NEURAL NETWORKS IN COMBUSTION SIMULATIONS

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Keywords: Computational Fluid Dynamics (CFD), Combustion simulation, Furnace, Finite-volume-model.

Abstract: The design process of commercially available combustion engines is often based on real experiments which is expensive concerning to fuel consumption, men power and environmental pollution. It is possible to replace complex experiments by computer simulations. The prediction of the velocity field, the mixing process of fuel and oxidiser and the temperature field is a wide range of research subjects. In case of turbulent flow simulations with combustion the chemical reactions and the coupling have to be calculated at the same time. With regard to computer time the used chemical reaction mechanism has a big influence on the performance of the whole simulation. Therefore optimisation procedures often improve the representation of the chemistry. The suggestion made in this paper, is the use of artificial neuronal networks for approximation of complex chemistry in turbulent combustion simulations.

1 INTRODUCTION

The prediction of minority species in the flow field of a turbulent combustion simulation like CO- or NO_x-formations depend on the used reaction mechanism. Often more complex chemical reaction mechanism contain hundreds of reactions and fifty or more species. Only optimised mechanisms contain these species of interest and in general the evaluation is computer time intensive. Further information can be found in Große and Joos (2009).

Former studies by Blasco, Fueyo, Dopazo and Ballester (1998) and Chen, Blasco, Fueyo and Dopazo (2000) show the use of ANN for representation of reduced chemical systems. Further studies by Große and Joos (2009, 2010) show the feasebility of the use of ANN for complex chemistry representation.

2 COMPLEX CHEMISTRY REPRESENTATION

A complex chemical reaction mechanism like the Gas Research Institute Mechanism 3.0 (GRIMech3.0) which consists of 325 reactions with 53 species is optimised for methane combustion in a wide pressure and temperature range. So the use of the GriMech3.0 means to solve the ordinary differential equation (ODE) system with 53 variables, which are the species, for each statistic representation (particle) in the flow field. The smallest eigenvalue of the Jacobian matrix of the ODE system is fixing the integration step, which means practically to integrate the system in smallest steps until the solution is reached:

$$\frac{dy_i}{dt} = \dot{r}_i(\bar{y}, T, p) . \quad (1)$$

In equation (1) $\dot{r}_i$ denotes the chemical reaction rate of species i, $\bar{y}$ the mass fraction vector, T the temperature and p the pressure. In general it is computer time intensive to evaluate this system of ODE for each species.

When the effects of turbulent flow are calculated at the same time during a simulation process the required CPU-time limits the evaluation of the stiff ODE system to simple problems with less finite-volume-elements in the model approximation.

3 TURBULENT FLOW SIMULATION WITH COMBUSTION

Turbulent flow is characterised by continuous velocity fluctuations, the resulting fluctuations of

Große L. and Joos F..
NEURAL NETWORKS IN COMBUSTION SIMULATIONS.
DOI: 10.5220/0003073904060410
In *Proceedings of the International Conference on Fuzzy Computation and 2nd International Conference on Neural Computation* (ICNC-2010), pages 406-410
ISBN: 978-989-8425-32-4

scalars lead to complex interactions between the turbulent flow field and the chemical reactions. Therefore deterministic approaches describe the interaction with probability density functions (PDF) as stated in Harder (2007).

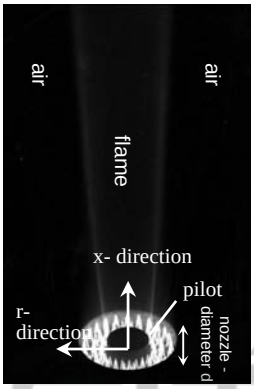

Figure 1: Picture of the Flame (Sandia, 2003) with description (added).

For this study a stochastically equivalent system in a Lagrangian framework is used. A high number of stochastic particles which is called stochastic particle ensemble represents the real distribution of scalars. The particles have the same initial distribution as the physical scalar values and are calculated in the flow field. For a piloted methane/air flame (Barlow and Frank, 1998; Barlow, Frank, Karpetis and Chen, 2005) the calculation was performed by connecting a three dimensional CFD solver with a PDF approach and the use of the commercially available computer program CHEMKIN for calculating the progress in complex chemical reactions with GRIMech3.0.

