15th Triennial World Congress, Barcelona, Spain

OPTIMISATION OF STEEL PRODUCTION INCORPORATING ECONOMIC FACTORS

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Abstract: Over the last four years efforts have been devoted towards the development and validation of mechanical test result models relating to a range of alloy steels. Several neural-network based models have been developed, two of which are related to the mechanical test results of Ultimate Tensile Strength (UTS), Reduction of Area (ROA), Elongation, etc. The ultimate aim of developing these models is to pave the way to process optimisation through better predictions of mechanical properties. In this research we propose to exploit such neural network models in order to determine the optimal alloy composition and heat treatment temperatures required, given certain predefined mechanical properties such as the UTS by including certain economic factors relating to the price of composites and the energy necessary for tempering. Genetic Algorithms, with their power of searching a relatively large space without requiring the gradient of a function, are used for this purpose. The results obtained are very encouraging in that steels with adequate properties and optimised costs are obtained. Copyright © 2002 IFAC

Keywords: Steel, mechanical properties, optimisation, genetic algorithms, economics.

1. INTRODUCTION

Heat treatments are commonly used to develop the required mechanical properties in a range of alloy steels. The heat treatment process consists of a hardening stage and a tempering stage. During the hardening stage, the steel is soaked at a temperature of typically 850 ^{0} to achieve full transformation to austenite, followed by quenching in an oil or water medium. Tempering is performed to improve ductility and toughness, by heating the steel to typical temperatures in the ranges 500-670 ^{0} and then air-cooling. The mechanical properties of the material are dependent on many factors, including the tempering temperature, quenchant, composition of the steel, geometry of the bar, etc. Metallurgical research has led to the understanding of the mechanical properties generated by the heat treatment process. However, this physical knowledge does not allow one to readily compute the mechanical properties that would be obtained through the heat treatment of a range of alloy steels. A heat treatment metallurgist usually balances the process parameters through the application of metallurgical knowledge, but would also use process experience, to obtain the required mechanical properties. Over the last few years, empirical models using neural networks have been built to predict mechanical test results for steels covered by a wide range of training data. Such models have been shown to improve product reliability and process efficiency (Tenner, 1999). The ultimate aim of developing such mechanical test result models is to facilitate process optimisation. In this research work, we investigate the exploitation of such models for optimal alloy design using target values for the Ultimate Tensile Strength (UTS). The Genetic Algorithm (GA) approach is applied to a set of input variables which will produce pre-specified mechanical test result values. Moreover, such algorithm is shown to be able to incorporate economic and qualitative factors such the price of composites as well as energy costs. This paper is organised as follows: Section 2 will give a brief introduction to Genetic Algorithms (GA), while Section 3 will show how a hybrid structure combining this evolutionary search method and the neural-network based predictive models was achieved. Section 4 will present and analyse the results obtained with such a structure. Finally, Section 5 will draw conclusions in relation to this overall study.

2. INTRODUCTION TO GENETIC ALGORITHMS (GA)

Genetic Algorithms (GA) are exploratory search and optimisation methods that were devised on the principles of natural evolution and population genetics. Holland (1973, 1975) first developed the technique of GA, and several other research studies provided a comprehensive review and introduction of the concept (Goldberg, 1989). Unlike other optimisation techniques, GA does not require gradients, but instead relies on a function, better known as a "fitness function", in order to assess the fitness of a particular solution to the problem in question. Possible solution candidates are represented by a population of individuals (generation) and each individual is encoded as a binary string containing a well-defined number of chromosomes (1's and 0's).

Initially, a population of individuals is generated and the fittest individuals are chosen by ranking them according to an a priori-defined fitness-function, which is evaluated for each member of this population. In order to create another better population from the initial one, a mating process is carried out among the fittest individuals in the previous generation, since the relative fitness of each individual is used as a criterion for choice. Hence, the selected individuals are randomly combined in pairs to produce an offspring by crossing over parts of their chromosomes at a randomly chosen position of the string. The new offspring is supposed to represent a better solution to the problem. In order to provide extra excitation to the process of generation, randomly chosen bits in the strings are inverted (0's to 1's and 1's to 0's). This mechanism is known as mutation and helps to speed up convergence and prevents the population from being predominated by the same individuals. All in all, it ensures that the solution set is never empty. A compromise, however, should be reached between too much excitation and none by choosing a small probability of mutation.

