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.

Acknowledgments

The authors are grateful for the financial support provided for this work by the US Department of Energy under the grant DE-FC07-01ID14252 and by the US Army Research Office under the grant DAAD 19-02-1-0363. They are also grateful for the in-kind support provided by their employing institutions.

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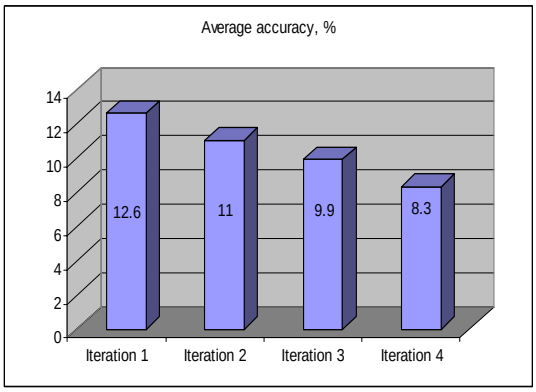

Figure 1. Average error of response surfaces representing experimental data.

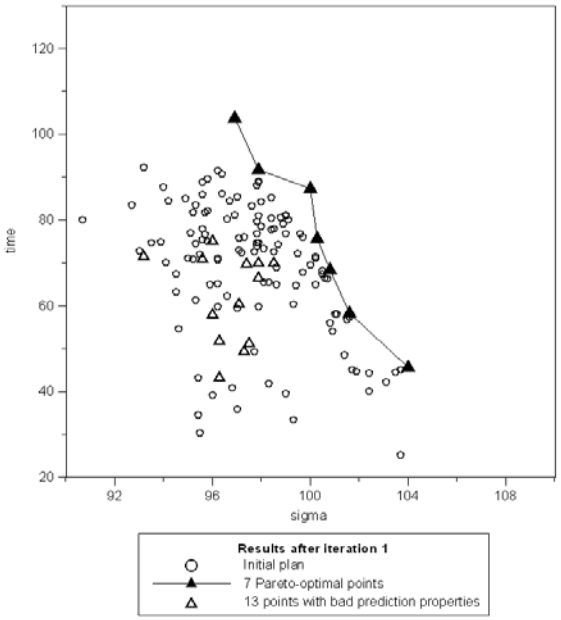

Figure 2. Initial 120 nickel based alloys and 20 alloys predicted by the 1st iteration with IOSO optimizer and consequently experimentally tested for maximum strength and time-to-rupture at 975 degrees Celsius.

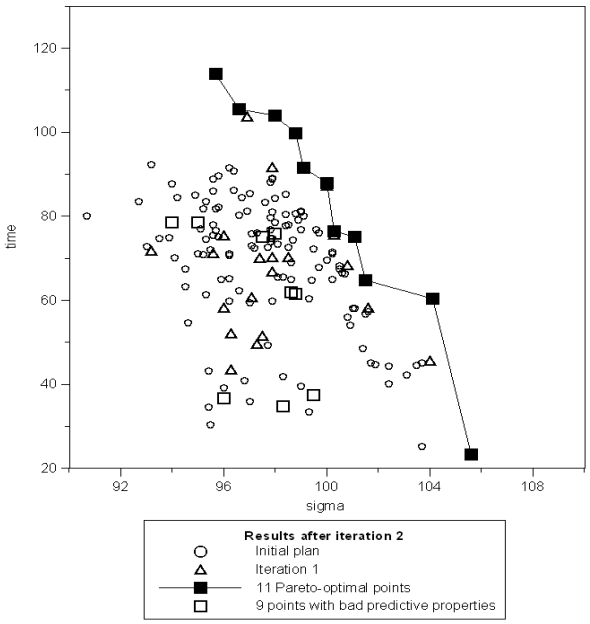

Figure 3. Initial 120 alloys plus 20 alloys from first iteration and 20 alloys predicted by the 2nd iteration with IOSO optimizer. All were then experimentally tested for maximum strength and time-to-rupture at 975 degrees Celsius.

