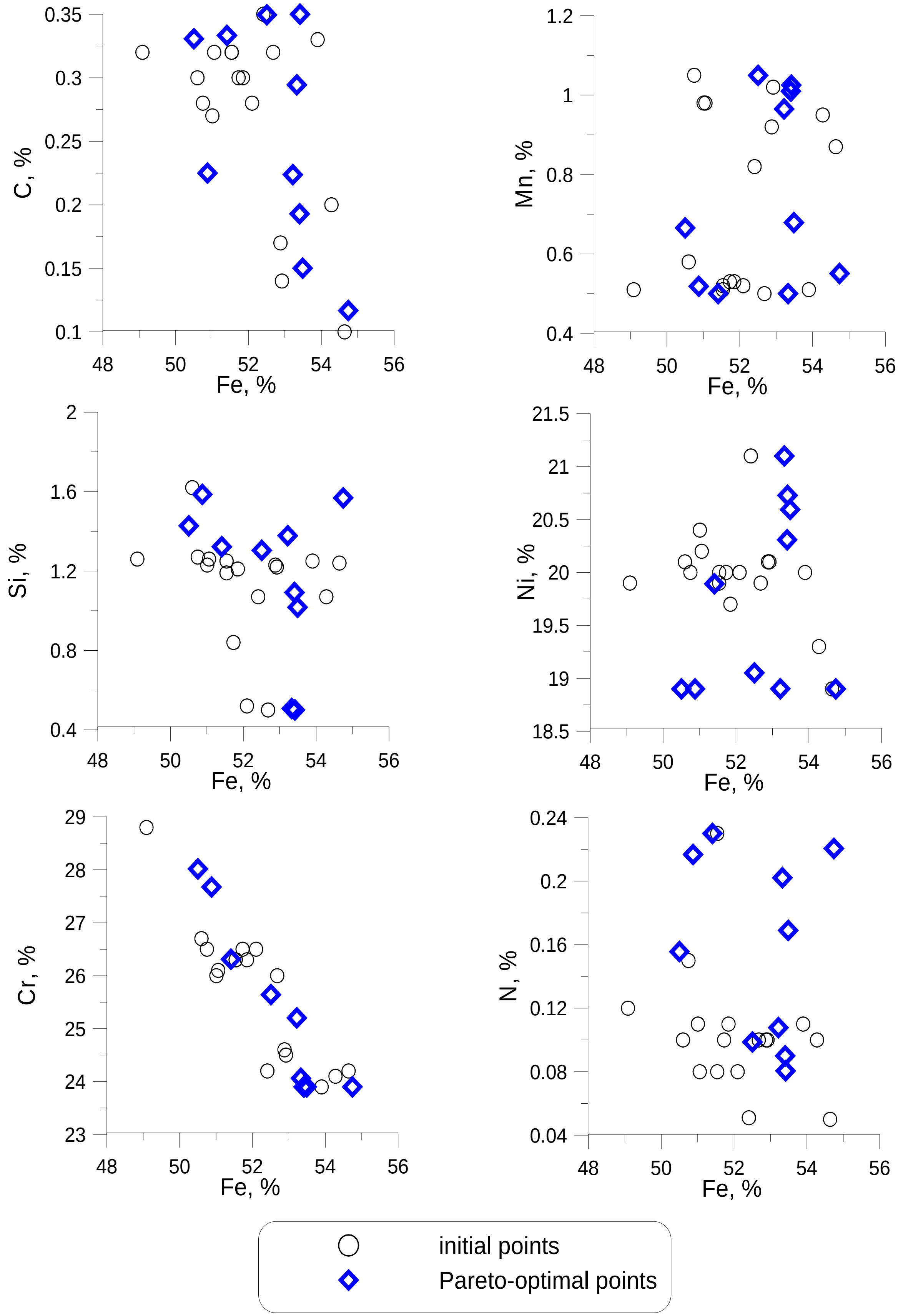

Figure 3: Result of the first iteration of steel composition optimization.

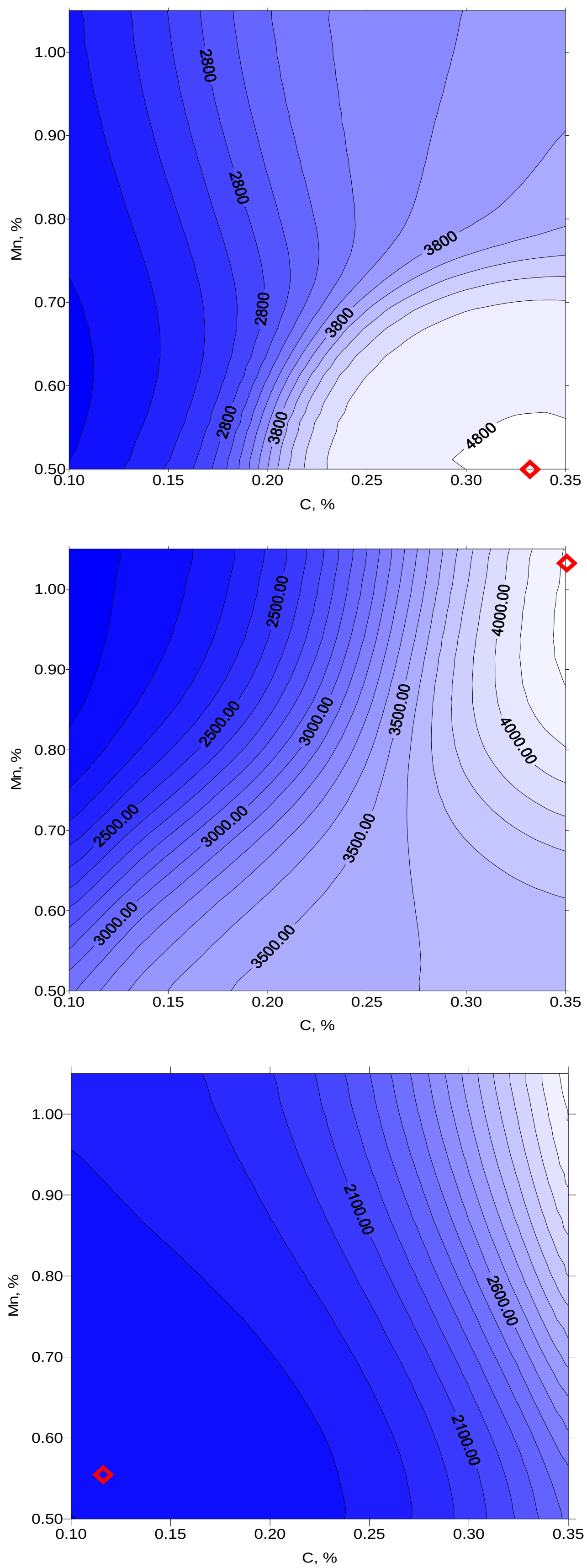

Figure 4: Topology of the ANN2-based response surface in the vicinity of 1st, 2nd and 10th Pareto-optimum points for C – Mn.

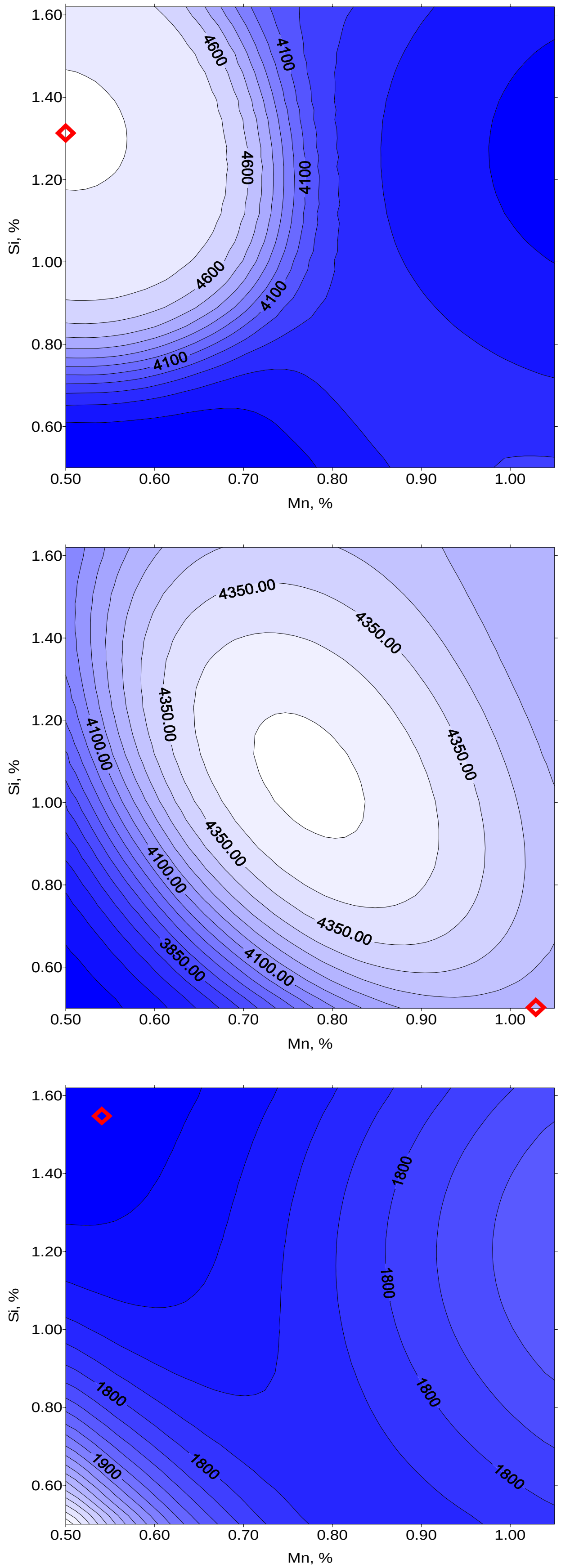

Figure 5: Topology of the ANN2-based response surface in the vicinity of 1st, 2nd and 10th Pareto-optimum points for Mn – Si.

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INVERSE DESIGN OF ALLOYS FOR SPECIFIED STRESS, TEMPERATURE AND TIME-TO-RUPTURE BY USING STOCHASTIC OPTIMIZATION

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ABSTRACT

The inverse problem in design of alloys is determination of chemical composition(s) of alloy(s) that will provide specified levels of, for example, stress at a specified temperature for the specified length of time. The inverse problem can be then formulated as, for example, a multi-objective optimization problem with a given set of equality constraints. This paper offers several formulations for the multiple objective functions and comparatively evaluates these models when using optimization to solve this *de facto* inverse problem.

INTRODUCTION

Our research recently concentrated on the inverse method in predicting chemical composition of steel alloys. It is a highly innovative approach that has received a warm welcome by some of the materials engineering experts from industry. For example, this formulation allows a structural design engineer who designed a machine part to ask a materials scientist to provide a precise chemical composition of an alloy that will sustain a specified stress level, at a specified temperature, and last until rupture for a specified length of time. This inverse method uses a variant of Prof. Yegorov-Egorov's optimization algorithm known as IOSO [1,2,3] to determine not one, but a number of alloys (Pareto front points) each of which will satisfy the specified properties while having different percentages of each of the alloying elements (a different "recipe"). This provides the user of the alloy with increased flexibility when deciding to create such an alloy, because he/she can use the "recipe" which is made of the most readily available and the most inexpensive elements on the market at that point in time.