Hence, for a given population of trials and set of operators together with procedures for evaluating each trial, a GA proceeds as follows:

An initial random population of trials, $\Pi(0) = A_m(0),\ m = 1, ..., M$, where M is the number of trials in the population, is generated.

For successive sample instances:

a) The performance of each trial, $\mu(A_m(T))$, $T = 0, 1, ...,$ is evaluated and stored.

b) One or more trials are selected by taking a sample of $\Pi(T)$ using the probability distribution:

$$\rho(A_m(T)) = \frac{\mu(A_m(T))}{\sum_{i=1}^{M} \mu(A_i(T))} \tag{1}$$

c) One or more genetic operators are applied to the selected trials to produce new offspring, $A_m^{\ o}(T),\ m = 1, ..., N$, where N is the number of offspring which is usually equal to the number of selected trials (parents).

d) The next generation of population, $\Pi(T+1)$, is formed by selecting $A_j(T) \in \Pi(T),\ j = 1, \ldots, N$ to be replaced by the offspring, $A_j^{\ o}(T)$; the criterion for selecting which trials should be replaced may be random, on the basis of the least fit or some other fitness basis.

e) The GA process is terminated after a pre-specified number of generations or on the basis of a criterion which determines convergence of the population.

It was pointed out that the successful running of a GA involves having to set a number of control parameters, which include population size, the nature and rates of the recombination operators; crossover, mutation and reproduction. Reproduction is defined as the process through which ‘parent structures’ are selected to form new offspring, by applying the above genetic operators, which can then replace members of the old generation. The method of selecting an individual to produce offsprings (or to be deleted from the population) determines its lifespan and the number of its offsprings. For example, if ρ_1 is the probability that an individual $A \in \Pi$ is selected to produce offspring during a sample step and ρ_2 is the probability that it will be deleted during that sample step, then the expected number of offspring of A is $\frac{\rho_1}{\rho_2}$ (Holland, 1975). The most common reproduction techniques are Generational Replacement (GR), Steady-State (SS), Generational Gap (GG), and Selective Breeding (SB). Only one of these will be the subject of this study, i.e. SB, which is described below.

2.1 Selective-Breeding reproduction technique

The Selective Breeding reproduction technique is designed to overcome some of the deficiencies in the other methods. In the steady-state breeding method, a sampling error still occurs in the selection of the parents and deletion of individuals from the population, and often good individuals can appear and be deleted without a chance of recombination. Selective breeding introduces determinism in order to eliminate stochastic sampling error in deletion of candidates. The method operates as follows:

1. An initial population, $\Pi(0)$ is created in the usual manner.
2. The population is evaluated to determine the performance of each individual, $\mu(A_m, m = 1, \ldots, M)$.
3. For successive generations, thereafter:

a) An entire population of offspring, $\Pi^o(T)$, is produced by selecting parents and applying genetic operators.
b) The offspring population is then evaluated.
c) The next generation of population is obtained by choosing the best M individuals from both $\Pi(T)$ and $\Pi^o(T)$.

2.2 Evaluation of trials

Each individual (genotype) in a population is a hypothetical candidate solution to the optimisation problem under consideration. The procedure of evaluating these candidate solutions consists of submitting each to a simulation model, and returning an assessment value according to a given fitness function. A controlled process is defined by a set of state variables $X = \{x_1, x_2, \ldots, x_n\}$ which are controlled by a set of control variables $C = \{c_1, c_2, \ldots, c_m\}$. The genotypes are trial 'control policies' for selecting C as a function of X. The role of the adaptive plan is to derive an optimal policy A_{opt} which minimises a given performance function. Such a performance function is very much dependent upon the optimisation process itself and can be expressed in terms of:

- Function minimisation;
- Goal achievement;
- Interval specification.

In the case of this research a combination of goal achievement and parameter minimisation was chosen as will be seen in the next sections.

3. COMBINING GA'S WITH NEURAL NETWORKS

The various routines relating to the Genetic Algorithm, previously written in 'C' programming language, had to be linked to the neural models developed using MATLAB . Initially, the GA is used to find a set of input values to the neural model to give certain target UTS values. The neural models hence developed include a relatively large number of inputs (22 in total for the UTS model) and there are many factors which can influence the UTS of steel. Although the GA can determine optimal values for all those inputs to reach a target UTS value, the present study is limited to five variables only which are:

- Carbon
- Manganese
- Chromium
- Molybdenum
- Tempering temperature

The remaining inputs would not affect the UTS values for the steel. To ensure that that these values do not prevent the GA from converging to an optimal solution, they were set to that of the median 1%CrMo values (Tenner, 1999).

