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Approximation of chemical reaction rates in turbulent combustion simulation

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Abstract. It is essential to increase the efficiency of the commercially available combustion engines because of the limitations in fossil energy resources and environmental pollution Also the emission standards are a challenging aspect. If one succeeds in designing the combustion process, in particular the chemical reactions, it would be feasible to partly replace complex experiments by computer simulations. The suggestion made in this paper, is the use of artificial neuronal networks for approximation of complex chemistry in turbulent combustion applications. The use of complex chemistry is computationally expensive and limited to simple geometry, therefore it is replaced by trained ANNs.

1 Introduction

Commercially available combustion engines like gas turbines are often used for decades. Often old robust engines can not fulfil current emission standards. Environmental pollution rises with the number and the age of these engines. Therefore the efficiency in relation to the decrease of emissions has to be examined. The design process of current combustors already is based on simulations while the former engines have a big potential for simulation based optimisation. The main focus is on the prediction of the velocity field, the mixing process of fuel and oxidiser, the emissions (exhaust gas) in general and the temperature field, for variable fuels, varying boundary conditions and modifications of the geometry. An optimum solution for a given parameter set can be validated by real experiment, but the complex variation of different parameters for cost-intensive experiments can be deferred. The research in the field of turbulent flow simulation consists of different subjects. For turbulent flow simulation with combustion, the chemical reactions and the coupling with turbulent flow have to be performed at the same time. Especially the reaction progress for prediction of emissions, like NO_x- and CO-formation, depends on the chemical reaction mechanism used. Optimised mechanisms designed to model natural gas combustion, including NO formation and reburn chemistry, contain hundreds of reactions and more than fifty species. Complex hydrocarbon fuels have more than

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1000 reaction steps with over 200 species [6]. The finite rate chemistry requires integration of ordinary differential equations (ODEs) of the form:

$$\frac{dy_i}{dt} = \dot{r}_i(\bar{y}, T, p)$$

Where $\dot{r}_i$ is the chemical reaction rate of species i, $\bar{y}$ is the mass fraction vector, T is the temperature and p is the pressure. It is in general computer time intensive to evaluate this system of ODEs for each species. And because of the wide spectrum of characteristic evolution timescales, the system has to be integrated quite often. The required CPU-time limits the evaluation of integrals of the stiff equations to simple problems or to strongly reduced numbers of species when turbulent flow is performed at the same time.
So the use of databases for storing chemical reactions and several storage-based techniques are widely described in literature to tackle that problem. The so-called look-up tables require large storage capacities and grow exponentially with the number of species [9].

2 Turbulent flow simulation with combustion

The continuous fluctuation of velocity is a characteristic property of turbulent flow. The resulting fluctuations of scalars lead to complex interactions between the turbulent flow field and the chemical reaction. Therefore the description often is realised by a deterministic approach [4]. The interaction between turbulent flow and chemical reaction is described with probability density functions (PDF) to conform to the stochastic nature of highly turbulent combustion processes. A stochastically equivalent system in a Lagrangian framework is used for the solution procedure. A so called stochastic particle ensemble which has the same initial distribution like the physical scalar values is used to solve the problem. A high number of stochastic particles which are calculated in the flow field, should represent the real distribution of scalars like the mass fraction of the species [4].
Using complex chemistry the exponentially growing requirements of storage capacities limits the look-up tables [9] for representing the chemical reactions with more than a few supporting points per species. Therefore the complex chemical reaction mechanism like the GRIMech3.0 [5] that consists of 325 reactions with 53 species is trained in ANNs. So the evaluation of the complex chemistry with marginal CPU-time and memory resources is introduced.

2.1 Approximation of complex chemistry with the use of ANN

For a given test set of boundary conditions it is possible to calculate the reaction progress. That means to calculate the progress in composition space of species in discrete time steps. For example with methane air combustion the brutto reaction is:

$$CH_4 + 2(O_2 + 3{,}76N_2) \rightarrow CO_2 + 2H_2O + 7{,}52N_2 .$$

For a piloted CH_4/Air Flame (Flame C) the calculation was performed by connecting a three dimensional CFD solver with a PDF approach and the use of Chemkin [10] (standard software tool) for calculating the progress in complex chemical reaction. Fig. 1 depicts the configuration of the burner and the test set [1]. The GRIMech3.0

was used for calculating the species mass concentrations in the flow field. The finite-volume-model has about 1.000 elements and is a rotational symmetric slice. Per element eight particles were used to represent the stochastic distribution of the PDF approach.

