

Assessment of neural network-based predictions of chemical production rates in CFD solvers

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Abstract

This paper outlines different implementation strategies of neural networks for the prediction of chemical source terms in CFD solvers and discusses their limitations based on the solution of generic reactor problems. Further, a robust and consistent neural network-based method to optimize existing global mechanisms for specific thermodynamic conditions and mixture compositions is introduced. This method is tested using stirred reactor problems and the CFD analysis of a lifted methane air-flame.

1. Introduction

The numerical simulation and analysis of chemically reacting flows often requires the evaluation of detailed reaction mechanisms. This is the case, for example, with lifted flames in combustors or with complex mixtures which can not be described with a mixture fraction scalar. An examples is the engine and gas generator exhaust in combination with the ambient air around a rocket base flow. In the case of hydrocarbons in particular, chemistry is complex, mathematically stiff and requires many reactions and species to be considered. This results in the need of significant additional CPU resources which are considerably larger than those required for the solution of the fluid transport equations alone.

Popular options to reduce the CPU demand of reacting flow simulations are the application of simplified combustion models such as flamelet or eddy breakup models or the use of reduced skeletal or global reaction mechanisms. However, this results in a limited range of applicability concerning the complexity of gas mixtures, the range of applicable thermodynamic states or the ability to predict kinetics driven lift-off or extinction phenomena. Another possibility to reduce the CPU cost and stiffness of the evaluation of the chemical source terms is the application of neural networks.^{1,6,7} In the present work we consider the general case being applicable to compressible and incompressible solvers and arbitrary gas mixtures. Here, the input of the network would be the mixture composition and the thermodynamic state and the output are the rates of change of species concentrations (source terms). Training data can be easily obtained from the exact evaluation of the law of mass action in conjunction with a detailed and accurate reaction mechanism. However, the mathematical stiffness of the problem imposes a severe challenge for the applicability of this approach.⁵

After a brief introduction to the source term calculation in CFD codes in section 2 and to the model problem of an isochoric reactor in section 3, different layouts and structures of neural networks for the direct prediction of chemical source terms are discussed in section 4. Due to systematic deficiencies of classical neural networks concerning the treatment of stiff combustion problems, an alternative approach is developed in section 5. The main idea is to predict global reaction rates instead of chemical source terms. The advantage of this method is a considerably reduced numerical stiffness and physical consistency concerning the preservation of the equilibrium state with zero net production rates. An application of the new method to a lifted air-methane flame shows promising results.

All implementations of neural networks were done with the tensorflow package.²

2. Finite rate chemistry modeling in CFD

Finite rate chemistry CFD solvers requires the implementation of a set of transport equations for the partial densities or concentrations of the different species in the reacting gas mixture. These transport equations contain a source term which models the chemical production or destruction rates. The goal of this study is to find an approximation for the production rate $\dot{\omega}_s$ of species S in the transport equation of the partial density, ρ_s , in equation 1:

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$$\frac{\partial}{\partial t} \int_V (\rho_s) dV + \int_S (\rho_s \vec{u}) \vec{n} dS - \int_S \frac{\mu}{Sc} \vec{\nabla} T \frac{\rho_s}{\rho} \vec{n} dS = \int_V \dot{\omega}_s dV \quad (1)$$

with the velocity vector, \vec{u} , the mass diffusion coefficient, μ/Sc and the control volume V with its surface S . The exact computation of this chemical source term is done using the law of mass action (equation 3) for a set of chemical reactions r (equation 2) with the participating species X_s and the passive collision partner M :



$$\dot{\Omega}_s = M_s \sum_r (\beta_s^r - \alpha_s^r) \left\{ k_r \prod_s \left(\frac{\rho_s}{M_s} \right)^{\alpha_s^r} [\tilde{M}_r] - \frac{k_r}{K_{EQ}} \prod_s \left(\frac{\rho_s}{M_s} \right)^{\beta_s^r} [\tilde{M}_r] \right\} \quad (3)$$

Here, α and β are the stoichiometric constants, k is the reaction rate and K_{EQ} is the equilibrium constant. The effective molar concentration of passive collision partners in three body reactions $[\tilde{M}_r]$ is.

$$[\tilde{M}_r] = \sum_s E_s \left(\frac{\rho_s}{M_s} \right) \quad (4)$$

with the third body efficiencies, E_s . For two body reactions we have $[\tilde{M}_r] = 1$.

The rate of the forward reaction, k_r , is usually calculated using an Arrhenius equation, which leads to an exponential dependence on temperature. The reverse reaction rate, k_r/K_{EQ} , is calculated from the forward rate and the equilibrium constant, K_{EQ} .