We have developed several mathematical formulations and corresponding software packages for different ways how to achieve inverse determination of chemical compositions of alloys that simultaneously satisfy several specified mechanical and cost/availability properties. These different formulations were then compared and analytically evaluated in an attempt to determine the most appropriate formulation. This way, the customer can choose the optimized alloy composition that is the most available and the least expensive at a moment when it is ordered from the alloy manufacturer.

It should be pointed out that inverse problem of determining alloy chemical composition is different from a direct optimization problem [4,5,6] of designing alloys that will have extreme properties.

FORMULATIONS

In particular, the objective was to determine chemical composition(s) of high temperature steel alloys that will have specified (desired) physical properties. Design variables were concentrations (percentages) of each of the following 14 alloying elements ***C, S, P, Cr, Ni, Mn, Si, Mo, Co, Cb, W, Sn, Zn, Ti***

No mathematical analysis was used to evaluate the objectives. The evaluations were performed using classical experiments on candidate alloys. In other words, we used an existing experimental database [4,5,6]. Optimization criteria was formulated as a multi-objective statement with three simultaneous objectives: minimize the difference between the specified and the actual stress, minimize the difference between the specified and actual maximum temperature, and minimize the difference between the specified and actual time to rupture (Table 1).

Table 1. Eight formulations for objective functions and constraints

		Objectives (minimize)				**Constraints (minimize)**
Model number	**Number of objectives**	**Stress**	**Operating temperature**	**Time until rupture**	**Low cost alloy**	
1	3	$(\sigma-\sigma_{spec})^2$	$(T-T_{spec})^2$	$(\theta-\theta_{spec})^2$		
2	1	$(\sigma-\sigma_{spec})^2+(T-T_{spec})^2+(\theta-\theta_{spec})^2$				
3	3	$(\sigma-\sigma_{spec})^2$	$(T-T_{spec})^2$	$(\theta-\theta_{spec})^2$		$(\sigma-\sigma_{spec})<\varepsilon$ $(T-T_{spec})<\varepsilon$ $(\theta-\theta_{spec})<\varepsilon$
4	1	$(\sigma-\sigma_{spec})^2+(T-T_{spec})^2+(\theta-\theta_{spec})^2$				$(\sigma-\sigma_{spec})<\varepsilon$ $(T-T_{spec})<\varepsilon$ $(\theta-\theta_{spec})<\varepsilon$
5	1	$(\sigma-\sigma_{spec})^2$				$(T-T_{spec})<\varepsilon$ $(\theta-\theta_{spec})<\varepsilon$
6	1		$(T-T_{spec})^2$			$(\sigma-\sigma_{spec})<\varepsilon$ $(\theta-\theta_{spec})<\varepsilon$
7	1			$(\theta-\theta_{spec})^2$		$(\sigma-\sigma_{spec})<\varepsilon$ $(T-T_{spec})<\varepsilon$
8	10	$(\sigma-\sigma_{spec})^2$	$(T-T_{spec})^2$	$(\theta-\theta_{spec})^2$	Ni, Cr, Nb, Co, Cb, W, Ti	

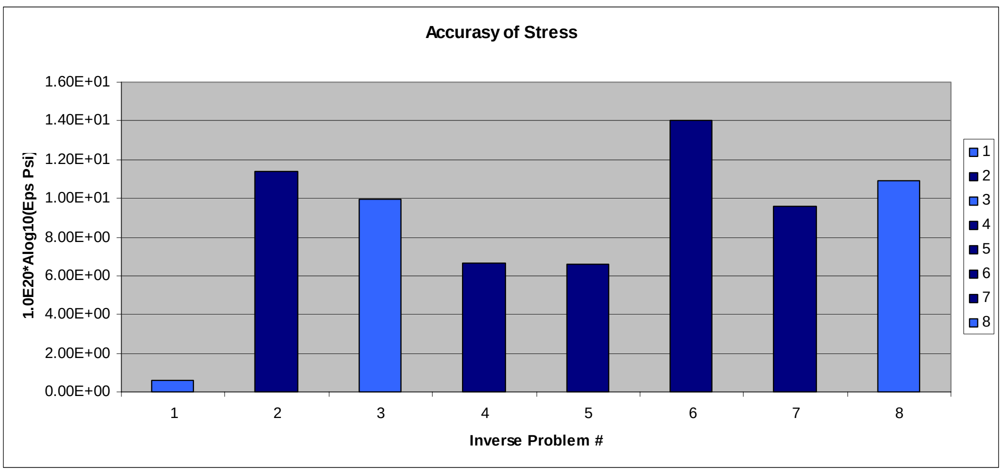

Fig. 1 Accuracy of satisfying the specified stress for eight formulations

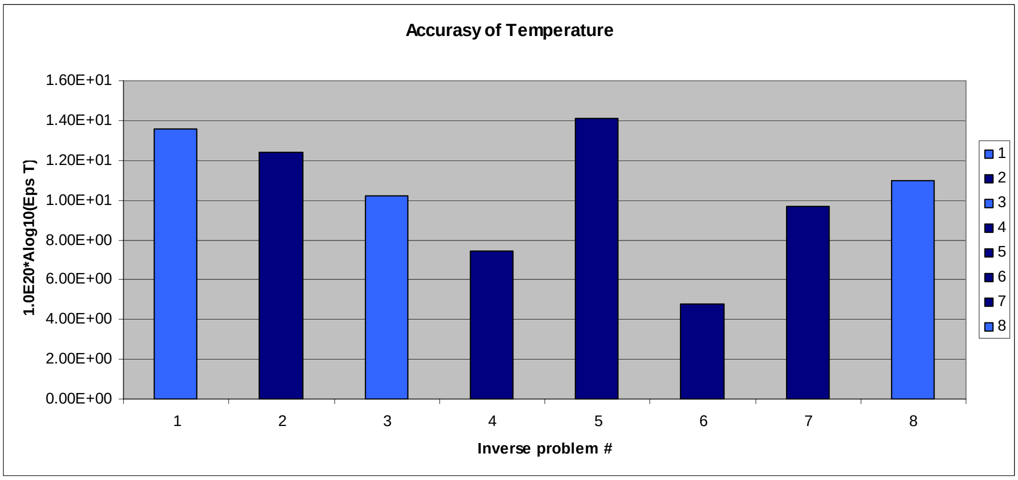

Fig. 2 Accuracy of satisfying the specified temperature for eight formulations

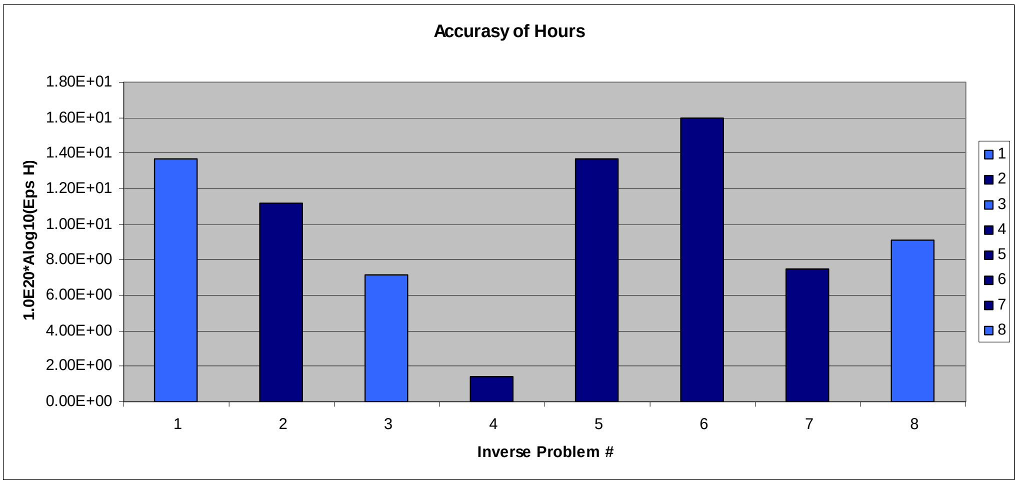

Fig. 3 Accuracy of satisfying the specified time-to-rupture for eight formulations

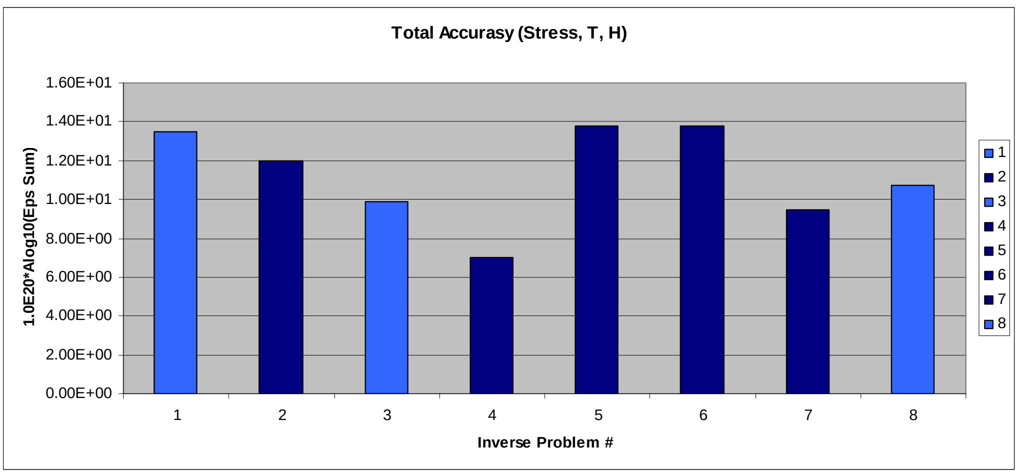

Fig. 4 Combined accuracy of satisfying the specified values for eight formulations

$$\Delta\sigma = \left(\sigma - \sigma_{spec}\right)/\,\sigma_{spec}\,, \quad \Delta T = \left(T - T_{spec}\right)/\,T_{spec}\,, \quad \Delta\theta = \left(\theta - \theta_{spec}\right)/\,\theta_{spec}$$

$$K_1 = 10\,N_{objectives} + N_{constraints} + N_{variables} \qquad K_2 = 100\,\Delta\sigma + \Delta T + \Delta\theta \qquad K_3 = N_{calls}\,/\,N_{Pareto}$$

$$\text{EPS}=\sum \; 1/[\left(\sigma - \sigma_{spec}\right)^2 + \left(T - T_{spec}\right)^2 + \left(\theta - \theta_{spec}\right)^2\,]$$

Maximize: $SCORE = K_1 K_2 \exp(EPS)\,/\,K_3$

Fig. 5 An ad hoc analytical formulation for the overall performance evaluation of the various inverse design formulations

