A new holistic systems approach to the design of heat treated alloy steels using a biologically inspired multi-objective optimisation algorithm

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Highlights

- We model mechanical properties of heat treated alloy steel using interpretable fuzzy models.
- We demonstrate how to locate the ‘best’ processing parameters and chemical compositions.
- We demonstrate how to achieve certain mechanical properties.
- We demonstrated a holistic systems approach to achieve ‘right-first-time’ production.
- We unravel the power of multi-objective optimisation and interpretable fuzzy modelling.

Abstract

The primary objective of this paper is to introduce a new holistic approach to the design of alloy steels based on a biologically inspired multi-objective immune optimisation algorithm. To this aim, a modified population adaptive based immune algorithm (PAIA2) and a multi-stage optimisation procedure are introduced, which facilitate a systematic and integrated fuzzy knowledge extraction process. The extracted (interpretable) fuzzy models are able to fully describe the mechanical properties of the investigated alloy steels. With such knowledge in hand, locating the ‘best’ processing parameters and the corresponding chemical compositions to achieve certain pre-defined mechanical properties of steels is possible. The research has also enabled to unravel the power of multi-objective optimisation (MOP) for automating and simplifying the design of the heat treated alloy steels and hence to achieve ‘right-first-time’ production.

Abbreviations

Abs, antibodies; AIS, artificial immune systems; Al, aluminium; BEP, back-error-propagation; C, Carbon; Cr, chromium; FRBS, fuzzy rule-based systems; IMOFM, an immune inspired multi-objective fuzzy modelling approach; Mn, manganese; Mo, molybdenum; MOP, multi-objective optimisation problems; Ni, nickel; PAIA2, a modified population adaptive immune algorithm; RMSE, root mean square error; ROA, reduction of area; S, Sulphur; Si, silicon; UTS, ultimate tensile strength; V, vanadium

Keywords

Multi-objective optimisation; Fuzzy modelling; Artificial Immune Algorithm; 'Right-First-Time' production of alloy steels

1. Introduction

As stated in the Steel Industry Technology Roadmap: Barriers and Pathways for Yield Improvements (Energetics, Inc., 2003) "making the steel and internal products correctly the first time minimises waste oxide generation, in-plant returns and, most importantly, customer rejects". Nearly 1% of all production is returned from the customers because it does not meet certain specifications, and in-house scrap represents another 8 million tons per year that must be reprocessed. Both types of scrap represent significant yield loss since the energy consumed in the production of these is lost (Energetics, Inc., 2003). Faced with increasing competitive markets and economic demands, metal producers are forced to 'rethink' their short and long term strategies when it comes to producing metal in order to meet tighter customers' specification and to more efficiently provide steels with more consistence and higher quality. Therefore, more research work is required to improve microstructure control and reduce defects.

The properties of the end product can be improved mainly through: (a) heat treatment process and, (b) thermomechanical processing. In this paper, we will focus on the first method which involves using specialist heat treatments to develop the required mechanical properties in a range of alloy steels. Traditionally, a heat treatment metallurgist would attempt to balance these factors using their metallurgical knowledge and experience in a bid to obtain the desired mechanical properties. However, due to the increasing complexity of the underlying system, this may still prove difficult even for the metallurgists to tune these parameters. Given the lack of mathematical models which can account for these complex systems and a large amount of available industrial process data associated with the systems, data-driven modelling becomes more and more vital for assisting the metallurgist to predict the mechanical test results without actually doing it. Based on these models, further operations of optimisation of the heat treatment process can also be developed, which is envisaged to be able to automate the steel design process and reduce the experimental costs (Chen, 2009).

In the light of the above considerations, finding out a suitable optimisation framework, which is more flexible to accommodate multiple objectives and more effective in search towards the new optimal design methodology is key to steel design. A more holistic framework is proposed to deal with these problems, which is based upon a modified Population Adaptive Immune Algorithm (PAIA2) (Chen, 2009 and Chen and Mahfouf,). An Immune inspired Multi-Objective Fuzzy Modelling (IMOFM) approach (Chen and Mahfouf, 2012) for prediction of steel properties is also devised based on PAIA2. The elicited mechanical property models are then incorporated into the framework of PAIA2 to automate and simplify the design of the heat treated alloy steels. The overarching aim of this research is to unravel the powers of multi-objective optimisation for automating and simplifying the design of the alloy steels and hence to achieve ‘right-first-time’ production. The work was part of the research activities which were previously carried out in the Institute for Microstructural and Mechanical Process Engineering: The University of Sheffield (IMMPETUS).

