UTILISING ARTIFICIAL NEURAL NETWORK AND REPRO-MODELLING IN TURBULENT COMBUSTION

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ABSTRACT

Two techniques, Artificial Neural Network (ANN) and Repro-Modelling (RM), are successfully used to represent the chemistry in turbulent combustion simulations. This is a novel application of both methods which show satisfactory accuracy in representing the chemical source term, and good ability in capturing the general behaviour of chemical reactions. The ANN model, however exhibits better generalisation features over those of the RM approach. In terms of computational performance, the memory demand for handling the chemistry term is practically negligible for both methods. The total Central Processing Unit (CPU) time for Monte Carlo simulation of turbulent jet diffusion flame, which is dictated mainly by the time required to resolve the chemical reactions, is smaller if the RM method is used to represent the chemistry, in comparison to the time required by the ANN model. The potential and capabilities of these techniques are extendable to handle the chemistry of different fuels, and more complex chemical mechanisms.

1. Introduction

The adequate representation of chemistry in reacting systems is one of the outstanding problems in turbulent combustion. This is mainly due to the complexity and highly non-linear nature of high temperature chemical reactions. A proper kinetic mechanism to describe the chemistry of a simple fuel like hydrogen, for example, may contain several tens of reactions and more than ten species. Although the systematic reduction of chemical kinetic sets to a manageable size of about 3-5 global reactions is possible [1], the numerical simulation of turbulent combustion remains computationally prohibitive. If look-up tables are used to store the changes in composition due to chemical reaction over specified time intervals, then the computer memory (storage) requirements would become extremely large. Alternatively, the computational run time would increase dramatically if the Ordinary Differential Equations (ODEs) representing the production rates of species are directly integrated during the simulation.

The objective of this paper is to outline a novel approach for representing chemical reactions in turbulent combustion simulations with a modest requirement of memory storage and CPU time. The principle is to produce mathematical equations which describe the chemical behaviour of a system given a set of compositions and reaction time scales. Two methods are used to describe such formulation: Artificial Neural Networks (ANN) and Repro-Modelling (RM). This is yet another genuine application of ANN which are widely used in many aspects of science and engineering. The intrinsic capability of ANN in approximating non-linear systems [2, 3] is essential for representing chemical reactions which are highly

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non-linear functions of temperature and species concentrations. The Repro-Modeling approach establishes functional relations in the form of high-order multivariate polynomials between a set of inputs and outputs. This method has recently been used for combustion simulation by Turányi [4]. Both ANN and RM methods use a training set of inputs and outputs which is generated separately and corresponds to chemical compositions that are accessible during the actual simulation. Since the problem is geared toward accounting for chemical reactions in turbulent combustion simulations, the training set is generated from the chemical system of $H_2/CO_2/O_2$ mixtures using a three-step reduced chemical mechanism [5]. A representative set of values for four scalars (mixture fraction, and molar abundance of CO_2, H, and H_2O) are used here as input and the output represents the change in composition of the reactive scalars; CO_2, H, and H_2O; over a certain reaction time. Although a specific fuel and chemical kinetic scheme is used here, the method can be extended to other fuel mixtures and more complex chemical kinetic mechanisms.

2. Artificial Neural Network Training

The neural network architecture used for this study is a multi-layer perceptron (MLP) that consists of an input layer, an output layer, and two intermediate (*hidden*) layers. A hyperbolic-tangent function is used as a transfer (activation) function. An equal number of neurons in each hidden layer is used as it proved (by trial and error experiments) that it is easier to train MLP network if the number of neurons in the internal layers are balanced. Significant differences in the number of neurons causes a 'bottleneck' junction of information that severely affect the convergence of the algorithm [7]. Similar observations

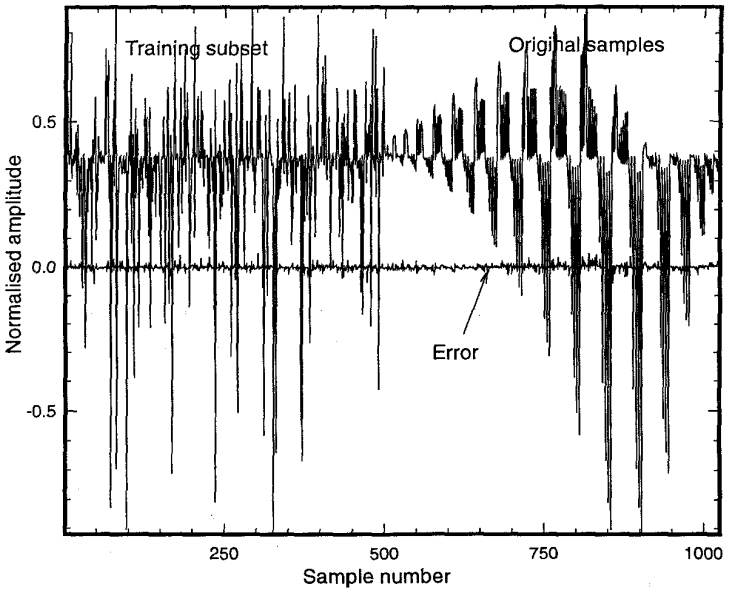

Figure 1: A typical neural network prediction (in normalised units) showing the training subset, the original samples, and the associated errors.

