MULTI-OBJECTIVE PARTICLE SWARM OPTIMISATION FOR ALLOY TOUGHNESS DESIGN USING A FUZZY PREDICTIVE MODEL

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Abstract: Alloy design is a challenging multi-objective optimisation problem, which consists of finding the optimal processing parameters and the corresponding chemical compositions to achieve certain pre-defined mechanical properties of steels. In this paper, we combine fuzzy modelling and Particle Swarm Optimisation (PSO) to address the multi-objective optimal alloy design problem. An adaptive weighted PSO algorithm is introduced to improve the performance of the standard PSO. Based on the established impact toughness fuzzy prediction models, the proposed optimisation algorithm has been successfully applied to the optimal design of heat-treated alloy steels. The experimental results have shown that the algorithm can locate the constrained optimal solutions quickly and provide a useful and effective guide for alloy steels design.

Keywords: Alloy Design, Multi-objective optimisation, Particle Swarm, Fuzzy modelling, Economic Factors

1. INTRODUCTION

Multi-objective Optimisation (MO) problems are commonly encountered in science and engineering areas, due to the multi-criteria nature of many application problems. In complex engineering design, such as development of alloy steels, two or more, sometimes competing and/or incommensurable objective functions have to be considered simultaneously. In the development of alloy materials, the conjoint design and control of chemical composition and details of thermomechanical processing schedules to develop optimum mechanical properties always lead to a complex exercise. The required mechanical properties of modern alloy steels are achieved by obtaining an optimum microstructure through a careful combination of alloy compositions, rolling schedules and heat treatment. In the steel industry, heat treatments (containing hardening and tempering stages) are commonly used to develop the required mechanical properties in a range of alloy steels. The mechanical properties of the material are dependent on many factors, including the tempering temperature, the quench temperature, the types of quench medium, the content of chemical compositions of the steel, the 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 challenge for the steel industry. To address this problem, a metal design paradigm which combines mechanical property prediction and an optimisation mechanism has been established as shown in Fig. 1. As the available physical knowledge of the heat treatment process is not enough to allow one to compute the mechanical properties, it is crucially important to establish reliable property prediction models. These will be obtained through elicited data-driven models, such as Neural Network models (Tenner, Linkens, et.al. 2001) and neural-fuzzy models (Chen & Linkens, 2001). These predictive models are then used to predict the mechanical properties of steel such as the Tensile Strength (TS), the Reduction of Area (ROA), Elongation and Impact Toughness. The predicted properties can be used as the objectives of the optimal metal design. In this study, the emphasis is on impact toughness property oriented alloy design. Fuzzy models for impact toughness prediction are used to facilitate the optimisation process for multi-objective approaches. For optimisation, the new paradigm of Particle Swarm has been used as an optimisation mechanism for alloy design.

The remaining parts of the paper are structured as follows: Section 2 presents the data-driven fuzzy modelling approach for Charpy impact toughness prediction. Section 3 describes the adaptive weighted non-dominated sorting PSO algorithm and its application to multi-objective optimal alloy design. Finally, results discussions and conclusion will be given in Section 4.

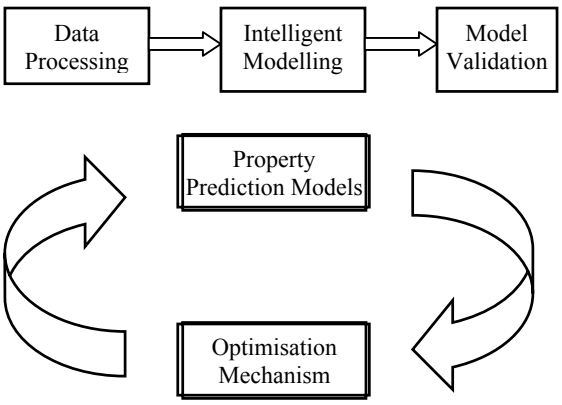

Fig. 1. Metal Design Optimisation

2. FUZZY MODELLING FOR MECHANICAL PROPERTY PREDICTION

Fuzzy modelling is one of the most active research fields in intelligent computation, which combines the facility of explicit knowledge representation in the form of if-then rules (the mechanism of reasoning in human understandable terms) and the ability of approximating complicated non-linear functions. A fuzzy model is a system description with fuzzy quantities, which are expressed in terms of fuzzy numbers or fuzzy sets associated with linguistic labels. Consider a collection of N data points $\{P_1, P_2,..., P_N\}$ in a m+1 dimensional space that combines both input and output dimensions. A generic fuzzy model is presented as a collection of fuzzy rules in the following form