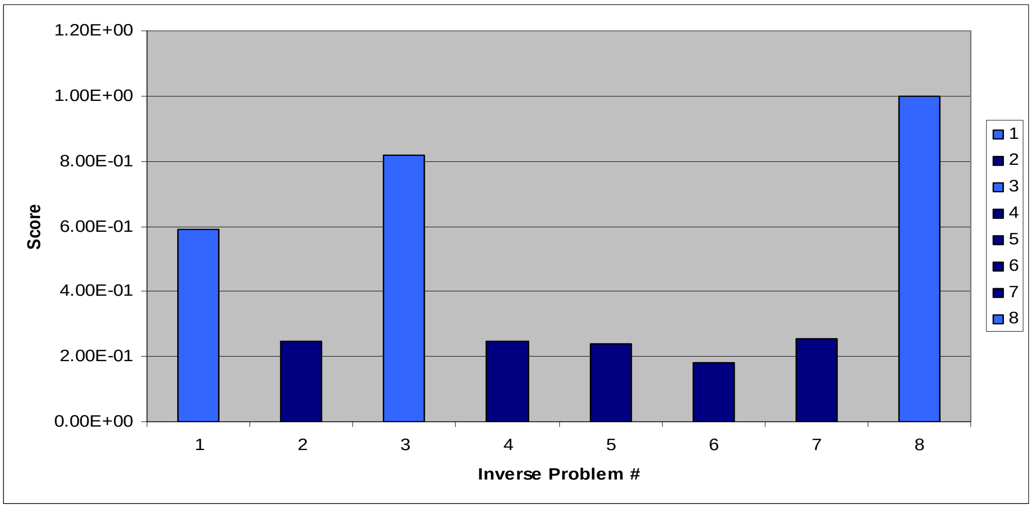

Fig. 6 Comparison of overall performance of the eight inverse formulations

	Eps str	Eps t	Eps h	Eps sum	N Const	N Obj	N Point (Pareto)	N Calls	Score
Prob. 1	.408E-19	.356E-06	.536E-06	.297E-06	0	3	50	417	0.590
Prob. 2	.269E-08	.267E-07	.172E-08	.104E-07	3	1	1	703	0.246
Prob. 3	.897E-10	.143E-09	.134E-12	.777E-10	3	3	50	445	0.817
Prob. 4	.434E-13	.289E-12	.244E-18	.111E-12	3	1	1	1020	0.246
Prob. 5	.413E-13	.139E-05	.549E-06	.646E-06	2	1	1	601	0.239
Prob. 6	.954E-06	.576E-15	.980E-04	.646E-06	2	1	1	774	0.180
Prob. 7	.408E-10	.515E-10	.299E-12	.309E-10	2	1	1	776	0.256
Prob. 8	.714E-09	.928E-09	.127E-10	.552E-09	3	10	46	834	1.000

Fig. 7 Summary of accuracies in satisfying objectives, number of constraints, number of simultaneous objectives, number of Pareto points generated, number of optimization algorithm calls required, and the final performance scores of the eight formulations

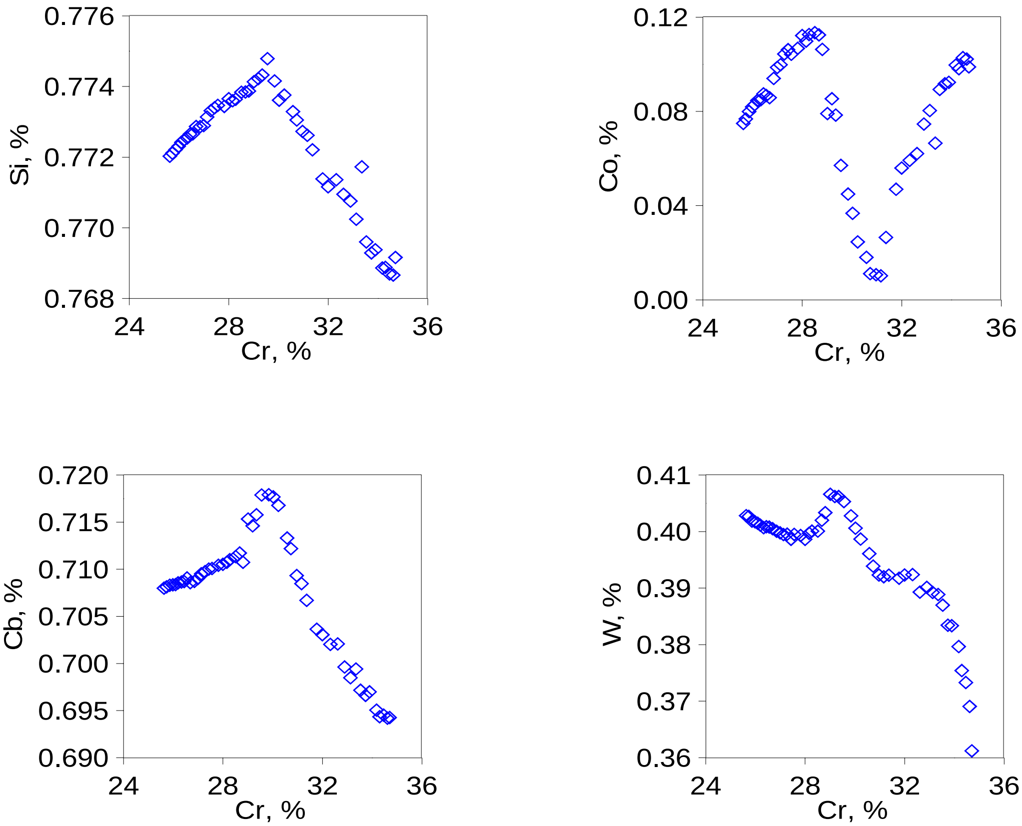

Fig. 8 Allowable variations of concentrations of several alloying elements with respect to Cr when specifying stress (230 N mm^{-2}), temperature (975 C) and time-to-rupture (5000 hours)

RESULTS

In the case of inversely determining concentrations of each of the 14 chemical species in steel alloys when using the eight mathematical formulations for the objective function(s) and constraints (Table 1), it is apparent that IOSO optimization algorithm offers consistently high accuracy in satisfying the specified stress (Fig. 1), operating temperature (Fig. 2), time-to-rupture (Fig. 3) and an overall combined accuracy (Fig. 4). When the suggested eight formulations were evaluated using an *ad hoc* evaluation procedure (Fig. 5), only a few formulations appear to offer an overall superior performance (Figs. 6 and 7). The predicted combinations of concentrations of alloying elements vary rapidly (Fig. 8) suggesting that only robust non-gradient based optimization algorithms could handle these types of problems.

This methodology of inversely designing chemical compositions of alloys offers a significant freedom to the designer to choose from a relatively large number of possible chemical compositions that satisfy the same specified physical properties.

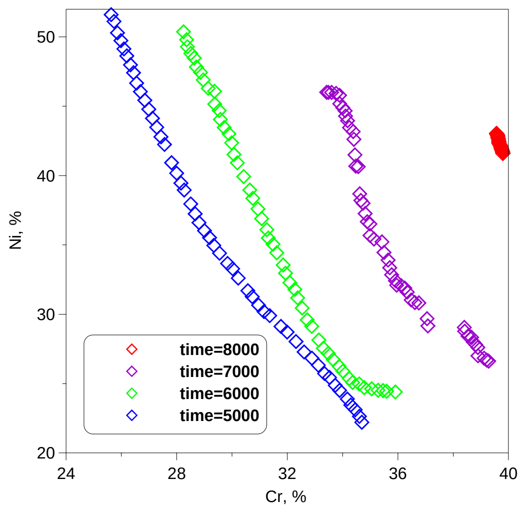

Fig. 9 Allowable ranges of Ni and Cr concentrations for a specified level of stress and temperature and different life expectancies.

For example, if the designer specifies the desired stress level of 230 N mm^{-2} and the desired temperature of 975 C, there will be 50 possible combinations of Ni and Cr concentrations that will all provide life expectancy of 5000 hours. If the life expectancy is specified by the designer to be 6000 hours for the same stress and temperature levels, the allowable range of possible combinations of Ni and Cr concentrations will decrease. This will become increasingly more noticeable as the specified life expectancy is increased further to 7000 and eventually to 8000 hours (Fig. 9).

The results of this multiple simultaneous least-square constrained minimization problem cannot be visualized for more that two alloying species at a time. For example, when concentrations of only two alloying elements like Ni and Cr are visualized, and temperature and life expectancy are unconstrained (unspecified) the optimizer will give a fairly large domain for possible variations of the concentrations of Cr and Ni. But, as the constraints on temperature level are introduced and progressively increased, the feasible domain for varying Cr and Ni will start to shrink (Fig. 10). Similar general trend can be observed when the life expectancy is specified and progressively increased.

Finally, when temperature level and the life expectancy are prescribed simultaneously and progressively increased simultaneously, the feasible domain for concentrations of Cr and Ni reduces rapidly (Fig. 11). Similar trends could be observed when looking at any other pair of alloying elements.

CONCLUSIONS

A new concept has been developed for designing alloys having specified multiple physical properties. This inverse problem was formulated as a constrained multi-objective optimization problem and solved using a robust evolutionary optimizer of IOSO type. As a result, multiple choices are obtained for combinations of concentrations of alloying elements whereby each of the combinations corresponds to another Pareto front point and satisfies the specified physical properties. This alloy design methodology does not require knowledge of metallurgy or crystallography and is directly applicable to alloys having arbitrary number of alloying elements.

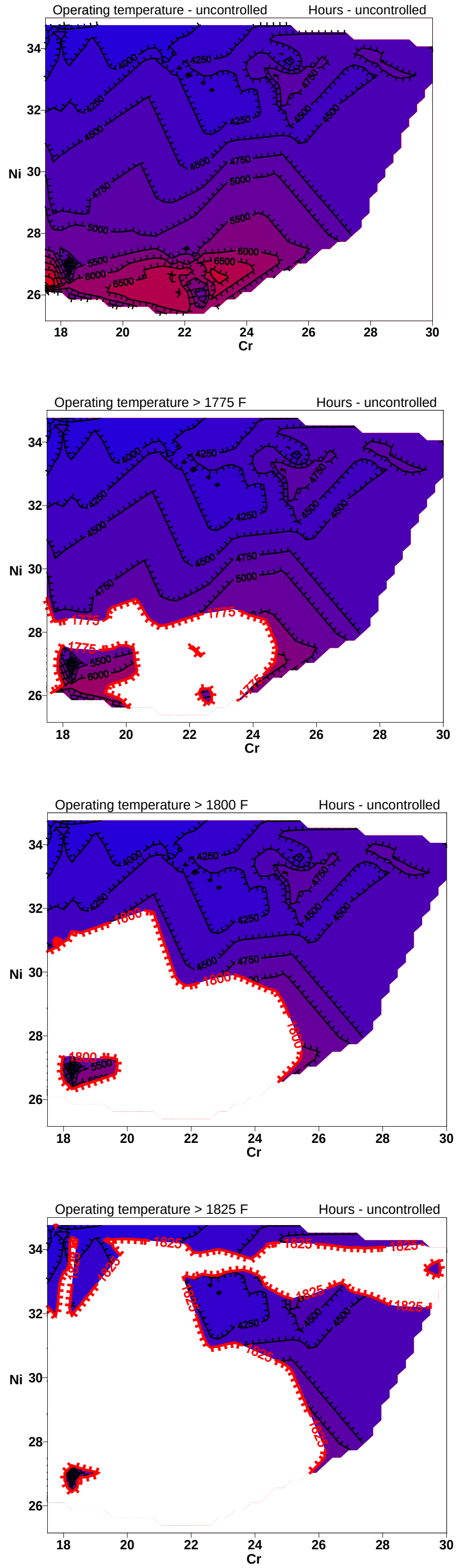

Fig. 10 Effect of increasing the temperature

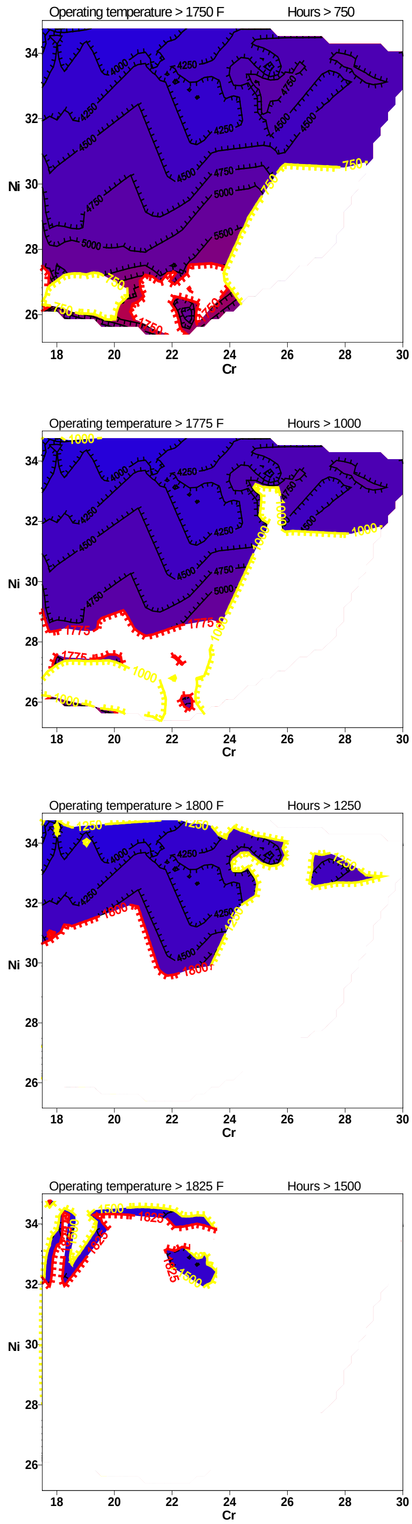

Fig. 11 Efect of simultaneously increasing temperature and life expectancy

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ROBUST OPTIMIZATION OF CONCENTRATIONS OF ALLOYING ELEMENTS IN STEEL FOR MAXIMUM TEMPERATURE, STRENGTH, TIME-TO-RUPTURE AND MINIMUM COST AND WEIGHT

