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

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

subject to a vector of inequality constraints

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

and a vector of equality constraints

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

In general, the solution of this problem is not unique. With the introduction of the Pareto dominance concept the possible solutions are divided into two subgroups: the *dominated* and the *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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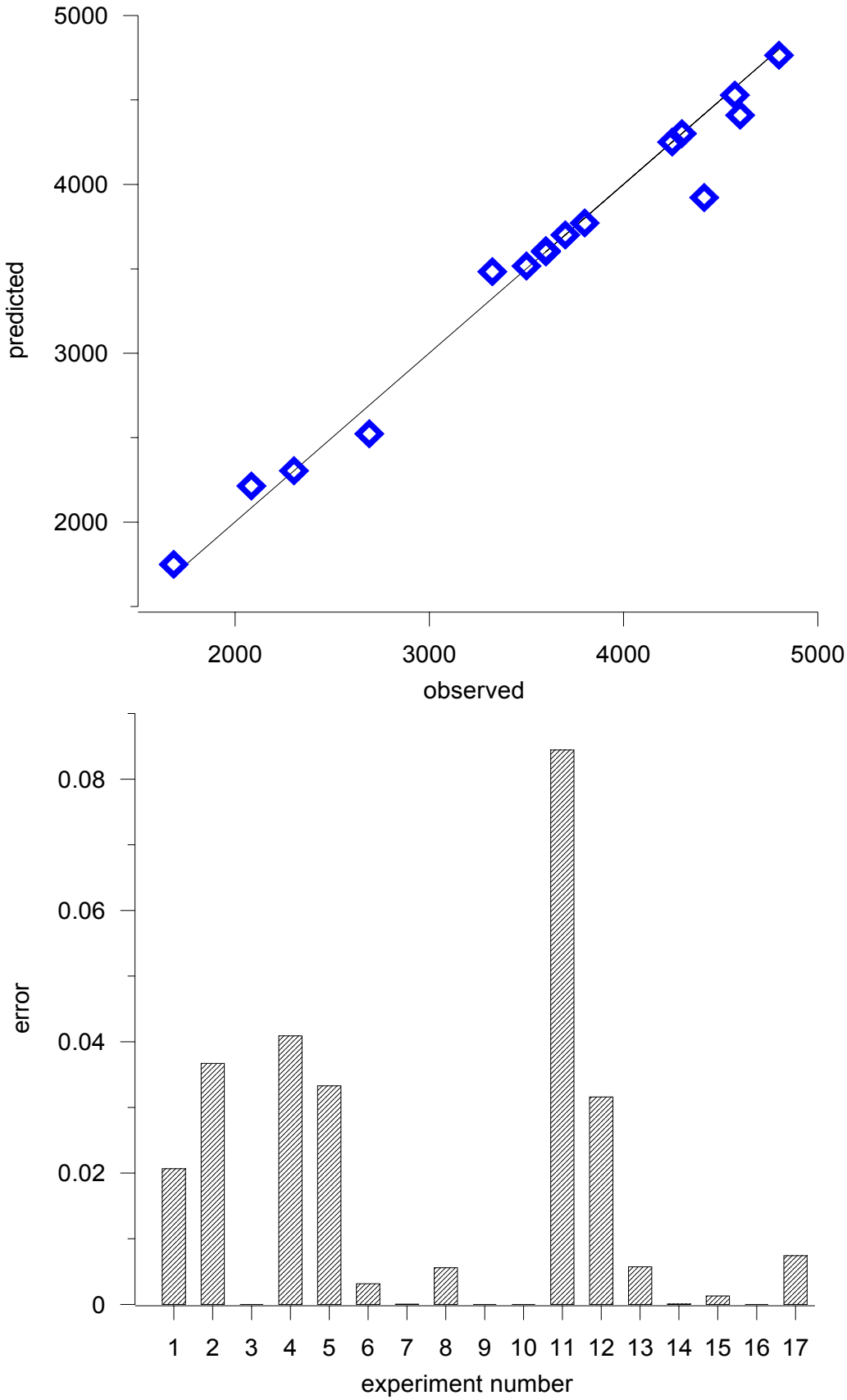

Figure 1: Accuracy of the ANN1.

