1. Introduction

The hull structure of a large ship is generally constructed from carbon-manganese ferritic steels. It is well known that at sufficiently low temperatures and high loading rates, all ferritic materials become susceptible to brittle fracture. A review of the fracture properties of ship steels was conducted in 1958 by Boyd, following investigations into the failure by brittle fracture of the welded Liberty ships during World War II when a requirement of minimum manganese to carbon ratio of 2.5 was implemented to improve toughness. However, until Boyd’s review, no toughness requirements for mild steel had been quantified, and requirements merely stated that ship steel should demonstrate ‘adequate notch toughness’. Boyd defined toughness requirements based upon the Charpy impact test (considered to be the most practical method for mass-production testing), at a test temperature of 0°C (close to the minimum sea water temperature a vessel might encounter in service). Boyd’s measurements showed that the vast majority of brittle failures in ships had occurred in steels with Charpy impact energies of less than 47 J, with a fracture surface more than 70% crystalline at the casualty temperature. An acceptance criterion of a minimum Charpy impact energy of 47 J at 0°C was introduced into Lloyd’s Register’s Rules in 1957. However, a requirement for a maximum 70% crystallinity was not adopted because of the difficulty in measuring this parameter consistently. In 1961, Lloyd’s Register introduced standard grades with minimum toughness controlled by differences in the Charpy impact requirements. The current requirements are: Grade A, no certified Charpy value, grades B, D and E, 27 J at 0°C, −20°C and −40°C, respectively. Higher strength steels may be specified but have increased Charpy energy requirements.

Following the implementation of toughness graded ship steels, the incidence of brittle fractures declined. However, no enforced checks were made for Grade A steel which forms the majority of material within the shell structure of many ships. It was presumed that the compositional requirements of LR Grade A guaranteed a notch toughness of 27 J at 0°C. However, this has not always been the case and some brittle failures have occurred. Following continued concern within the shipbuilding industry, Lloyd’s Register introduced a Rule requirement in 1997 for in-house checks for every 250 t of Grade A plate produced by the steel maker, to ensure that an impact energy of 27 J at 0°C is achieved.

However there are still some concerns especially regarding the occurrence of steels showing high crystallinity while showing acceptable energy values. Therefore in the period between 1997 and 1998, Lloyd’s Register instigated a review of the fracture properties of ship steels, in order to evaluate the improvement in properties and hence consider whether any Rule changes were necessary. A total of 38 Grade A plates with a thickness range of 12 to 16 mm and 22 Grade AH36 plates with a thickness range of 15 to 22 mm were obtained from steelmakers world-wide, these thicknesses at typical of that for the shell structure of a...
large vessel. The chemical composition of each plate was determined, together with the Charpy toughness, fracture appearance transition temperature and susceptibility to strain-ageing embrittlement.

This study revealed that the toughness of modern steels far exceeds the minimum required energy values given in the Rules. This confirms the improved Charpy toughness of such steels over the past 40 years. Therefore, it is concluded that no changes in the Rule requirements for minimum Charpy toughness are necessary. However, the use of a non-impact tested steel is still being criticised and a predictive method to estimate toughness to production variables could be a useful tool. The aim of the present work is to establish the link between composition, microstructure and Charpy toughness for high strength structural steels by applying multi-disciplinary expertise and fuzzy modelling techniques.

Companies in the steel industry value highly the achievement of required levels of toughness properties of hot rolled steel products, with recent years having seen work attempting to unravel this through Charpy impact test modelling, such as instrumented Charpy test modelling,\(^1,2\) modelling Charpy impact energy data using statistical analyses\(^3,4\) and numerical modelling of the ductile-brittle transition.\(^1,2,10\)

However, these studies have focused on specific test conditions and specific steel, whereas little work has been done to establish generic composition-processing-impact toughness models. The work described here aims at linking steel composition and microstructure to a prediction of Charpy impact energy for Grade A and AH36 ship steels.

In this paper, after the introduction of the general scheme of the adaptive fuzzy modelling method, Charpy impact properties prediction for ship steels is presented in Sec. 3. The effects of chemical composition and microstructure on impact toughness properties are also studied and discussed here. In particular, the paper highlights the interactions between some key elements such as C, Mn and S, which are highlighted through fuzzy model response surfaces.