R_i: **If** x_1 is A_{i2} **and** x_2 is A_{i2} ... **and** x_m is A_{im}
then $y = z_i(\boldsymbol{x})$ (1)

where $\boldsymbol{x} = (x_1 , x_2 , ... , x_m)) \in U$ and $y \in V$ are linguistic variables, A_{ij} are fuzzy sets of the universes of discourse $U_i \in R$, and $z_i(\boldsymbol{x})$ is a function of input variables. Typically, z takes the following three forms: a singleton, a fuzzy set or a linear function. Fuzzy logic systems with the centre average defuzzifier, the product-inference rule and the singleton fuzzifier are of the following form:

$$y = \sum_{i=1}^{n} z_i [\prod_{j=1}^{m} \mu_{ij}(x_j)] \Big/ \sum_{i=1}^{n} \prod_{j=1}^{m} \mu_{ij}(x_j) \quad (2)$$

where $\mu_{ij}(x)$ denotes the membership function of x_j belonging to the ith rule.

According to the fuzzy modelling paradigm proposed by Chen and Linkens (2001), the data-driven fuzzy modelling consists of the following tasks: 1) generating an initial fuzzy rule-base from data, including initialising the membership function parameters; 2) determining the number of fuzzy rules; and 3) optimising the parameters both in the antecedent and consequent parts of the rules. All membership function parameters in the antecedent part and the linear weights in the consequent part of the fuzzy rules are optimised via a gradient-descent learning algorithm. The acquired fuzzy model should be validated under certain performance indices, such as accuracy, generality, complexity, interpretation, etc. Once the model performance achieves the pre-defined criteria, the final model is produced.

In materials engineering, it is important to establish an appropriate composition-processing-property model for materials development. As one of the most important characteristics of alloy steels, toughness is assessed by the Charpy V-notch impact test. The absorbed impact energy and the transition temperature defined at a given Charpy energy level are regarded as the common criteria for toughness assessment. However, not much work has been done to date on establishing generic composition-processing-impact toughness models. In this study, the aforementioned fuzzy modelling approach has been used to establish generic toughness prediction models which link materials compositions and processing conditions with Charpy impact properties. To build a Charpy toughness prediction model, 3804

heat treatment process data were collected and used for modelling. The data set contains chemical compositions, processing parameters and Charpy energy *Cv*(J) tested at different temperatures (between -60 and 23 ^{o}C). 50% of the data were used for model training and the remaining 50% of the data were used as testing data. The model inputs include chemical compositions (C, Si, Mn, S, Cr, Mo, Ni, Al, V), the geometry of the bar (width and thickness) and processing variables (Quench.T, Temp.T and Charpy test Temperature). The model output is the predicted Charpy impact energy *Cv*. Based on the obtained 3804 heat treatment process data, the fuzzy model with 6 rules was developed to predict Charpy impact energy using the fuzzy modelling procedure described in the previous section. The predicted result with a Root-Mean-Square-Error of RMSE=18 is shown in Fig. 2. This prediction model is then used for toughness assessment in optimal alloy design.