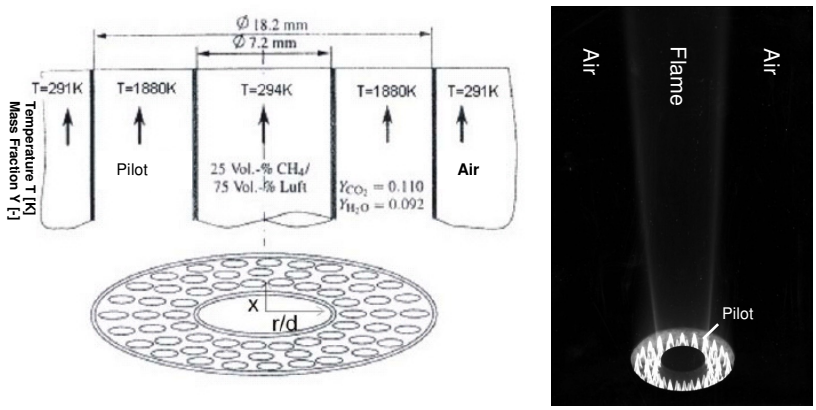

Fig.1: Boundary conditions of the test set [4] and close-up of the pilot flame [1]

In order to train the ANN the input and output chemical states of the stochastic particle ensemble, which were calculated with the GRIMech3.0 and Chemkin were saved. An almost complete dataset consists of 1.000.000 in and output samples. The integration of the ODEs represented by the system of 325 reactions is expensive with regard to computer time. The solution for the whole finite-volume-model needs about 168h CPU-time (CPU Q6850, 8GB, WIN XP64bit).

Because of accuracy reasons the dataset of in- and output concentrations of the species were subdivided into several clusters. Each cluster consists of the training base for one ANN which is a simple feed-forward-net with two hidden layers and six in- and output neurons for the four main species CH_4, CO_2, H_2O, O_2, the temperature and CO as an important minority species of the whole dataset. The number of neurons in the hidden layer is variable in the range of 12 to 50 depending on the number of data in one cluster. A bias neuron is set for the hidden layer and the output neurons. For the training the Resilient-Backpropagation-Algorithm with weight-backtracking and the mean squared error was used [8]. In the first step six of the 53 species were analysed. After the training process the Chemkin solver is replaced by the ANNs. A rerun of the simulation shows the overall good approximation of the ANNs and the applicability of ANNs for complex chemistry representation. Furthermore the enormous reduction of CPU-time in comparison to the calculation with ODEs.

2.2 **Results**

The main axial profiles (x-direction, r/d=0, Fig.1) of the regarded species and the temperatures are shown in Fig. 2-4. A comparison of ANNs and ODEs solution show that there is only a small difference of about 0,5% in species mass fractions and temperature. If one takes into account that only eight particles per element were used to represent the stochastic ensemble in the flow field the difference is in the range of fluctuation during the calculation steps.

