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Inverse modelling for optimal metal design using fuzzy specified multi-objective fitness functions

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Abstract

This paper presents the results which relate to the development and application of evolutionary multi-objective optimisation algorithms for the design of alloy steels using crisp as well as fuzzy logic based objective functions. The applied optimisation algorithms aim at determining the optimal heat treatment regime(s) and the required weight percentages for the chemical composites to obtain the pre-defined mechanical properties of steels, such as the ultimate tensile strength (UTS) or better known as tensile strength (TS) and elongation (ELO). During this process, the targeted mechanical properties and the reliability of their predictions are considered simultaneously in the above objective functions. Results show that for the multi-objective case the use of fuzzy logic based functions, as opposed to crisp ones, is beneficial especially when the application can tolerate a relatively low degree of discrimination between the so-called multi-objective '*pareto*' solutions.

Keywords: Metals; Mechanical Properties; Optimisation; Evolutionary computing; Multi-objective; Neural-networks

1. Introduction

In the steel industry, heat treatments are commonly used to develop the required mechanical properties in a range of alloy steels. The heat treatment process consists of hardening and tempering stages. During the hardening stage, the steel is soaked at a temperature of typically 850 °C to obtain a fully austenitic microstructure. This is followed by quenching in an oil or water medium to achieve the transformation to martensite. Tempering is performed to improve ductility and toughness by heating the steel to typical temperatures in the ranges 500–670 °C and then air-cooling. The mechanical properties of the material are dependent on many factors, including the tempering temperature, quenchant, chemical composition of the steel, geometry of the bar, etc.

Determining the optimal heat treatment regime and the required weight percentages for the chemical composites to obtain the pre-defined mechanical properties of steel is a vital challenge for the steel industry. Because the available physical knowledge of the heat treatment process is not enough to allow one to compute the mechanical properties, these will be obtained through elicited data-driven models. To this end, and over the last few years, empirical models using neural networks (NNs) have been developed and validated based on industrial data relating to a range of alloy steels (Tenner, 1999; Mahfouf, Jamei, & Linkens, 2004). These predictive models are utilised for the prediction of the mechanical properties of steel, namely the tensile strength (TS) and the elongation (ELO), although the study can also be extended to other mechanical properties such as the reduction of area (ROA) and the Charpy toughness.

In this current research work, the above models are used to facilitate the optimisation process for single and multi-objective approaches. In addition, two sets of crisp and fuzzy objective functions are defined to compare the performance of the optimisation algorithms. With this in mind, evolutionary multi-objective (EMO) algorithms are

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applied to a set of decision variables, which include the chemical composition of the steel as well as the tempering temperature profile to obtain the pre-specified mechanical properties. As will be seen later, the study was confined to four (4) chemical compositions, namely carbon (C), manganese (Mn), cromium (Cr), molybdenum (Mo), and the tempering temperature, although such a set can be extended easily to include more decision variables. Fig. 1 shows that the optimisation mechanism consists of two important components: a reliable prediction model and an efficient optimisation paradigm, which is in fact equivalent to an inverse modelling problem or a 'reverse engineering' problem.

One way of realising such optimisation operation is to 'simply' invert the original forward model (see Fig. 1) and obtain the one single solution. However, such a solution is not always unique, especially when more than one objective are taken into consideration. Moreover, the CORUS metallurgists, who were consulted in relation to this study, expressed the view that not only would they be interested in those solutions which were more familiar to them, but also in the other solutions which they had never encountered before, i.e. new chemical compositions and new tempering temperature which would apparently lead to similar mechanical properties. While the metal industry so far used 'know-how' to arrive at what is considered to be 'acceptable outcomes, several other authors tackled this problem within the context of mathematical formulations (Yegerov & Dulikravich, 2004). In this work, the authors used a large experimental database to search for the solution(s) in response a set of optimisation criteria. Hence, the number and the quality of the solutions will very much depend on the size of the database itself. In this present study, it is proposed to solve this optimisation problem using evolutionary computing (EC) techniques which have the distinct advantage of searching relatively large solution spaces. These spaces would be searched within the domain of single-objective as well as multi-objective optimisations. Recently, many evolutionary-based algorithms were proposed to tackle multi-objective problems (MOPs), nevertheless some of these proved more effective than others for a range of applications (Zitzler & Thiele, 1999). In this research work, the strength pareto evolutionary algorithm 2 (SPEA2) proposed by Zitzler, LaumaNN, and Thiele (2002) is implemented and the obtained results are presented and discussed.

This paper is organised as follows: Section 2 will introduce briefly the models which were elicited to describe the mapping between the alloy compositions, tempering and quenching temperatures and the corresponding mechanical properties. Section 3 will present and discuss the obtained results from applying a single-objective optimisation algorithm using genetic algorithms (GA) (Goldberg, 1989). Section 4 will give a brief introduction to EMO and will present and analyse the results obtained following the application of such techniques. In this section, the results which relate to the use of fuzzy objective functions will also be presented and discussed. Finally, Section 5 will draw conclusions in relation to this overall study.

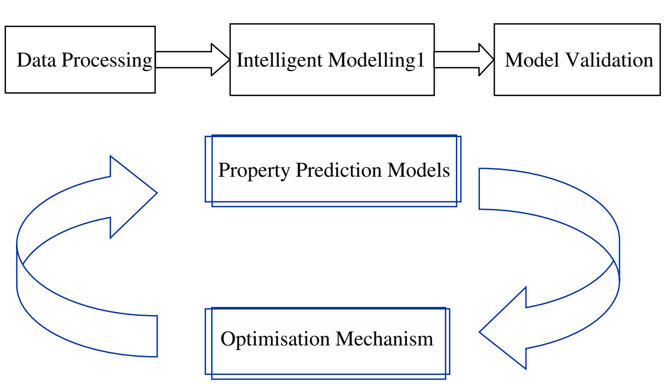

Fig. 1. Modelling and optimisation of material properties.

2. Intelligent modelling of mechanical properties of alloy steels

Since the available physical knowledge of the heat treatment process is not enough to allow one to compute the mechanical properties, these will be obtained through the elicited data-driven models. Over the last few years, empirical models using NNs have been built to predict mechanical test results for steels covered by a wide range of training data (Tenner, 1999), Jones and MacKay (1996), Badmos, Bhadeshia, and Mackay (1998) and Dulikravich, Egorov, Sikka, and Muralidharan (2003). These models are used to facilitate the finding of the optimal heat treatment regime and the weight percentages for the chemical composites to obtain the desired TS, ROA, and ELO.

The multi-layer perceptron (MLP) NN (Bishop, 1995) is used for developing all the prediction models, due to its flexibility and universal approximating capability (Hornik, Stinchcombe, & White, 1989; Kurkova, 1992). The training of a MLP network typically involves three stages: initialisation, forward processing, and backward processing. The initialisation sets up the NN architecture and the number of hidden layers, the activation functions, the training algorithms, and the weighting matrices initialisation. The forward processing calculates the network outputs according to the inputs. The backward processing takes care of the network weights based on the error performance with a selected training algorithm, which is the backbone of NN modelling.

The NN models used for this research consist of an Ensemble of 10 NN based models which used 5707 data sets for ELO, 5559 data sets for ROA, and 5711 data sets for TS. An ensemble model development involves two stages: generation of individual candidate NNs and combining the NNs into an ensemble model. In the first stage, one should to determine what variations are to be introduced to generate the individual NNs, such as the initial weights, the training algorithms, the training data etc. It is worth noting that some discretion needs to be