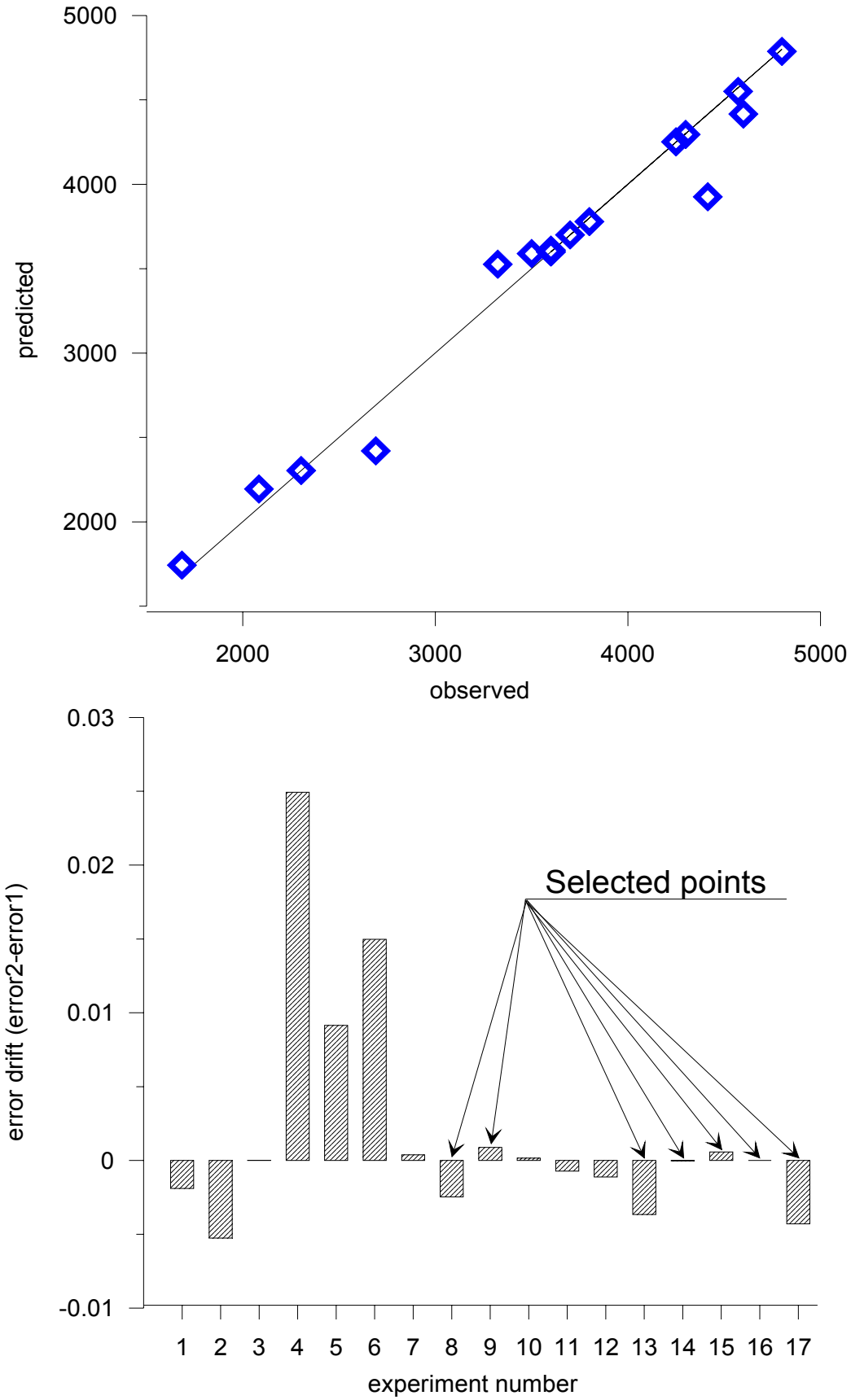

Figure 2: Accuracy of the ANN2.

