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Review

Applications of soft computing techniques in materials engineering: A review

Odetunji A. Odejobi[1]* and Lasisi E. Umoru[2]

[1]Cork Constraint Computation Centre, Computer Science Department, University College Cork, Cork, Ireland.
[2]Materials Science and Engineering Department Obafemi Awolowo University, Ile-Ife, Osun State, Nigeria.

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Within the last two decades, a substantial amount of research efforts has been directed at the application of Soft Computing (SC) techniques in engineering. This paper provides a systematic review of the literature emanating from these efforts with particular focus on materials engineering. The primary aim is to provide background information, motivation for applications and an exposition to the methodologies employed in the development of soft computing technologies in engineering. Our review shows that all the works on the application of SC to materials engineering have reported excellent, good, positive or at least encouraging results. In our opinion, the lack of negative results might be due to the simplification of materials engineering problems to manageable and predictable situations. We draw particular attention to the strengths and weaknesses of soft computing techniques in the context of materials engineering applications. Our appraisal of the literature suggests that the interface between materials engineering and intelligent systems engineering techniques, such as soft computing, is still blur. The need to formalise the computational and intelligent systems engineering methodology used in materials engineering, therefore, arises. We also provide a brief exposition to our on-going efforts in this direction. Although our study focuses on materials engineering in particular, we think that our findings applies to other areas of engineering as well.

Key words: Composite materials, fuzzy logic, soft computing, intelligent systems engineering, formal methods.

INTRODUCTION

The pervasive use of soft computing in various engineering applications makes it an indispensable tool in the development of products that have implications for the human society. A case in hand, which is the focus of this paper, is soft computing applications in the areas of materials engineering. The significance of engineering materials to the functioning and technological development of human society is well documented (Dobrzanski, 2006). Natural materials have physical, chemical and mechanical properties that have been studied and well documented in the materials science literature. Materials science literature also documents knowledge that aids the understanding of the causative relationships between materials constituents, structure and properties at a level that allows composition and processing parameters to be selected to create composite materials with target properties (Zhang et al., 2008; Ashby, 2000). Such relationships can be discerned by empirical experiments or by the use of mathematical and/or computational models.

Modern engineering materials, from those used to make simple things such as our tooth brush to complex things such as the computer and the airplane, do not occur naturally. The need to engineer materials that meets specific human needs then arises. To achieve this, materials engineers apply the knowledge generated in materials science. Materials engineering encompasses the science and art involved in the conceptualisation, specification, design, analysis, fabrication and evaluation of generic materials in their various forms and in different operating conditions with the aim of developing materials for an application. The materials engineer's job is constrained by the technology available, the environment in which the materials will be used as well as the type of application that the materials will be put. For example, nuts and bolts that will be used in computer hardware will have different requirements from those that will be used in commercial vehicles. The requirements for the computers and

*Corresponding author. Email: t.odejobi@4c.ucc.ie. Tel: +353-21-4902795 Fax: +353-21-4274390.

vehicles meant for civil applications are different from those meant for military applications. The same requirements will not apply if the nuts and bolts will be used in different environment: for example those that will be used in warm and humid weather, such as sub-Saharan Africa, and those meant for cold and wet weather, such as some European countries or Canada. The nature, frequency and kinds of loading and unloading of the materials are another crucial component of the materials engineering decision. For example, the crash of BOAC Flight 781 in 1954 was attributed to ”metal fatigue” caused by the repeated pressurisation and de pressurisation of the aircraft cabin". The job of the materials engineer is to develop new materials by taking into consideration these very complex constraints, while bearing in mind non-functional constraints, such as price and aesthetic values emanateing from cultural preferences. Another interesting dimension to the constraint is the current trend in technological advances and the need to develop more user friendly technologies that is functional, economical, and easy to dispose as well as with low environmental footprint.

There is a huge and growing amount of materials (Ermolaeva et al., 2002; Mates, 2008) available to modern materials engineers. The many features used to describe these materials, together with the confounding nature of the interaction between these features, makes manual or adhoc approach to materials engineer impractical. Also, the volume of output suggest the need to reduce fabrication costs by deploying tools and techniques that will reduce the gaps between users' requirements and the specifications of fabricated materials. These complexities, and the accompanying rapid rate of change in the demand for new materials, present new challenges to materials engineers (Dobrzanski, 2006). This motivates the development and application of more versatile techniques on the one hand; and on the other hand, the need to automate specific aspects of the materials engineering process. At the moment, soft computing (SC) based techniques and methods are becoming more popular as they are gaining prominence in various areas of engineering. In materials engineering, SC techniques have been successfully applied in materials design, improvement, and selection as well as in the control of the processes for materials fabrication. This paper has three main objectives, which are to:

- Provide a short background to the SC methods that are relevant to materials engineering.
- Provide a review of the state of the art in the application of these methods in materials engineering.
- Present a brief discussion on our proposed framework within which the SC methods could be more productively deployed in materials engineering.

In the following Subsection 1.1, we describe the materials engineering problem, from a computational perspective, as a multi-criteria decision process and we discuss the limitations of the analytical approach at adequately addressing this problem in Subsection 1.2. We provide a background to the soft computing approach to materials engineering in Section 2. In Sections 3, 4, 5 and 6 we provide a review of the artificial neural networks, fuzzy logic and genetic algorithms and the hybrid techniques, respectively, as applied in materials engineering. Section 7 documents our ongoing work on the formalisation of SC for application in materials engineering while Section 8 concludes this paper.

The materials engineering problem

The processes that underlay the materials engineering decisions can be recast as a linear programming problem (Sen and Yang, 1995; Balcom and Curtner, 2000; Ermolaeva et al., 2002; Goupee and Vel, 2007). Suppose that there are a set of *n* generic or constituent materials, M = $\{m_1, m_2,.., m_n\}$, from which a composite, C, is to be created. Let $(a_1, a_2,.., a_n)$, be the amount of each materials. For each combinations of $\{m_1, m_2,.., mn\}$ we can determine properties, e.g. tensile strength, young modulus, that will give a desired attribute of the composite C. For example, if our goal is the tensile strength, we can use the above information to mathematically express the tensile strength, t, of the target material C as follows:

$$t_1a_1 + t_2a_2 +, \ldots, + t_na_n \quad (1)$$

Where each t_i is a quantitative representation of the tensile strength of materials mi.

The salient assumption here is that the tensile strength of materials is additive. Note that some of the t_i may actually be zero, for example if a material does not exhibit the property of interest. The aim is to choose only from among those materials which meet the minimum requirement, say t units of tensile strength, in the target composite materials C. We, therefore, demand that Equation 1 satisfies the linear inequalities of the form:

$$\sum_{i=1}^{n} t_i a_i \geq t. \quad (2)$$

The above expression is only for one attribute of the composite *C*, that is, tensile strength. To account for other attributes, similar mathematical expressions must be constructed. Of course Equation 2 can be solved easily by choosing sufficiently large quantity of material values. However, when engineering constraint (Gutteridge and Waterman, 1986) such as materials cost and weight, are factored in, then the problem becomes a combinatoric one. For example, if the aim is to reduce material cost in terms of price, *P*, and the unit price of each material amount $(a_1, a_2,..,a_n)$, is $(p_1, p_2,..,p_n)$, then the aim will be to solve Equation 2 subject to the constraint in the linear cost expression given by:

$$P = p_1a_1 + p_2a_2 +, \ldots, + p_na_n. \quad (3)$$

The problem is to choose a combination of generic materials so as to satisfy the requirement (that is, the linear inequalities) of the composite at the minimum cost (that is, linear cost expression). This is clearly a multi-objective optimization problem and there are analytical tools that can be used or adapted for its solution (Goupee and Vel, 2007; Balcom and Curtner, 2000; Ermolaeva et al., 2002; Akinola, 2001). For example, if we use the following objective compound function (Ashby, 2000):

$$C = \alpha_1c_1 + \alpha_2c_2 +, \ldots, + \alpha_nc_n \quad (4)$$

Where α_i and c_i are weight coefficient and material index, respectively, for the i^{th} objective, then each of the objectives can be viewed as a constraint on the property of the desired composite material, that is, C.

This problem generally involves three engineering decision tasks:

- The acts of generating design options, each of which consist of the specific choice of n generic materials and fabrication processes;
- The design feasibility conditions, which constraint the possible design options generated;
- An index associated with each design option, which represents a weighted average of cost (in terms of benefit) for the design options.

The problem is to find a design that satisfies 2 and minimises 3.

Analytical approach to materials engineering

In the analytical approach to materials engineering, the properties of materials are measured and specified as numbers or points, which then become data reflecting certain states of materials. Mathematically, such data are modelled as a realization of an appropriate variable using a suitable data type (Bandemer and Lorenz, 1998). Although, the process for generating the data is not random, random or pseudo-random data are frequently used when building models in materials engineering.

Analytical approach to materials engineering uses techniques developed around mathematical models. This includes finite elements method (FEM) (Jeffreys, 1988; Zienkiewicz and Taylor, 1994; Sampath and Zabaras, 1999), statistical approach based on the Analysis of Variance (ANOVA) as well as regression analysis techniques (Montgomery, 1997). The limitations of these approaches to materials engineering arose from the low cardinality (Freeman, Antonucci, and Lewis, 2000) of materials data as well as the set of *a priori* assumptions for their application. It is well known that analytical methods are poor at handling data with low cardinality or data expressed in linguistic form (Graebe, Goodwin, and Elsley, 1995). The materials data provided in materials science literature must, of necessity, be augmented with material behaviour information which agrees closely with experimental observations, for them to be useful in materials engineering. These observations are expressed linguistically and the complexity of the problem requires simplification, resulting in a manageable but less accurate models. In Rao and Mukherjee (1996), for example, it was shown that analytical models for simulating the macromechanical behaviour of ceramic-matrix composite is difficult, necessitating the use of simplifying assumptions which compromised accuracy. The design approach employed by materials engineers in real-life involves conception and reasoning about abstract objects using their cognitive ability, which is neither numerical nor random. This process is best modelled linguistically as such is closer to the uncertainty, imprecision and vagueness that characterises natural materials properties. Indeed Lee and Kopp (2001a) argued that it is difficult to construct a mathematical model when automating metal forming processes, owing to their non-linear and non-stationary characteristics. Also Elishakoff and Ferracuti (Elishakoff and Ferracuti, 2006) observed that:

> "On one hand, most engineers, as it were, neglect uncertainty, but on the other hand, the allowable stress level was introduced long time ago as a ratio of the yield stress to the so-called safety factor to provide the region for the safe utilization of the structure. Thus the uncertainty is introduced into practice by the back door" (Elishakoff and Ferracuti, 2006).

The discussions above indicate that the materials engineering process is complex as design decisions have to be based on incomplete and uncertain information or data. Sometime, the design decisions are based on uncertain and incomplete understandings of the process through which the final product will result. Most of such process are intuitive and cannot be described in a definitive manner that facilitates mathematical rendering. For example, the mechanical properties of metals reveal the elastic and inelastic reaction when force is applied. This involves relationship between stress and strain, as represented by elasticity, tensile strength as well as fatigue limit. In the metal industry, these variables are typically derived from a micro-structural investigation of materials, usually analyzed visually (Voracek, 2001a). The behaviour of composite, for example, is highly sensitive to a number of design variables such as percentage reinforcement, interface shear strength, geometrical and material properties of the constituent materials and how they map onto the mechanical behaviour of the composite. This behaviour cannot be accurately modelled using simple linear relations, even when the number of the design variables is small. The degree of non-linearity and the extent of interaction of the constituent is also not clearly known (Rao and Mukherjee, 1996).

The sensitive behaviour of materials and their processing, as highlighted above, account for why the materials engineering process employs design judgments and expert opinion that are qualitative, often combinatorial and, in most cases, can only be represented heuristically (Trawlers et al., 1995a). Computer simulations have become essential in the development of modern materials (Abreu, 2007) as they facilitate experimentation with various ideas before the final product is fabricated. In recent times, however, tools from Artificial Intelligence (AI) have become popular in materials engineering. This includes: artificial neural networks and fuzzy logic. In Wang, Feng, Yan, and Fuh (1996) neural networks representing the mapping function for an expert system was used for production rules in materials design. It was shown that, compared with the traditional production rule based expert systems, neural network based expert systems are more effective in approximate reasoning. In Voracek (2001b), a method based on inductive learning and classification principle was selected and justified as a suitable tool for predicting the mechanical properties of cast irons. It was shown that the intelligent approach to materials prediction is a good alternative to the traditional ways of laboratory investigations and processing of experimental data. In the domain of optimisation and nuclear production processing, Trauwaert, Reynders, and Roy (1995b) have also shown that classical clustering problems are better modelled using fuzzy logic rather than with a crisp based method.