A calculation using the PDF approach presented in this work was conducted with 8 particles per finite-volume-element. The whole model has 1000 elements. The model is a rotational symmetric slice of the whole flame. Figure 1 depicts the flame (Sandia, 2003). Because of CPU-Time reasons a more detailed model with more volume-elements or the increase of the stochastic particles is limited. 8 particles with 1000 elements require 8000 integrations of the ODE system per iteration step.

3.1 PDF CFD Simulation

The general approach for the calculation is shown in figure 2.

The convergence in the probability distribution of the particle is reached after 1700 iteration steps. The input and output chemical states of the stochastic particle ensemble were saved. So the species mass concentrations in the flow field and their change in the 53 dimensional state during the simulation is known. A complete dataset of about 1.000.000 in and output samples in the form ($\bar{y}$ (t),T(t); $\bar{y}$ (t+dt),T(t+dt)) where t is the absolute time and dt the time of the reaction progress which is calculated with the complex chemistry mechanism is the basis for the training of the ANNs. A simple chess-board cluster algorithm is used for clustering the dataset in six dimensions. The data in each cluster consists of the training base for one ANN.

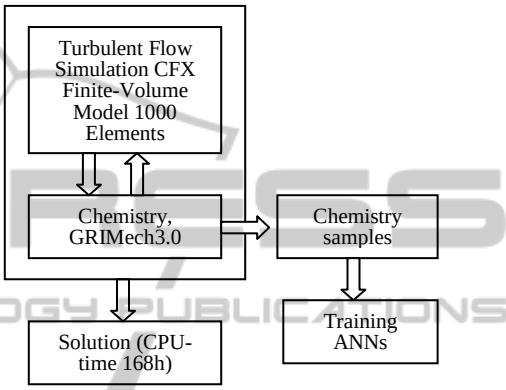

Figure 2: Approach for the PDF CFD simulation.

168h of CPU-time is needed for the calculation of the solution and the chemistry samples for the whole finite-volume-model (CPU Q6850, 8 GB, WIN XP64bit).

Former studies (Große und Joos, 2010) show that the calculation with ANNs yields a good approximation of the ODE system solution. Furthermore the ANNs solution requires only $1/14^{th}$ of the CPU time, which is about 12h for the 1000 finite-volume-element model. So several parameter studies with ANNs are applicable during a full ODE simulation. Moreover the possibility of more precise calculations is given.

3.2 CFD Simulation with ANNs

The clustered dataset is used to train ANNs which are able to reproduce the change in species mass concentrations during the simulation. The ANNs are simple feed-forward-nets with two hidden layers with up to 50 neurons and six in- and output neurons for four main species (CH_4, CO_2, H_2O, O_2), the temperature and one important minority species (CO). Because of complexity reduction only five of the saved dataset of 53 species were analysed. The stoichiometric global reaction of complete methane/air combustion is given in equation (2).

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

With the closure condition that sum of mass fractions of the species has to be one, N_2 is the closure condition species. A more detailed combustion description includes hundreds of reaction steps with several intermediate species like the GRIMech3.0 with more than 50 species.

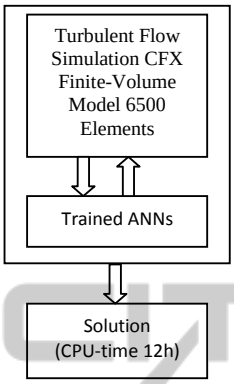

Figure 3: Approach for the PDF Simulation with ANNs.

For each ANN a bias neuron is set for the hidden layers and for the output neurons. As learning algorithm the Resilent-Backpropagation by Igel and Husken (2003) with weight-backtracking and the mean squared error was used.

The rerun of the simulation with ODE replaced by 1500 ANNs (figure 3) show the ability of ANNs for complex chemistry representation (Große and Joos, 2010).

The reduction of CPU-time in comparison to the ODE calculation makes it possible to simulate a high resolution model of the flame with about 6500 finite-volume-elements and up to 26 stochastic particles per element to describe the stochastic particle ensemble. Precise simulation solutions allow the comparison with measurements and are therefore a tool for optimisation tasks.