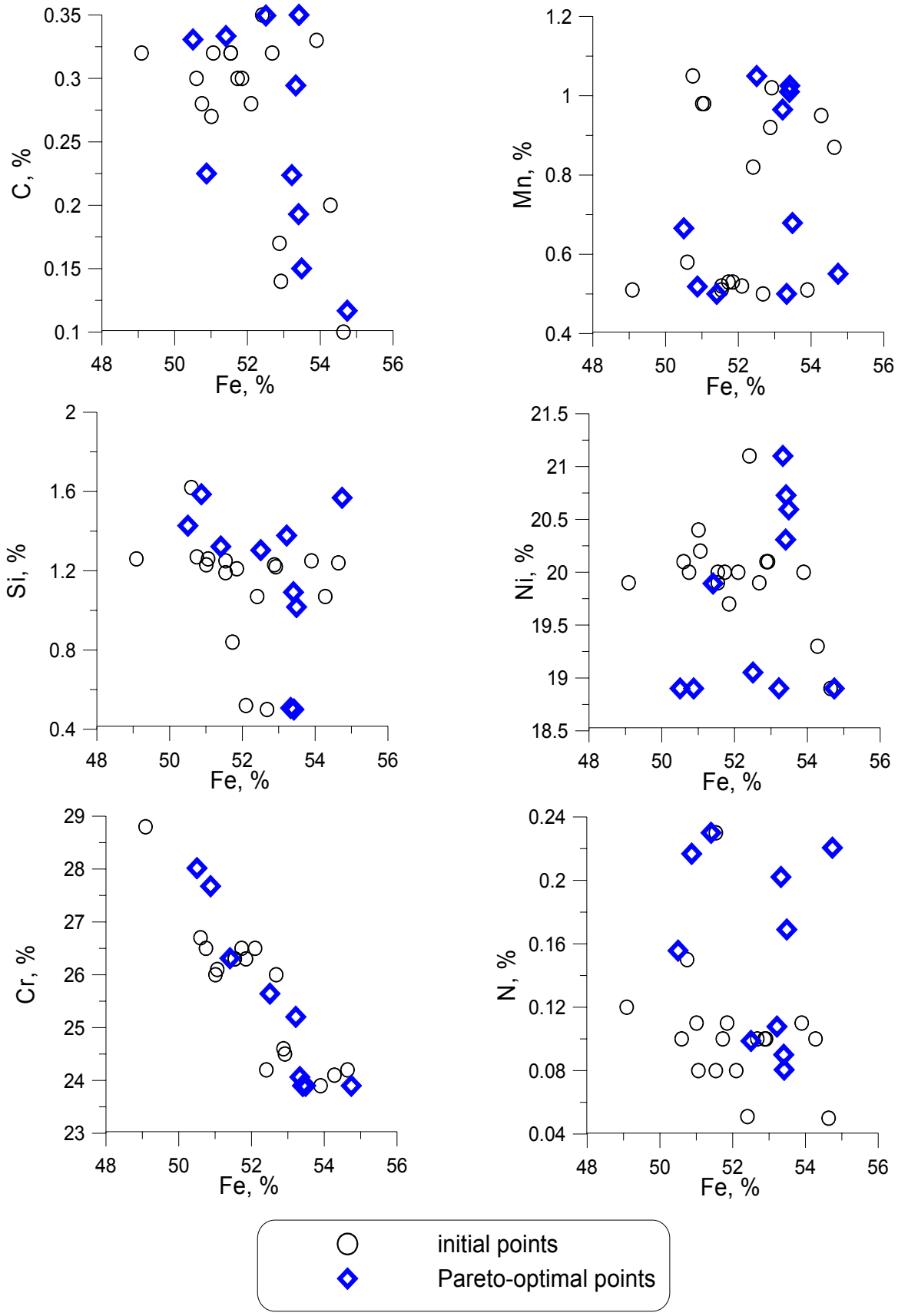

Figure 3: Result of the first iteration of steel composition optimization.