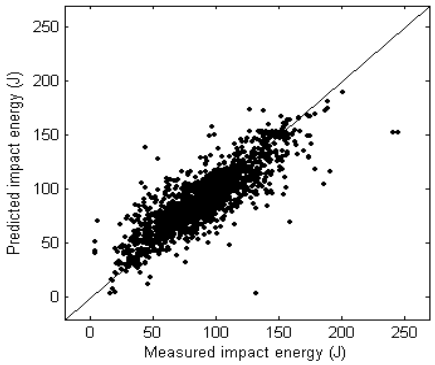

Fig.2 Charpy impact energy prediction using fuzzy model

3. MULTI-OBJECTIVE OPTIMAL ALLOY DESIGN USING PARTICLE SWARM OPTIMISATION

As mentioned in the previous section, alloy design is a challenging multi-objective optimisation problem, which consists of finding the optimal chemical compositions and processing parameters for pre-defined property requirement. The PSO is a relatively new technique for finding the optimal regions of complex search spaces via the interaction of individuals in a population of particles. It was originally introduced by J. Kennedy and C. Eberhart in 1995. Unlike evolutionary algorithms, which are based on the principle of survival of the fittest, the PSO is motivated by the simulation of social behaviour of flocks. As Kennedy stated (Kennedy J. 1997), the algorithm is based on a metaphor of social interaction, searches a space by adjusting the trajectories of individual vectors, called "particles" as they are conceptualised as moving points in multidimensional space. The individual particles evaluate their positions relative to a goal at every iteration. They are drawn stochastically towards the positions of their own previous best performance and the best previous performance of their companions. The PSO algorithm has been shown to be a successful optimiser in a wide range of functions. It is easily implemented and usually results in faster convergence rates than the GA (Eberhart R. and Shi Y. 1998). In this paper, an improved PSO algorithm is introduced to address this multi-objective alloy optimal design problem.

3.1 Improved Particle Swarm Optimisation algorithm

The PSO algorithm defines each particle as a potential solution to a problem in a dimensional space, with particle i represented as: $\boldsymbol{x}_i=(x_{i1}, x_{i2}, \ldots, x_{id})$, $i=1, 2, \ldots N$. Where d is the search dimension and N determines the number of particles in the population. The original formula developed by Kennedy and Eberhart was improved by Shi and Eberhart by introducing an inertia weight w into PSO algorithm (Shi Y. and Eberhart R. 1999). During each iteration, the particles' position is modified according to the following equations:

$$\boldsymbol{v}_i(t) = w\, \boldsymbol{v}_i(t\text{-}1)+c_1 r_1(\boldsymbol{p}_i- \boldsymbol{x}_i(t\text{-}1))+ c_2 r_2(\boldsymbol{p}_g- \boldsymbol{x}_i(t\text{-}1)) \quad (3)$$

$$\boldsymbol{x}_i(t) = \boldsymbol{v}_i(t)+ \boldsymbol{x}_i(t\text{-}1) \quad (4)$$

where $\boldsymbol{v}_i$ is the velocity, w is the inertia weight, c_1 and c_2 are positive constants, and r_1 and r_2 are random numbers obtained from a uniform random distribution function in the range [0, 1]. $\boldsymbol{p}_i$ represents the best previous position of the ith particle and $\boldsymbol{p}_g$ denotes the best particle among all the particles in the population. The inertia weight w plays the role of balancing the global and local searchers and its values may vary during the optimisation process. A large inertia weight encourages a global search while a small value pursues a local search. Shi and Eberhart (1999), suggested to change the inertia weight linearly from 1 to 0.4 to restrict the global search ability of the PSO algorithm at the end of a run.

To improve the performance of the PSO for multi-objective optimisation problems, we proposed an Adaptive Weighted PSO (AWPSO) algorithm (Mahfouf and Chen, 2004), in which the velocity in Eq. (3) is changed as follows:

$$\boldsymbol{v}_i(t+1) = w\, \boldsymbol{v}_i(t)+\alpha\, [r_1(\boldsymbol{p}_i- \boldsymbol{x}_i(t))+ r_2(\boldsymbol{p}_g- \boldsymbol{x}_i(t))] \quad (5)$$

The second term in Eq. (5) can be viewed as an acceleration term, which depends on the distances between current position $\boldsymbol{x}_i$ and personal best $\boldsymbol{p}_i$ and global best $\boldsymbol{p}_g$. The acceleration factor α is defined as:

$$\alpha=\alpha_0+ t/N_t \quad t=1, 2, \ldots, N_t \quad (6)$$

where N_t denotes the number of generations, t represents the current generation, $\alpha_0 \in [0.5, 1]$ is a constant. As can be seen, the acceleration term will increase as the iteration increases, which will

enhance the global search ability at the end of run and will help the algorithm to jump out of the local optimum especially in multi-modal problems.