Coding of the genetic algorithm is based on defining the number of individuals in the population and the chromosome length of each one using the so-called 'concatenated binary mapping'. This coding is usually realised by joining segment codes of all the parameters into one composite string.

In this study, the GA was set with the following parameters:

Population size = 60
Chromosome length (in bits) = 60
Probability of Crossover = 0.95
Number of Crossover Points = 5
Probability of Mutation = 0.09
Fitness Scaling: Function Normalisation

Each individual (candidate solution) was then organised into 60 bits, with each block of 16 bits representing the following parameters to be optimised: carbon (C), manganese (Mn), chromium (Cr), molybdenum (Mo), and tempering temperature. Figure 1 summarises the organisation of the chromosome.

4. STANDARD AND PARTIALLY CONSTRAINED OPTIMISATION

4.1 Using GA to Find a Target UTS Value

The first experiment using GA consisted of setting a target UTS value (868 N/mm^2). The following fitness function was used to guide the GA to an optimal solution:

$$J_{UTS} = (UTS - UTS_{trgt})^2 \qquad (2)$$

The final UTS value obtained after 50 generations was 867.99 N/mm^2 with a Chromium composition of 2.60%! knowing that chromium is a relatively expensive element compared to carbon, metallurgists would certainly not favour this composition.

4.2 Using GA to find a target UTS value with model standard deviation

In the previous experiment the GA had provided a (non-unique) solution which is different to that of the median analysis. Particularly, it would not make financial sense to use less carbon and more chromium if the only mechanical test requirement was a predefined UTS target value. Hence, a more reliable solution can be obtained if the standard deviation (SD) between all predictors was included in the fitness function as a penalty parameter, i.e.

$$J_{UTS,\,SD} = \lambda_1 \left(\frac{UTS_{Target} - UTS}{UTS_{Target}}\right)^2 + \lambda_2 \left(\frac{SD}{1000}\right)^2 \qquad (3)$$

The standard deviation value is that related to the ensemble member's predictions for a given set of input variables, and the constants λ_1 and λ_2 will allow one to obtain all the *pareto* solutions to the problem by expressing priorities. It is worth noting that the standard deviation term is very important as its presence means that the UTS target value will not be met unless it lies in a dense area of the data (low SD values).

The GA was allowed to run for 2000 generations with $\lambda_1 = 90$ and $\lambda_2 = 70$. Figure 2 shows the evolution of the alloy steel composition throughout this number of generations. In turn, Table 2 displays the GA adjusted values against the 1%CrMO values, which appear to be much closer now.

Table 1 GA-based optimal composition *versus* 1%CrMo analysis for run of Figure 4.

Variable to be Optimised	**1%CrMo Value**	**GA-Adjusted Value**
C(%)	0.41	0.3302
Mn(%)	0.78	0.7878
Cr(%)	1.08	1.0552
Mo(%)	0.22	0.2167
Tempering Temperature (^oC)	630	580

5. CONSTRAINED OPTIMISATION INCLUDING ECONOMIC FACTORS

The factors contributing to the cost of heat treatment operation are shown in Tables 2a, 2b[1] and are related mainly to the price of composites and the energy costs incurred through tempering. In this study, only these factors have been considered although other composites and temperatures can also be included:

Table 2a Contribution of composites to the cost of heat treatment

Composite	**Cost ($ per tonne)**
Manganese (Mn)	18
Chromium (Cr)	42
Molybdenum (Mo)	52

Table 2b Contribution of annealing (tempering) to the cost of heat treatment

Item	**Cost ($: 1.3GJ/tonne at 600 ^{o} C)**
Annealing (tempering)	4.88

Taking into account the above data we conducted three more experiments with the GA by modifying the fitness function as follows:

$$J_{UTS,SD,ECONOMY} = \lambda_1 \left(\frac{UTS_{Target} - UTS}{UTS_{Target}}\right)^2 + \lambda_2 \left(\frac{SD}{1000}\right)^2 + \lambda_3 \left[\frac{Mn\_Cost + Cr\_Cost + Mo\_Cost}{10000}\right]^2 \qquad (4)$$

Depending on the relative values given to λ_1, λ_2, and λ_3, priority will be given to achieving the desired mechanical property with a minimum standard deviation or having the total costs (for composites and/or energy) down.