The paper is organised as follows: Section 2 introduces PAIA2, which gives the basis and framework for further alloy design tasks; also in this section, PAIA2 is applied to multi-objective fuzzy modelling for prediction of steel properties; Section 3 is devoted to the optimal design of heat treated alloy steels in a multi-objective optimisation sense; experimental results relating to the prediction of mechanical properties, such as Ultimate Tensile Strength (UTS) and Reduction of Area (ROA) of the end product, are presented; with such a knowledge and PAIA2 in hand, simultaneous optimisation of several conflicting objectives, such as the strength, the ductility of steels and the costs of the heat treatment process, is carried out; finally, discussions and conclusions are given in Section 4.

2. Bio-inspired multi-objective optimisation and modelling

The increasing interest in applying biological inspired optimisation to real engineering problems lies in the fact that the apparently simple structures and organizations in nature are capable of dealing with most complex systems and tasks with relative ease. Compared to classical optimisation techniques which aim at exact optimal solutions, bio-inspired (heuristic) search methods propose instead to locate the near optimal solutions and do not rely on availability of analytical models. The flexible structure of such a search mechanism can not only handle different knowledge representations in a single framework, but can also provide pragmatic solutions in a more efficient way. Given the fact that optimal alloy design problem requires different types of models to fully describe the whole process and is more often than not of a multi-objective nature, a heuristic search method represents a salient tactic to fuse different models and produce Pareto solutions. Among many biological optimisation paradigms, Artificial Immune Systems (AIS), as a relatively new research area dating back to Farmer and Packard (1986)’s paper, lends itself to represent a viable candidate to the problems investigated in this paper for its more flexible structure and enhanced search power.

2.1. A modified population adaptive immune algorithm (PAIA2)

In (Chen, 2009 and Chen and Mahfouf,), Chen and Mahfouf proposed a modified Population Adaptive Immune Algorithm (PAIA2) for Multi-objective Optimisation Problems (MOP). The algorithm is the synthesis of the four human immune metaphors for the creation of novel solutions to real world problems, which are the Clonal Selection Principle (Burnet, 1959); the Network Hypothesis (Jerne, 1974 and Perelson, 1989); the adaptive antibody’s concentration (Chen and Mahfouf, 2006), and the vaccination and the secondary response (Chen and Mahfouf, 2006). The main stages of PAIA2 are shown in Fig. 1.

Full-size image (32 K)

Fig. 1.

Main stage of PAIA2 for MOP solving (NCR: the number of current non-dominated Abs; NPR: the number of non-dominated Abs in the last iteration; IN: the initial Abs size; Stop: at least one iteration step is executed).

Two types of fitness evaluation methods (Activation) are used in PAIA2 so that the algorithm receives environmental information from both the objective space (through non-dominated sorting) and the decision variables space (through the distance measured in the variable space between the two chosen solutions). Such information combined with the density information in the decision variable space provides adequate selective pressure to effectively advocate the most promising and evenly distributed solutions into the next iteration. On the one hand, the Clonal Selection and Clone prefer good solutions by providing them with more chances to be cloned so that they always dominate the whole population. On the other hand, the Clone itself contributes significantly to the diversity of the population. Affinity Maturation includes hypermutation, receptor editing and recombination. The former two increase the diversity of the population so that more objective landscape can be explored. The hypermutation rate of the cloned solutions decreases when the optimization process evolves so that a more focused search is introduced in the later iterations. This decreasing rate can be controlled through a predefined Dirac's parameter. The Simulated Binary Crossover (SBX) (Deb and Agrawal, 1994) is utilised as the recombination operator which efficiently uses the information contained in the solutions so that fine search can be executed in the late stage of the optimization. Reselection ensures that good mutants are inserted into the memory set and bad solutions apoptosis. Network Suppression regulates the population so that it is adaptive to the search process. Newcomers are used to further increase the diversity of population. For more details of the implementation of PAIA2, readers are referred to (Chen, 2009 and Chen and Mahfouf,).