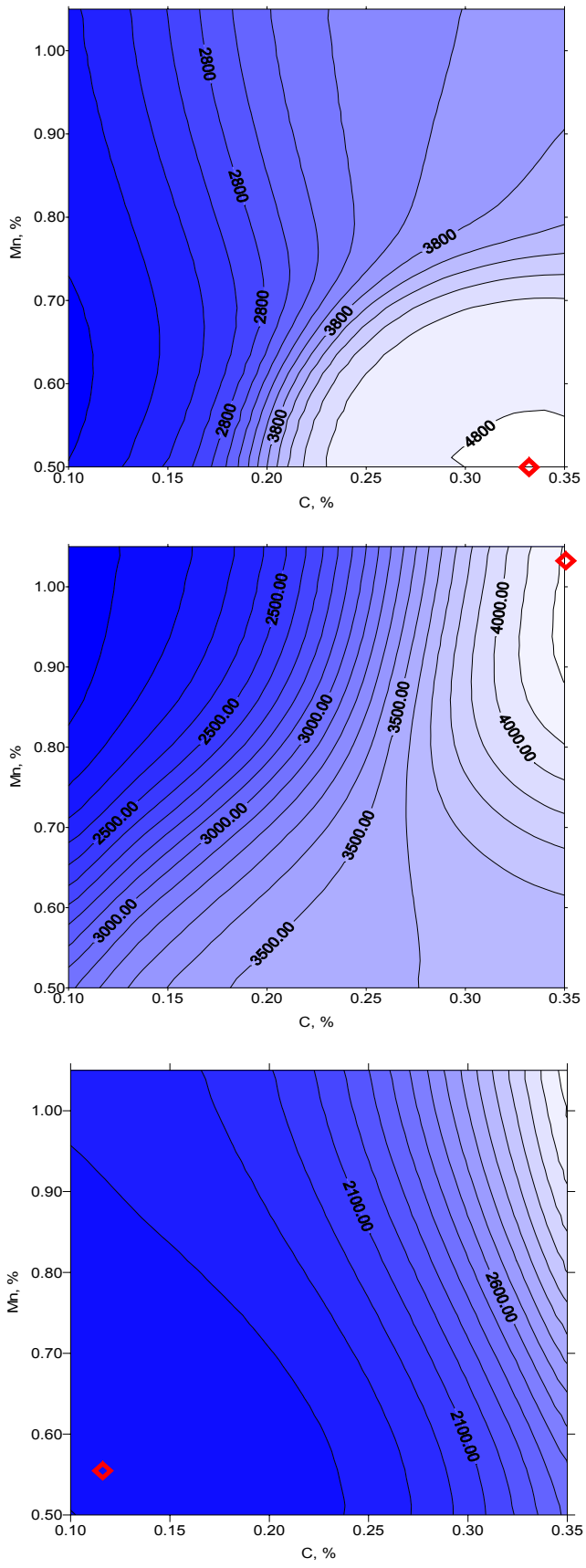

Figure 4: Topology of the ANN2-based response surface in the vicinity of 1st, 2nd and 10th Pareto-optimum points for C – Mn.

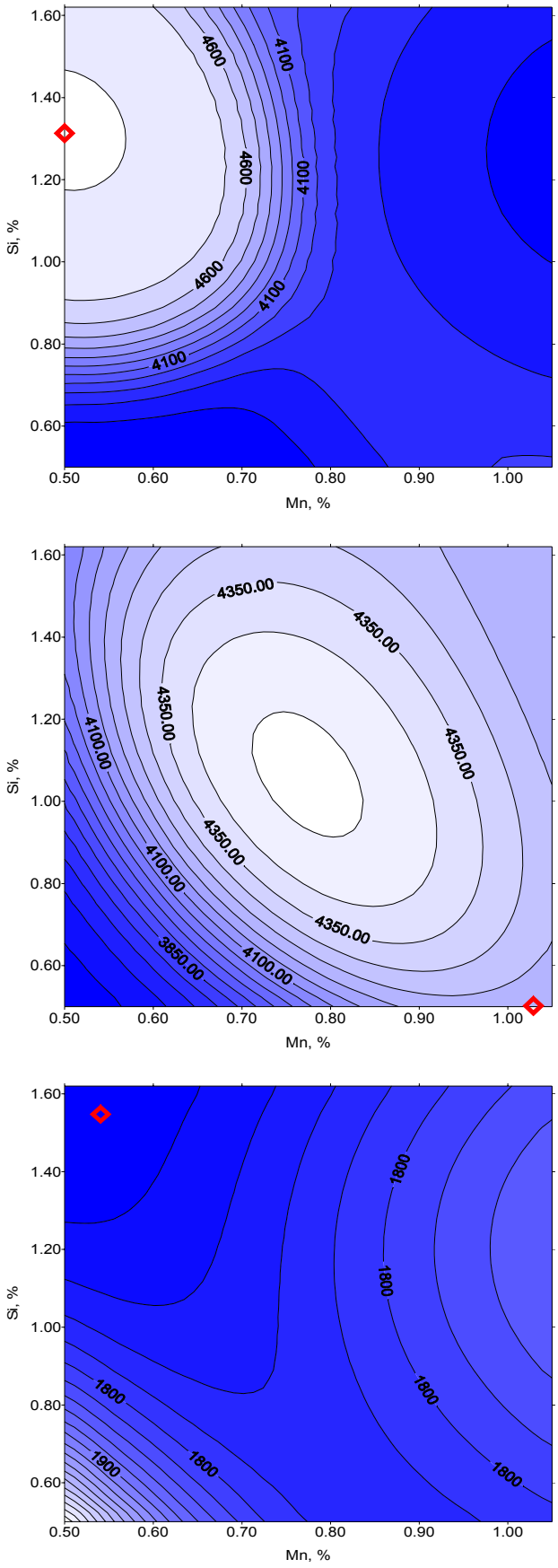

Figure 5: Topology of the ANN2-based response surface in the vicinity of 1st, 2nd and 10th Pareto-optimum points for Mn – Si.