Equation 3 represents an algebraic system for calculating the formation rates ($\dot{\Omega}_s$) of the species involved in the reaction mechanism. Due to the exponential temperature dependence and the nonlinear relation to the molar concentrations of the participating species, this system tends to be mathematically stiff and difficult to evaluate for complex reaction mechanisms.

In the following sections, two basic solution approaches for the treatment of equation 3 with the help of neural networks are described and evaluated. In the first, the source terms, $\dot{\Omega}_s$, are calculated directly with different layouts and structures of neural networks. In the second, the equation is still evaluated algebraically, but with a greatly reduced number of chemical reactions and correspondingly adjusted and optimized reaction rates, k_r . The evaluation of the properties of the neural networks and the quality of the predictions is carried out with the help of the simple model problem of a perfectly stirred isobaric or isochoric reactor (see section 3). To further reduce the complexity of the problem, hydrogen/oxygen chemistry is used for initial bench-marking. In the last section 5, the optimization of a reduced hydrocarbon reaction mechanism and the test case of a lifted axisymmetric flame are considered as more complex validation cases.

3. Model problem: perfectly stirred reactor

An isochoric or isobaric reactor with a hydrogen/oxygen mixture was selected as a simple model problem to assess the performance of neural networks to calculate chemical production rates. A fixed volume with closed adiabatic walls (isochoric) or a variable volume with constant pressure (isobaric) is considered. A hydrogen/oxygen mixture is initially set under self-ignition conditions. The temporal evolution of the mixture towards the equilibrium state is computed and serves as the test case for the source term prediction. The results to the exact (law of mass action with Arrhenius rates) approach are used as training data for the neural networks and as the benchmark result for accuracy assessment. A schematic representation of a reactor is given in Fig. 1.

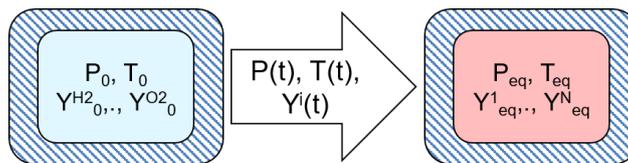


Figure 1: Schematic of an isochoric reactor

An example result for an isochoric reactor with a stoichiometric mixture is given in Fig. 2. The initial reactor conditions are given in the picture. The various curves refer to results calculated with the flow solver TAU⁸ and the

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software package CANTERA⁴ using the Jachimowski reaction mechanism.³ The reference results from the flow solver and Cantera calculations were also used to train the neural networks for the chemical production rates. A typical set of support points for training data is marked with the round symbols.

The time history of the chemical source terms is given in Fig. 2(b). These values are to be reproduced by the neural network approach. In general, the source terms vary over many orders of magnitude. Positive and negative values are possible.

From these results, 3 characteristic regions within the temporal evolution of the reacting gas mixture in the reactor can be identified:

1. Ignition delay, up to approx. 16 μs : This is where chemical radicals such as atomic oxygen or OH are formed. The corresponding source terms (and radical concentrations in the mixture) are very small. This area is important for the correct reproduction of the ignition delay time.
2. Ignition, between 16 and 26 μs : After a critical concentration of radicals has been reached, the mixture ignites. This region is characterized by extremely large source terms and fast chemical reactions.
3. Equilibrium: after 26 μs : After the completion of the ignition phase, chemical equilibrium conditions are established. Here, the net source terms of all mixture components vanish (production = destruction). In section 4 it becomes clear that the consistent prediction of this state with exactly vanishing source terms is a considerable challenge for neural networks.