The work summarised above suggests that researchers are becoming more aware of the uncertain characteristics of natural materials and the limitations of mathematical and analytical tools at modelling them realistically. In addition to numerical data, modern methods also integrate verbal and textual expression, graphics as well as objects and frames (Dym, 1998) into the materials properties description process. A new trend, evolving in material engineering, is a paradigm which exploits a systematic integration of the traditional analytical and modern intelligent techniques in the development of computational solutions. The relevance of this paradigm is documented in the literature, which indicates that the number of successful computing-based materials engineering applications is increasing (Oduguwa, Tiwari, and Roy, 2005; Mantere and Alander, 2005; Hoffmann et al., 2005; Kamiya et al., 2005; Mellit and Kalogirou, 2008; Flintsch and Chen, 2004).

Soft-computing techniques

The term Soft Computing (SC) encompasses many techniques which include: Fuzzy Logic (FL), Neuro-Computing (NC), Probabilistic Reasoning (PR), Evolutionary Computing (EC) or Genetic Algorithms (GA), Chaotic Systems (CS), Belief Network (BN) and part of Learning Theory (LT) (Zadeh, 1965, 1994, 1995; Mellit and Kalogirou, 2008). SC techniques are different from analytical approach in that they employ computing techniques that are capable of representing imprecise, uncertain and vague concepts (Voracek, 2001a; Kulak et al., 2005; Kahraman, 2007; Guarino et al., 2009). Analytical, also called hard computing, approaches on the other hand use binary logic, crisp classification and deterministic reasoning. In their editorial review, (Hoffmann et al., 2005) observed that:

> "In contrast with hard computing methods that only deal with precision, certainty, and rigor, soft computing is effective in acquiring imprecise or sub-optimal but economical and competitive solutions. It takes advantage of intuition, which implies the human mind-based intuitive and subjective thinking is implemented here".

Techniques in SC are able to handle non-linearity and they offer computational simplicity when compared with the analytical methods. These techniques have been shown to be able to manage large amount of information and mimic biological systems in learning, linguistic conceptualisation, optimisation and generalisation abilities. Soft computing techniques are finding growing acceptance in materials engineering and three of them are popular, namely: (i) Fuzzy Logic (FL), (ii) Artificial Neural Networks (ANN) and (iii) Genetic Algorithms (GA). There are well established methodologies for integrating SC techniques to realise synergistic or hybrid models with which better results could be obtained (Zadeh, 2001). The use of hybrid techniques is also growing. The literature on the application of soft computing to materials engineering (ME) is so vast and so rich that it will be impractical to attempt a complete review in a journal article. To this end, we focus on those papers that we consider to be of interest, not only in terms of their contribution to knowledge and good practice, but also those that help us to draw attention to some observed or perceived lapses in the application of SC techniques.

Specifically, we consider papers written in the English language and of the following types:

i) Journals
ii) Con-ference proceedings and preceding
iii) Workshop pre-sentations and
iv) Standard text-books.

The majority of the work cited in this paper is journal articles. The reason for this is that we want to report on soft computing applications that are established in ME. Our review methodology focuses on:

i) The justification for the application of SC method.
ii) The specification of the problem and its significance.
(iii) The model development (design, implement and evaluation).
v) The outcomes and values of the solutions developed.

In the following subsections, we summarise the funda-

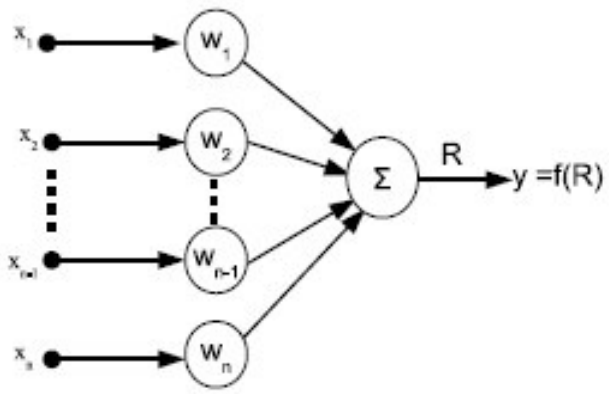


Figure 1. Model of a neuron.

Table 1. Artificial neural network activation functions.

Function name	Mathematical expression
Sigmoid	$f(y)=\frac{1.0}{1.0+\exp^{y}}$
Linear	$f(y)=ay+b$
Gaussian	$f(y)=\exp^{-\|m+y\|^2\alpha}$
Exponential	$f(y)=\exp(y+m)$
Bipolar sigmoid	$f(y)=\frac{1.0-\exp^{y}}{1.0+\exp^{y}}$

mentals of each of the SC techni-ques and review their applications in modern materials engineering tasks (Eichhorna et al., 2005) based on the above stated criteria.

ARTIFICIAL NEURAL NETWORKS

Artificial Neural Network (ANN) is also called connectionist model, neural net, or parallel distributed processor (PDP) model (Wang, 1997). Underlying the computational power of the ANN is the motivation to model the neurological activity in the human biological system. However, the ANN is a gross simplification of the human neurological system as the human nervous system comprises billions of various types of neurons whose structure, length and functionality depend on their location in the body (Schalkoff, 1997). Good reviews of the ANN technique are documented in (Basheer and Hajmeer, 2000; Waszczyszyn and Ziemianski, 2001; Mellit and Kalogirou, 2008) from which much of the materials presented here are drawn. The ANN comprised of interconnection of simple, non-linear computational elements (Wang, 1997; Lippmann, 1989) which are called nodes or neurons. A neuron typically consists of three components: (i) a group of weights, (ii) a summation function, and (iii) a non-linear activation function f(R) (Figure 1). An ANN can contain a large number of neurons. These neurons are linked with variable weights.

The computational behaviour of an ANN model is determined by the values of the weight associated with each neuron. To derive the behaviour of an ANN, it is usually trained on sample data. The sample data is normally represented in the form of an input matrix, X, and the corresponding output vector, Y. The job of the ANN is to learn the input-output relations embedded in X → Y through a learning process. The operations of the processing units consist of a number of steps. First, each input field xi is multiplied by a corresponding weight $w_i \in \mathbf{W}$. The product of each input field and its corresponding weight are then summed to produce the cumulative weighted combination *R*, as shown in Equation 5:

$$R = w_1x_1 + w_2x_2, \ldots w_nx_n = \sum_{i=1}^{n} w_ix_i \quad (5)$$

In order to adjust the behaviour of the neurons a quantity θ, called the bias, can be used as threshold. In that case Equation 5 will take the form:

$$R = w_1x_1 + w_2x_2, \ldots w_nx_n + \theta = \sum_{i=1}^{n} w_ix_i + \theta \quad (6)$$

The result, *R*, is further processed by an activation function f (:) to produce one output signal y. We can express the computation of y mathematically as:

$$y = f\left(\sum_{i=1}^{n} w_ix_i + \theta\right) = f(R) \quad (7)$$

Depending on the behaviour of the system being modelled, the function f() can take many forms, e.g. linear, sigmoid, exponential (see Table 1). The sigmoid, linear, and Gaussian functions are popular in materials engineering (Haykin, 1999; Mellit and Kalogirou, 2008; Tsai and Wang, 2001).

The computed value of y can serve as input to other neurons or as an output of the neural network depending on its position in the network configuration. Each node in the ANN is responsible for a small portion of the processing task and they are able to perform this task after a training session. The training process usually involves minimising the sum of square error between actual and predicted output. The ANN captures the behaviour in the available training data by continuously adjusting and finally determining the weight connecting neurons in adjacent layers. The most commonly used learning algorithm

is the backward error propagation (also called the back-propagation or back-prop) algorithm. This algorithm uses the gradient descent method in its implementation (Anaraki et al., 2008). Theoretically, a limited amount of training data points does not guarantee that a neural network will generalise the “true" behaviour desired. In order to verify the result of generalization, therefore, cross-validation (Jeffreys, 1988) is used.

The cross-validation process involves the sectioning of the parent database into three subsets (Basheer and Hajmeer, 2000): training, test, and validation. The training subset usually includes all the data belonging to the problem domain and is used in the training phase to update the weights of the network. The test subset is used during the learning process to check the network response for untrained data. The data used in the test subset are usually distinct from those used in the training. Based on the performance of the ANN on the test subset, the architecture may be changed and/or more training cycles applied. The third portion of the data is the validation subset which usually includes sample data different from those in the other two subsets. This subset is used after selecting the best network to further examine the network or confirm its accuracy before being implemented in real-life systems. There are no definitive rules for determining the required sizes of the various data subset; however a rule of thumb is to use the ratio 60: 20: 20 for sectioning of the parent database into the training, test, and validation subsets.

ANN with one hidden layer have been found to be effective for most practical applications in ME. Several ANN architectures and algorithms have been developed and documented in the literature (Haykin, 1999; Cheroutre-Vialette and Lebert, 2000; Mellit and Kalogirou, 2008). Three of such architecture that was used in the materials engineering include: (i) the multilayer perceptron (MLP); (ii) the radial basis function network (RBN); and (iii) the recurrent neural network (RNN). The structure and algorithm for these ANN architectures are briefly discussed in the following subsections.

Multilayer perceptron

The Multi-layer Perceptron (MLP) is perhaps the most popular ANN model in materials engineering. This is probably due to its simplicity and the availability of software for its implementation. MLP has been described as a universal approximator (Hornik, Stinchombe, and White, 1989) due to its robustness at approximating real-world data. The structure of a typical MLP is shown in Figure 2. The basic MLP networks consist of neurons arranged in layers. Connections are established between two successive layers only and from neurons in a preceding layer to another in a succeeding layer only. The connections have weights associated with them and their operations as discussed in artificial neural networks

The first layer is the input layer, and it establishes the first contact points to the data. The output layer is the last

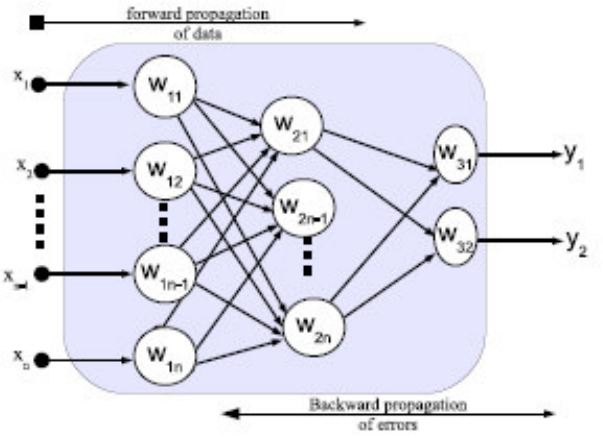


Figure 2. Multi-layered perceptron architecture.

layer in the network and it is responsible for presenting the result of the ANN to the outside world. There is at least one layer, called the hidden layer, between the input and the output layers. In a chain-like formation, the output of the neurons in the input layer is fed into the input of the neurons in the hidden layer neurons. The output of the last hidden layer neurons are fed into the input of the output layer neurons. Succeeding layers in the network sums the inputs of previous layers, adds a bias to the sum and apply the activation function to produce its own output. The last layer in the MLP architecture often has linear activation function.

Radial basis function network

The Radial Basis Function (RBF) Network is a 2-layer network in which the learning process is achieved in two different stages (Lippmann, 1989; Schalkoff, 1997; Wang, 1997). In the first stage, the input data set **X** alone is used to determine the parameters of the basis functions, that is, the first-layer weights. As only the input data are used, this training method is called unsupervised. The first layer weights are then kept fixed while the second layer weights are determined in the second phase of the training. The second stage is supervised as both input and target data are required. Optimal training parameters are achieved using the classic least squares approach. Figure 3 shows the configuration of a typical RBF.