As argued in (Chen, 2009, ch. 3), an ineffective search could be introduced in the MOP context due to many search attempts being wasted to locate more dominant solutions in the current non-dominated front rather than progressing to a more optimised front. Therefore, the most efficient way to deal with MOP problem is to divide the search process into two separate stages. In the first stage, a single objective optimization algorithm is used to locate any solution on the Pareto front. The solution which is identified in the first stage serves as the vaccine (initial population) in the MOP stage to quickly expand the rest solutions on the Pareto front. In doing so, one maximises the possibility of choosing the right direction for the mutants in both stages, hence, saving precious computational resources. Such a mechanism has been adopted in Section 2.2 in the search for the optimal fuzzy models, where the search space is relatively large.

PAIA2 possesses the following strengths which cannot be found in the conventional evolutionary algorithms (Chen, 2009).

(1)

Adaptive population. PAIA2 possesses an adaptive population size which can be adjusted to an adequate size according to need of the problem. This adaptive rather than a fixed population leads to the following two advantages: (a) Initial population size is not problem dependent; and (b) more solutions can be obtained without significantly increasing the number of evaluations by tuning the network suppression threshold.

(2)

Good jumping-off point. By using the multi-stage optimization procedure, an optimized solution can be included in the initial population to bias the search process, which reduces the computational load of the whole optimization process.

(3)

Good and fast convergence. A good balance between exploitation and exploration, due to the adoption of Hypermutation operator, and an adaptive population size make good and fast convergence possible for PAIA2.

A comprehensive experimental study has been carried out in (Chen, 2009) to compare PAIA2 with other state-of-the-art MOP algorithms, such as NSGAII (Deb, 2002), SPEA2 (Zitzler et al., 2001) and VIS (Freschi and Reetto, 2005). The results confirmed that PAIA2 outperformed its counterparts in most cases in terms of the convergence and distribution measures. In the following section, PAIA2 is applied to multi-objective fuzzy modelling with the aim of finally automating the steel design process based on the elicited models.

2.2. An immune inspired multi-objective fuzzy modelling (IMOFM)

In order to account for the enlarged search space due to the simultaneous optimization of the fuzzy rule-base structure and its associated parameters, Chen and Mahfouf (2012) adopted a multi-stage optimisation procedure as discussed in Section 2.1 and a variable length coding scheme. Due to space constraint, only Mamdani Fuzzy Rule-based Systems (FRBS), namely IMOFM_M is presented here. A typical rule in a Mamdani FRBS reads as follows:

equation(1)

where, View the MathML source is the ith linguistic value (fuzzy set) for the j th linguistic variable (input) xj defined over the universe of discourse Ʊj; the function View the MathML source associated with View the MathML source that maps Ʊj to [0, 1] is the corresponding membership function; Ri represents the i th rule in the rule base, and yi is the output of the i th rule. Zi is the linguistic value of the output, and its associated membership function is µBi(y). In this paper, IMOFM_M uses

Gaussian membership function (2) and (3) for the premises View the MathML source and bell-shape membership function (4) for the consequents Zi.

equation(2)

equation(3)

equation(4)

Hence, a Mamdani FRBS after centre of gravity defuzzification can be formulated as follows:

equation(5)

where, bi is the centre of area of the membership function μBi(y) and is the peak (View the MathML source) if μBi(y) is symmetric. View the MathML source denotes the area under View the MathML source over the output interval View the MathML source. View the MathML source is the parameter vector in which each individual parameter is linked directly to centres and spreads of the corresponding membership functions. This parameter vector is extracted initially from data via G3Kmeans clustering algorithm (Chen et al., 2012) and is refined further using a constrained Back-Error-Propagation (BEP) algorithm (Chen and Mahfouf, 2012). These first two stages are implemented to improve prediction accuracy so that a 'vaccine model' can be obtained for the MOP stage.

The FRBS extracted via G3Kmeans and the constrained BEP need further a multi-objective optimisation to simultaneously simplify its structure and tune the corresponding parameters. To this aim, two objectives are formulated.

equation(6)

where, Nrule is the number of fuzzy rules in FRBS; Nset is the total number of fuzzy sets; RL is the summation of the rule length of each rule. Simplifying FRBS structure will result in a variable-length parameter vector θ, and tuning parameters in θ will cause a so-called 'unordered sets of rules' problem (Cooper and Vidal, 1994 and Magdalena, 1998). In both cases, the decision variable space is constantly changing. Therefore, a fixed-length coding scheme, which comes very naturally in most heuristic search algorithms, may not be feasible anymore in this case. In order to still utilise PAIA2, a variable length coding scheme is needed along with a new distance index (Chen and Mahfouf, 2012). The basic idea is to find the distance of the closest rules in different FRBSs rather than the distance of corresponding rules. Such a distance measure forms the basis for the fitness evaluation (Activation) step in PAIA2 so that one can freely delete or merge rules and move membership functions without noticing the changing nature in each candidate solution caused by such manipulations. The whole framework of IMOFM_M is shown in Fig. 2.