Instead of using a linearly decreasing inertia weight, we use random number as the inertia weight and change the inertia weight at every generation using the following formula:

$$w=w_0+(1-w_0)\,r \;; \tag{7}$$

where $w_0 \in [0, 1]$ is a positive constant, r is a random number uniformly distributed in [0, 1]. In this paper we set $w_0 = 0.4$, which produces a randomly varying weight between 0.4 and 1 with a mean value of 0.7.

To evaluate the performance of individual particles, an appropriate evaluation function should be defined. We simply use the weighted aggregation approach to construct the evaluation function F for multi-objective optimization as follows:

$$F=\sum_{i=1}^{m} w_i f_i \;; \qquad \sum_{i=1}^{m} w_i = 1 \tag{8}$$

where m is the number of objectives, i=1, 2, …, m, f_i denotes the ith objective function. To approximate the Pareto front instead of a certain Pareto solution, the weights w_i for each objective are changed systematically and normalised as follows:

$$w_i = \lambda_i \Big/ \sum_{i=1}^{m} \lambda_i \;; \qquad \lambda_i=U(0,1) \tag{9}$$

The function $U(0,1)$ generates a uniformly distributed random number within [0,1]. In this way, we can get a uniformly distributed random weight combination, which are generated at every generation. The idea is to use dynamic weights instead of fixed weights to achieve the Pareto solutions. This dynamically weighted aggregation approach was introduced for the selection of best $\boldsymbol{p}_g$. To improve the convergence of the multi-objective optimisation, the non-dominated sorting technique, which was proposed and improved by Deb et. al. (Deb K., Agrawal S., et.al. 2000, Deb K. and Goel T. 2001) and then introduced into the PSO algorithm by Li X. (2003) has been also used in the modified PSO algorithm. The effectiveness of the AWPSO algorithm has been demonstrated (Mahfouf and Chen, 2004). Compared to several widely recognised evolutionary algorithms, such as NSGA II and SPEA, the proposed algorithm achieved better convergence and diversity when tested challenging functions, such as ZDT1~ZDT4.

3.2 Optimal design for heat-treated alloy steels

The proposed algorithm has been applied for the optimal design of heat-treated alloy steels. In this section, details relating to the optimisation of Charpy impact toughness using the AWPSO algorithm are presented and discussed. The decision vector consists of the weight percentages for the chemical composites, namely: Carbon (C), Silicon (Si), Manganese (Mn), Chromium (Cr), Molybdenum (Mo), and Tempering temperature (Temp) respectively. As aforementioned, all optimisation experiments are based on the fuzzy property prediction models.

3.2.1 Toughness oriented optimal design

Companies in the steel industry value highly the achievement of the required levels of toughness properties of hot rolled steel products. The optimal alloy toughness design aims at finding the appropriate chemical compositions and tempering temperature with the criterion of a minimum Charpy impact energy of 54J at -20°C, which is equivalent to the ductile-brittle transition temperature at 54J energy level which is below -20°C. In order to achieve the pre-defined toughness requirement, the model prediction error band should be taken into account in the selection of objectives. It is worth noting that the error band, which depends on the model accuracy and training data density, provides an accurate guide to the model prediction error. The objective functions for alloy toughness design are defined as:

$$\text{Minimise: } f_1 = \begin{cases} 100Cv & if\ Cv < 1.5Cv_0 \\ 2Cv_0 / Cv & if\ Cv \geq 1.5Cv_0 \end{cases} \tag{10}$$

$$\text{Minimise: } f_2 = \mathrm{EB_c} \tag{11}$$

Where Cv_0 =54J, which stands for the required Charpy energy level, and $\mathrm{EB_c}$ is the 95% confidence error band for the prediction model. The objective functions f_1 and f_2 represent the requirement for Charpy toughness and the corresponding model prediction error band. Fig. 3 illustrates the optimisation results with Charpy energy values against error band corresponding to the obtained Pareto solutions with the target value Cv_0 =54J. It indicates that the two objectives are in conflict, as any improvement in one objective causes deterioration in the other. Table 1 displays different solutions selected from the Pareto solutions. It can be seen that the algorithm converged to a specific area that minimised the objective functions and provided optional solutions (with different combinations of chemical compositions and tempering temperature), which meet the pre-defined toughness requirement even when taking the error band into account.