Recurrent neural network

The Recurrent Neural Networks (RNN) is not as popular as the MLP and RBF network architecture in ME applications. RNN have however, been shown to possess powerful computational capabilities for modelling behaviour commonly associated with materials dynamics (Haykin, 1999; Elman, 1990; Draye et al., 1996; Parlos et al., 1994; Seker et al., 2003; Giles et alk., 1995). Several RNN architectures have been proposed in the literature,

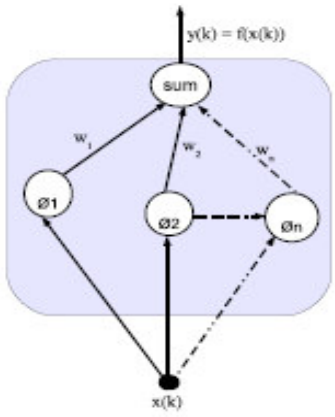


Figure 3. Radial bias architecture (Haykin, 1999)

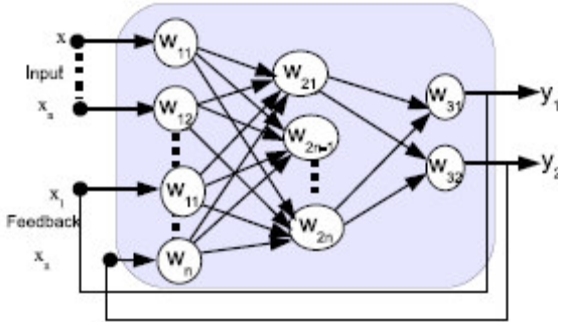


Figure 4. RNN-Jordan architecture.

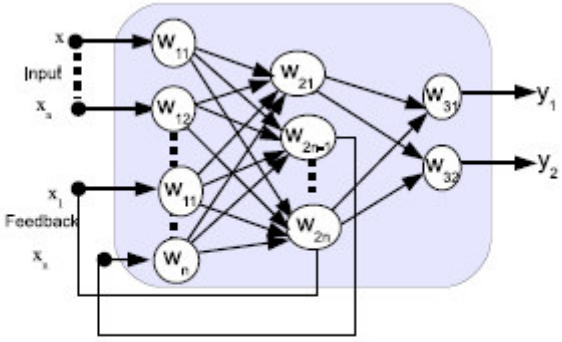


Figure 5. RNN-Elman architecture

however three of them are more commonly used in engineering applications: Fully RNN, Jordan, and Elman (Giles et al., 1995; Cheroutre-Vialette and Lebert, 2000; Seker et al., 2003). The basic structures of these RNNs (Figures 4,5 and 6). The important aspect of RNN is that, unlike the MLP and RBN, it allows the output of neurons in succeeding layers to be connected to those in the preceding ones. The learning process in RNN comprises input neurons, processing neurons, feed-forward and re-

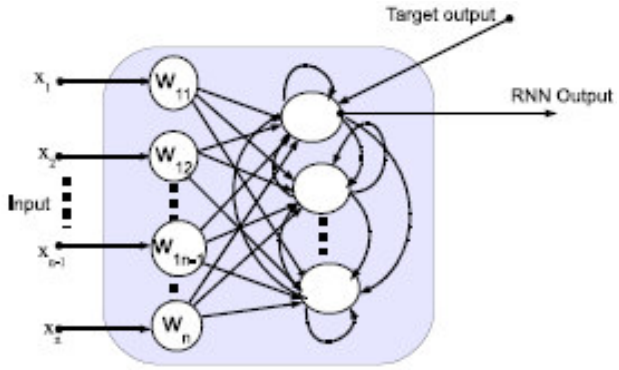


Figure 6. RNN-fully connected architecture.

current connections. Some of the processing neurons are assigned as output neurons. The output of a processing neuron may be connected to all processing neurons in the model. For example, in a fully connected recurrent network, every processing neuron is connected to all processing neurons including itself. The training and operation of the RNN is dynamic in that it depends on time step. The output of a processing neuron at the current time step depends on the input signals and feedback signals in the previous time step.

Applications of the ANN technique

As shown in Figure 7 the application of ANN in materials engineering is increasing in popularity from only about 3 papers in 1995 to more than 20 papers reporting the application of ANN in 2007. In most of the papers we reviewed, the process of developing an ANN based model consists of the following stages (Rao and Mukherjee, 1996; Basheer and Hajmeer, 2000):

- Generation of training data.
- Selection of a network type.
- Selection of the input and the output for the network.
- Design of a suitable network configuration.
- Selection of a suitable training strategy.
- Training and validation of the resulting network.

As shown in Figure 8, ANN based tools have been applied in prediction, modelling, control, identification design and optimisation areas of materials engineering. The majority of the applications we reviewed, about 48%, have been in the area of materials properties prediction. This is closely followed by materials properties modelling, about 37%. Works in the areas of materials properties optimisation and design account for 5 and 3%, respectively, and model identification and materials process control represent 1% each of the reviewed work (Table 3). Most of the publications used the parameters in Table 2 to describe their models. The majority of the work review used the MATLAB software for implementing their models. For example, in some work, (Chakraborty, 2004), the number of input to the

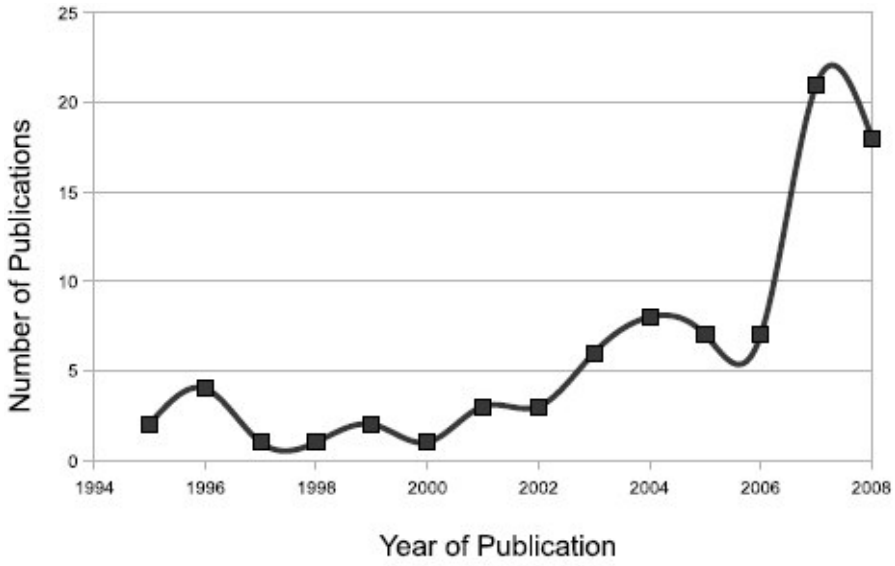


Figure 7. Graph of number of publications by year.

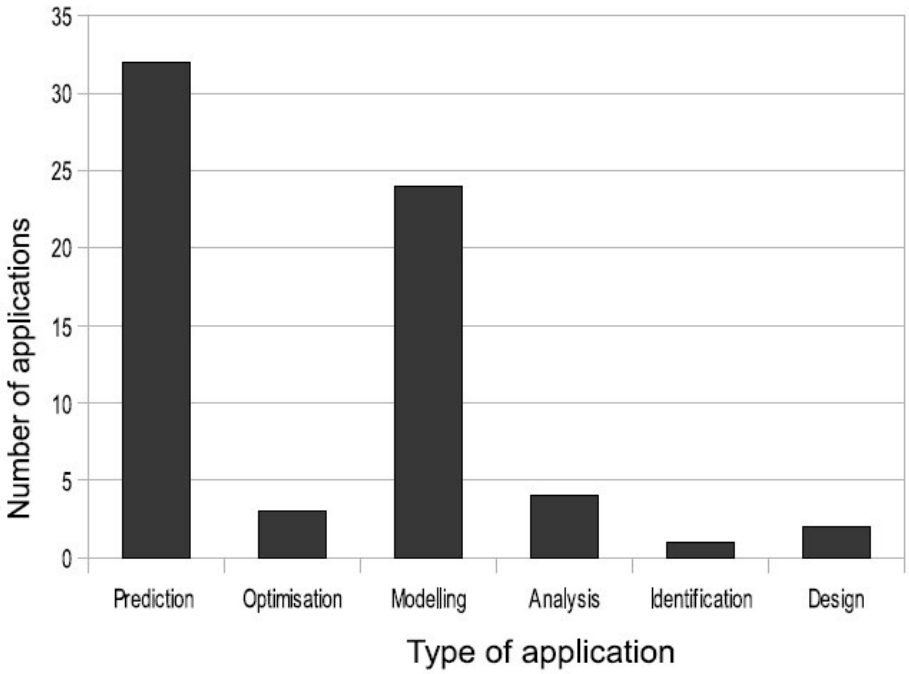


Figure 8. Application of ANN in ME

ANN is very large. This choice of ANN design makes it difficult to adequately analyse the model behaviour and explain its operation. We are of the opinion that, if the input to an ANN model is more than five, the model should be modularised for effective analysis. Some work (Guessasma et al., 2004; Guler and Artir, 2007) used ANN architecture with more than two hidden layers. The practicability of such model in materials engineering application in terms of economy of tool is diff cult to justify as it is well known that ANN with one layer will produce a good approximation. In most of the work we reviewed, however, ANN models have been shown to generate better predictions than the classical linear regression (Rao and Mukherjee, 1996; Cai et al., 2008). One of the reasons frequently cited for the use of ANN in materials engineering is its ability to recognise and learn the underlying nonlinear relations between input and output without the need to construct an explicit mathematical model. This is

Table 3. Applications of ANN in ME.

Applications	Publications	% of Total
Prediction	(Luong and Spedding, 1995; Rao and Mukherjee, 1996; Wang et al., 1996; Waszczyszyn and Ziemianski, 2001; Chen, 2001; Lu et al., 2003; Genel, 2003; Fotovati and Goswami, 2004; Altinkok and Koker, 2004; Seyhan et al., 2005; Song et al., 2005; Chakraborty, 2005; Durmus and Ozkaya, 2006; Altinkok and Koker, 2006; Cai et al., 2007; Col et al., 2007; Erzurumlu and Oktem, 2007; Guler and Artir, 2007; Yilmaz and Ertunc, 2007; Forouzan and Akbarzadeh, 2007; Selvakumar et al., 2007; Ates, 2007; Umbrello et al., 2008; Martn et al., 2008; Ozerdem and Kolukisa, 2008; Kazan, Firat, and Tiryaki, 2008; Jiang et al., 2008; Raj and Daniel, 2008; Lin et al., 2008; Altun and OKisi, 2008; Bezerra et al., 2008; Zhang et al., 2008).	48
Modelling	(Malinov et al., 2001; Zeng et al., 2002; Smith et al., 2002; Wong and Hamouda, 2003; Guessasma et al., 2004; Guessasma and Coddet, 2004; Guo and Sha, 2004; Parlos et al., 1994; Guo et al., 2005; Altinkok and Koker, 2005; Koker et al., 2007; Su et al., 2005; Bahrami et al., 2005; Saltan and Sezgin, 2007; Demirhan et al., 2007; Kafkas et al., 2007; Karatas et al., 2007; Nemati and Moetakef, 2007; Okuyucu et al., 2007; Karnik et al., 2008; Mirzadeh and Najafizadeh, 2008; Anaraki et al., 2008; Karatas et al., 2008; Zhao et al., 2008)	37
Control	(Guessasma et al., 2003)	1
Identification	(Xu et al., 2004)	1
Design	(Dym, 1998; Cai et al., 2005)	3
Optimisation	(Liujie et al., 2007; Xu et al., 2007 ;Cui et al., 2008)	5
Critique	(Sha and Edwards, 2007; Smets and Bogaerts, 1992; Cottis et al., 1999)	5

Table 2. Important ANN architecture description variables.