2. Methodology of Adaptive Fuzzy Modelling

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. Adaptive fuzzy systems can be viewed as fuzzy logic systems whose rules are automatically generated through fuzzy neural network training. The major advantage of fuzzy modelling is its ability to integrate the logical processing of information with attractive mathematical properties of general function approximators capable of representing complex non-linear mappings. Also, the if-then rule mechanism is easy to manipulate, understand and, to a certain extent, is domain independent. In materials engineering, it is beneficial to develop accurate, transparent and computationally efficient structure-property models for materials development.

Consider a collection of \(N\) data points \(\{P_1, P_2, \ldots, P_N\}\) in a \(n+1\) dimensional space that combines both input and output dimensions. Without loss of generality, we consider a multi-input-single-output fuzzy logic system as a general presentation of fuzzy systems. A generic fuzzy model is presented as a collection of fuzzy rules in the following form:

\[
R_i: \text{If } x_1 \text{ is } A_{1,i} \text{ and } x_2 \text{ is } A_{2,i} \ldots \text{ and } x_n \text{ is } A_{n,i} \text{ then } y = \mu(x) \text{ is } B_{i,\text{rule}} \text{ with } i = 1, \ldots, p
\]

where \(x=(x_1, x_2, \ldots, x_n)\in U\) and \(y\in F\) are linguistic variables, \(A_i\) are fuzzy sets of the universes of discourse \(U_i\subseteq R\), and \(z(x)\) is a function of input variables. Typically, \(z\) takes the following three forms: singleton, fuzzy set or linear function. Fuzzy logic systems with centre average defuzzifier, product-inference rule and singleton fuzzifier are of the following form\(^15\):

\[
y = \sum_{i=1}^{p} z_i \left[ \prod_{j=1}^{n} u_{ij}(x_j) \right] / \sum_{i=1}^{p} \prod_{j=1}^{n} u_{ij}(x_j) \ldots \ldots (1)
\]

where \(u_{ij}(x)\) denotes the membership function of \(x_i\) belonging to the \(i\)th rule. Very commonly, a radial basis function, especially the Gaussian function, is chosen as the membership function, i.e. \(u_{ij}(x) = \exp(-(x-a)^2/\sigma_i^2)\).

According to the fuzzy modelling paradigm proposed Chen and Linkens,\(^1,15\) a fuzzy modelling problem is equivalent to satisfying the following requirements: 1) generating an initial fuzzy rule-base from data; 2) determining the optimal number of fuzzy rules; and 3) optimising the parameters both in the antecedent part and consequent part of the rules. The above objectives can be achieved by incorporating fuzzy c-means clustering associated with a new partition validity index and parameter self-learning algorithms, which will be described below.

2.1. Rule-base Self-generation

It is generally acknowledged that classes or clusters of the data which have a similar geometrical location should be formed. Fuzzy clustering is a well recognized paradigm to generate the initial fuzzy model. Numerous clustering algorithms have been developed. The most widely used algorithm is the fuzzy c-means (FCM) due to its efficacy and simplicity. However, the number \(c\) of clusters must be predetermined. The FCM algorithm partitions a collection of \(n\) data points \(\{X=(x_1, x_2, \ldots, x_n)\}\) into \(p\) fuzzy clusters such that the following objective function is minimized.

\[
J_m = \sum_{i=1}^{c} \sum_{j=1}^{p} u_{ij}(x) \| x_j - v_i \|/m \quad 1 < m < \infty \ldots \ldots (2)
\]

where \(m\) is a fuzzy coefficient, \(v_i\) is the prototype of the \(i\)th cluster generated by fuzzy clustering, \(u_{ij}\) is the membership degree of the \(i\)th data belonging to the \(i\)th cluster represented by \(v_i, u_{ij} \in U, \text{ with } U \) being a \(p \times n\) fuzzy partition matrix which satisfies the constraints:

\[
0 \leq u_{ij} \leq 1 \quad \forall i, j \text{ and } \sum_{j=1}^{p} u_{ij} = 1 \quad \forall k.
\]