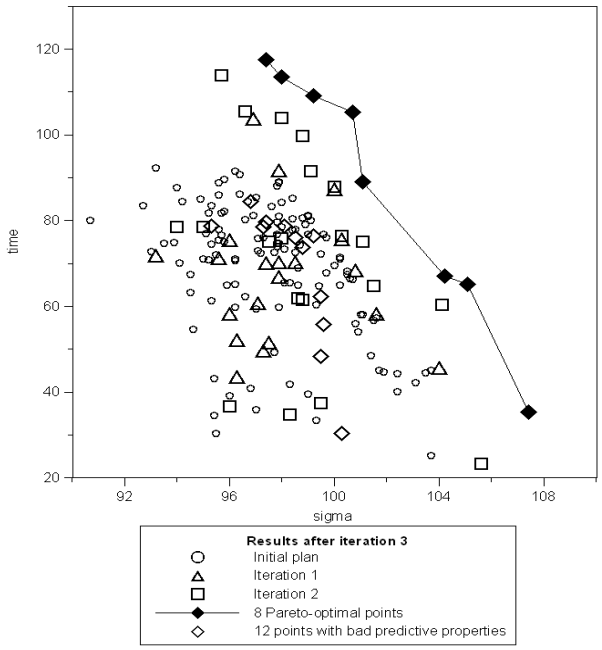

Figure 4. Initial 120 alloys plus 20 alloys from 1st iteration, plus 20 alloys from 2nd iteration, plus 20 alloys predicted by the 3rd iteration with IOSO optimizer. All were then experimentally tested for maximum strength and time-to-rupture at 975 degrees Celsius.

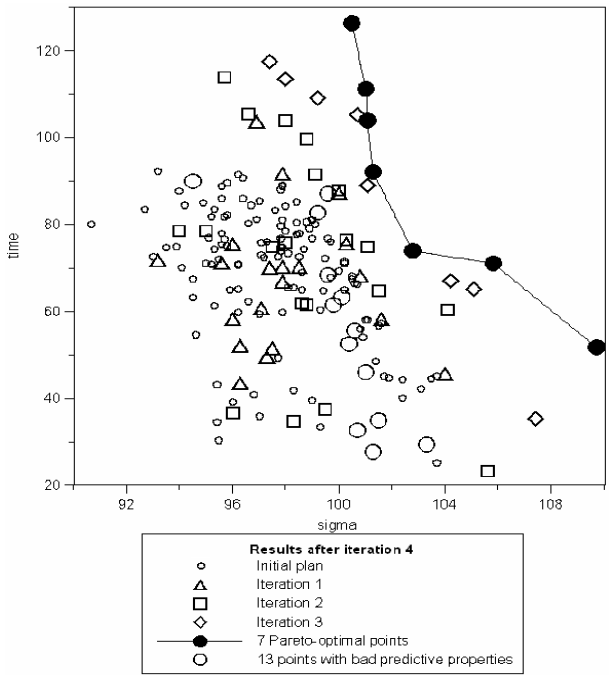

Figure 5. Initial 120 alloys plus 20 alloys from 1st iteration, plus 20 alloys from 2nd iteration, plus 20 alloys from 3rd iteration, plus 20 alloys predicted by the 4th iteration with IOSO optimizer. All were then experimentally tested for maximum strength and time-to-rupture at 975 degrees Celsius.

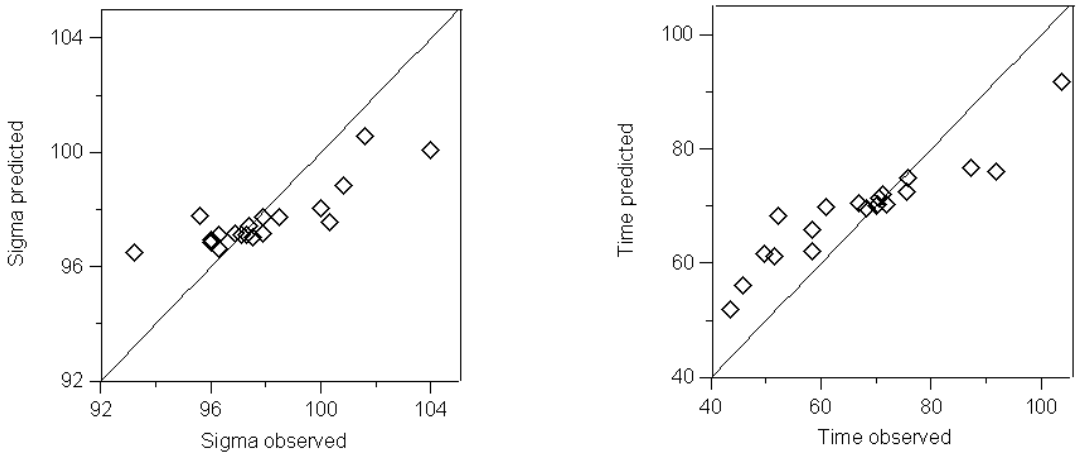

Figure 6. Predicted and observed values of two optimization criteria after first iteration.