Parameter	Data type
Number of layers	Integer
Number of input layer neurons	Integer
Number of hidden layer neurons	Integer
Number of hidden layers	Integer
Number of output layer neurons	Integer
Momentum rate	Real
Learning rate	Real
Error after learning	Real
Learning cycles or Epoch	Real

This is why the ANN technique is considered to be model-free and useful in the modelling of complex input-output relationships. Also the ANN is tolerant to data containing noise and measurement errors. Conventional ANNs have a number of limitations which must be borne in mind when applying them in materials engineering. First, there is the need to manage a large number of parameters used for controlling variable in ANN model. This process is not systematic but intuitive. Inability to appropriately manage ANN model parameters accounts for the difficulty in obtaining stable solutions and danger of overfitting resulting in the lack of generalization capability In addition, ANN models are not expressive as they could not be used to explain, in a comprehensible manner, the process underlying their results. ANN, therefore, results in “black box" models which are not very useful in situation when it is important to understand the operation of the system, such as in the design of materials meant for use in safety critical systems.

FUZZY LOGIC

Zadeh (1965, 1973) laid the foundation for the engineering applications of fuzzy logic (FL). FL has been applied in diverse areas like control systems, pattern recognition, forecasting, reliability engineering, signal processing, monitoring, and medical diagnosis (Zimmermann, 1996; Takagi and Sugeno, 1985; Bezdek, 1993; Perzyk and Meftah, 1998; Arroyo-Figueroa et al., 2000; Karray and silva, 2004; Mellit and Kalogirou, 2008). Fuzzy logic, upon which fuzzy models are based, is a generalization of the binary logic. Unlike the binary logic, however, truth-values in the range (0*;* 1) are assigned to variables. The membership of element in classical set theory is binary, that is an element x *must* belong to a set *S* or not. In fuzzy set, on the other hand, a class admits the possibility of partial membership in itself. For example, if X = {x} denotes a space of objects, the fuzzy set A over X is a set of ordered pairs $A = \{x; \mu_{A(x)}\}$, where $A(x)$ is the degree to which x belongs to A. If the function $\mu_{A(x)}$ returns the value 0:0

Table 4. Tropical screw specification.

A screw for fasting computer components together should have shafts and blades made of *high* carbon steel. Steel is used because it has *high modulus*; the modulus measures the resistance of the materials to elastic deflection or bending. The shafts must also have *high yield strength*; this will prevent the screw from bending plastically or permanently if used to drive bolts against a hard or dusty casing. Such situation arise when the bolts is stuck into a casing that has become rusty due to *high humidity* and dust. The blade must have a *high hardness*; this will prevent the screw from being indented by the materials of the computer bolts. The screw materials must also have a *high fracture toughness* to prevent it from breakage when twisted. In addition, it must have *low tendency* for rust in humid environment.

Table 5. A comparison of materials properties for different fibres (Chen et al., 1995).

	E-glass	**S-Glass**	**Carbon / graphite H.M.)**	**Carbon / graphite (H.S.)**
Specific tensile strength	Low	Moderate	Moderate	High
Specific Young's modulus	Low	Low	Very High	High
Specific compress strength	-	Low	Moderate	High
Specific shear strength	-	Good	Fairly-good	Good
Impact strength	Fair	Fair	Poor	Poor
Elongation	Moderate	Moderate	Low	Moderate
Fibre cost	Very-Low	Very-Low	High	Moderate

then x does not belong to A at all. If the value returned is 1.0 then x is totally a member of A. Partial membership of an element x to a set A is modelled by numbers between 0.0 and 1.0. The closer $\mu_{A(x)}$ is to 1.0, the more x belongs to A. For example, a $\mu_{A(x)}$ of 0.5 indicate that x's membership in A is 50%.

Fuzzy set, therefore, provides a powerful computational paradigm for extending the capability of binary logic in ways that enables a much better representation of knowledge in materials engineering. This is because fuzzy logic facilitates the expression of continuum by way of assigning numerical grade of membership. The multi-value attribute of FL allows intermediate values to be defined between conventional binary evaluation points, such as the degree of presence or absence of a material constituent in a composite. This facilitates the intuitive assignment of numerical values in obtaining exact solutions even when vague or imprecise concepts are used to describe materials properties.

While designing materials for computer hardware repair tools meant for use in topical areas, the description in Table 4 formed part of the requirement we generated based on our interactions with technicians. As can be seen in that table, all the variables were expressed without stating specific numerical values, but their degree of strengths. In (Chen et al., 1995) the comparison of materials properties for some fibres and matrices in aerospace structures are described as having high strength-to- weight and stiffness-to-weight ratio properties (Tables 5 and 6). The FL technique facilitates the development of a powerful method for modelling this kind of vague and imprecise knowledge. Fuzzy values are different from probability values. For example, when we say that a material with stress value of 210.00 MPa has a fuzzy value $\mu(x = 210.00) = 0.95$ in the High class we do not mean that there is 95% chances of the stress been categorised as High. What this implies is that on a scale of 0.0 to 1.0, a stress value of 210.00 MPa is 0.95 compatible with the linguistic description High. This is similar to classifying a student that scores 95% in an examination as among the very best in a class. The value 0.95 is therefore not an expression of the probability of occurrence but a confidence value which allows us to represent the compatibility between a linguistic label and a numerical value.

Table 6. A comparison of materials properties for different matrices (Chen et al., 1995).

	Epoxy	**Peek**	**Polyimide**
Service temperature	Low	Moderate	High
Water absorption	Fair	Excellent	-
Electrical properties	Excellent	Good	Excellent
Thermal expansion	Excellent	Excellent	-

To develop a FL based model, there is the need to first design the membership functions (MF). MFs convert crisp inputs into linguistic terms. The membership functions can take different forms depending on the model design

strategy and how the behaviour of the materials is described. Trapezoidal, triangular, and sigmoid functions are most commonly used in materials engineering. In some situation the membership functions are determined automatically by using data summarisation or optimisation techniques (Mohamed et al., 2004). Linguistic variables are the core element of concept description in fuzzy logic. Formally, a linguistic variable, defined over a continuous universe of discourse UoD, can be characterised by five attributes and formally defined by a 5-tuples;

$$\langle x, T(x), U, G, M \rangle$$

where x is the name of the variable; $T(x)$ is the term set of x, that is, the set of linguistic values of x with each value being a fuzzy number on U; G is the syntactic rule for associating the names of values x; and M is a semantic rule for associating with each value its meaning.

For example, if x is the tensile strength as represented in Table 5 then the linguistic terms Low, Moderate, and High, will form the term set, $T(x)$. Hence $T(x)$ = (Low, Moderate, High). If $T(x)$ is characterised by a fuzzy UoD with numerical values in the range U = [90.00; 400.00] g/mm^2 then a membership functions can be defined over UoD with each linguistic variable occupying portions of the UoD. A triangular membership function defined over this UoD is shown in Figure 9(a). The tensile strength with values 120.50 g/mm^2 is computed as μ (120.50) = 0.5 in the fuzzy class Medium as shown in Figure 9(b).

Membership function can overlap. Usually, the UoD is normalised into the interval [0.0; 1.0] for convenience and ease of membership function derivation. As the tensile strength property of materials is a vague concept that it is difficult to represent by a numerical measure, especially for a higher temperature (Tien, 2005), the use of such linguistic description can be most useful. Membership functions that are popularly used in materials engineering are listed in Table 7. A description of a FL based model is shown in Figure 10. The model comprises four principal components: a fuzziffication process, fuzzy knowledge base, decision-making logic and de-fuzziffication unit. Crisp data in the form of numerical values are usually the input and output of fuzzy logic based systems.

Input fuzzification process

The fuzziffication process performs a scale mapping that transfers the range of numerical or crisp input values into linguistic values using the membership function. The membership function actually converts the numerical values into suitable values which are associated with some linguistic terms. The mapping is done over the universe of discourse of the respective input variable. The fuzzification process uses predefined membership functions to map input into linguistic terms. Specifically, the fuzzification process permits a binding to take place between linguistic terms and membership functions, making the terms amendable to fuzzy computation.

Inference process

The inference process uses a fuzzy knowledge base (FKB) to compute the output corresponding to the fuzzy input. The FKB comprises of a knowledge base for the application domain in the form of fuzzy membership function (FMF) database and linguistic rules. The FMF database provides the necessary definition that must be used by the linguistic rules to generate decision. The fuzzy rules characterises the decision goals, usually, as specified by a domain expert. A set of predefined rules are applied to the output of the fuzzification process. The rules are in the form of if-then statement. The inside of a rule contains one or more conditions, called antecedence. The then side contains one or more implications or actions call precedence. The inference process evaluates the rules by computing the degrees to which each of the rules should activated to form the output. The then part of a fuzzy rule can be a mathematical function that computer crisp value as in the Takagi and Sugeno, 1985 model. The choice of process state variables, the fuzzy partition of the input space and the choice of membership function in this case is done using a trial-and-error approach. The fuzzy decision process is done using computations over linguistic terms. Each rule in the FKB is considered and its output is activated in accordance with the degree of truth that is evidence in its premise. To infer the output of the fuzzy system, the output of each rule is combined in a process called aggregation.

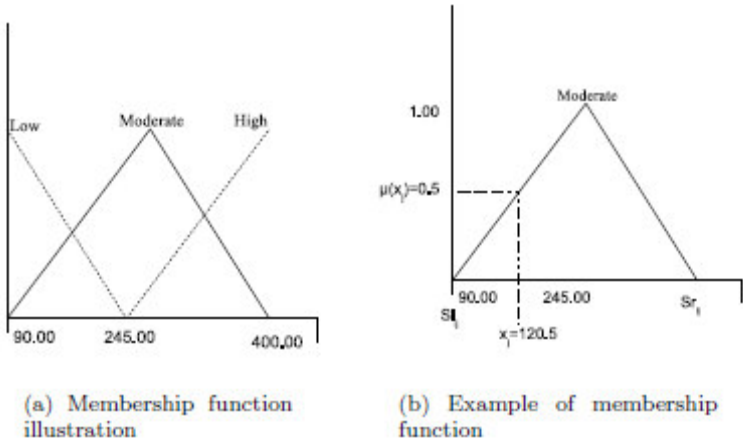
Defuzzification process

The output of the inference process is in linguistic form. To be useful, this output must be converted to its crisp or non-fuzzy form. The defuzzification process computes the outputs by mapping the rule strengths computed by the predefined rules (D'Errico, 2001) to real number values. The Mean of Maximum (MOM) and the Center Of Gravity (COG) formulae are commonly used in the defuzzification process used in materials engineering. To illustrate the COG, assuming that the discrete fuzzy set Af = ($\mu(x_1)$, $\mu(x_2)$…μ (x_n)), is given and the following function is used to weight its membership functions;

$$K(\bar{x}) = \sum_{i=1}^{n} (x_i - \bar{x})^2 \mu(x_i). \tag{8}$$

If we consider Equation 8 as cost function, then we can minimise it by taking its first derivative and equating it to zero as follows:

$$\frac{dK(\bar{x})}{d\bar{x}} = 2.0 \times \sum_{i=1}^{n} (x_i - \bar{x}) \mu(x_i) = 0.0. \tag{9}$$



(a) Membership function illustration

(b) Example of membership function

Figure 9. Fuzzy membership functions illustration.

Table 7. Fuzzy membership functions.

Function name	Mathematical expression
Triangular	$f(x,a,b,c)=\max\left\{\min\left(\frac{x-a}{b-a},\frac{c-x}{c-b},0.0\right)\right\}$
Trapezoidal	$f(x,a,b,c,d)=\max\left\{\min\left(\frac{x-a}{b-a},1.0,\frac{d-x}{d-c},0.0\right)\right\}$
Bell-shaped	$f(x,a,b,c)=\frac{1.0}{1.0+\left\|\frac{x-c}{a}\right\|^{2b}}$
Gaussian	$f(x;\alpha,c)=\exp^{\frac{-(x-c)^2}{2\alpha^2}}$
Sigmoid	$f(x,a,b,c)=\frac{1.0}{1.0+\exp^{-a(x-c)}}$

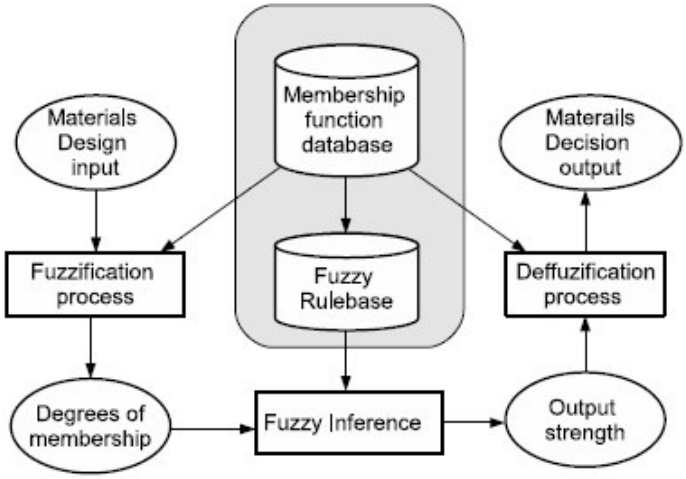


Figure 10. Fuzzy logic model.