Full-size image (31 K)

Fig. 2.

The Proposed IMOFM_M Framework.

Figure options

IMOFM_M does not suffer from the curse of dimensionality and a set of FRBSs representing the trade-offs between interpretability and accuracy are obtained through a single run, and only the maximum allowable number of rules is required a priori, which reduces any user intervention during the whole design process to a minimum level. For more details of IMOFM_M, readers are referred to (Chen and Mahfouf, 2012). In the next section, the detailed results of UTS modelling are presented, where, IMOFM_M is used to predict mechanical properties of alloy steels which serve as the objectives to be minimised in PAIA2 in order to automate the heat treated alloy steel design process.

3. Optimal design of heat treated alloy Steels

3.1. Problem description

The mechanical properties of the alloy steels depend on several factors of which the following are believed to represent the most crucial ones: tempering temperature, quench type, chemical compositions (alloying elements) of the steel, the bar size, test sample location on the bar (test depth), batch distribution in the furnace, measurement tolerances and variations in the process equipment and operators (Tenner, 1999), of which the last dependent factor is mostly dependent on the treatment site. Due to the limited physical knowledge, computing the mechanical properties, such as Ultimate Tensile Strength (UTS) and Reduction of Area (ROA) of the end product, based on these dependent factors is proved to be hard. However, having such a relationship is vital in deciding the optimal heat treatment regime and weight percentage of chemical compositions. In the past, several mechanical property models were developed which were mainly based on linear regression methods (Pickering, 1978) or artificial neural networks (Tenner, 1999). The linear models are only designed for specific classes of steels and specific processing routes, and not sophisticated enough to account for more complex interactions, while neural networks are black-box modelling techniques and one cannot have a deep insight into the model. Hence, a transparent data-driven modelling framework for material property prediction, such as IMOFM_M presented in Section 2.2, is still needed so that further design of weighted chemical compositions and heat treatment regime can be developed. The prediction performances of IMOFM_M are presented in Section 3.2. Due to space constraints, only the UTS modelling is presented. The optimal design of heat treated alloy steels is discussed in Section 3.3.

3.2. IMOFM_M modelling results

The UTS data set consists of 3760 data samples and includes 15 inputs and one output as shown in Table 1.

Table 1.

The inputs and output of Tensile Strength data set.

Inputs	Test depth		Size	Site	C (%)
Max.	140	381	6	0.62	
Min.	4	8	1	0.12	

Inputs	Si (%)	Mn (%)	S (%)	Cr (%)
Max.	0.35	1.72	0.21	3.46
Min.	0.11	0.35	5e-4	0.05

Inputs	Mo (%)	Ni (%)	Al (%)	V (%)
Max.	1	4.16	1.08	0.27
Min.	0.01	0.02	5e-3	1e-3

Inputs	Hardening temperature			Cooling medium	Tempering temperature
Max.	980	3	730		
Min.	820	1	170		

Output	Tensile strength
Max.	1842 N/mm2
Min.	516.2 N/mm2

To test the efficacy of IMOFM_M, the UTS data set is randomly divided into two parts: 75% of the data are used for training and the remaining data are used for testing. Another 12 more recent samples are used as the unseen data set to validate the generalisation properties of the model. The maximum number of rules is set to 12. The number of iterations for the constraint BEP and PAIA2 are set to 500 and 1200 respectively. As shown in Fig. 3, without any prior knowledge as to how to simplify the model and to what degree, the proposed method provides a set of 47 Pareto FRBSs, which represents various degrees of simplification.

Full-size image (67 K)

Fig. 3.

The Pareto fronts obtained using IMOFM_M.

Among these options and after the investigation of the trade-off of these elicited FRBSs, the steel designers can finally decide their preferred degree of model simplification. For the illustration and further steel design purposes, a 7-rule simplified Mamdani FRBS has been chosen for its good prediction accuracy and interpretability. Fig. 4 shows the performance of the initial 12-rule FRBS and the simplified 7-rule FRBS.

Fig. 4.