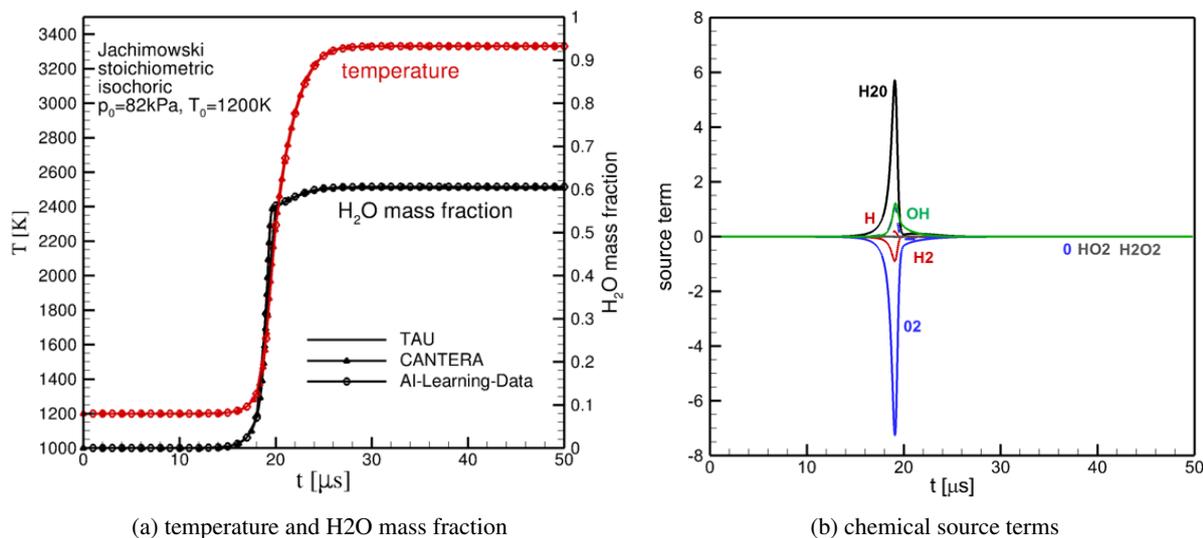


Figure 2: Example time histories in an isochoric reactor

4. Application of neural networks for the direct prediction of chemical source terms

4.1 Classic neural network

A standard structure was chosen as the first variant for describing the reaction kinetics using the species source terms with the help of neural networks. The input variables are the mixture composition (mass fractions, Y_i) as well as the pressure and the temperature of the gas. To improve the accuracy and reduce the overall stiffness of the problem, each output (the chemical source term expressed by the time derivative of the mass fraction) was calculated by its own dedicated network. The computational setup as used for calculating a reactor test case is shown schematically in Fig. 3. The neural network for the source term prediction was coupled with a thermodynamic mixture model and an ODE solver for time integration. The investigated neural networks feature 2 to 5 layers of 10 to 200 nodes each. RELU and sigmoid activation function were used. As common with interpolation problems, a linear activation function was always chosen for the output layer.

Typical results for a network size of 5 layers of 200 nodes each with RELU activation are shown in Fig. 4 and 5. The networks were trained with a set of reactor data as described in section 3.

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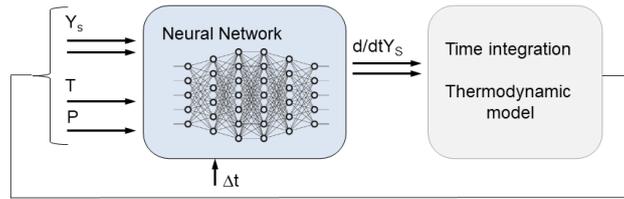


Figure 3: Computational setup

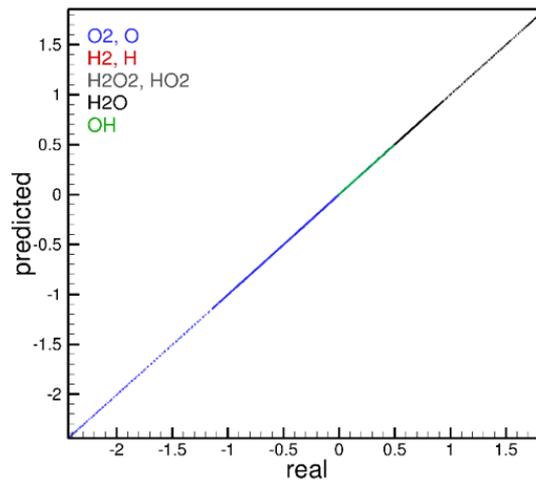


Figure 4: Source terms: predicted vs. exact

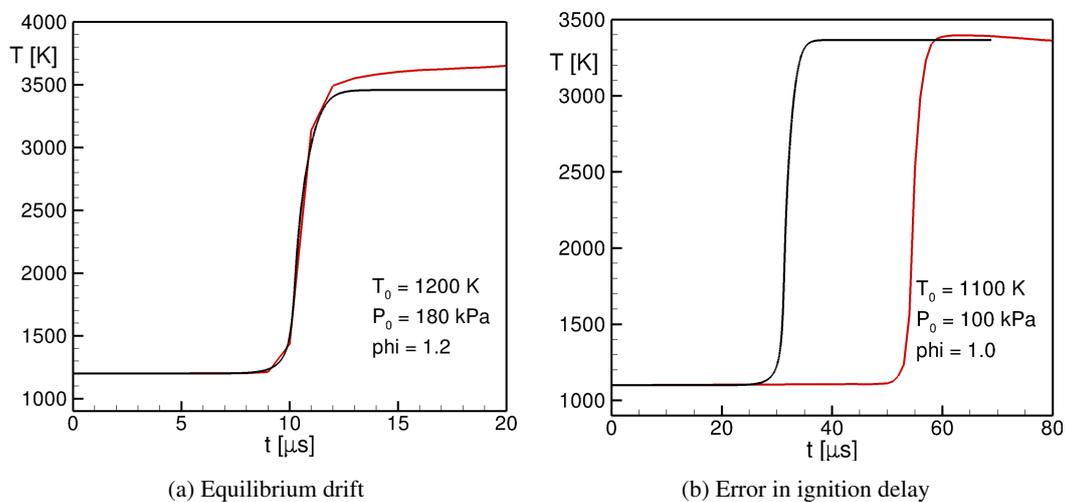


Figure 5: Examples of temperature histories with neural network predicted source terms