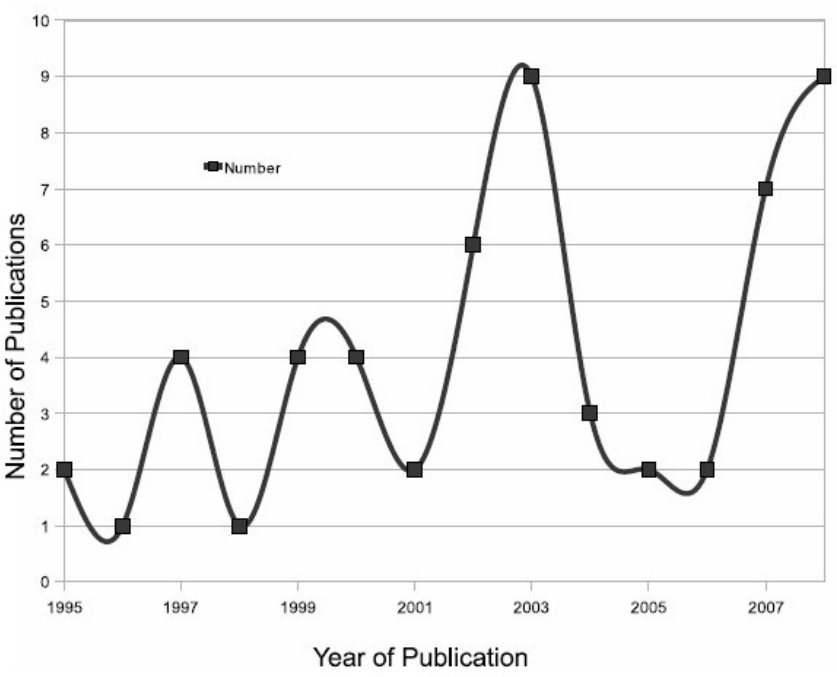


Figure 11. Graph of fuzzy logic based models in materials engineering.

Making $\bar{x}$ the subject of Equation 9 we have:

$$\bar{x} = \frac{\sum_{i=1}^{n} x_i \mu(x_i)}{\mu(x_i)}. \quad (10)$$

Equation 10 is the center of gravity (COG) defuzzification formula. This formula has been extended to obtain the weighting function COG (WFCOG) defuzziffication method, which can represent subjective attitude of design decision. An expansion of the COG method using a parameterized defuzzification method with maximum entropy weighting function was proposed in (Liu, 2007).

Application of fuzzy logic in materials engineering

As shown in Figure 11 the application of FL in materials engineering is increasing but not as popular as ANN. There are about 3 papers in 1995 which increased to 9 papers reporting the application of FL in 2008. As shown in Figure 12 fuzzy logic has been applied in the areas of materials properties modelling, selection, prediction, evaluation, design, clustering, optimisation, control, monitoring and model identification. The majority of the paper follows the procedure we described above for the membership function generation and defuzziffication module design. As shown in Table 13 FL technique is more frequently applied in materials properties model and selection, which account for 21% each of the paper we reviewed. This is followed closely by materials properties prediction which accounts for 20% of the paper reviewed. The application of FL in materials process control accounts for 13% and applications in materials properties optimisation accounts 8%. Few publications have also reported the application of ANN in materials properties evaluation and clustering, about 2%. In all the publications we reviewed, the use of FL in materials engineering, particularly in materials properties modelling and prediction, seems to be motivated by the fact that it makes the materials development process more expressive and its solution easier to interpret. Fuzzy modelling makes certain types of problems easier to handle and often yields more information than does the ANN. However, in some of the work reviewed, (Wong et al., 1999; Wong and Hamouda, 2002; Zhu et al., 2003), the number of input variables is large making the justification for the application of FL as a solution that is easier to interpret, difficult. The confounding nature of variable interaction, when their number is larger, that is greater than five makes it difficult to analyse the effect of the input on the output obtained from the model. We think that when the number of input is large a good engineering option is to modularise the model.

Apart from the limitations we highlighted above, the FL technique has some inherent limitations that should be considered when being applied to materials engineering. First, the process for membership functions generation is context dependent and may be influenced by many design preferences adopted by the engineer. This is not a good enough process as it is desirable in practical applications of materials to use a systematic technique that has a well laid out structure. Second, the design of the defuzzification process is dependent on experience and it is often accomplished by a trial-and-error method (Borto-

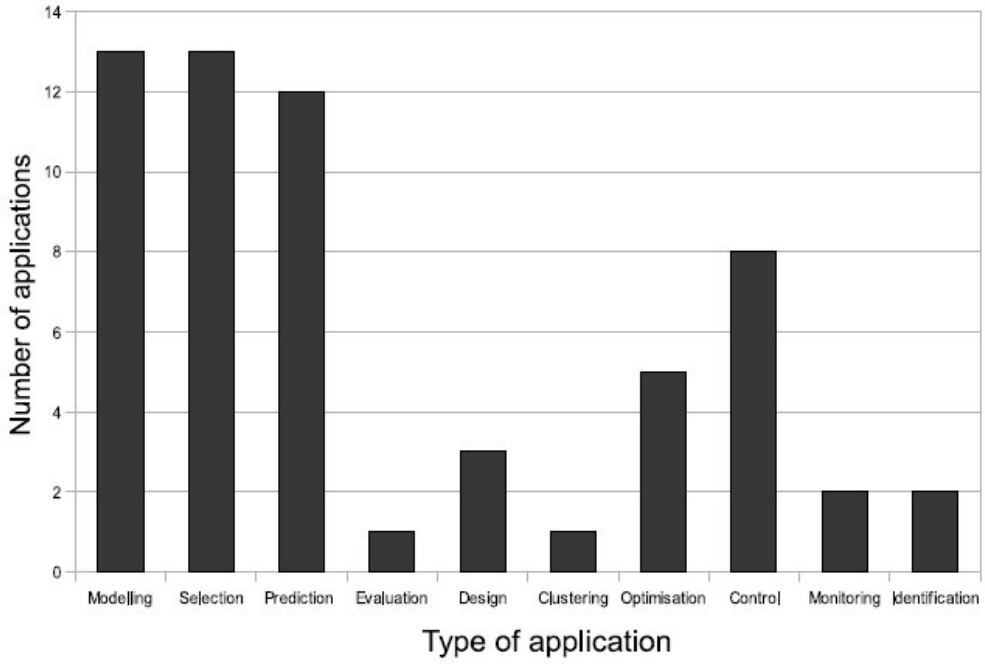


Figure 12. Application of fuzzy logic based models in materials engineering.

Table 13. Applications of Hybrid in ME.

Applications	Publications	% of Total
ANN-Fuzzy	(Tsai and Wang, 2001; Shuiping et al., 2002; Hancheng et al., 2002; Miaoquan et al., 2002; Lin et al., 2002; Kuo et al., 2002; Lezanski, 2001; Lu et al., 2003; Chen et al., 2003; Zhu et al., 2003; Jalham, 2005; Vitanov and Voutchkov, 2005; Garca, 2005; AsiltÄurk and UnÄuvar, 2008; Uros et al., 2008; Topcu et al., 2008)	57
Fuzzy-GA	(Tarng et al., 1997; Kojima et al., 2001; Zhao and Zhang, 2002; Nandi and Pratihar, 2004a; Yan and Fang, 2008)	18
GA-ANN	(Aijun et al., 2004; Oktem et al., 2006; Anijdan et al., 2006 ; Zakeri et al., 2007; Zhou et al., 2008)	18
ANN-Fuzzy-GA	(Tuma et al., 1996; Inal 2008)	7

lan and Pedrycz, 1997; Roychowdhury and Pedrycz, 2001). It is well known that defuzzification process can produce counter-intuitive results even when they have been carefully designed (Wang, 1996; Mizumoto, 1988). Although fuzzy logic provides an effective tool for linguistic knowledge representation and manipulation which is transparent, an efficient, definitive and systematic method for capturing this knowledge into practical systems is yet to be developed. In addition to this, the number of rules in a fuzzy rule base can quickly grow and become complex to manage if the number of inputs or the fuzzy sets defined of the inputs is large. These situations make it difficult to guarantee certain fundamental engineering materials properties, such as consistent performance. To this end, we posit that the fuzzy logic based technique should be used bearing in mind that it only provide a paradigm to manage some kind of fuzziness observed in human cognition. Its application to materials engineering should, therefore, not be misconstrued as definitive in conception and absolute in practicality.

The prototype and exemplar theories (Rosch et al., 1976; Wang, 1996) in psychology portend that people judge some instances to be better examples of a concept than some other, and can intuitively assign a number equivalent to degree of membership relation. This finding could be exploited for formalising fuzzy model in order to achieve the level of consistence required in materials engineering.

GENETIC ALGORITHM

The principles of Genetic Algorithms (GA) and the mathematical framework underlying it were developed in the

late 1960s (Holland, 1962; Kristinson and Dumont, 1992; Koppen et al., 2006). GA is normally discussed in the context of Evolutionary Computing (EC). The core methodologies of EC are Genetic Algorithms (GA), Evolutionary Programming (EP), Evolution Strategies (ES) and Genetic Programming (GP) (Oduguwa et al., 2005). In GA, attempt is made to model the processes underlying population genetic theory by using random search. GAs uses the survival-of-the-fittest strategy, where stronger individuals in a population have a higher chance of creating an offspring. To achieve this, the current input (population) is used to create a new and better population based on specified constraints. The inputs are normally represented as string and they model chromosome in human genetics. In materials engineering, for example, the input string will represent some properties of materials that are of interest.

The success of GA application in materials engineering task is dependent on the encoding of variables that describe materials attributes in the form of strings. The number and types of the variables that will be encoded as string depends on the resolution of the data and scale of the problem. Each input variable can be viewed as a gene in the chromosome that represents the input space. It seems more intuitive to represent the genes as real-numbers since the representation is close to how variable are used in engineering. In that case a chromosome will be a vector of floating point numbers and the length of the chromosome is the vector length of the solution to the problem. In many applications of the GAs including those in materials engineering, however, the input variables are encoded as integers or binary strings. Encoding multiple real-value continuous variables consists of converting the numbers into integer and concatenating them. The resulting integer values then become the input variables to the GA process. After the GA processes is completed, the resulting integer string are decoded using a complimentary data conversion process. A four level data processing scheme that could be used to achieve this is depicted in Figure 13. The four levels comprised of: real number, normalised number, integer and binary strings. Real numbers representing the two variables Variable1 and Variable2 with values 12.50 and 0.72, respectively, are first normalised. The normalised values are converted to integer and then encoded as binary strings. The GA processes the binary strings and its output is converted back to real numbers. The input string is subjected to a number of processing steps before the final output is generated, namely: selection, crossover or mating and mutation (Figure 14). The selection process determines which string in the current generation will be used to create the next generation. This is usually achieved through a bias random-selection (BRS) method (Chen et al., 2007; Baumes and Collet, 2008). In the BRS method, parents are randomly selected from the current population in such a way that the best strings in the population have higher chances of being selected. By using the best points to determine the next population, the algorithm is expected to move in the most promising direction towards an optimal solution.

Table 9. Fitness function types.