The prediction performances of the initial 12-rule FRBS and the simplified 7-rule FRBS for the training and testing data using IMOFM_M.

Fig. 5 shows the prediction performances of the 'vaccine FRBSs' and the simplified FRBSs on the 12 validation data (an unseen 12-data set independently obtained from a Tata-steel Europe Site in Sheffield-UK). As indicated by the graph, the refined FRBSs obtained from the second modelling stage (constrained BEP) could not fit the newly collected samples as some predictions are very close to or even outside the ±10% error bands. Conversely, the generalization capability of the simplified FRBSs is very much improved due to the simultaneous optimisation of the two objectives.

Fig. 5.

The prediction performances of the 12-rule FRBSs after the constraint BEP and the 8-rule and 7-rule simplified FRBSs after the multi-objective optimisation.

Figure options

Fig. 6 shows 3 selected rules from the 7-rule simplified FRBS. This rule-base reveals certain heat treatment knowledge relating to the UTS, which may or may not be fully understood by the metallurgist, although it is reckoned to be transparent enough.

Fig. 6.

The selected rules from the 7-rule simplified Mamdani FRBS.

To facilitate the metallurgist to further understand the hidden knowledge, the three-dimensional response surfaces of the UTS model can be employed by plotting two varying input variables against the output while keeping other input variables constant. The constant variables are set to the 'median' values of the dominant steel grade. Using this method, one insight gained by inspecting Fig. 7 is that the strength of the modelled steel is greatest at low tempering temperature and high carbon content, and is lowest at high tempering temperature and low carbon content. Furthermore, with high carbon content, the effect of tempering temperature is much more non-linear than the one with low carbon content. A similar analysis can be conducted using the other variables and mechanical properties.

Fig. 7.

Response surfaces of the 7-rule simplified Mamdani UTS model.

Table 2 summarises the prediction performance of the simplified Mamdani FRBSs for the UTS, and ROA. The ROA data includes 3710 data samples. It has 15 inputs, which are the same as the UTS data with the same ranges, and 1 output, which is the ROA in the range of 21.8–79.4%. A randomly selected 75% of data samples are used as the training set and the rest as the testing set. The models listed in Table 2 are chosen for their good interpretability and prediction accuracy. These models will be used later in Section 3.3 to locate the optimal heat treated regime and weighted percentage of chemical compositions.

Table 2.

The prediction performance of IMOFM_M for UTS and ROA.

IMOFM_M models	No. of rules	Training (RMSE)	Testing (RMSE)	Validation (RMSE)
UTS	7	34.70	36.44	37.80
ROA	6	3.30	3.40	–

3.3. Optimal design of heat treated alloy Steels

Well-designed alloy steels often need to satisfy a set of targets, such as the desired mechanical properties, the economic cost and the environmental concerns. Sometimes, a solution is not as good as one may think it initially to be if the whole set of targets has to be considered simultaneously. For example, as discussed in Section 3.2, lower tempering temperature and higher carbon content often deliver higher tensile strengths. However, as shown in Fig. 8, if the ductility reflected by the ROA of the end product needs to be considered as well, a high carbon content and a low tempering temperature make the product less ductile.

Fig. 8.

Response surfaces of the 6-rule simplified Mamdani ROA model.

Furthermore, the steel making process is highly nonlinear. Hence, the interactions between different targets, such as the costs and the mechanical properties, are even more involved and often difficult to analysis. The cost for production depends on the amount of the added chemical compositions and the temperature for the heat treatment. Increasing the use of certain chemical compositions and temperature will significantly level up the cost, hence, being in contradiction with the target values of the UTS and ROA. The challenging task of designing alloy steels lies inherently in its multi-objective nature, and can only be elegantly dealt with in a MOP framework. MOP offers more flexibility and also reduces the necessary level of expertise in understanding complex interactions between different objectives, hence, the weights setting to integrate different objectives. In the following two case studies, we show how PAIA2 is exploited to simultaneously achieve different mechanical properties, and also in a cost-effective way.

3.3.1. Case study 1: the optimal design of both UTS and ROA

To achieve certain alloy steels with a predefined target UTS value and a predefined ROA value, PAIA2 together with the 7-rule UTS FRBS and the 6-rule ROA FRBS shown in Section 3.2 are employed here to search for the optimal weighted chemical compositions and the heat treatment regime. However, these two often competing objectives are not always in conflict. This can be observed from the response surfaces in Fig. 9.