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Key words: Multi-objective optimization; Robust optimization; Inverse design; Metal alloys; Alloy design.

Abstract: *This paper is based on the use of experimental data and a new evolutionary truly multi-objective optimization algorithm for simultaneously optimizing several properties of steel alloys while minimizing the number of experimental evaluations of the candidate alloys. This approach has been shown to have the potential of identifying new chemical compositions for significantly superior performance alloys requiring as few as 80 new alloy samples that otherwise could not be identified with classical techniques without requiring thousands of new alloys. Furthermore, this approach has been demonstrated to have the potential for determining concentrations of alloying elements for a specified set of alloy's properties for specific applications, thereby maximizing their utilization. Cost and weight are two of the objectives in addition to the more standard objectives such as maximized operating temperature, tensile stress and time-to-rupture.*

1 INTRODUCTION

The most prominent center for research activity in certain aspects of predictive modeling using artificial neural networks and regression analysis in materials science is at Cambridge University in the U.K.[1-4]. However, use of neural networks and regression analysis does not provide for the capability to search significantly outside of a given data set for possibilities of even more extreme solutions.

Therefore, this paper is based on the use and a special adaptation of a multi-objective constrained Indirect Optimization based upon Self-Organization (IOSO)[5-7]. This multi-objective optimization algorithm allows for concentrations of a number of alloying elements to be optimized so that a finite number of properties (maximum tensile strength, maximum operating temperature, maximum time-until-rupture, minimum weight, minimum cost, etc.) of the alloy are simultaneously extremized, while satisfying a number of equality and inequality constraints.

IOSO multi-objective optimization algorithm is of a semi-stochastic type incorporating certain aspects of a selective search on a continuously updated multi-dimensional response surface[5-7]. Objective function evaluations in this particular project were obtained utilizing experimental testing and verification of the initial alloy samples and all newly created alloys in order to determine optimum concentrations of each of the alloying elements. This novel alloy design tool is expected to minimize the need for the addition of expensive alloying elements and still obtain the optimum properties needed to design the components. The main benefits of IOSO 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 gradient-based and genetic optimization algorithms. Also, the self-adapting multi-dimensional response surface formulation used by IOSO allows for incorporation of realistic non-smooth variations of experimentally obtained data and allows for accurate interpolation of such data.

However, the properties of the alloys strongly depend not only on the alloys' chemical compositions, but also on their microstructure. For instance, the heat resistance of the austenitic stainless steel product can be entirely different from super alloys. Thermal processing of the alloys can also significantly change the actual properties of the alloys. Without taking these aspects of the alloys' design and production into account the proposed design optimization method will be of only marginal practical utility. Therefore, inclusion of the microstructure aspects directly or indirectly into the design optimization set of design variables should be the next phase of this research effort.

2 INDIRECT OPTIMIZATION BASED UPON SELF-ORGANIZATION (IOSO) ALGORITHM

IOSO algorithm consists of two stages. The first stage is the creation of an approximation of the objective function(s). Each iteration in this stage represents a decomposition of the initial approximation function into a set of simple approximation functions (Fig. 1) so that the final response function is a multi-level graph (Fig. 2).

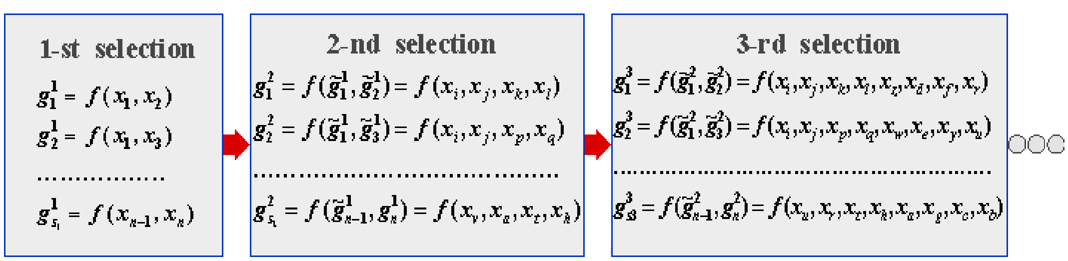

Figure 1: Approximation functions used in building objective function(s) in IOSO.

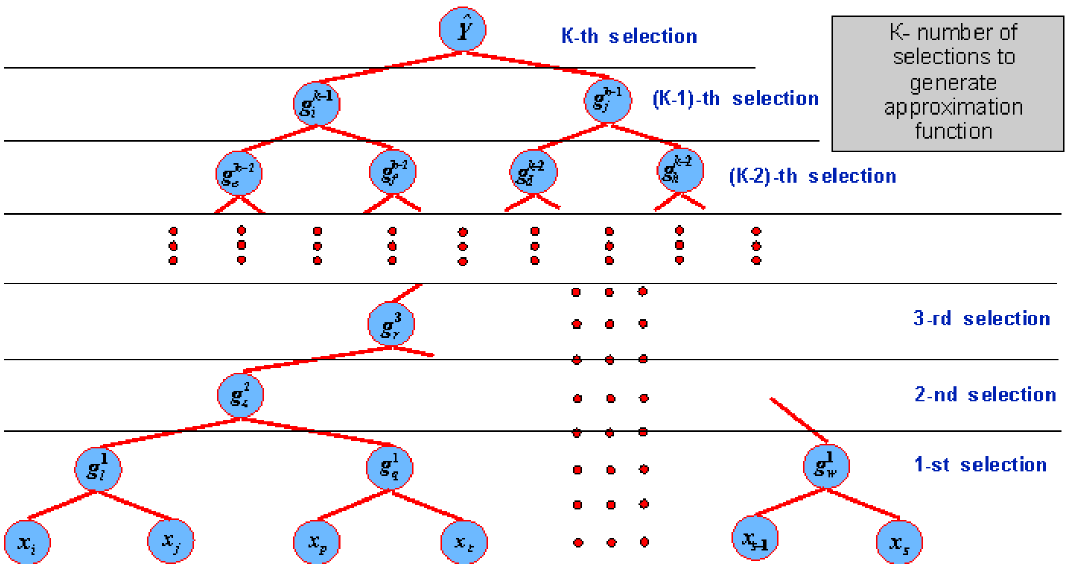

Figure 2: Example of the IOSO response surface structure.

The second stage is the optimization of this approximation function (Fig. 3). 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.

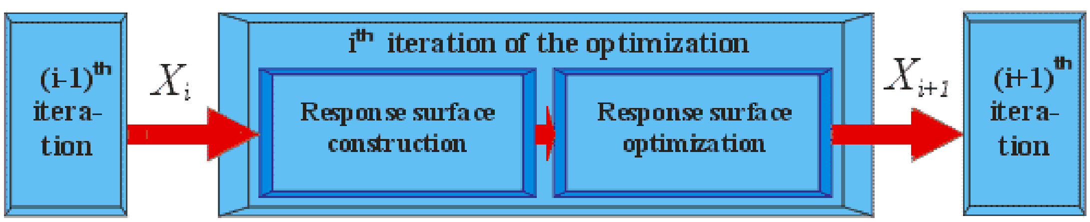

Figure 3: Global IOSO iteration scheme.

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 for a particular objective is built. These functions differ from each other according to both structure and definition range.

The optimization of these approximation functions allows us to determine a set of vectors of optimized variables. IOSO uses Sobol's algorithm[8] for redistribution of the initial points in the multi-dimensional function space. IOSO algorithm also includes algorithms of artificial neural networks 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 artificial neural networks parameters at the stage of their training that are based on the minimal curvature of the response surface and a provision of the best predictive properties for a given subset of test points.

A preliminary proof of this alloy optimization concept was published recently by Dulikravich et al.[9] and expanded more recently to a larger data set[10-12].

3 OPTIMIZING ALLOYS FOR MAXIMUM PERFORMANCE BY UTILIZING AN EXISTING DATABASE

An initial database was obtained containing experimentally measured mechanical properties on 201 H-type cast steel alloys[10]. However, certain alloys did not have complete information on alloy chemical composition. These alloys were deleted from the set. Besides, certain alloying elements (V, Bi, Se, Zr, Sb, Cd) were present in a very small number of alloys provided, which makes it impossible to assess their effect from information in this database. Such alloys were also excluded from further analysis. Furthermore, an evaluation of uniformity of distribution of the percentage values of different elements in the existing range was made since certain alloying elements had concentrations differing very strongly from the universal set. This resulted in the final database having only 158 steel alloys.

Concentrations of the following 17 elements were taken as independent variables: *C, S, P, Cr, Ni, Mn, Si, Cu, Mo, Pb, Co, Cb, W, Sn, Al, Zn, Ti.*

The minimum and maximum values for the concentrations of each element were determined from the existing set of experimental data ($Exp\_min_i, Exp\_max_i,\ i=\overline{1,17}$). Then, new minimum and maximum values for each of the 17 elements were obtained as follows: $Min_i = 0.9 \cdot Exp\_min_i,\ Max_i = 1.1 \cdot Exp\_max_i,\ i=\overline{1,17}$ (Table 1).

Table 1. Ranges of concentrations of 17 independent design variables (chemical elements in the steel alloy)

	C	**S**	**P**	**Cr**	**Ni**	**Mn**	**Si**	**Cu**	**Mo**
min	0.063	0.001	0.009	17.500	19.300	0.585	0.074	0.016	0.000
max	0.539	0.014	0.031	39.800	51.600	1.670	2.150	0.165	0.132

	Pb	**Co**	**Cb**	**W**	**Sn**	**Al**	**Zn**	**Ti**
min	0.001	0.000	0.000	0.000	0.000	0.001	0.001	0.000
max	0.006	0.319	1.390	0.484	0.007	0.075	0.015	0.198

The following parameters were then used as optimization objectives:

- Stress (PSI – maximize);
- Operating temperature (T – maximize);
- Time to "survive" until rupture (Hours – maximize).