Typical fitness function
Number of Hits
Sensitivity/Specificity
PPV/NPV
R-square
MSE (mean squared error)
RMSE (root mean squared error)
MAE (mean absolute error)
RSE (relative squared error)
RRSE (root relative squared error)
RAE (relative absolute error)

To determine the fitness of a chromosome, a fitness function is used. Fitness functions are objective functions that quantify the optimality of a chromosome. It facilitates the ranking of a chromosome against all the other chromosomes. Generating a robust fitness function for an application is a major challenge in the development of GA based models. For example, a minimisation problem that has the fitness function *F*(c), for chromosome variable c, can take the form:

$$F(c) = O(c) + P(c), \tag{11}$$

Where O(c) is the objective function and P(c) is the penalty function.

The determination of O() and P() require the use of intuitive, and often non-trivial trial-and-error, approach which are difficult to test. Their usefulness can only be determined based on the results they produce during experimentation and simulation. The fitness function is some kind of error minimisation function over a set of input data modelled using one or more of the error functions listed in Table 9. GAs models do not require the optimization function to be continuous or derivable, or even be a mathematical formula (Mantere and Alander, 2005). For example, it is possible to define a fitness function f (m_e) = $1/m_e$, where m_e is the mean absolute error in the training set. In that case the best individual in the population would be the chromosome with the minimum error.

During the mating process, the strings that describe materials properties are selected and paired. This pair is called the parent string. In the basic crossover operator, if the length of the parent strings is l, an integer number between 1 and l is randomly selected. Assuming that the randomly selected number is s, the mating process swaps bits s + 1 through r of the first parent with string s+1 through l of the second parent. This swapping process is called also crossover (Figure 15). In this way, two new strings (called offsprings) are created for the current generation. More complex crossover operators such as, flat, arithmetic, and blend (Herrera et al., 1998) can also be used to achieve the operation but the basic crossover

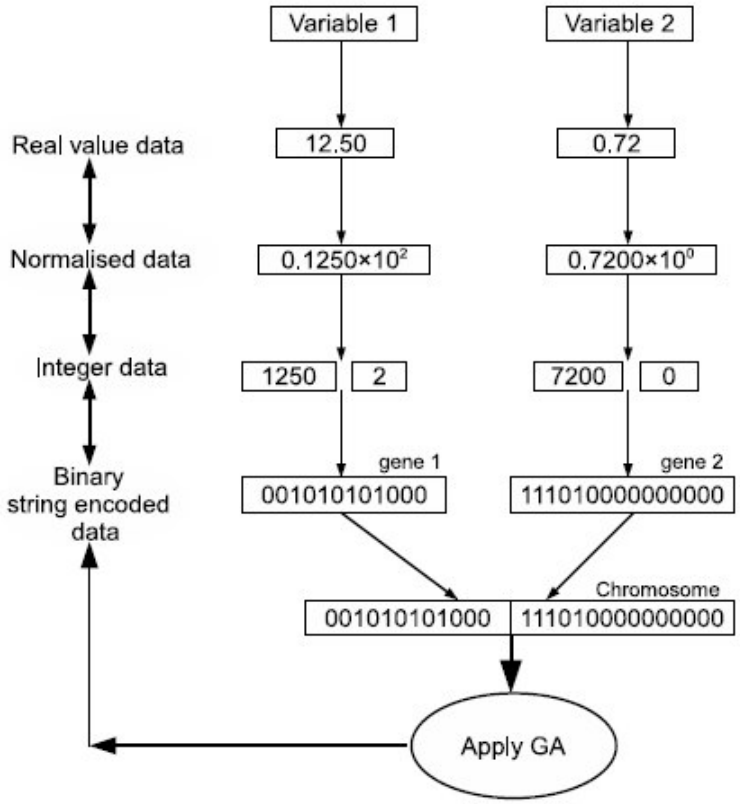


Figure 13. Variable processing in genetic algorithms.

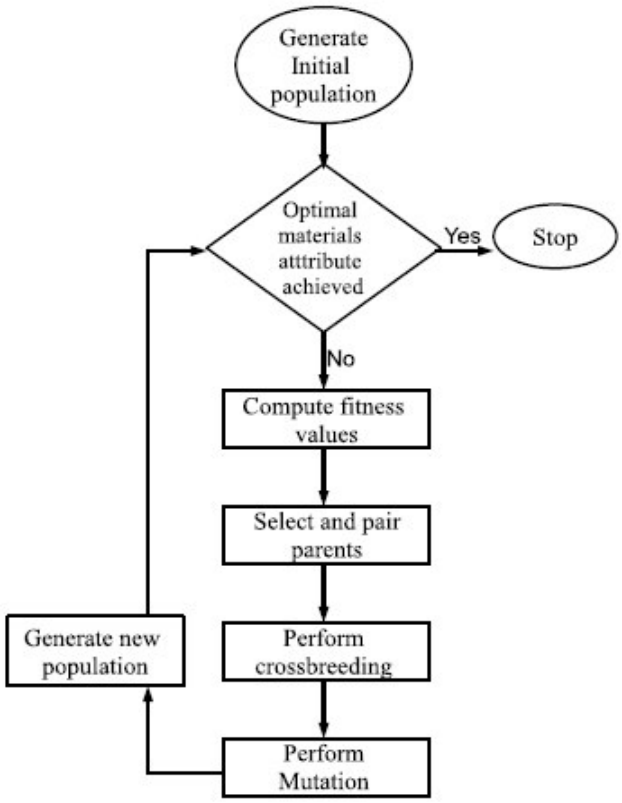


Figure 14. Genetic algorithms process

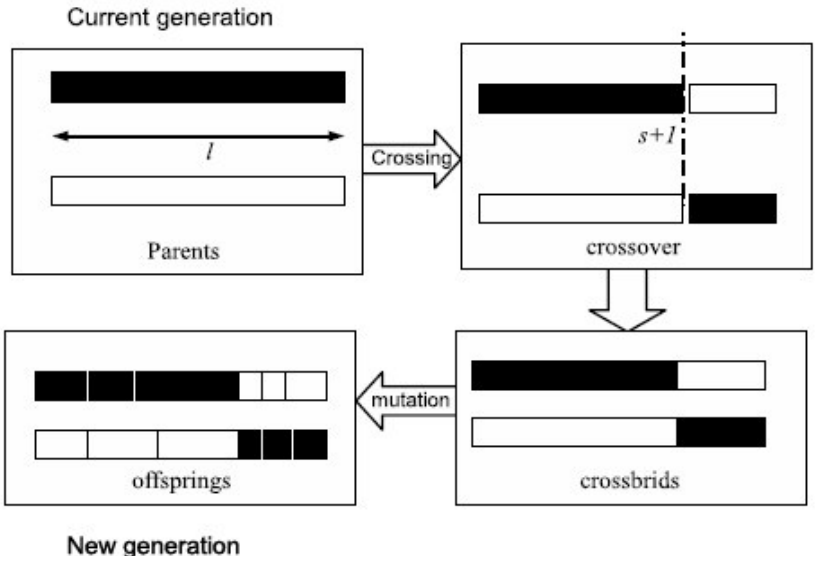


Figure 15. The crossover process

operator described above is frequently used in materials engineering. In the final step called mutation, bits in all the new strings or chromosome are subjected to changes based on a mutation probability. A fixed small mutation probability is usually set at the beginning of the algorithm. The bits at specific location in the chromosome are flipped by replacing the 0s by 1s and the 1s by 0s. To illustrate this process, given a chromosome;

$$C = (c_1, c_2, \ldots, c_n), c_i \in [0,1]$$

and the gene cj is a gene to be mutated. A simple mutation algorithm computes $c_i' = c_i$ using the formula:

$$C_i' = \begin{cases} 0 & = \text{if } \ c_j = 1 \\ 1 & = \text{if } \ c_j = 0 \end{cases} \qquad (12)$$

There are other more complicated mutation operators such as non-uniform mutation and random mutation but the fixed number bit swapping operator discussed above is frequently used in materials engineering. The resulting strings from this process forms the new population for the next generation of the GA process. Mutation is conducted to prevent the premature convergence of the design variables. Convergence occurs when the bit structures of strings in the mating pool become identical in an early stage of the GA evolution process. The GA process continues until a set of stop criteria are met. Such stop criteria may be when an individual recognises all the examples or when a maximum number of generations have been run. In materials engineering such criteria may correspond to specified material yield strength or hardness of a composite.

Applications of the genetic algorithm in materials engineering

As shown in Figure 16 the application of GAs in materials engineering is increasing but not as popular as FL. There are about 4 papers in 2004 which increased to 20 papers 2008. The majority of the papers in 2008 appear in the special issue of Computational Materials Science Journal. As shown in Figure 17, the GAs techniques have been applied in the areas of materials properties modelling, optimisation, identification, prediction and design. The majority of the application is in materials properties modelling and optimisation which account for about 32% each of the total paper reviewed. Model identification accounts for 10% while materials properties prediction and design accounts for 4%. From all the papers reviewed, it was shown that GAs have proven effective in the materials properties optimisation problems and areas that require parameter training such as function optimization, materials processing and system identifications (Holland, 1962; Goldberg, 1989; Michalewicz, 1996; Fang et al., 2008). Since the GA process proceeds from several points, the method has a better probability of locating a global minimum as opposed to ANN and FL models that proceed from one point to another. Also GAs work on a coding of design variables rather than on the variables themselves, which allows for an extension of these algorithms to design space consisting of a mix of continuous, discrete, and integer variables (Tarng et al., 1997). The application of GA in materials engineering is growing although not as popular as those of ANN and FL. Two reasons account for the limitations of the application of the GAs in materials engineering. The first is the use of randomness in obtaining optimal solution. From an engineering point of view, the concept of randomness is difficult to explain and justify in real-life applications, particu-

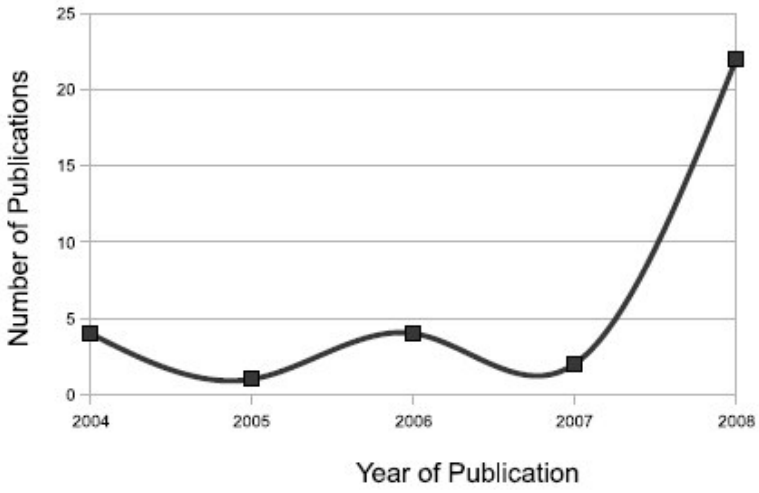


Figure 16. Graph of GA application by year.

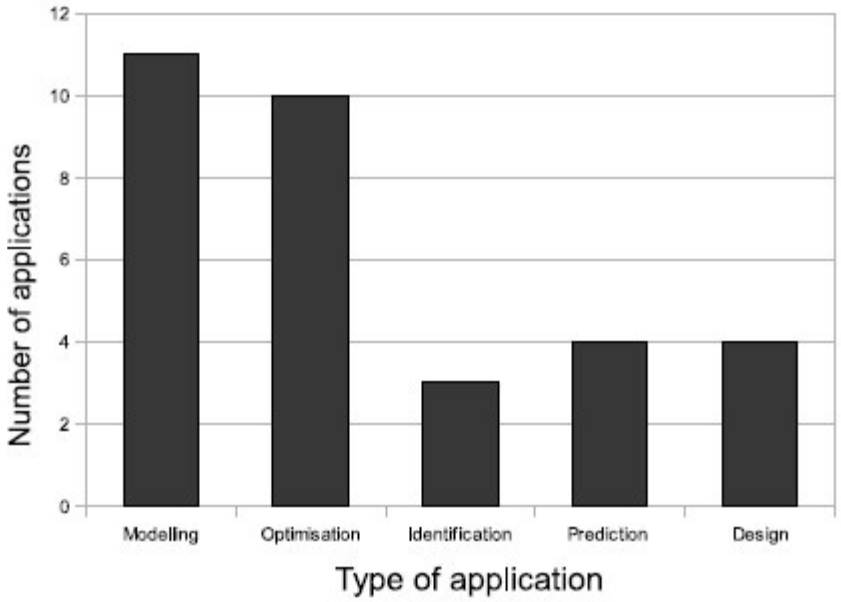


Figure 17. GA application histograms.

larly in safety critical systems. The second limitation relates to the intuitiveness of evolution theory in problem solving. FL and ANN seem intuitive as a model for human learning and linguistic knowledge used in solving real-life problems. How the theory of human genetic factors into human problem solving is not very clear.