have been reported by deVilliers and Bernard [6]. The learning algorithm used is the backpropagation scheme with an individual adaptive learning rate factors for the weight matrices and bias vectors. A constant value for the momentum term factor is used. The details of the optimisation process and sensitivity analysis of the architecture and topology of the network are described by Christo et al. [7].

In order to reduce the possibility of being trapped in local minima, the training of the ANN is carried

out using a subset of the original training samples. The training subset is generated randomly during the learning process. To achieve smooth behaviour of the algorithm, the size of the subset should be 70%-80% of the size of the training set (see Fig. 1). This continuous (dynamic) randomisation of the subset of the training samples is found to give superior performance, in terms of convergence rate, over using a fixed set of preselected training samples.

Figure 2 shows the actual and the associated errors of the ANN model in approximating the incremental changes $\Delta\Gamma_{CO_2}$ (kmol/kg) of the reactive scalar, CO_2 over reaction time $\Delta t \approx 1.56\mu s$. The small

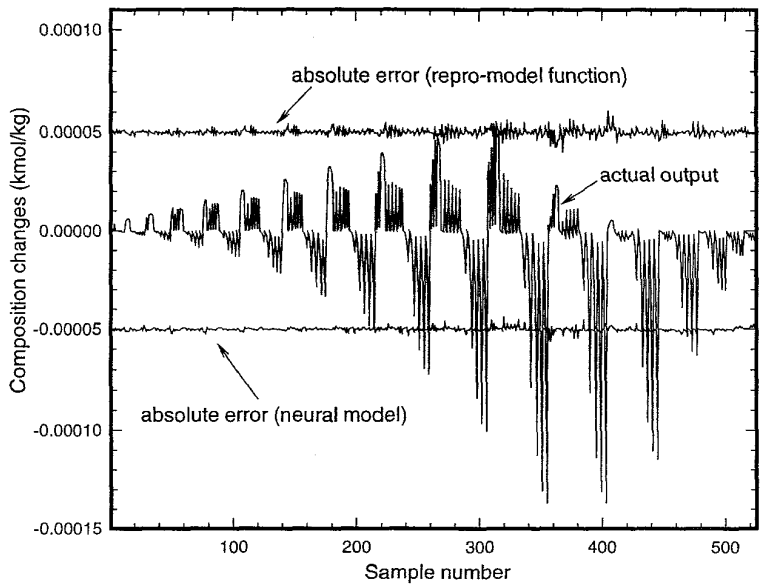

Figure 2: Neural network and Repro-modelling approximation of composition changes of Carbon dioxide, $\Delta\Gamma_{CO_2}$, over reaction time of 1.56 μs, and the associated absolute errors (for clarity, the errors distributions are shifted by a fixed interval).

magnitude of the errors and their uniform distribution implies that satisfactory convergence of the ANN algorithm is achieved over the entire range of the training set, and is not confined only to the subset domain.

3. Repro-Modelling Training

Repro-modelling (RM) means the approximation of a sophisticated, time consuming computational model by a simple empirical model consisting of one or several explicit functions. In the special case of the RM approach called 'parameterisation' technique, an explicit algebraic formulation is obtained by numerical fitting of functions to the numerical solution of the differential equations which describe the chemical reaction. The input-output samples are fitted by a least-square approximation with high order multivariate orthonormal polynomial using the Gram-Schmidt algorithm [8]. To reduce the computational cost in evaluating the multivariate polynomials due to unnecessary multiplications, an appropriate factorisation, *i.e.* Horner equation, is used. The algorithm used does not ensure an optimal factorisation, but the result is close to optimal.

The accuracy of the RM functions in representing the compositional changes $\Delta\Gamma_{CO_2}$ (kmol/kg) over

reaction time of $\approx 1.56\mu s$ is shown in Fig. 2. The figure clearly shows good approximation indicated by small and uniformly distributed errors across the entire samples space.