Cluster validity is the problem of finding the best value for \(p\) subject to minimisation of \(J_m\). Since \(J_m\) monotonically decreases with \(p\), an efficient criterion for evaluating the partition performance is required. In this paper, a simple and effective fuzzy partition measure\(^15\) is used as a cluster validity criterion associated with the FCM algorithm, which is defined as follows:
$V_p = \frac{1}{n} \sum_{k=1}^{n} \max_{i} (u_{ik}) - \frac{1}{K} \sum_{k=1}^{p} \sum_{j=1}^{P} \left[ \frac{1}{n} \sum_{k=1}^{n} \min (u_{ik}, u_{jk}) \right].$

where $K = \sum_{j=1}^{p} i$ ............(3)

It can be seen that the cluster validity measure $V_p$ is composed of two items. The first item reflects the compactness within a cluster while the second item indicates the separation between clusters. The validity $V_p$ criterion tends to indicate a good cohesion within clusters and a small overlap between pairs of clusters.

The FCM algorithm attempts to classify the given set of data vectors into a certain number of clusters by searching for local minima of $V_p$. The procedure of the fuzzy clustering algorithm associated with the validity measure (3) is carried out through an iterative optimization of $V_p$ according to the following steps:

Step 1. Choose the maximum cluster number $c_{max}$, iteration limit $T$, fuzzy exponent $m$, and termination criterion $\varepsilon$.

Step 2. With $p=2, 3, \ldots, p_{max}$; initialize the positions of cluster centres: $V_0 = (v_{10}, v_{20}, \ldots, v_{p0})$.

Step 3. For $i=1, 2, \ldots, T$;

- Calculate $u_{ik} = \left[ \sum_{k=1}^{p} (d_a^k / d_b^k)^{2/(m-1)} \right]^{-(m-1)/2}$ ...........(4)
- where $d_a^k = \| x_i - v_k \|$, $i=1, 2, \ldots, p$; $k=1, 2, \ldots, n$;

- Calculate $v_{ij} = \frac{1}{n} \sum_{i=1}^{n} (u_{ik} x_i)^{1/n} / \left( \sum_{i=1}^{n} (u_{ik}) \right)$ m .......(5)

If $\| V_{n} - V_{n-1} \| < \varepsilon$, go to next step, otherwise repeat step 3.

Step 4. Calculate $V_p(c)$ by (3); if $p<p_{max}$, repeat from Step 2. Otherwise, stop the program and set the optimal cluster number $p=p_{max}$, where $c_{opt}$ meets the following condition:

$V_{p_{opt}} = \max \{ V_p(p) \} \; \; \; p=2, 3, \ldots, p_{max}$

After cluster validation, both the number of rules and the prototypes of the clusters $v_j = (v_{j1}, v_{j2}, \ldots, v_{jm}, v_{j+1})$, are obtained, where $j=1, 2, \ldots, p$. Let $a_j = (v_{j1}, v_{j2}, \ldots, v_{jm})$, then the vector $a_j$ denotes the prototype of the $j$th fuzzy partition in the input space, and it can also be viewed as the centre of the Gaussian membership functions in the antecedent of the $j$th rule, while $z_j$ is the prototype of the $j$th fuzzy partition in the output space, and denotes the fuzzy output value in the consequent part of the $j$th rule. Therefore, the rule-base which is composed of $p$ fuzzy rules can be represented as:

$R_j$: IF $x_i$ is $A_{j1}$ and $x_j$ is $A_{j2}$ and ... and $x_m$ is $A_{jm}$ THEN $y$ is $z_j$

where $R_j$ denotes the $j$th rule, $A_i$ is the fuzzy set defined by the Gaussian membership function; and $z_j = \Sigma_{k=1}^{n} b_{jk} x_k$, is the $j$th rule output with respect to a relational fuzzy model or a functional fuzzy model with $x_n=1$, respectively.