[1] Professor M C Sellars: Private Communication

Hence, in the first experiment the GA relied on a fitness function where $\lambda_2 > \lambda_3 > \lambda_1$ which translates into: "we would not mind if the UTS is slightly away from the target, but we would like the GA to look into a dense region of the model with the cost of composites being taken into account". At the end of this experiment the GA converged to the following values:

$$UTS = 878 N/mm^2; \quad SD = 2.62; \quad Costs = \$\,73.54.$$

It is worth noting that such a cost is lower than the one obtained using the experiment of Section 4.2 which was \$ 74.54, a saving of \$ 1 per tonne!

The second experiment consisted of the following combination of the weights: $\lambda_3 > \lambda_2 > \lambda_1$, which translates to the same linguistics as above with not so much emphasis on the standard deviation but on the costs. The result of the experiment led to the following values:

$$UTS = 867 N/mm^2; \quad SD = 4.50; \quad Costs = \$\,72.41.$$

A final experiment was conducted in which a penalty on the energy costs was also included as follows:

$$J_{UTS,SD,ECONOMY} = \lambda_1\left(\frac{UTS - UTS_{Target}}{UTS_{Target}}\right)^2 + \lambda_2\left(\frac{SD}{1000}\right)^2 + \lambda_3\left[\frac{Mang\_Cost + Cr\_Cost + Mo\_Cost}{10000}\right]^2 + \lambda_4\left(\frac{Annealing\_Cost}{1000}\right)^2 \tag{5}$$

In this experiment the following combination of the weights was adopted: $\lambda_3 > \lambda_4 > \lambda_2 > \lambda_1$, which ensures that a reliable model is elicited (through a low SD) but with a composition and a tempering temperature which will drive the total costs down. Hence, the result of the experiment, also shown in Figure 3, led to the following values:

$$UTS = 869 N/mm^2; \quad SD = 3.99; \quad Costs = \$\,71.17.$$

Table 3 summarises the various compositions and costs obtained under various optimisation strategies (costs include energy costs); it is worth noting that the number allocated to each case can be identified as follows:

- Case 1: the standard 1%CrMo composition.
- Case 2: as per Section 4.2.
- Case 3: as per Section 5 with priority given to SD.
- Case 4: as per Section 5 with priority given to composite costs, energy costs not included.
- Case 5: as per Section 5 with energy costs included.

Table 3 Summary of compositions and costs after GA-based optimisation.

Case	Mn	Cr	Mo	Temp.	SD	Costs (\$)
1	0.78	1.08	0.22	630	N/A	76.02
2	0.79	1.06	0.22	580	3.68	74.54
3	0.79	1.05	0.20	579	2.62	73.54
4	0.71	1.08	0.18	585	4.50	72.41
5	0.76	1.04	0.18	573	3.99	71.17

6. CONCLUSIONS

In this research work we have proposed a novel method to find optimal model inputs given certain constraints using genetic algorithms. The ability of GA to adjust a number of variables (a total of 5) to meet a target UTS value was initially demonstrated. It was also shown that if the model standard deviation was included in the fitness function as a penalty term, the GA can provide a reliable and generally more practical solution, in terms of lower tempering temperatures (energy savings) and practical composition levels (reasonable percentage composition of chromium for instance). Further experiments, which include the Reduction of Area (ROA) mechanical test and the corresponding SD, were also conducted which pointed to the same conclusion. The work was later extended to include economic factors, such the costs associated with the composites and annealing (tempering), and showed that through a careful choice of weights (penalties), priorities can be set *vis-à-vis* the optimisation of the mechanical properties, model accuracy, and also the overall costs incurred. Future experiments will consider the use of other mechanical properties such as the ROA and Elongation together with the inclusion of all composite costs and temperatures in a multi-objective context.