The following parameters were then used as optimization objectives: stress (PSI – maximize); operating temperature (T – maximize); time to "survive" until rupture (Hours – maximize). During this research the solution of a simultaneous three-objective optimization problem and a series of two-objectives problems were accomplished when one of the considered parameters was constrained.

During the first stage, the problem of simultaneously optimizing three objectives was solved with 100 points of Pareto optimal solutions (Fig. 4). Analysis of this result allowed us to extract an area of admissible combinations of different optimization objectives since results were distributed in the admissible part of the objectives' space quite uniformly.

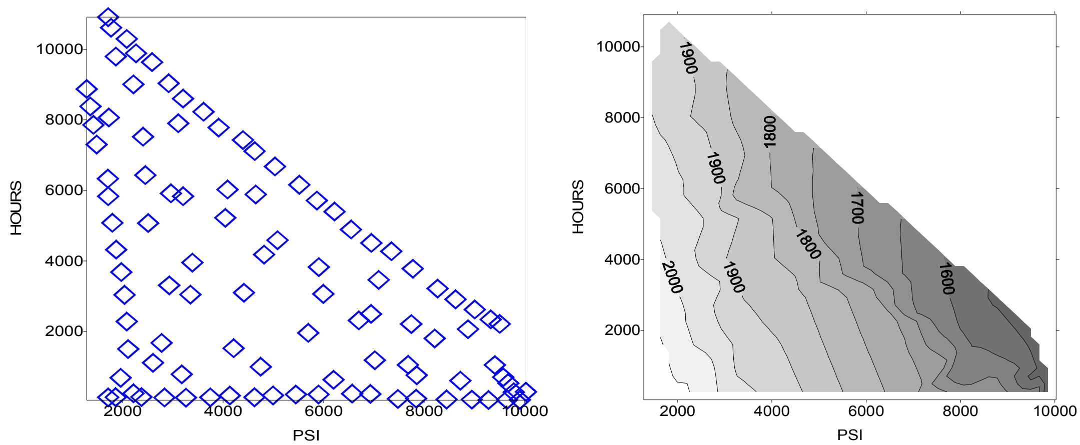

Fig.4. Time-to-rupture vs. strength for three-objectives Pareto set using 17 design variables. Constant temperature contours are also indicated in degrees Fahrenheit.

Such a distribution offers a possibility for a significant improvement of accuracy of response surfaces on condition that the experiments will be carried out at the obtained Pareto optimal points. Then, in accordance with the elaborated technique, it is necessary to conduct experiments at the obtained Pareto optimal points, evaluate accuracy of prediction of values of partial optimization objectives, and either complete the process or perform another iteration.

However, it can be seen that the ranges of variation of optimization objectives for 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.

In our case, a decision was made to perform five separate two-objectives alloy optimizations with 17 and 9 variables where temperature will serve not as an objective, but as an inequality constraint (Fig. 5 and Fig. 6). It can be seen that maximum achievable values of PSI and HOURS, and possibilities of compromise between these parameters largely depend on temperature. For instance, the increase of minimum temperature from 1600 F to 1900 F leads to the decrease of attainable PSI by more than 50 percent. At the same time, limiting value of HOURS will not alter with the change of temperature.

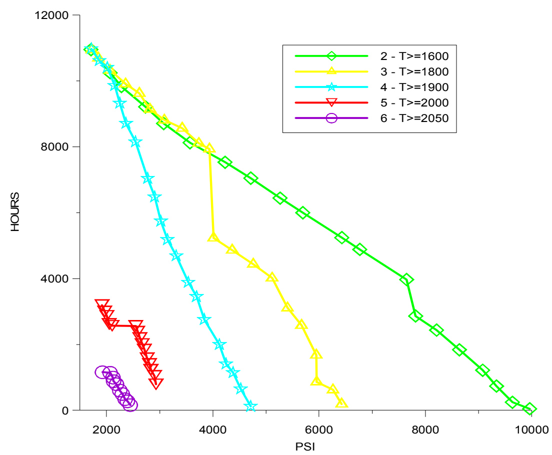

Figure 5: Pareto-optimal sets for five different (temperature) constraints using 17 design variables.

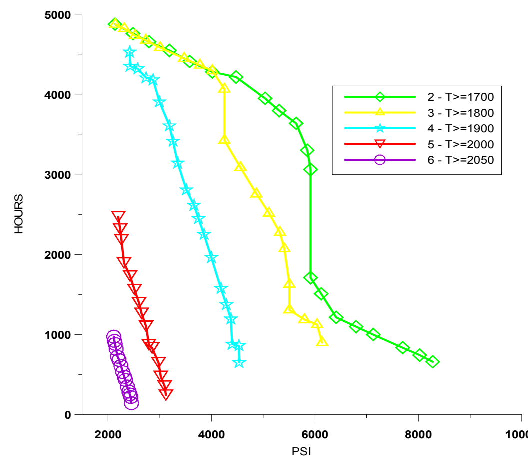

Figure 6: Pareto-optimal sets for five different (temperature) constraints using 9 design variables.

4 DESIGN OPTIMIZATION OF NEW GENERATIONS OF STEEL ALLOYS UTILIZING EXPERIMENTAL VERIFICATION

This work represents the first experimentally verified attempt to step out of the initially available database when optimizing nickel based heat-resistant alloy castings[11] containing ***Ni, C, Cr, Co, W, Mo, Al, Ti*, *B, Nb, Ce, Zr, Y***, and ***S, P, Fe, Mn, Si, Pb, Bi*** as trace elements. Heat treatment of the samples of such alloys involved heating to 1210 C, holding for 4 hours, and air cooling to room temperature. During these tests the maximum stress at room temperature (sigma) and the time to survive until rupture at 975 C and 230 N/mm^2 load were measured. Manufacturing of all of the alloys involved in this case and experimental testing of their properties were carried out in the same certified metallurgical institute. Chemical compositions of these alloys differed by varying concentrations of the following seven elements: ***C, Cr, Co, W, Mo, Al, Ti*** (Table 2). The concentration of ***Nb*** in all tests was 1.1%, while concentrations of ***B, Ce, Zr, Y*** were 0.025%, 0.015%, 0.04%, and 0.01% respectively. The concentration of nickel made the rest of 100% of the alloy. Average percents of the addition agents were negligible.

Table 2. Ranges of design variables (concentrations of 7 major alloying elements)

	C	Cr	Co	W	Mo	Al	Ti
min	0.13	8.0	9.0	9.5	1.2	5.1	2.0
max	0.20	9.5	10.5	11.0	2.4	6.0	2.9

During each IOSO iteration, a two-criterion optimization task with 20 Pareto optimal points was solved. The two simultaneous optimization objectives were: maximize stress and maximize time-to-rupture at elevated temperature. The initial database contained 120 experimentally tested steel alloys whose concentrations were specified using Sobol's algorithm[8] so that they are as uniformly distributed as possible. After that, 4 iterations were conduced using IOSO with 20 new (Pareto optimal) alloys predicted and consequently experimentally tested after each iteration. Thus, the total number of experimentally tested alloys during the solution of the entire optimization problem using IOSO was only 200 which is considered a significant improvement over the current alloy design methodologies. The accuracy and predicting capabilities of the self-adapting response surfaces generated by IOSO were constantly improving during the optimization process (Figs. 7-16). A summary of the evolution of the Pareto front through four IOSO iterations (Fig. 17) demonstrates that IOSO is capable of reliably predicting concentrations of alloying elements that create superior performance steel alloys after each application of IOSO. Notice that all data presented in these figures are the results of experimental evaluations involving 120 original database alloys and four sets of 20 alloys each predicted by the IOSO algorithm.

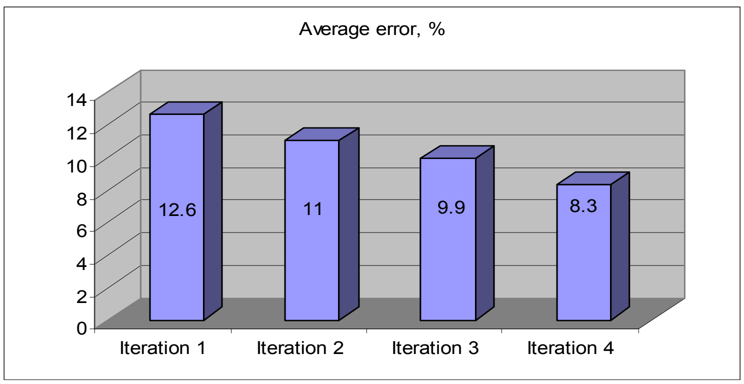

Figure 7: Accuracy evolution of IOSO response surfaces.

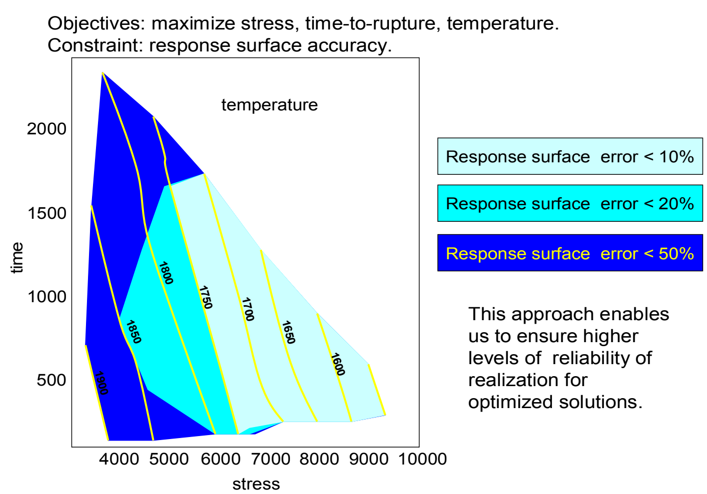

Figure 8: Accuracy of IOSO response surface representation and its effect on the results of optimization.

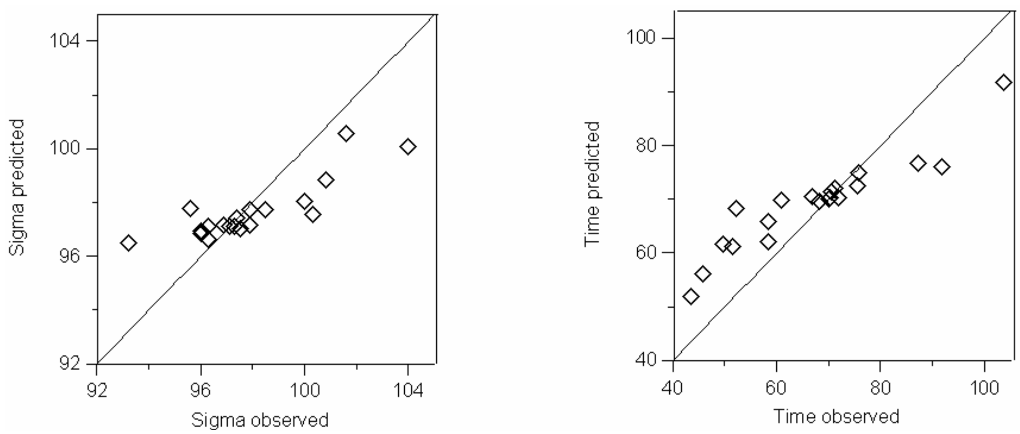

Figure 9: Predicted and observed values of the criteria after first iteration.