2.2. Parameter Optimisation

When a fuzzy model has been constructed in the process of rule-base generation, a parameter learning procedure is subsequently applied to obtain a more precise fuzzy model in the process of parameter identification. There are several methods for training the fuzzy model, that is, to learn the optimal membership function parameters $a_{ij}, \sigma_j$, and linear weights $b_{ij}$ here. We adopt the gradient-descent-based approach to optimize the parameters $a_{ij}, \sigma_j$, and $b_{ij}$ in combination using a performance index of Root Mean Square Error (RMSE). Using gradient-descent algorithms, the parameter learning algorithms can be derived as:

$\Delta b_{ij} = \eta (y_{ij} - y_i) q_j(x)$ ..............(6)

$\Delta a_{ij} = \eta (y_{ij} - y_i) \frac{(x_j - a_{ij})}{\sigma_j^3} (z_j - y_i) q_j(x) ...........(7)$

$\Delta \sigma_j = -\eta (y_{ij} - y_i) \frac{(x_j - a_{ij})^2}{\sigma_j^3} (z_j - y_i) q_j(x) .......(8)$

where $\eta$ is the learning rate, and $q_j(x) = u_j(x) / \sum_{i=1}^{n} u_j(x)$.

Once the parameter learning is completed, the final model is obtained. The acquired fuzzy model should be validated under certain performance indices, such as accuracy, generality, complexity and interpretability. If the model performance is not good enough, further modification including structure and parameter optimisation will be required. Once the model performance achieves the pre-defined criteria, the final model is produced.

3. Charpy Toughness Modelling for Ship Steels

The above fuzzy modelling approach has been used to construct composition-microstructure-property models for Charpy impact properties prediction of Grade A and AH36 ship steels. The ranges of main chemical compositions of ship steels are listed in Table 1. In the process of modelling, 60% of the data were used for model training and 40% data were used for testing.

3.1. Charpy Modelling for Ship Steel Grade A

A total of 38 Lloyds Register certified Grade A plates

<table>
<thead>
<tr>
<th>Composition</th>
<th>C</th>
<th>Si</th>
<th>Mn</th>
<th>Al</th>
<th>S</th>
<th>P</th>
<th>Ni</th>
<th>Mo</th>
<th>Cr</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grade A</td>
<td>0.08–0.18</td>
<td>0.01–0.03</td>
<td>0.4–0.5</td>
<td>0.001–0.003</td>
<td>0.06</td>
<td>0.032</td>
<td>0.037</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Grade AH36</td>
<td>0.11–0.178</td>
<td>0.013–0.463</td>
<td>0.98–1.555</td>
<td>0.064</td>
<td>0.001–0.012</td>
<td>0.022</td>
<td>0.03</td>
<td>0.01–0.05</td>
<td></td>
</tr>
</tbody>
</table>
were tested at temperatures of −20, 0 and 20°C using longitudinal specimens. The thickness of the individual plates was in the range 12 to 16 mm. Most of the plates were delivered in the as-rolled condition and the plates were all satisfactorily fine-grained with a typical ferrite/pearlite microstructure. The database available for the analysis contains chemical composition, ASTM grain size, tensile strength, measurements of Charpy impact energy and corresponding test temperature. A total of 342 data for Grade A ship steels were used to develop the prediction models.

As mechanical processing information was not available for this ship steel data set, microstructure and tensile strength were used for impact property prediction. Firstly, a composition-microstructure-impact property fuzzy prediction model with inputs of C, Mn, S, P, Al, grain size, test temperature was developed for Grade A ship steels. The prediction result with Root Mean Square Error RMSE=22.19 is shown in Fig. 1. It is seen that Charpy impact energy can be predicted well based on the chemical composition and microstructure. Since tensile strength strongly links to composition, processing conditions and microstructure, it is beneficial to introduce UTS (Ultimate Tensile Strength) in the toughness prediction model due to the lack of processing information. Figure 2 shows the prediction result with UTS as an added input variable in the fuzzy prediction model. Clearly, the prediction accuracy was improved compared with the model without UTS. In the case of UTS data not being available, a tensile strength prediction model can be developed first, and then used further to predict impact energy. Figure 3 shows the tensile strength prediction result using C, Si, Mn, Al, and grain size as input variables. Using the predicted UTS to predict impact energy, a very similar prediction result was obtained with RMSE=21.11.