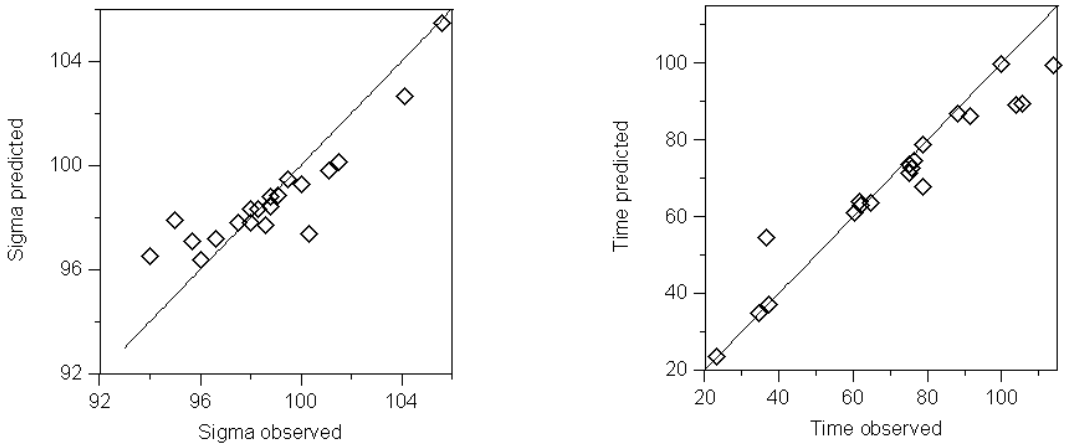

Figure 7. Predicted and observed values of two optimization criteria after second iteration.

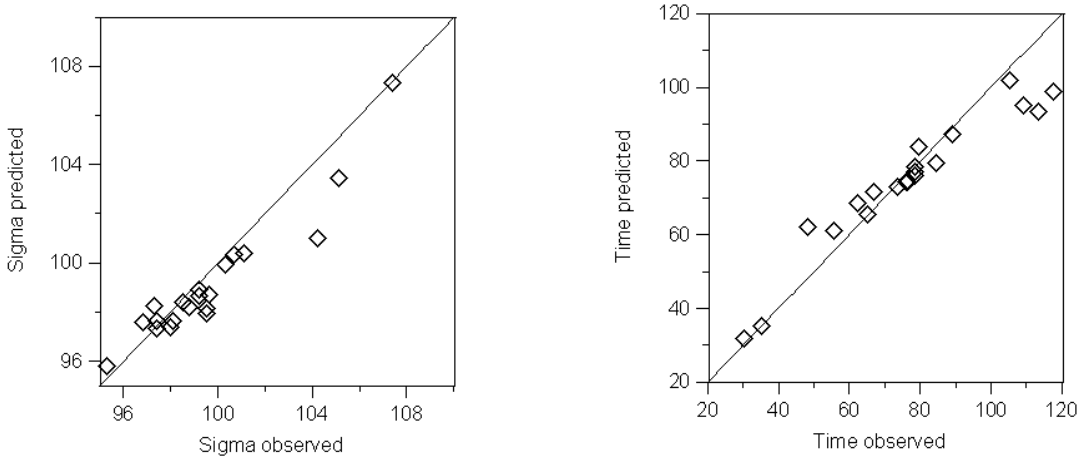

Figure 8. Predicted and observed values of two optimization criteria after third iteration.

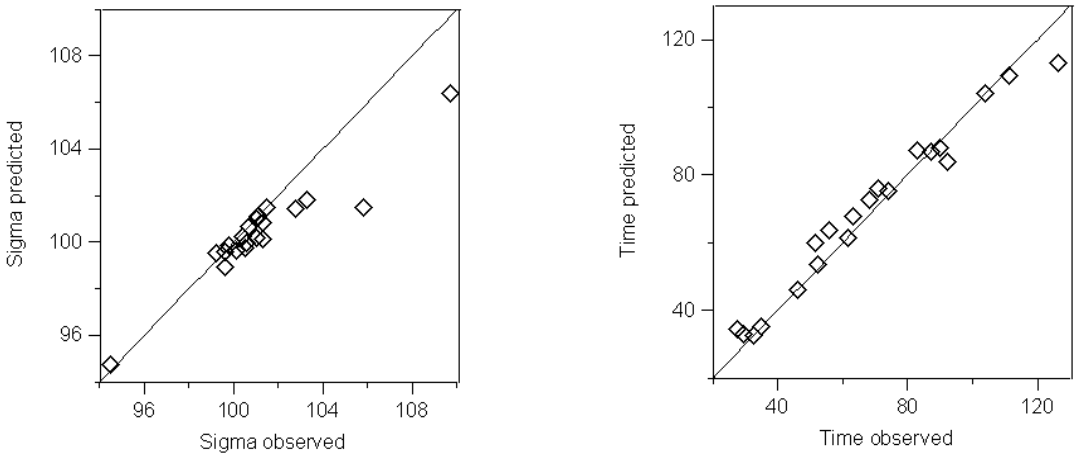

Figure 9. Predicted and observed values of two optimization criteria after fourth iteration.