3.3 Results

The comparison of measurements and simulation solutions of the calculation with ANNs and the ODE system on the main axis (r=0mm, see figure 1) is shown in figures 4-7, with d=7,2mm as nozzle diameter. The high resolution finite-volume-model of the flame with 6500 elements was used with different numbers of particles (8 or 26) per element.

The configuration and the boundary conditions of the flame and the scalar measurements are adopted by (Barlow and Frank, 1998). The calculation with the ODE system is used as reference application but in general it is not analysable because of a summarized calculation time of 100 days as well as convergence problems during the solution iterations.

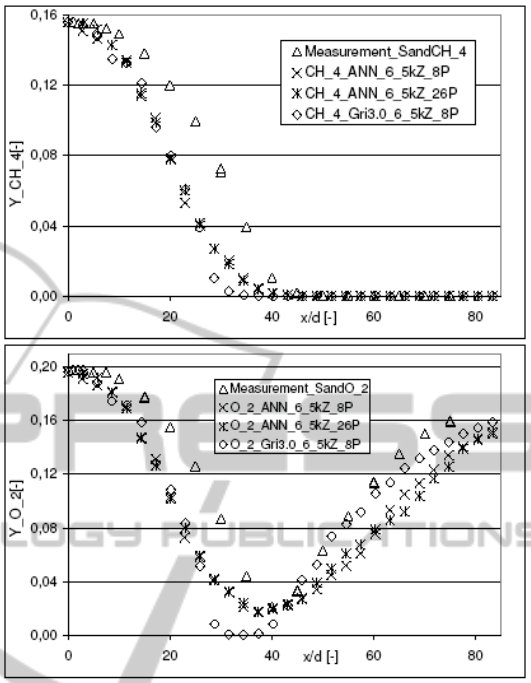

Figure 4: Comparison of measurements, ANNs and ODE system simulation solutions of the educts of the flame.

The educts in figure 4 show a good approximation of the measurements. There is a small downstream shift of methane and oxygen. The maximum and minimum is within the range of the measurements. The calculations with 8 (8P) and 26 (26P) particles for representation of the stochastic particle ensemble of the ANNs simulation are almost similar. Using a finite volume-model with a higher resolution will probably yield further improvement. The calculation with the ODE system and the high resolution model with 8 particles show the same trend. The extreme points became apparent and the drop of the species is marginal faster. Physical observed the strong gradient of educts between 15 to 40[x/d] is an indicator for the position of the flame.

The products shown in figure 5 show also a matching behaviour. Measurements and calculation diverge only in form of a small shift, which is connected with the shift of the educts. The values of carbon dioxide are slightly higher with a maximum difference of 0,02. The calculation with the ODE system shows the same behaviour. Only the extreme points have a higher difference to measurement values.

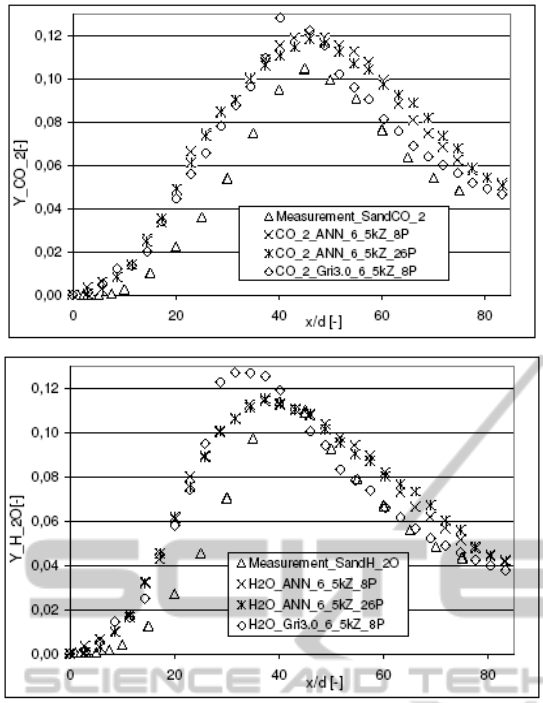

Figure 5: Comparison of measurements, ANNs and ODE system simulation solutions of exhaust gas components of the flame.