Fig. 9.

Normalised response surfaces of the UTS and ROA with respect to carbon content and tempering temperature (all other variables are kept as the mean value in their respective range).

Fig. 9 shows the normalised response surfaces with respect to the carbon content and the tempering temperature for the UTS and ROA. The UTS and ROA values have been normalised to better illustrate the intersection between the two. The intersection shown in Fig. 9 indicates that there may exist some region in which both objectives can be met simultaneously. In the above case, both mechanical properties can be improved simultaneously within the normalised range between 0.25 and 0.42. This effectively means as long as the target UTS value is between 847.65 N/mm2 and 1073.04 N/mm2 and the target ROA value is between 36.2% and 46.0%, both objectives can be improved all at once. However, when more variables are taking into account, such a region can be very hard to understand and visualised. Due to a very high dimensionality normally involved in the heat treatment process, such as 15 inputs in this paper, identifying such a region is not a straightforward task. Zhang (2008) proposed to use a MOP algorithm to obtain the lower and upper boundaries of this region by simultaneously optimising two sets of objectives. In this paper, the same method is employed. In order to find out the lower mechanical property boundary of this region, the following two objectives are formulated:

equation(7)

To obtain the higher mechanical property boundary of this region, the following two objectives are considered instead:

equation(8)

The most interesting weighted chemical compositions and heat treatment conditions in this work are: weighted percentages of Carbon (C), Manganese (Mn), Chromium (Cr), Molybdenum (Mo) and tempering temperature. All other input variables are kept as constant to their respective mean values. The parameters of PAIA2 are set to: initial population size is 7, Clonal selection threshold is 0.4, network suppression threshold is 0.005, the maximum clone size is 95, and the Dirac's effect parameter is 1. Due to the stochastic nature of PAIA2, 10 independent runs were executed for both the lower and upper boundaries. Empirically, 200 iterations are set in order for PAIA2 to fully converge for this problem, which is equivalent to an averaged 42,336 evaluations for the lower boundary and 31,498 for the upper one. The algorithm is implemented in MATLAB and executed on a standard computer (Intel(R) Core(TM) i5 CPU, 2.27 GHz). The average execution time is 5.19 s for the lower boundary and 2.92 s for the upper boundary. The speed of convergence of PAIA2 is far more satisfactory for the off-line optimisation task like this. Fig. 10 shows the obtained Pareto fronts from one of the 10 typical runs.

Fig. 10.

The upper and lower boundaries (Pareto fronts as depicted by circles) and design regions for the simultaneously design of the UTS and ROA.

Figure options

Comparing to the results reported in (Zhang, 2008), Fig. 10 reveals a wider Region I, where both the UTS and ROA can be improved simultaneously. Due to more accurate predictions in mechanical properties by using IMOFM_M and the enhanced search power given by PAIA2, the lower boundary has been pushed to the extreme and both boundaries have been extended to cover the whole range of the UTS and ROA. This effectively means that the UTS and ROA only compete with each other when they are above the upper boundary and in Region II. Also, caution must be taken for regions close to the boundaries as small variation in optimised decision variables may cause big variation in either the ROA or UTS. Hence, when designing a metal alloy, these regions should be avoided for a more robust design. The graph with different regions shown in Fig. 10 gives a clear indication to metallurgists for their initial assessment with respect to the feasibility of a potential steel design and the compromise which they may face if the target design falls into Region II.

As an illustration example, we demonstrate two steel design solutions, where the first design with the target UTS value is 900 N/mm2 and the target ROA value is 70% and the second design with the target UTS value is 900 N/mm2 and the target ROA value is 50%. For both designs, the objectives can be described as follows:

equation(9)

View the MathML source

The first design is above the upper boundary and in Region II. Hence only a set of trade-off solutions can be obtained. 10 independent runs have been executed and an average of 10,000 evaluation times is adequate for this problem. The average execution time is 0.72 s. The results obtained from different runs are consistent and one random result from the 10 runs is shown in Fig. 11. Table 3 provides details of one set of Pareto solutions from the 10 runs.

Fig. 11.

The obtained Pareto solutions when the View the MathML source and ROATarget=70%: (a) Objective View the MathML source; (b) UTS vs. ROA; and (c) all solutions found during the search process.

Table 3.

The details of the Pareto solutions for the first design problem.