4. Discussion

To examine the generalisation capabilities of both methods, the ANN model and RM functions are then used to approximate a set of compositions that are collected from a Monte Carlo (MC) simulation of a turbulent diffusion flame of H_2/CO_2 fuel using the probability density function approach [7, 9]. The absolute errors obtained in approximating $\Delta\Gamma_{CO_2}$ for a reaction time of 12.5 μs using ANN and RM methods are shown in Figs. 3(a) and 3(b), respectively. Reasonable accuracy is obtained except for a few

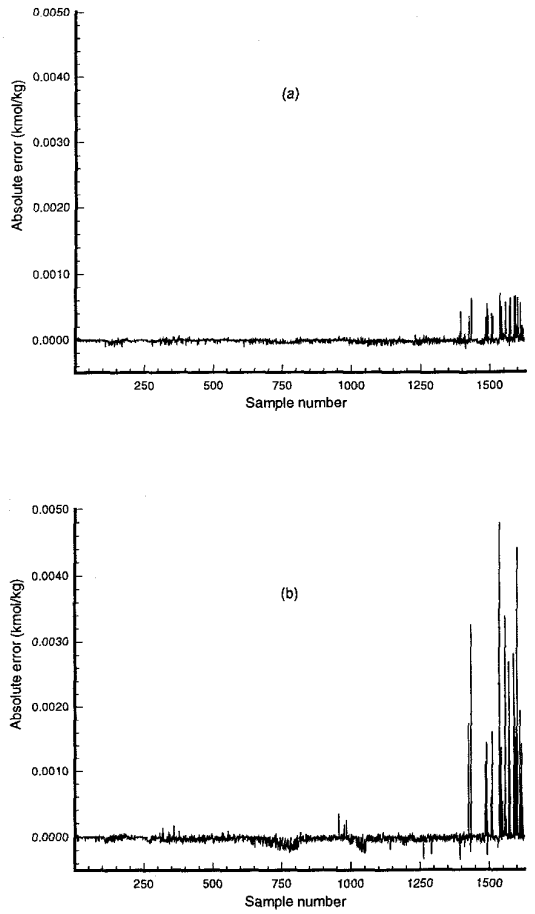

Figure 3: The absolute errors distribution in modelling the composition changes of Carbon dioxide, $\Delta\Gamma_{CO_2}$ over reaction time 12.5 μs: (a) neural network model, (b) repro-modelling function.

samples which constitute less than 10% of the sample space. The overall generalisation performance, measured in terms of the error function E_p [1], of both methods are very good. However, it is better (smaller error function) for the ANN model ($E_p \approx 10^{-7}$) than that obtained by the RM technique ($E_p \approx 10^{-6}$). It is also observed that both methods suffer some degradation in accuracy if the modelled compositions are far enough outside the working range of the model. This result highlights the importance of selecting training samples that are adequately represents the input/output combinations over a broad dynamic range. The appropriate selection of training set is currently an iterative trial and error procedure and

[1] $E_p \equiv \Sigma_{i=1}^{N}(d_i - y_i)^2$, represents the difference between the network's outputs, y_i and the desired outputs d_i, over the N training samples.

remains one of the major problems encountered during the development of the ANN and RM models. A new approach known as 'statistical mapping', to address the problem of the selection of training sets for chemically reacting systems, is currently under investigation.

The overall storage requirement for the MC simulation using 20,000 stochastic particles is $\approx$ 8.8 Mbytes, with less than 0.05% of that memory is required for handling the chemistry term (by either method). This is compared to 30% (at least) that would be required if look-up tables are used to store the chemical source term. The savings in storage become more pronounced as more complicated chemical schemes are used [7]. The CPU time required for the MC simulation when representing the chemistry using the RM