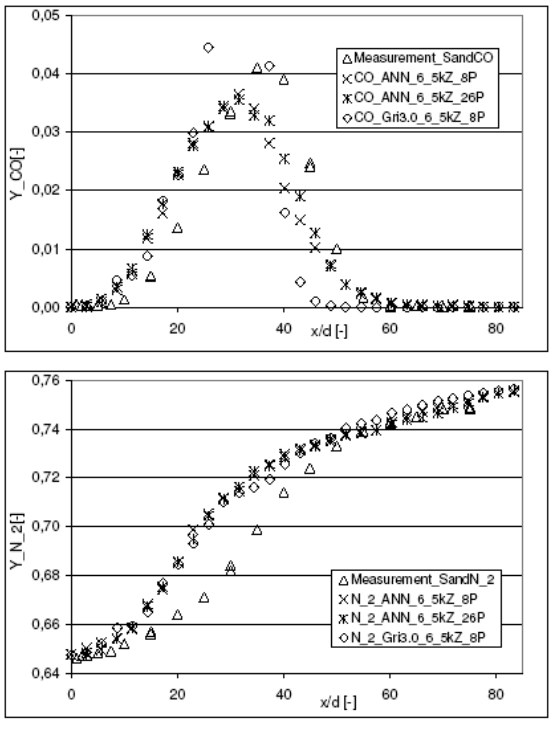

Figure 6: Comparison of measurements, ANNs and ODE system simulation solutions of carbon monoxide and nitrogen.

Carbon monoxide is an import minority species. Several reduced mechanisms can not calculate the values of that specific species. In comparison the values in figure 6 are within the same range. The maximum point for the ODE system is about 0,008 higher and the CO oxidation is faster than for the ANNs simulation. The measurements show a small shift to higher [x/d]-values which is in good correlation to the former discussed species values.

Nitrogen is the closure condition. The mass fractions of the species have to sum up to one, so that the CFD solver is able to compute the density for the flow field calculation. Therefore the overall error of the calculation results can be seen in the values of nitrogen in figure 6. In comparison of the ANNs and ODEs solution the error is marginal.

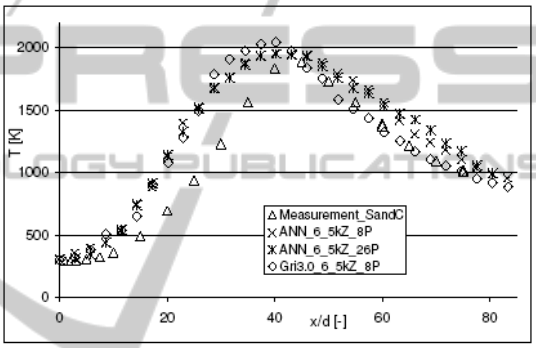

Figure 7: Comparison of measurements, ANNs and ODE system simulation solutions of the flame temperature.

In summary measurements and calculations of the examined species show good results. In physical description the flame front of the calculation with ANNs is shifted to lower x-values. But the same solution is also generated by the full GriMech3.0 solution.

Figure 7 depicts the temperature which shows the same shift in flame front position and the good trend in comparison of ANNs and ODE calculation.

Further comparison of the flow field and turbulence values show the performance of the ANNs simulation solutions. Because of the coupling of the turbulent flow field and the reactions, minor changes can result in convergence problems and species mass concentrations which are not physical. Whereas the ODE system is a physical model ANNs only represent the learned dataset within the given limits.

3.4 Future Prospects

In order to reach an improvement the chemistry samples which are generated with a model of about

1000 finite-volume-elements should be replaced by samples of the high resolution model. Further the use of a more fitting cluster algorithm will improve the performance regarding the number of used ANNs. The forecast of further minority species like NO_x or unburnt hydrocarbons can help to fulfil current exhaust emission directives.

ACKNOWLEDGEMENTS

The investigations were conducted as part of the joint research programme **COOREFF-T/COORETEC-turbo** in the frame of AG Turbo. The work was supported by the Bundesministerium für Wirtschaft und Technologie (BMWi) as per resolution of the German Federal Parliament under grant number **0327716L.** The authors gratefully acknowledge AG Turbo and **MAN Diesel & Turbo SE** for their support and permission to publish this paper. The responsibility for the content lies solely with its authors.

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