3.2.2 Optimal alloy design with economic factors

This experiment aims at finding the optimal chemical compositions and heat-treatment process parameters in order to obtain the required toughness while minimising the production costs. The production costs of heat-treated steels include the costs of addition of alloying elements, such as Cr, Mo, V, etc. and the costs of energy consumption during the heat-treatment process. Based on the expert's knowledge,

a new objective function to reflect such costs was introduced as follows:

f_3=18Mn+21Cr+52.25Mo3+4.88Temp/600; (12)

Fig. 4 displays the optimisation results of optimising f_1, f_2, and f_3 defined by Equations (10)-(12) using the AWPSO algorithm. Table 2 shows the five different solutions selected from all the Pareto-solutions. Again, it can be seen that the optimisation method produced well-converged and spread Pareto-optimal solutions.

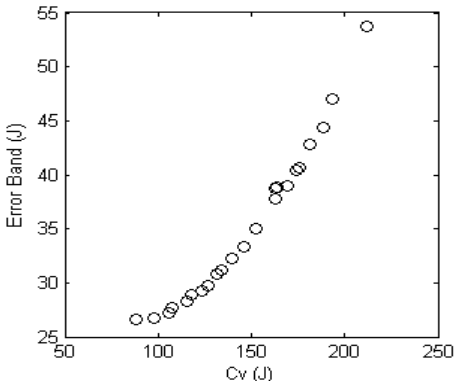

Fig. 3. Pareto-solutions for the two-objective alloy design

Table 1 Optional solutions selected from the Pareto solutions

	C	Mn	Cr	Mo	Temp	Cv	EB
1	0.447	0.811	1.002	0.291	697	88	26.6
2	0.385	0.865	1.243	0.279	706	105	27.3
3	0.337	0.933	1.044	0.342	730	127	29.7
4	0.264	1.024	1.315	0.335	726	146	33.3
5	0.212	1.197	1.123	0.420	725	169	39.0

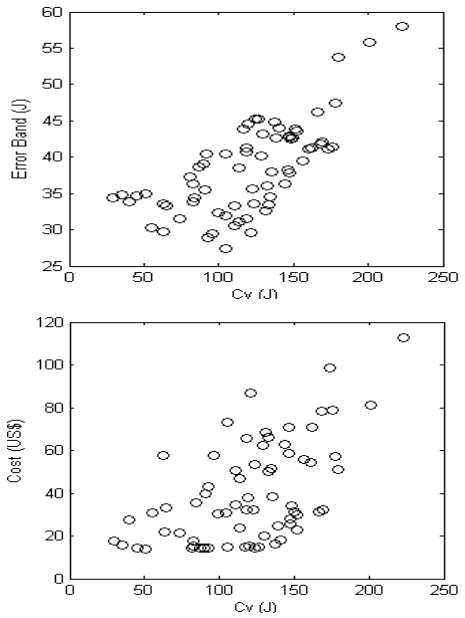

Fig. 4. Optimisation results for the three-objective alloy design.

Table 2. Optional solutions for three-objective optimal alloy design

	C	Mn	Cr	Mo	Temp	Cv	EB	Cost
1	0.39	0.82	0.94	0.25	730	105	27	73.2
2	0.37	1.06	0.39	0.17	730	111	30	50.4
3	0.25	1.03	0.49	0.12	730	135	34	51.4
4	0.30	0.89	1.03	0.01	730	118	31	65.7
5	0.40	0.83	0.31	0.17	719	93	29	42.9

4. CONCLUDING REMARKS

A multi-objective optimisation mechanism using fuzzy modelling and Particle Swarm Optimisation techniques has been successfully applied to the optimal design of heat-treated alloy steels. The main aim of the research was to determine the optimal heat treatment regime and the required weight percentages for the chemical composites to obtain the desired mechanical properties of steel. Based on the data-driven fuzzy model, the Charpy impact toughness can be predicted effectively and then used to facilitate optimal alloy design. The experimental results have shown that the optimisation algorithm can locate the constrained minimum design with very good convergence, and also provide a range of optional solutions which fit the pre-defined property requirement. The simulations also indicate that the algorithm produced very consistent solutions and can be effectively used in other industrial optimisation problems. Further investigations on multi-objective optimal alloy design involving more mechanical property criteria, such as Tensile Strength, Elongation, Reduction of Area, etc. should be beneficial for the steel industry as a whole.

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