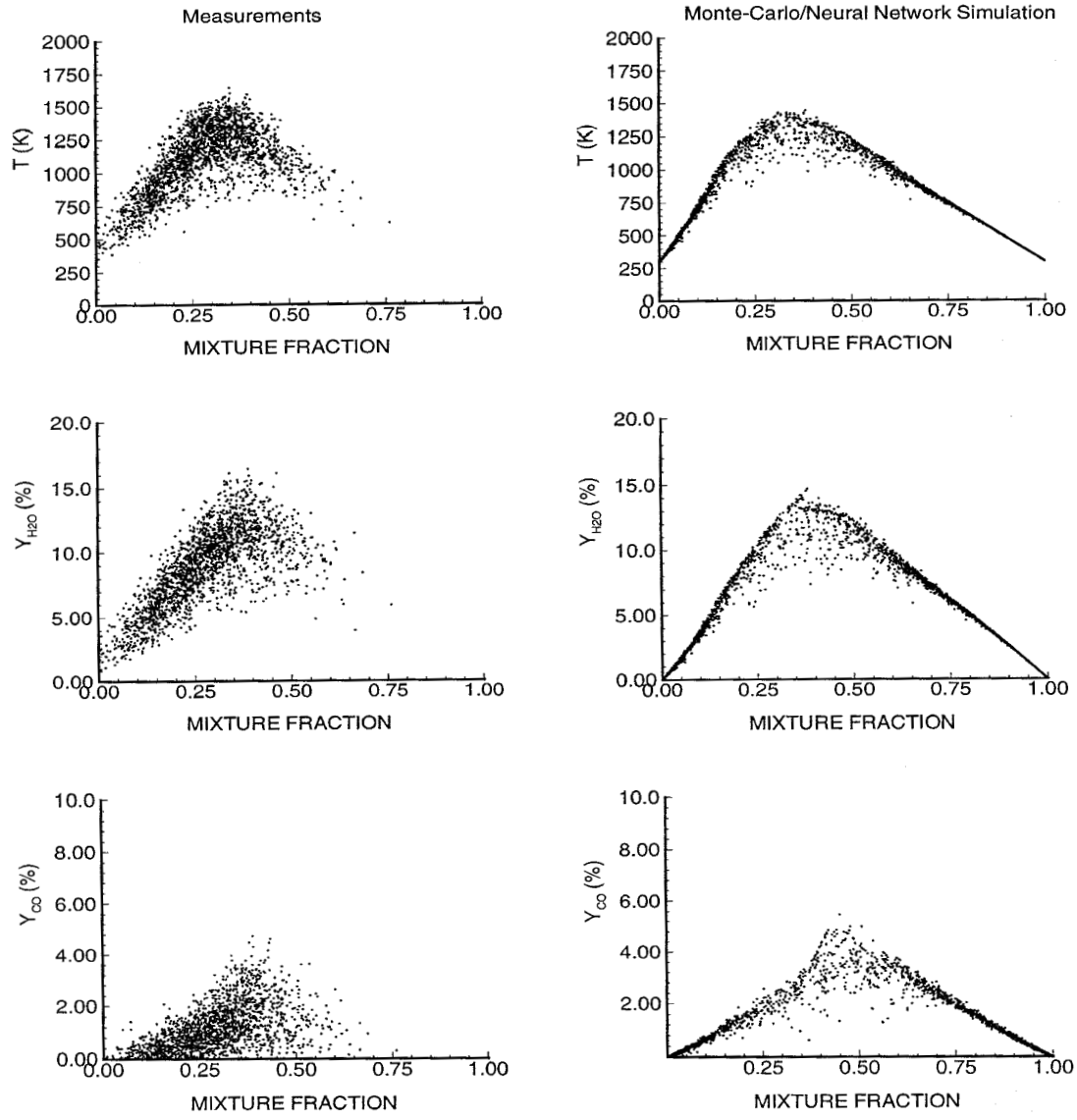

Figure 4: Measured (left) and calculated (right) scatter plots for temperature (T), and the mass fractions of H_2O, and CO plotted against mixture fraction ξ, for the H_2/CO_2 flame with jet velocity u_j=130 m/s, at axial location x/D_j=6.

method, is about five times smaller than that required if ANN modelling is used. The computation time required by either method, however is about one order of magnitude smaller than the CPU time required by the direct integration method. Comparable results in predicting the flow field and the composition field are achieved by both methods. This is clearly illustrated in Fig.4 which shows scatter plots for

the temperature (T) and mass fractions (Y) of H_2O and CO, obtained by MC simulation with ANN method compared favorably with experimental results. Whilst the current article is concerned with the application of ANN and RM to approximate chemical reactions in turbulent combustion simulations, the utilisation of these methods can be extended to applications for other non-linear system identification processes, such as the dynamics and control of a robotics arm.

5. Conclusions

- Artificial neural network and Repro-Modelling approaches are successfully used to represent the chemistry of $H_2/CO_2/O_2$ mixture, accurately and efficiently.
- In general, both methods show good generalisation features, but the ANN approach exhibits better generalization capabilities than the RM functions. However, some degradation in the performance of both methods become noticeable once the modelled samples deviate significantly from the model's dynamic range.
- Both methods require a modest amount of computer memory. The computational cost of the RM approach is less than that of the ANN modelling, however the generalization of this observation is not conclusive, and require further investigation. The computation cost of both methods is much less in comparison to the CPU time of the direct integration approach. The storage requirement is also negligible compared with the storage demand of look-up tables.

Acknowledgments

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