HYBRID MODELS

The soft-computing techniques, particularly those discussed here, are complementary rather than competitive (Zadeh, 2001, 1994). This implies that a hybrid model employing a combination of artificial neural networks, fuzzy systems, and/or genetic algorithms should produce better results. The various combinations of these approaches have proven useful in the development of robust intelligent systems (Zadeh, 2001). For example, the fuzzy logic based technique can be combined with neural networks to form neuro-fuzzy model. There are at least four hybrid models that can be created from the above SC techniques:

i) Neuro-fuzzy
ii) Fuzzy-genetic
iii) Neuro-genetic,
iv) Neuro-fuzzy-genetic.

Table 11. Soft computing constituents (Hoffmann et al., 2005).

	Methodology	Strength
1	Artificial neural networks	Learning and approximation
2	Fuzzy systems	Approximate reasoning
3	Evolutionary algorithms Systematic	random search/optimisation

Table 12. Comparison of soft computing techniques features.

Methods	Learning capacity	Knowledge representation capacity	Real-Time operation functionality	Optimisation capacity	Data requirements	Expert input level
ANN	VH	H	H	M	VH	VL
FL	M	VH	M	VH	M	VH
GA	M	M	H	VH	M	M
FL-ANN	M	H	M	L	M	VL
FL-GA	M	M	M	L	M	M
ANN-GA	M	M	H	M	M	VL
FL-ANN-GA	M	M	M	L	M	VL

V L = Very Low; L = low; M = medium; High= V; H = Very High

The strength of each of the SC techniques is summarised in Tables 11 and 12 summarises a subjective assignment of the capabilities of the hybrid SC techniques. We briefly summarise them in the following subsections.

Neuro-fuzzy

The neuro-fuzzy model, which involves the integration of ANN and FL techniques are perhaps the most popular hybrid technique used in materials engineering. Neuro-fuzzy models are able to take advantage of the fuzzy inference mechanism capabilities in fuzzy logic and the learning ability of neural networks. The ANN technique is usually used as the learning algorithm for the defuzzification process in FL based models. Neuro-fuzzy models are regarded as black-box models which provide little insight to help understand the underlying process. Figure 18(a) illustrates a simple configuration of a neuro-fuzzy model.

Fuzzy-genetic

When the FL and GA techniques are combined to develop a solution, the fuzzy-genetic model results. The aim here is to exploit the ability of the fuzzy logic at knowledge description and the optimisation capability of the genetic algorithm. Usually, the defuzzification process in fuzzy logic based model are developed using optimal selection of elements from a fuzzy set. Aside from GA, techniques that employ the concepts of interaction, variability, and voting techniques are also used to optimise the defuzzification and membership generation process. Figure 18(b) illustrates a simple configuration of a fuzzy-genetic algorithms model.

Neuro-genetic

When the ANN and GA techniques are combined to develop a solution, the neuro-genetic model results. The aim here is to take advantage of the learning ability of the ANN and optimisation ability of the genetic algorithm. Figure 18(c) illustrates a simple configuration of a neuro-genetic algorithms model. No application of neuro-genetic algorithms model in materials engineering has been reported in the literature we reviewed.

Neuro-fuzzy-genetic

When the three SC techniques discussed here are combined to develop a solution, the neuro-fuzzy-genetic model results. Usually, the GA approach is used to optimise the performance of a neuro-fuzzy system. The development of this approach is usually guided by heuristics, based on the experiences of an expert materials engineer. In (Huang, Gedeon, and Wong, 2001) the architecture in Figure 19 was proposed for developing a neuro-fuzzy-genetic model for predicting the permeability in petroleum reservoirs. The vector X^c and matrix Z^c are the training pattern and Y^c is the target output. The following heuristics was proposed for its realisation:

- Select appropriate well data set.
- Generate fuzzy rules by neural networks.
- Generate hyper-surface membership function by neural network.
- Optimise defuzziffication operator parameters by gene-

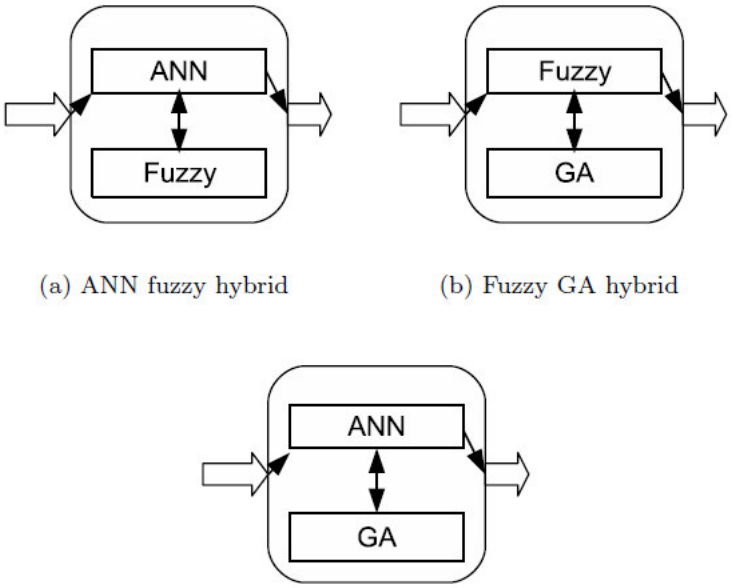


Figure 18. Hybrid soft computing models.

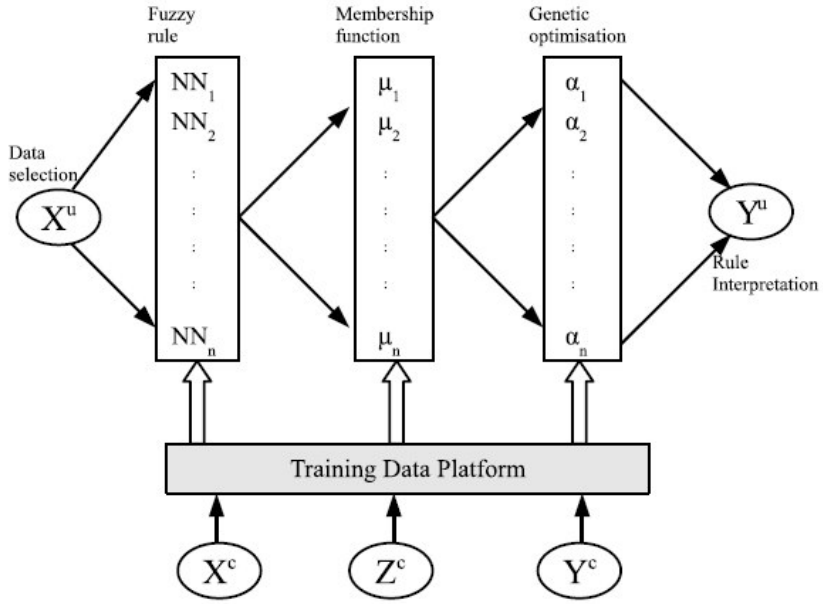


Figure 19. ANN –fuzzy-GA hybrid (Huang et al., 2001).

ric algorithms;
- Interpolate fuzzy rules to provide estimates.

Applications of the Hybrid methods in materials engineering

As shown in Figure 20 the application of SC hybrid techniques in materials engineering is increasing but not as popular as FL and ANN. There are about 3 papers in 2001 which increased slightly to 5 papers 2008. As shown in Figure 21 hybrid models have been used in materials properties modelling, optimisation, identification, prediction and design. ANN-fuzzy model is the most popular hybrid as it accounts for 57% of the total. The rea-

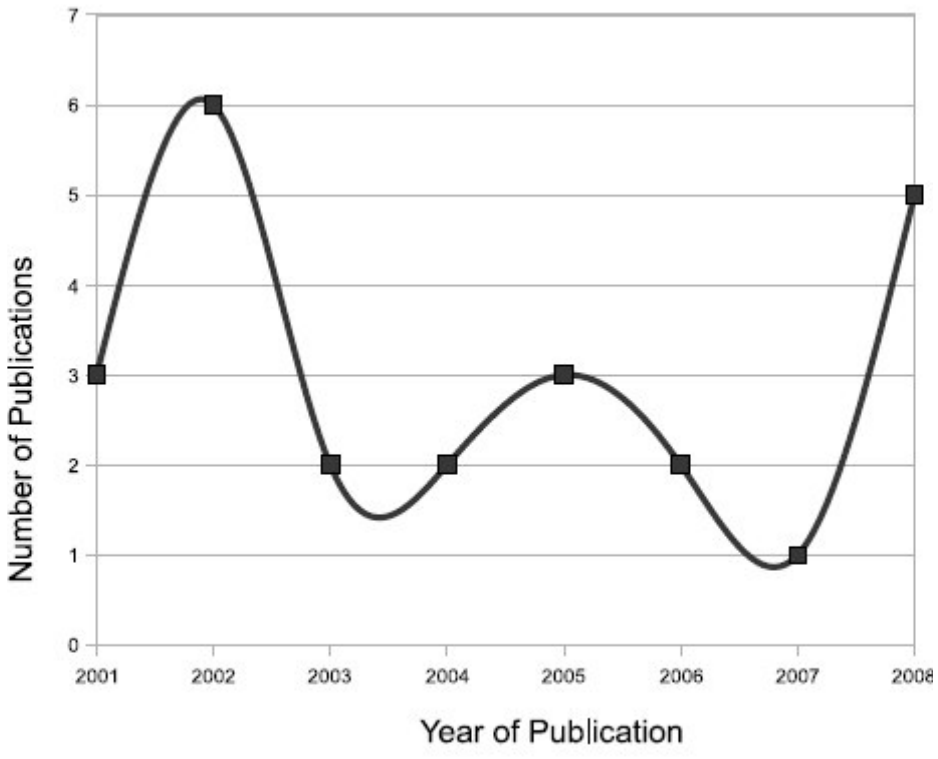


Figure 20. Graph of hybrid application by year.

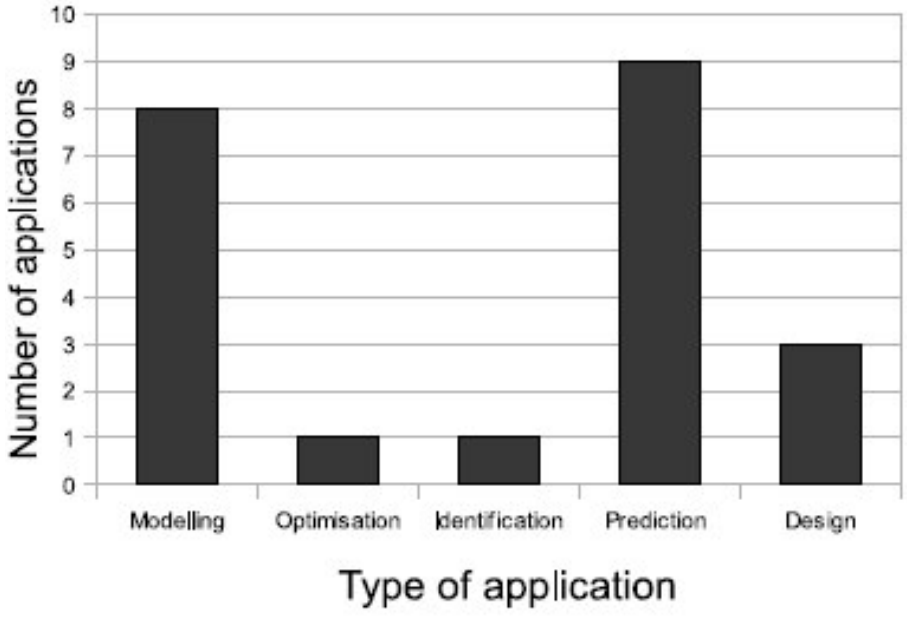


Figure 21. Histogram of hybrid application.

son for this is not far fetch as the aim in most engineering application is to produce an expressive system that is easy to understand and update. The ANN-fuzzy model facilitates these aims. The Fuzzy-GA and ANN-GA account for 18% each of the total applications while the neuro-fuzzy-genetic model accounts for 7% of the applications. Although the hybrid models in materials engineering has been shown to produce better results (Ermolaeva et al., 2004) the processes underlying the development and implementation of such models is very complex. There is no veritable method to guarantee that the methods will always perform well. Other intelligent sy-

stems engineering techniques that have been applied in materials engineering include, decision trees (Georgilakis et al., 2007; Shao et al., 2001), expert system (Long et al., 2004; Buggy and Conlon, 2004; Faura et al., 2001; Alitavoli and McGeough, 1998; Vitanov et al., 1995) and probability based decision model such as the Monte Carlo model (Lin et al., 1997).