In order to investigate the influence of chemical compo-

![Fig. 1. Impact energy prediction without UTS. RMSE=22.19.](image1)

![Fig. 2. Impact energy prediction with UTS. RMSE=20.75.](image2)

![Fig. 3. UTS prediction. RMSE=1.13.](image3)

![Fig. 4. Response surface of the fuzzy model for Grade A ship steels.](image4)
sition and microstructure on Charpy properties, model response surface analysis with respect to the link between two specific factors and Charpy energy has been conducted on the fuzzy models at a test temperature of 0°C for Grade A steel. Through the model response surfaces, the interactions between some specific factors such as C/Mn and Mn/S could be revealed. The corresponding response surfaces are displayed in Fig. 4. It can be seen that low carbon and high manganese usually produce better impact properties. Low sulphur residual and high Mn/S ratio generally improve impact toughness. An increase in aluminium generally increases Charpy impact energy. It is also clear that fine grain size generates good Charpy v-notch impact property, which is consistent with existing metallurgical knowledge.

3.2 Charpy Modelling for Ship Steel Grade AH36

The Charpy impact tests for Grade AH36 steel were undertaken on specimen sets from 22 different plates originating from worldwide steel makers. The test temperature ranged from 0°C to 80°C. A total of 214 data for Grade AH36, containing information on chemical composition, tensile strength and impact properties (including impact energy and 27 J transition temperature), were used to develop the fuzzy prediction model. Using the proposed adaptive fuzzy modelling method, a 6-rule fuzzy model with C, Mn, S, Cr, Mo, Ni, Al, UTS and test temperature as input variables was developed for the prediction of impact energy and ITT 27 J. The model prediction results are displayed in Figs. 5 and 6 respectively. It can be seen that both Charpy impact energy and ITT 27 J can be predicted well using a simple fuzzy model with a small number of rules.

To reveal the relationship between individual variables and Charpy toughness, model response surfaces were also obtained. Figure 7 shows the effect of composition and tensile strength on Charpy impact energy in the brittle-ductile transition region (here −40°C). It can be seen that lower sulphur residual improves Charpy properties. It is also seen that the addition of Ni is generally beneficial to Charpy toughness, and the addition of Cr, Mo and Al did not create significant changes in impact energy. In Grade AH36 ship steels, higher tensile strength generally corresponds to higher impact energy, which might be produced by finer grain size. It should be pointed out that different combina-
tions of elements have different effects in the transition region and upper shelf energies, hence making the problem very complex. Further investigation of influence factors on Charpy toughness in different regions is needed.

3.3. Charpy Fracture Surface Characterisation Prediction for Grade AH36 Ship Steels

The fuzzy modelling approach was also used to predict Charpy fracture surface characteristics, such as lateral expansion, and brittleness (fracture appearance). A six-rule fuzzy model (including 7 inputs: C, Mn, S, Nb, V, UTS, Test Temperature) was developed for the prediction of lateral expansion and percentage of brittleness.

The model prediction result with RMSE = 0.27 mm for lateral expansion of 214 tested specimens is shown in Fig. 8. Table 1 shows the prediction of the Charpy impact energy, brittleness and lateral expansion for eight different plates at a temperature of −20°C. It can be seen that using fuzzy modelling we can predict not only impact properties but also the corresponding fracture surface characteristics, which are useful for toughness assessment. Considering the scatter that may be expected with actual Charpy impact energy results, the values predicted in Table 2 for energy, crystallinity (brittleness) and lateral expansion can be considered to provide good predictions of the actual measured results. This provides confidence in the approach and would suggest that it can be used to predict results for grades of steel used in shipbuilding that are traditionally not impact tested.

4. Conclusions

Using the neural-fuzzy models obtained in this study it is possible to predict Charpy toughness for a given steel composition, microstructure and/or tensile strength, and also reveal useful qualitative information linking composition-microstructure to Charpy impact properties. Fuzzy modelling results also show that the impact energy of all test plates in Grade A steels is well above 27 J at 20°C. Also, 27 J transition temperatures (ITT27 J) for all plates in Grade AH36 steels are well below −20°C, and are well above the required Lloyds Register toughness criteria. It is clear that the proposed fuzzy modelling method is effective for Charpy toughness prediction and assessment. The trends predicted by the model are consistent with current metallurgical knowledge. It is possible with this approach to estimate the toughness of grade A ship steel that is not tested in production, giving a high level of confidence to the shipbuilding industry. Further investigation of interactive influence factors and incorporation of expert knowledge and data-driven modelling techniques will be beneficial in the prediction of Charpy properties.

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