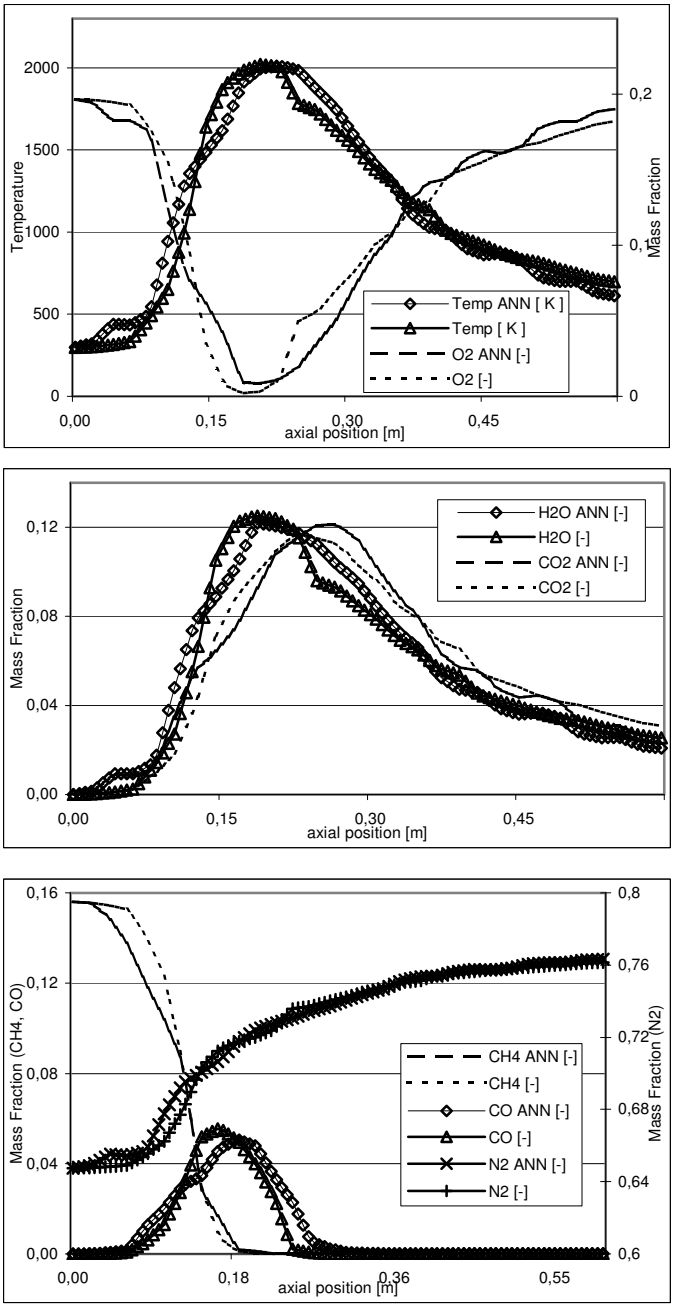

Fig. 2-4: Comparison of ODEs/ANNs calculation on the main axis; Temperature and O_2 (Fig. 2); H_2O and CO_2 (Fig. 3);CH_4, CO and N_2 (Fig. 4)

The trained ANNs calculate the output for temperature and mass fractions of the species with a fixed time step of dt=0,00003[s]. The net has learned the data and is able to reproduce the full dataset.
Nitrogen is used by the CFD solver as closure condition. The mass fractions of the species have to sum up to one, so that the density in the flow field can be calculated. Therefore nitrogen is an overall good indicator for the accuracy of the solution. If the analysed species by the ANNs calculation leave the high dimensional composition space, the mass fraction of nitrogen represents the sum of the error.
Fig 4. shows the trend of N_2. It is in good approximation of the ODEs calculation

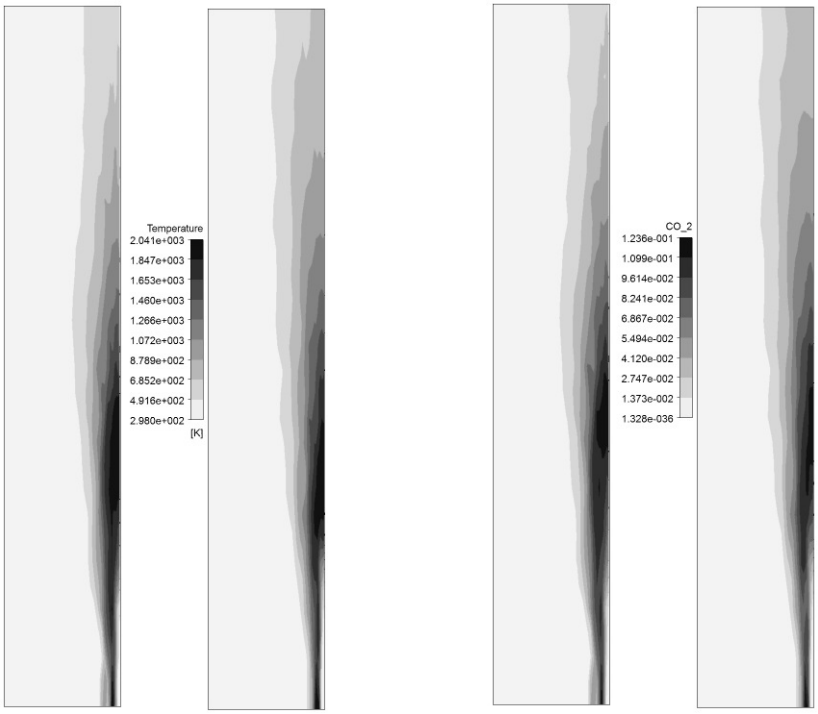

Fig. 5: Temperature and mass fraction of CO_2 in the flow field in comparison ANNs (left)/ODEs (right) calculation

The complete temperature and CO_2 fields which can be seen in the side view of the finite-volume-model slice in Fig. 5 show that both solutions have no significant difference.
The solution using ANNs requires only $1/14^{th}$ of the CPU time required by the solution using the ODEs, which equals 12h on the system used.

2.3 **Conclusion**

The computation of temperatures and concentrations of the main species and also minority species like CO in turbulent combustion can be approximated by the use of ANNs. Furthermore it is possible to reproduce complex chemistry within the range of the analysed inputs. A speed up factor of the simulation of more than 14 was shown.

It is therefore possible to use more than eight stochastic particles per volume element to represent the distribution of scalars in the flow-field, which is expected to yield a more precise solution. More than that to increase the number of volume elements.

3 Future Prospects

Because of the high dimension of the used chemical reaction mechanism the dataset has to be carefully examined. For this study more than 1200 ANNs were used. In order to reduce this number a more fitting clustering algorithm, than the high dimensional chess board, is needed. Moreover it would be interesting to examine the remaining species because of the possibility to predict NO_x formations which are nowadays of enormous interest by the appraisal of combustion engines.
The increase of finite volume elements and the increase of stochastic particles in the flow field can possibly improve the solution. The comparison to measurements data [1] of the used flame test set will show the solution quality.

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