Pareto solutions	C (%)	Mn (%)	Cr (%)	Mo (%)	Tempering Temperature (°C)	UTS (N/mm2)	ROA (%)
1	0.1200	1.2130	1.4518	0.2112	723.32	899.27	67.24
2	0.1200	1.2487	1.4897	0.1935	730.00	898.12	67.56
3	0.1200	1.2154	1.4876	0.2105	730.00	894.05	67.67
4	0.1200	1.1885	1.4830	0.1911	729.99	888.41	67.85
5	0.1200	1.1434	1.4831	0.1922	730.00	881.67	68.07
6	0.1200	1.0994	1.4934	0.2123	730.00	876.69	68.25
7	0.1200	1.0592	1.4863	0.1918	729.99	869.58	68.69
8	0.1200	1.0265	1.4793	0.1907	729.99	865.09	68.66
9	0.1200	0.9731	1.4856	0.1915	729.99	858.13	68.93
10	0.1200	0.9188	1.4921	0.2111	729.78	852.98	69.17
11	0.1200	0.8748	1.4543	0.1788	730.00	844.79	69.46
12	0.1200	0.8303	1.4832	0.2153	729.99	842.66	69.65
13	0.1200	0.7785	1.4558	0.1903	729.98	835.08	69.95

The Second design is within Region I. Therefore, both design targets can be achieved simultaneously. Again, 10 independent runs have been executed and, on average, 10,000 evaluation times are adequate. The averaged execution time is 0.68 s. The results are shown in Fig. 12. For this design, all candidate solutions finally converged to one point in the objective space and the details of the solution are shown in Table 4.

Fig. 12.

The obtained Pareto solutions when the View the MathML source and ROATarget=50%: (a) Objective View the MathML source; (b) UTS vs. ROA; and (c) all solutions found during the search process.

Table 4.

The details of the Pareto solutions for the second design problem.

Pareto Solutions	C (%)	Mn (%)	Cr (%)	Mo (%)	Tempering Temperature (°C)	UTS (N/mm2)	ROA (%)
1	0.1584	1.6430	0.4653	0.2745	633.20	900.00	50.01

3.3.2. Case study 2: the optimal design of both mechanical Properties and the cost

Economic factors form another important objective which may be in conflict with the predefined mechanical properties. As stated in (Mahfouf et al., 2006), the production costs of heat-treated steels include the costs of the addition of alloying elements, such as Mn, Cr, Mo and Tempering Temperature, although other composites and temperatures could also be included. The factors contributing to the cost of heat treatment operation are summarised in Table 5 (Mahfouf et al., 2006).

Table 5.

Contribution of composites and tempering (annealing) to the cost of heat treatment.

Composite and Annealing	Cost (US$ per tonne or US$ 1.3 GJ/tonne at 600 °C)
Mn	18
Cr	42
Mo	52
Annealing (tempering)	4.88

Table options

Therefore, the production costs can be formulated as follows:

equation(10)

View the MathML source

By taking into account such economic consideration, the problem of designing an alloy steel with the predefined target UTS and ROA properties becomes a three-objective optimisation problem described as follows:

equation(11)

View the MathML source

Fig. 13 displays the obtained Pareto front for an alloy steel design with the predefined View the MathML source and ROATarget=70%. Again, 10 independent runs have been executed and, on average, 60,000 evaluation times are adequate for this problem. The average execution time is 11 s.

Full-size image (57 K)

Fig. 13.

The obtained Pareto solutions when the View the MathML source and ROATarget=70%: (a) Objective View the MathML source; (b) UTS vs. ROA vs. production cost; and (c) all solutions found during the search process.

Figure options

Table 6 provides details of one set of Pareto solutions from 10 runs. As can be seen from Fig. 13 and Table 6, the most costly solution appears when both mechanical properties are close to the target values. In such a scenario, in order to produce metals with high toughness more Cr needs to be added. Furthermore, the metal needs to be tempered at a relatively high temperature in order to achieve high ductility. Both aforesaid factors increase the production costs.

Table 6.

The details of the Pareto solutions for optimal design of mechanical properties and the cost.