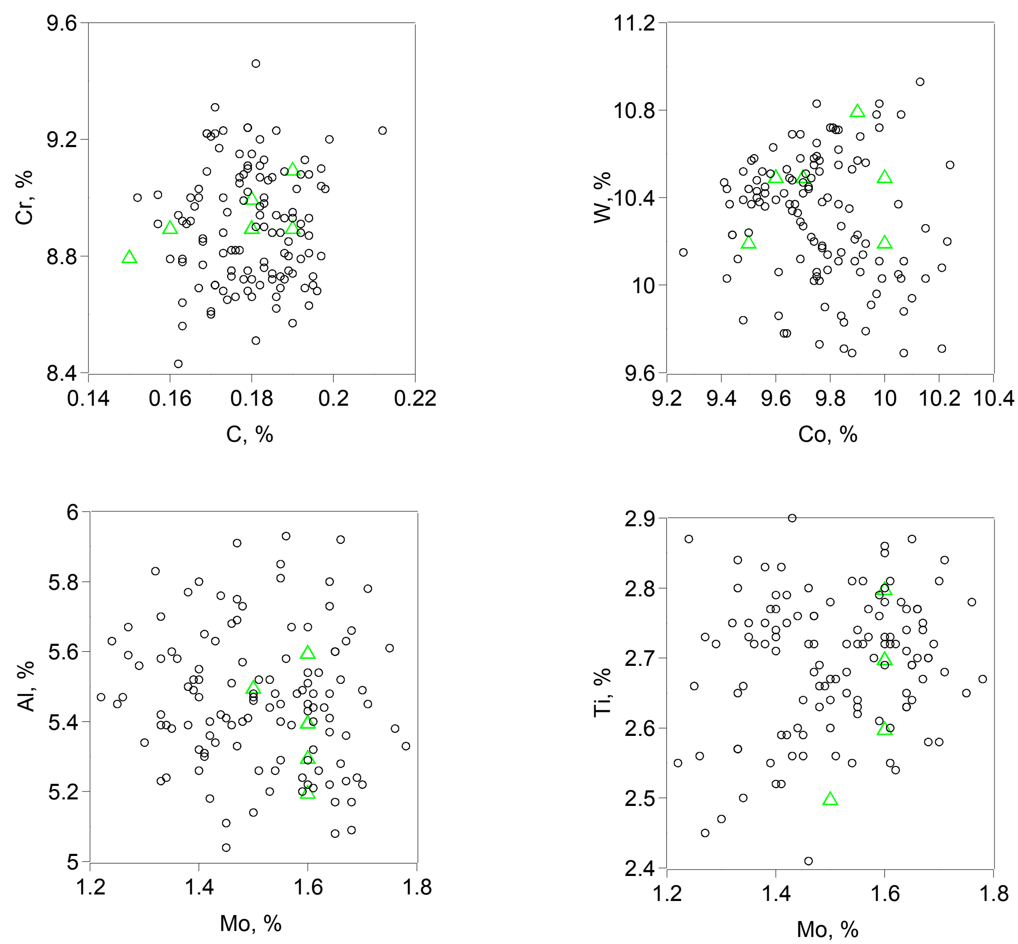

Figure 10: The number of Pareto optimal solutions by variable parameters after first iteration.

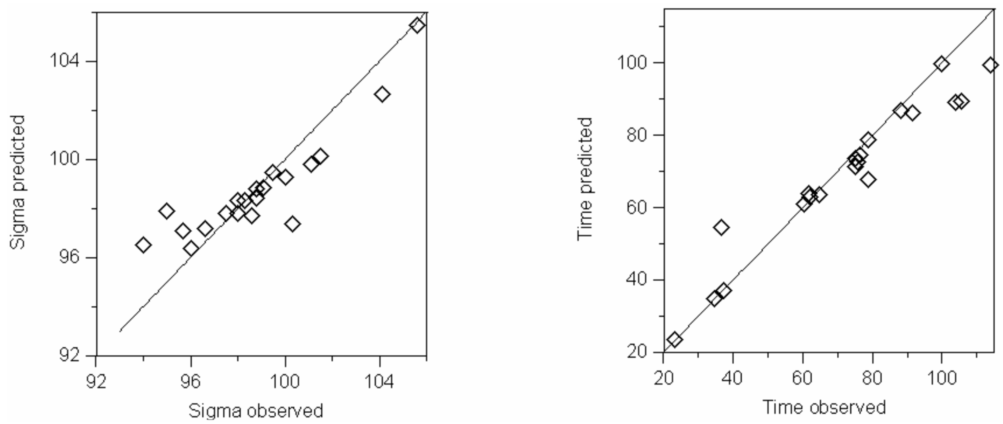

Figure 11: Predicted and observed values of the criteria after second iteration.

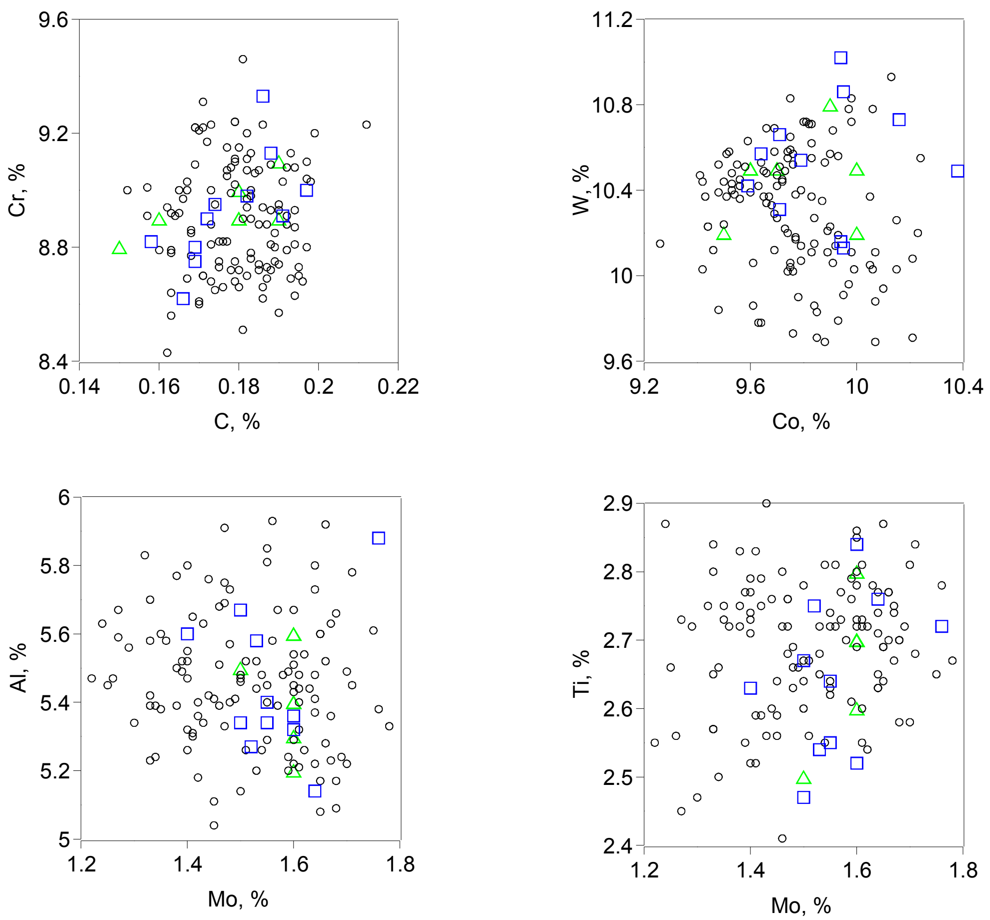

Figure 12: The number of Pareto optimal solutions for variable parameters after second iteration.

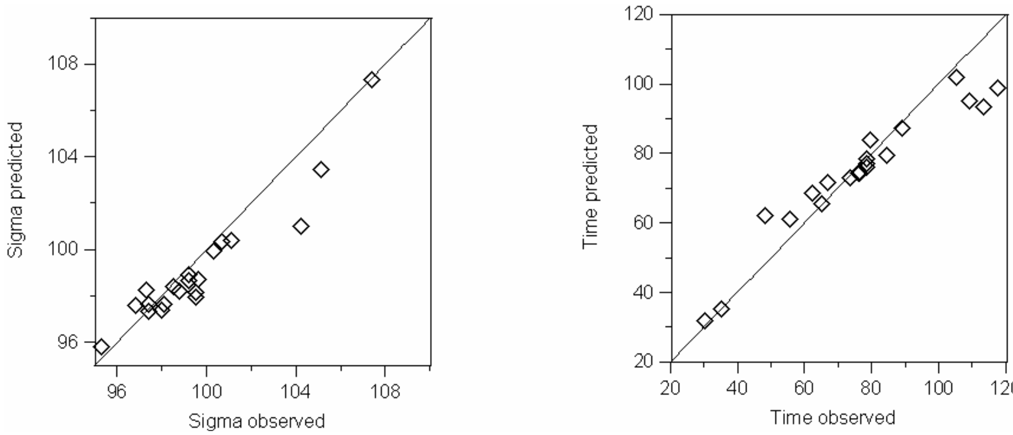

Figure 13: Predicted and observed values of the criteria after second iteration.

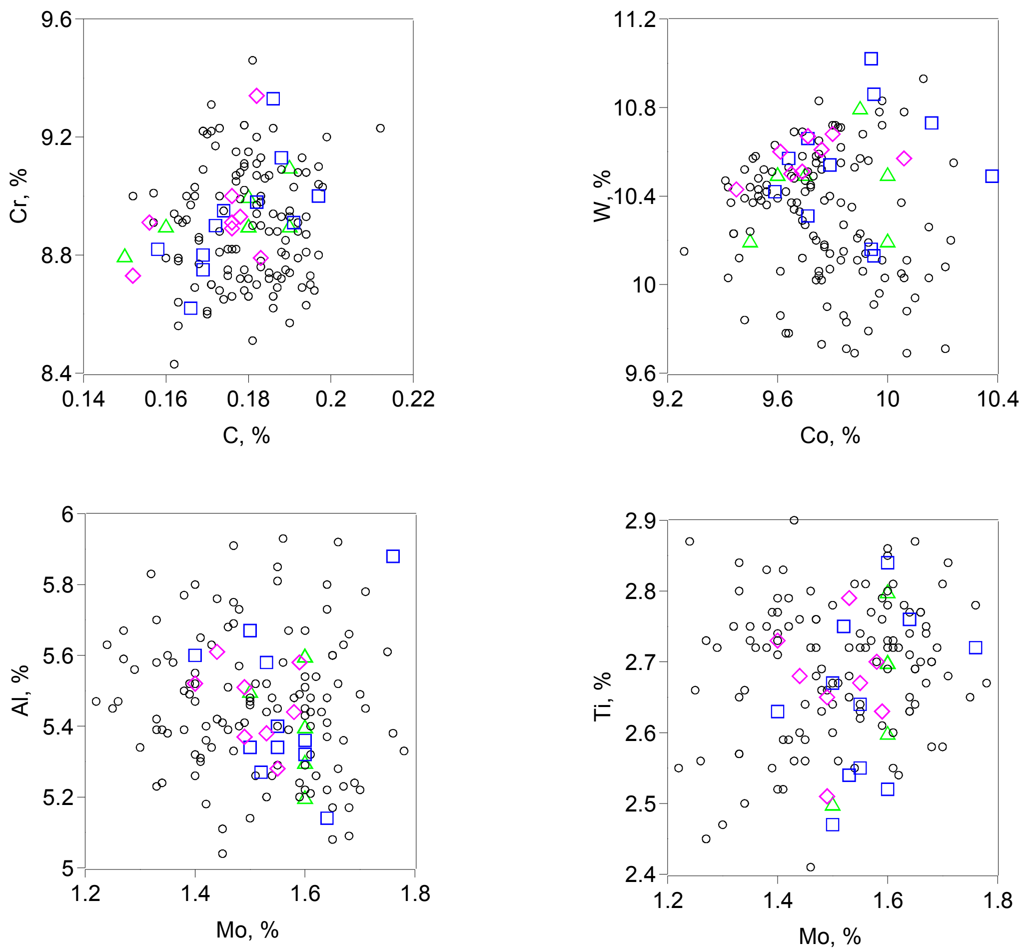

Figure 14: The number of Pareto optimal solutions for variable parameters after third iteration.