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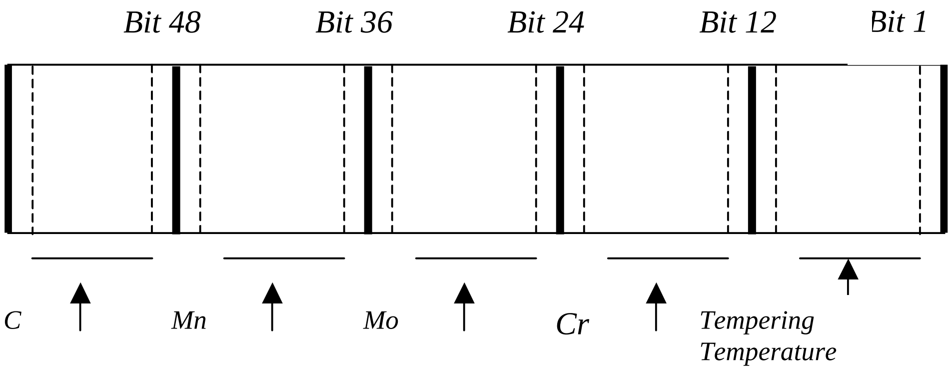

Fig. 1 A typical GA-coding of steel composition and temperature.

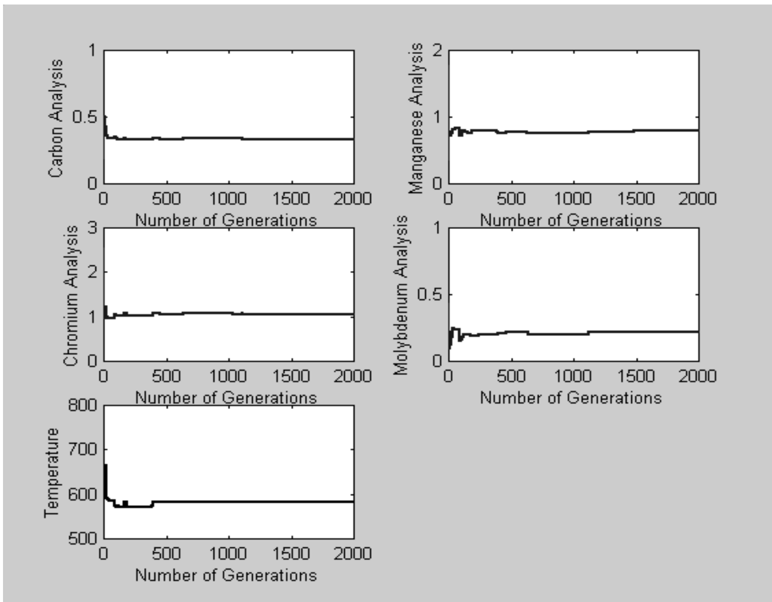

Fig. 2 Evolution of the 5 inputs throughout successive generations for constrained optimisation; no economic factors included.

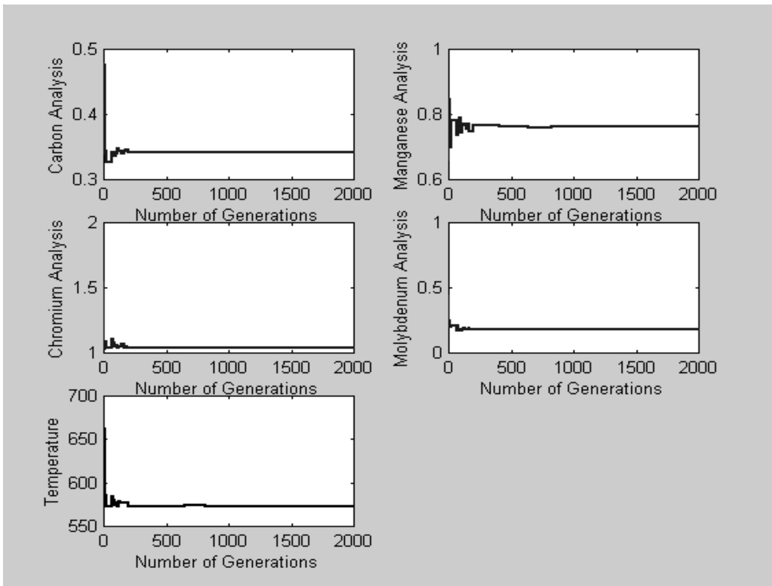

Fig. 3 Evolution of the 5 inputs throughout successive generations when composite and energy costs are taken into account.