Pareto solutions	C (%)	Mn (%)	Cr (%)	Mo (%)	Tempering Temperature (°C)	UTS (N/mm2)	ROA (%)	Cost ($)
1	0.1200	1.0331	1.5902	0.2185	710.90	881.29	67.31	102.52
2	0.1200	1.0301	1.4750	0.2125	715.64	878.83	67.69	97.36
3	0.1200	1.0332	1.2837	0.2158	726.12	867.58	68.34	89.64
4	0.1200	0.8772	1.2893	0.1925	720.19	850.71	68.89	85.80
5	0.1200	1.1985	0.9454	0.1937	720.35	865.71	67.16	77.21

6	0.1200	0.9496	0.9586	0.1465	660.23	884.99	63.87	70.34	
7	0.1200	1.2041	0.6754	0.1950	725.36	823.26	67.50	66.08	
8	0.1200	1.2104	0.6432	0.1603	661.30	870.82	62.48	62.52	
9	0.1200	0.8844	0.6754	0.1950	726.72	787.57	69.32	60.34	
10	0.1200	0.8907	0.6432	0.1603	662.66	830.29	64.84	56.77	
11	0.1202	0.8521	0.6116	0.1252	596.88	899.42	57.73	52.39	
12	0.1200	0.9147	0.5486	0.1375	692.54	786.32	67.25	52.29	
13	0.1200	0.4399	0.6233	0.1495	646.01	795.69	66.03	47.13	
14	0.1200	1.2108	0.2409	0.1607	661.88	786.03	63.16	45.65	
15	0.1200	0.3967	0.6037	0.1501	581.70	868.79	57.36	45.03	
16	0.1200	0.3826	0.6227	0.1374	552.25	916.95	53.21	44.67	
17	0.1200	1.2634	0.0799	0.1934	714.87	731.17	66.91	41.97	
18	0.1200	0.8474	0.0957	0.1676	593.56	805.47	58.73	32.82	
19	0.1200	0.4403	0.2195	0.1493	645.52	735.38	66.66	30.16	
20	0.1200	0.3913	0.2377	0.1441	555.55	828.52	55.47	29.04	
21	0.1200	0.5659	0.0557	0.0151	447.90	927.97	50.40	16.95	
22	0.1200	0.3586	0.0887	0.0117	566.14	736.34	57.94	15.39	
23	0.1200	0.3598	0.0597	0.0119	709.50	674.85	71.64	15.37	
24	0.1200	0.3518	0.0559	0.0141	285.54	1154.92		57.28	11.73

Table options

By investigating Table 6, one can also identify the most influential variables are Cr and tempering temperature. A variation in these two variables delivers a compromise between end product mechanical properties and normally change significantly the production cost. Hence, using PAIA2, a set of trade-offs could be obtained which provides metallurgists valuable information with regards to how to design steels in a more cost-effective way. Also, that by comparing Table 6 with Table 3, due to the addition of J3, it can be concluded that more diverse solutions can be found, from which more insights into the impact of different factors on the final product can be extrapolated.

4. Conclusions

Every scientific endeavour tries to find answers to the problems at hand and in doing so, raises several others. The work presented in this paper is not an exception. Since it proposed to answer the following 3 questions:

(1)

How to use bio-inspired paradigms to account for the problems involving multiple conflicting goals?

(2)

How to automate the process of acquiring transparent knowledge from high dimensional data without too much damage to the predictive performance of the extracted knowledge base?

(3)

How to automate the design of heat treated alloy steels in a holistic framework and achieve 'right-first-time' production?

To answer the first question, a new modified Population Adaptive based Immune Algorithm (PAIA2) and a multi-stage optimisation procedure for solving MOP were proposed. These two together form the basic framework of the whole work and provide answers to the rest two questions. A multi-stage immune based multi-objective fuzzy modelling (IMOFM) method was proposed in response to the second question and demonstrated abilities of not only being able to elicit accurate models but also revealing hidden knowledge which might not be noticed by the metallurgists. Also, due to structure simplification, the generalisation ability of the elicited model is greatly improved. With the accurate prediction and the heuristic search algorithm, 'right-first-time' production of steels is achievable.

As discussed in Section 3.3.1, some regions close to the identified boundaries are very sensitive to the small variation in optimised decision variables as it may cause big variation in the objective space, i.e. the UTS and ROA. This effectively means that a design falls into these areas may not be robust and reliable in practice. Hence, more research effort should be carried out for a MOP algorithm to produce reliable solutions through the study of the relationship between the decision variable space and the objective space. Also, as mentioned by Beyer and Sendhoff (2007), as the goal (objective) function always represent models and/or approximations of the real world, the question arises whether it is desirable to locate isolated, singular design point with a high precision. More research into robust optimisation should be carried out in future.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version.

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