FORMALISING THE SOFT COMPUTING APPLICATION METHODOLOGY

Soft computing techniques provide appealing alternatives for supporting the materials engineering process. Although the soft computing constituents have several advantages when used individually, a synergistic integration of these complementary techniques into hybrid models have the potential for the development of practical and efficient intelligent materials engineering tools. However, the application of SC in materials engineering is evolving. Our review of the literature revealed that different researchers are employing different views of concepts as well as varying implementation approaches. This makes it difficult to assess, in a definitive manner, the overall implications or outcome of a given implementation. There is no doubting the fact that materials are potentially life critical due to their pervasiveness. Qualities of engineering materials are crucial to the performance of modern safety critical systems and a number of materials related failures have been recorded in recent times. It will not be out of place to speculate that the root cause of a large number of these failures is the ambiguous, incomplete and/or inconsistent specification of materials. This factor includes inadequate consideration for the loading characteristics and physical environment where the materials could be used. During the development of new materials, there is the possibility of gaps between materials requirements and the engineers' conception of those requirements. This will result in the generation of compromised specification and hence an unrealistic application of SC solution. This misunderstanding could go undetected in the absence of a practical automated or formal method that adequately supports process life cycle activities in materials engineering. Some form of standardisation then becomes very crucial in order to achieve manageable and acceptable engineering practise (Zadeh, 2001; Hoole, Mascrenghe, and Navukkarasu, 2007; Erdik, 2008). In our ongoing research, we are developing a formal technique for eliciting and refining materials specification. The fundamentals of the specification process are similar to the principles used in modern software engineering. The aim of our formal approach to the engineering of materials is as follows:

- To support a framework for materials specification that is amenable to computational rendering.
- To achieve precise and consistent designs.
- To improve the accuracy and testability of the materials specification task.
- To improve the cost-effectiveness of the materials engineering process by reducing the disparity between users' requirements and materials design specification hence reducing the possibility of errors in the fabricated materials;
- To support the sharing of materials engineering knowledge between and among engineers, technicians and materials fabricator.

For computational conveniences, we viewed each engineering materials as an object which has properties or attributes that can take values, for example in the real or integer number space. An object can be subjected to events, as part of an engineering process. When an object is subjected to an event, the object changes state. The state change may results in another object with different properties from the original object. Objects are related to each other by way of attribute association predicates. For example, if the process P (.) is applied to object O_{Si} in state S_i, the object will eventually get to state O_{Si}. The relation between object O_{Si} and O_{Sf} is modelled by the process predicate P (.). This requirement can be formally specified as $O_{Sf} \leftarrow P (O_{Si})$ which can be processed computationally. Within the proposed framework (see Figure 22), materials design specifications namely: functional and non-functional, are extracted from the user requirements. The non-functional specifications, which have more consequence for materials design, seems to be the most difficult to formalise. The functional specification are less demanding, as the generic properties of materials on which they are based, are accurately documented in materials science and engineering physics. The procedural knowledge underlying materials engineering can be specified as a series of procedures, and represented in the form of rules. These rules can be imperative or heuristic. They can therefore be viewed as conceptualised information domain knowledge, attributes, relationships between attributes and the constraints on the attributes. A computational representation of this knowledge structure using a formal language model presents a number of interesting challenges. Our approach starts with the formulation of objectives and constraints about materials which are then translated into heuristics. Within this context, the materials engineering problems can be recast as constraint-satisfaction problem (Freuder, 1982; Nadel and Lin, 1991; Kumar, 1992) which can be stated as follows. Assuming we are given a set of variables that describe materials properties, a finite domain for each variable, and a set of constraints that must be satisfied. Each constraint is defined over some subset of the original set of variables and limits the combinations of values that the variables in this subset can take. We define four types of constraints on materials attributes and properties:

State dependent constraints

Once a material enter a state, say SF, the set of proper-

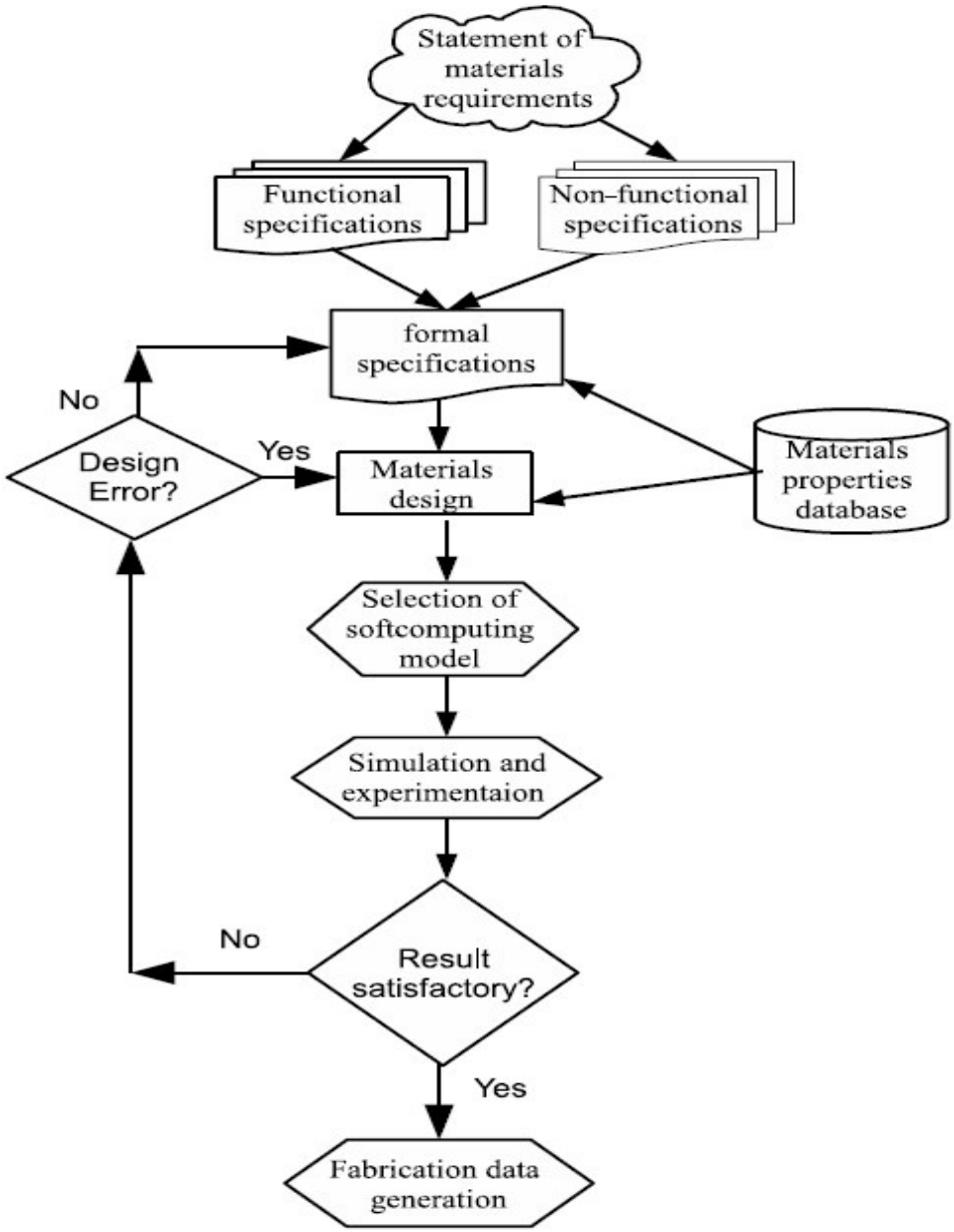


Figure 22. Overview of proposed framework.

ties F must be activated; conversely when the state SF has been left, the properties F are deactivated;

Causal dependent constraints

Once a materials property f1 is activated, another property or property set f2 must be activated, i.e. the activation of property set f1 causes f2;

Mutually exclusive constraints

Once a set of properties f1 is activated, another properties f0 cannot be activated;

Timing constraints

A set of properties *F* is to be activated before another property or set of properties are activated.

The activation or deactivation of materials properties can be triggered by a number of events, including the application of a process or change in environment. The goal is to find one assignment to variables such that all the constraints defined in a materials requirement are satisfied. In materials analysis problem, the goal could be to find all the assignments that satisfy a set of constraints.

Issues of soundness and completeness of materials specification is being addressed in the context of model verification and validation. Our on-going work employs the algebra of descriptive mathematics provided by CASL (Common Algebraic Specification Language) (Bidoit and Mosses, 2004) and the fuzzy automata (Gupta et al., 1977) to realise a formal method for materials engineering.

Conclusion

In this paper, we have presented a review of the applications of soft computing techniques focusing on materials engineering. Although, this paper is by no means an exhaustive review of the literature in the application of soft computing to materials engineering, we hope that we have given an adequate overview of what is currently happening in this evolving and dynamic area of research. As stated earlier in this paper, the decision process underlying the development of engineering systems requires that a compromise be struck between several, usually conflicting, objectives. This process involves decision that utilises intuitively obvious mental (or cognitive) models but that are difficult to articulate mathematically. The soft computing approach is appropriate to support this type of decision because its techniques are very efficient at handling imprecise, uncertain, ambiguous, incomplete, and subjective data and information. Soft computing techniques make it possible to create models and systems by exploiting the approximate reasoning and partial truth in order to mimic the remarkable decisions making ability of humans in real-life situations (Flintsch and Chen, 2004).

Three soft computing techniques are prominently used in materials engineering: artificial neural networks, fuzzy logic and genetic algorithms. The neuro-fuzzy systems seem to be the most popularly used hybrid of these techniques in materials engineering. However, neuro-genetic, fuzzy-genetic, and neuro-fuzzy-genetic applications are also emerging. All researchers that have used SC based approach in materials engineering have reported “excellent", “good", “positive" or at least “encouraging" results. The lack of negative results might be partly due to the fact that materials engineering problems are simplified to manageable and predictable applications.

Modern materials engineering tasks involves the development of products presenting design challenges that involves complex situation with overwhelming data and information which are further constrained by confounding materials processing and fabrication decisions. This complexity seems to have motivated the recent cross-fertilisation of ideas between diverse areas of research: such as materials engineering, computer engineering, intelligent systems engineering and engineering physics. The tool of the trade is also changing from the traditional mathematical and analytical approaches to modelling, simulation and computational approaches.

The interface between materials engineering and intelligent systems engineering techniques, such as the soft computing, is still blur. There is, therefore, the need to put in place some formal structure that remove or reduce grey areas. As the computer is becoming an indispensable tool in modern materials engineering, it becomes desirable to have a computational framework within which various materials could be explored from conceptual-ization, to design through evaluation to fabrication using the computer. How this can be achieved through computation and formal methods is the focus of our ongoing research. Our computational approach to materials engineering has the potential of making materials engineering process more effective and efficient. For example, in composite materials development, this approach can facilitate an algebraic exploration and experimentation, which includes proofs, with various composite models before the commitment of more important materials engineering resources. This will, in effect, facilitates an appropriate management of human efforts as well as natural materials and resources, particularly those that are susceptible to depletion.

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