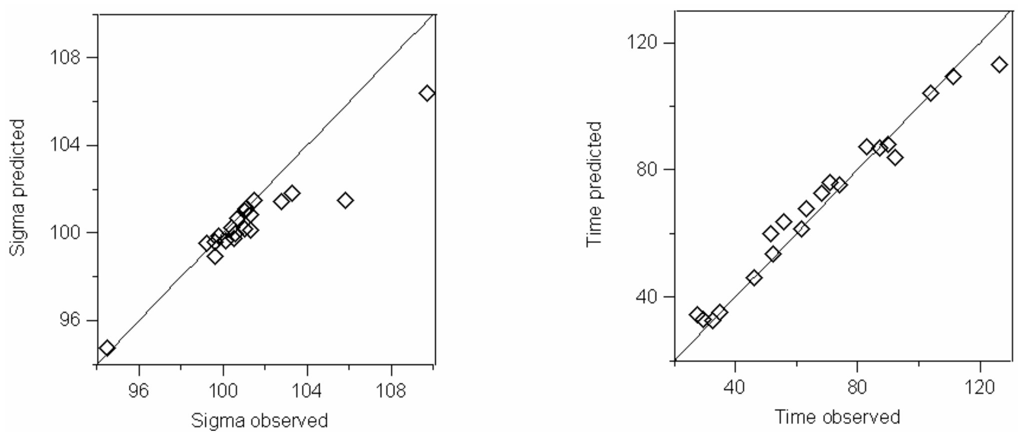

Figure 15: Predicted and observed values of the criteria after fourth iteration.

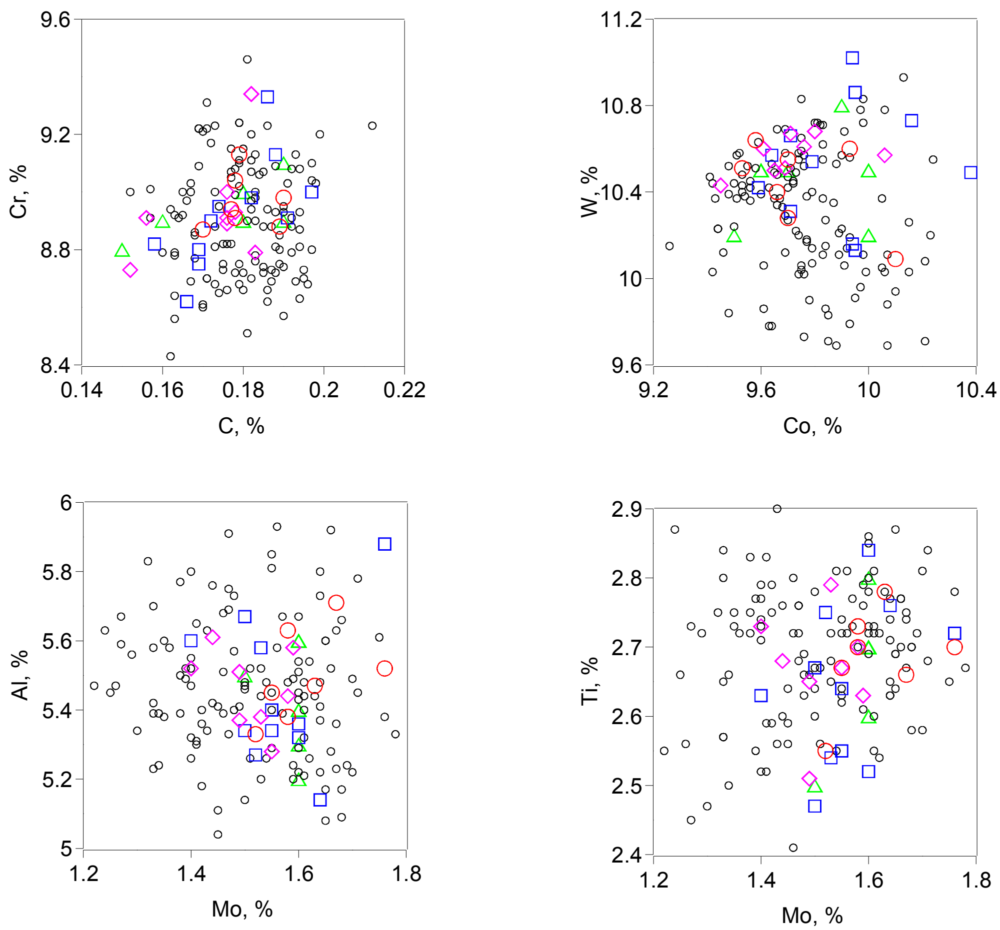

Figure 16: The number of Pareto optimal solutions for variable parameters after fourth iteration.

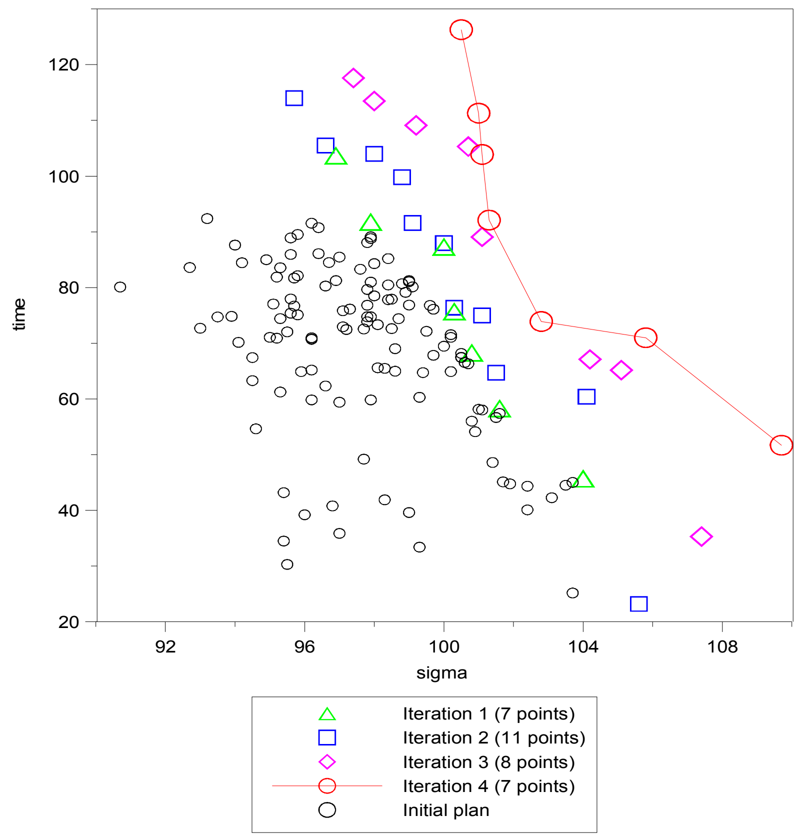

Figure17: The dynamics of change of Pareto optimal solutions after each of the four iterations with IOSO.

5 INCLUDING MINIMUM COST AND WEIGHT OBJECTIVES

In many applications it is highly desirable to use as light alloys as possible. Yet, it is well-known that high temperature resistant alloys require ingredients that have the highest melting points. However, these alloying elements are also very dense, thus heavy. This is an obvious example of a multi-objective optimization where some of the objectives (in this case high temperature resistance and weight) are highly opposing.

Furthermore, certain alloying elements are considerably more expensive than other elements. In direct response to a rapidly increasing demand from industry and military to develop high performance alloys that will also be affordable, we obtained a standard daily price list of typical alloying elements available on the metals market. We also obtained a list of densities of these alloying elements. The original idea was to optimize simultaneously the following five objectives: maximum stress, maximum temperature, time-to-rupture, minimum cost of the raw ingredients, and minimum volume-specific weight (density) of the resulting metal alloy. However, we reformulated it as a sequence of five different multi-objective optimization problems that are depicted in Fig. 18-21. Each symbol in these figures represents an alloy with its own chemical composition.

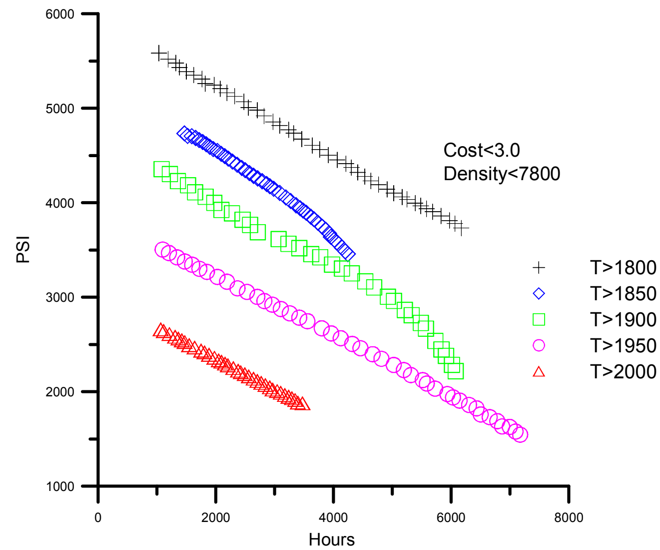

Figure 18: Pareto fronts for two primary constraints (minimum cost and minimum specific weight) and five secondary constraints (maximum temperature).

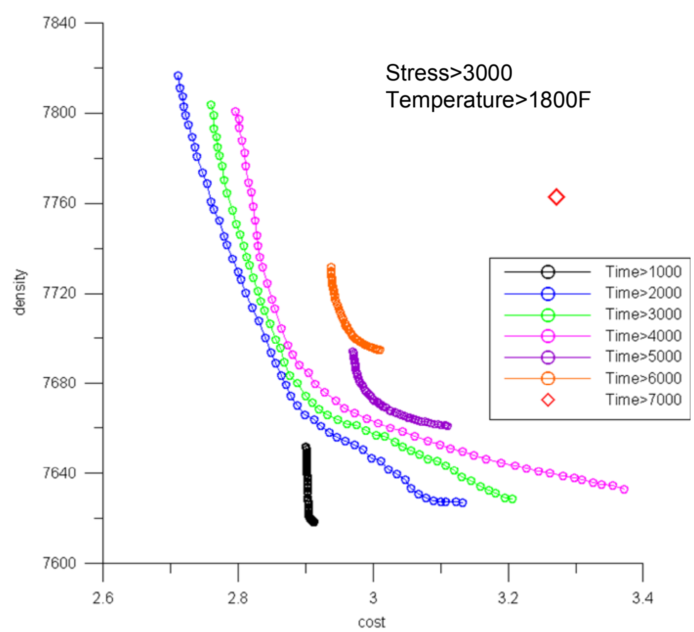

Figure 19: Pareto fronts for two primary constraints (maximum stress and maximum temperature) and seven secondary constraints (time-to-rupture).

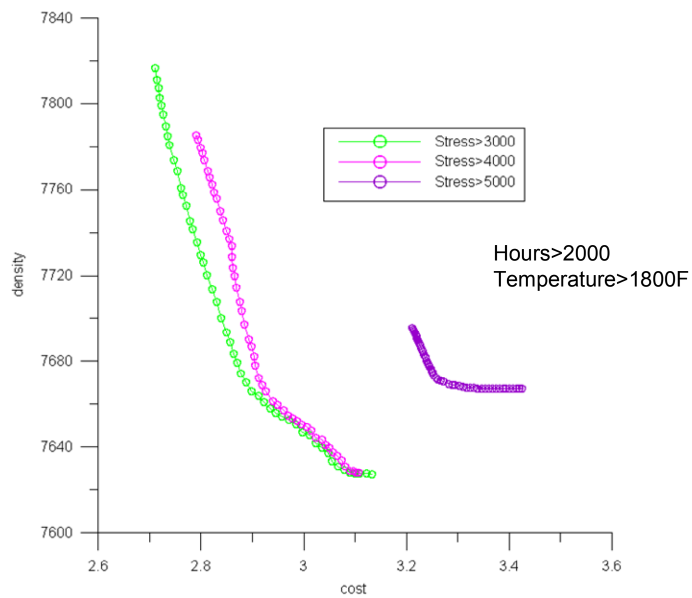

Figure 20: Pareto fronts for two primary constraints (time-to-rupture and maximum temperature) and three secondary constraints (maximum stress).

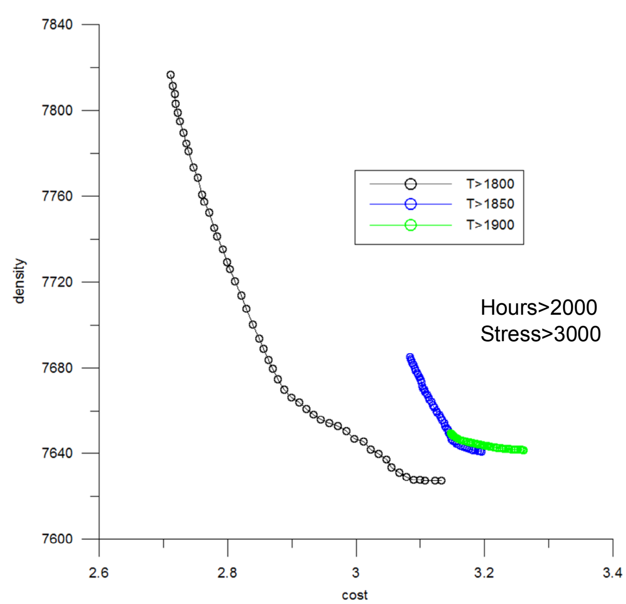

Figure 21: Pareto fronts for two primary constraints (time-to-rupture and maximum stress) and three secondary constraints (maximum temperature).

6 INVERSE DESIGN OF ALLOYS FOR SPECIFIED PROPERTIES

This is an entirely new concept in design of alloys. The inverse problem in this case is determination of chemical composition(s) of alloy(s) that will provide specified levels of, for example, stress at a specified temperature for the specified length of time. The inverse problem can be then formulated as, for example, a multi-objective optimization problem with a given set of equality constraints. We have used IOSO multi-objective optimization algorithm to achieve the solution of this type of inverse alloy design problem. The results (Fig. 22) demonstrate that it is possible to create a large number of alloy compositions that will satisfy the specified multiple properties. It should be pointed out that these are the visualizations of only two (Cr and Ni) of the 14 chemical elements whose concentrations were optimized in order to illustrate how the inverse design method works.

Notice that when the temperature and the life expectancy are introduced and progressively increased, the feasible domain for varying most of the alloying elements' concentrations will rapidly shrink[10]. Similar general trend can be observed when the life expectancy is specified and progressively increased.

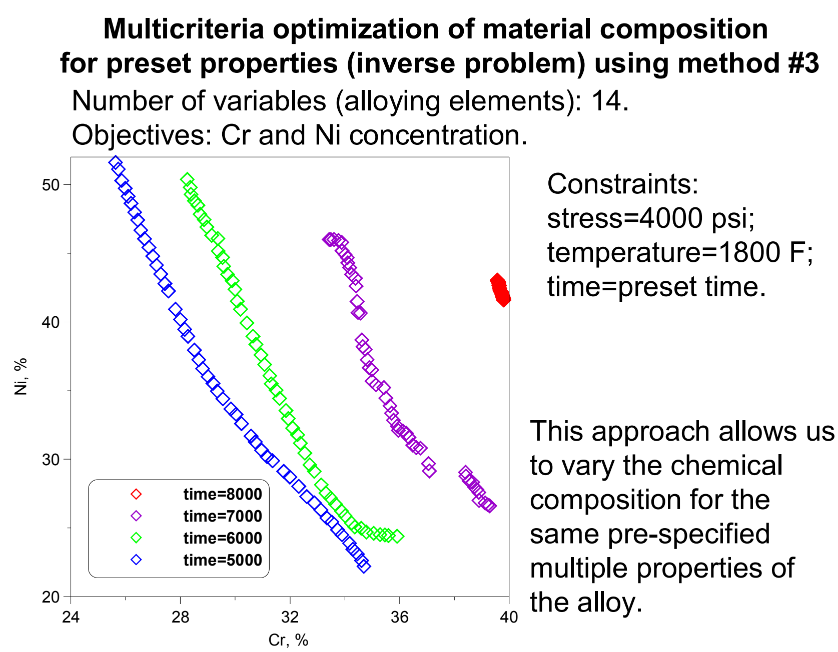

Figure 22: Inversely designed Pareto optimal concentrations of Ni and Cr as a function of time constraint.

7 ROBUST DESIGN OPTIMIZATION OF STEEL ALLOYS

Most publicly available databases contain 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 reported measured properties. These differences can be explained as errors due to the particular conditions existing during the experimental evaluations (measurement errors), and during certain operating conditions (for example, thermal condition during alloy processing) (Figs. 23 and 24).

IOSO Technology implements the new evolutionary response surface strategy. This strategy differs significantly from both the traditional approaches of nonlinear programming and the traditional response surface methodology. Because of that, IOSO have higher efficiency, provide wider range of capabilities, and are practically insensitive with respect to the types of objective function and constraints: smooth, non-differentiable, stochastic, with multiple optima, with the portions of the design space where objective function and constraints could not be evaluated at all, with the objective function and constraints dependent on mixed variables, etc.

The concepts of robust design optimization allow finding an optimal solution for the particular technology level thus assuring that such a technical solution could be realized in practice with high probability. It should be pointed out that several other approaches perform evaluation of probability parameters only after the deterministic optimal solution is found since they employ very simplified estimates of probability parameters during optimization process. The distinctive feature of the robust IOSO design optimization is that optimization problem is solved using stochastic formulation directly, where the evaluation of probability parameters is performed at each iteration. This results in reliable arrival to the truly robust optimal solution. High efficiency and accuracy of the IOSO robust design optimization is insured even when high level of noise is present in responses. This has been confirmed by the thorough testing of the IOSO algorithms using well-known test functions.

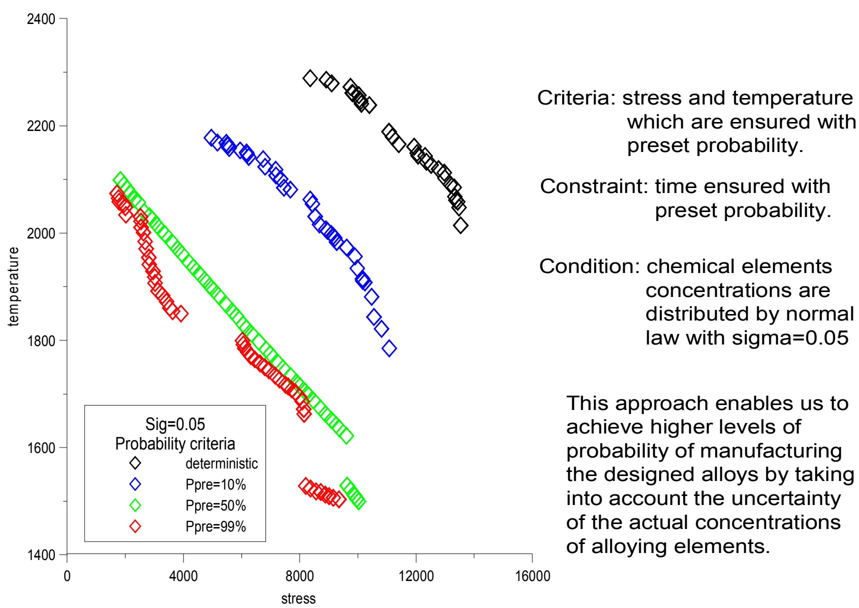

Figure 23: Multi-objective optimization of steel alloy properties including uncertainty of concentrations.

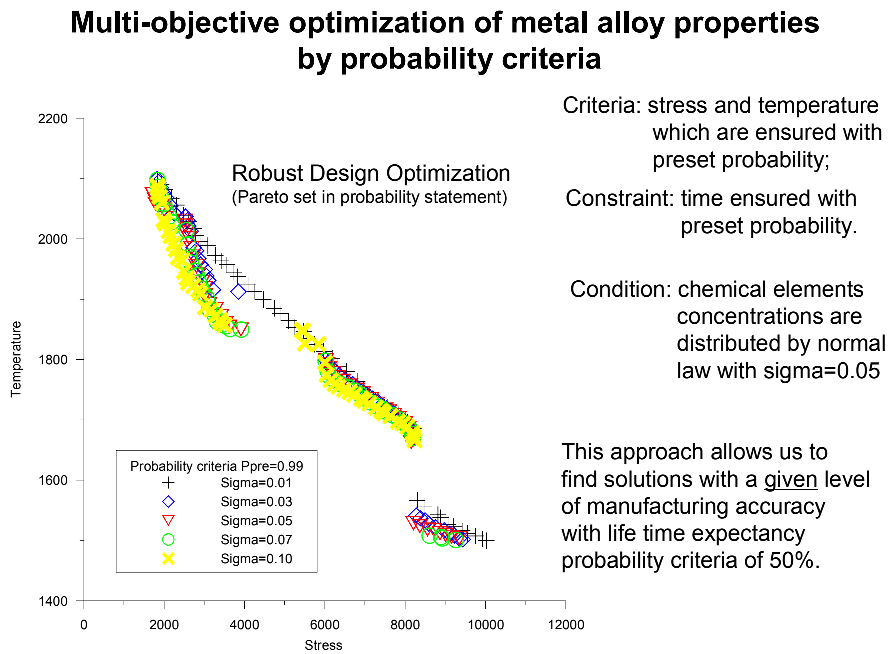

Figure 24: Multi-objective optimization of steel alloy properties including manufacturing inaccuracy.

CONCLUSIONS

The exposed alloy design methods use an evolutionary optimization algorithm that utilizes neural networks, radial basis functions, Sobol's algorithm, and self-adapting multi-dimensional response surface concepts based on graph theory. Evaluations of physical properties of all alloys (maximum stress at elevated temperature, maximum operating temperature, time-to-rupture at elevated temperature) were performed using classical experimental techniques thus automatically confirming the validity of the predictions of properties of the optimized alloys. Alloys were successfully designed for minimum weight and minimum cost of raw ingredients in addition to the multiple physical properties like maximum stress, time-to-rupture and operating temperature. These alloy design methods could also incorporate uncertainty of the alloy manufacturing and testing. These design methods are applicable to design of any type of alloys and could account for additional desired features of new alloys like corrosion resistance, microstructure features, thermal and mechanical treatment, manufacturing cost, etc.

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