The error of the scaled source terms in Fig. 4 is less than 2% compared to the exact value in almost the entire prediction range. Problems arise in the region of vanishingly small source terms. Here, despite the large neural networks and the small absolute deviation, the relative prediction error is too high to achieve a constant equilibrium composition (Fig. 5(a)) or the correct ignition delay time (Fig. 5(b)). Especially the equilibrium state requires source terms which are precisely equal to zero and even small errors cause non-physical drift phenomena. Due to the extremely high number of degrees of freedom required to simulate a reaction mechanism with a simple neural network, there are no significant advantages with regard to the required computational time or the memory requirements of the CFD method.

Since sufficient robustness, especially for the prediction of the chemical equilibrium, could not be guaranteed even in the limit against extremely large networks, this approach was discarded for further work. Scaling the input and

output quantities of the network with sigmoid functions or by taking the logarithm with prediction of the sign using a separate classification network did not lead to a significant improvement in the results.

4.2 Adapted neural networks

In order to improve the predictive ability of the neural networks in the limit areas of ignition delay and equilibrium, the mathematical structure of the neurons was adapted to typical terms which govern the law of mass action and the Arrhenius reaction rates. Here, the optimized degrees of freedom (neuron weighting factors) of the network correspond approximately to physical properties of the reaction system such as stoichiometric coefficients or Arrhenius constants.

The chemical source terms are calculated essentially by summation over products of the input concentrations of the species to the power of their stoichiometric coefficients. These products are multiplied by reaction rates, which in turn are described with the function $AT^n \exp(-b/T)$. Hence a typical structure of the sum terms in the evaluation of the exact law of mass action (equation 3) is

$$\dot{\Omega}_s = \sum_r \prod_s X_s^{\alpha_s} T^n A \exp(-b/T) + \dots \quad (5)$$

The structure of an example network with 2 nodes using the mathematically adapted structure is illustrated in Fig. 6. The concentrations and the temperature are first logarithmized in a preprocessing layer. In a further preprocessing layer, the temperature is inverted. The following Arrhenius nodes have an exponential activation function. In this way, in the present example, the product of the concentrations to the power of their stoichiometric coefficients is simulated via the summation of w_{n1} and w_{n2} with a subsequent exponential function. Furthermore, the multiplication with T^n is realized by the multiplication of w_{n3} with the logarithm of T . The term $\exp(-b/T)$ is modeled in the node by the exponential activation function with the inverted temperature (here, w_{n4} act as the constant b in equation 5). In the final summation layer, the summation takes place over all reactions, the weighting factors here correspond to the Arrhenius constants A .

With the help of this network structure, the number of required degrees of freedom could be reduced by 3 orders of magnitude while maintaining the same level of accuracy. This would potentially save computing time in the CFD solver. However, the problems associated to very low or vanishing production rates which are described in section 4.1 continued to occur even with a large number of neurons. This affects the prediction of ignition delay and equilibrium. Therefore, this approach was also discarded for further work.

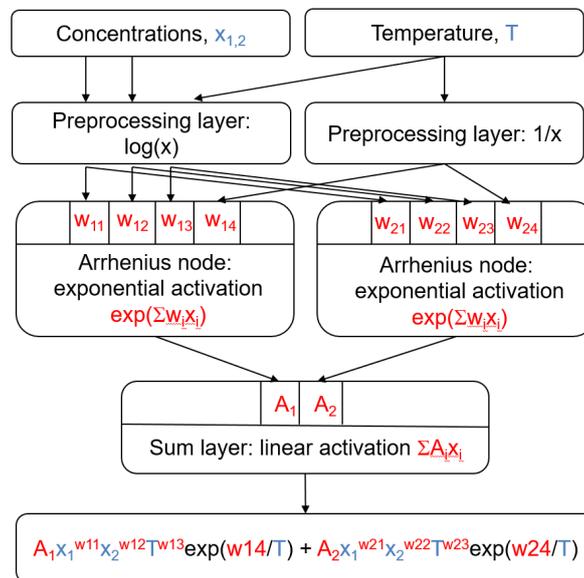


Figure 6: Adapted mathematical structure of the neural network

4.3 Exact Arrhenius-Neurons

Due to the observed deficits in the prediction accuracy of the previously tested neural network structures, the mathematical structure of the nodes was further adjusted. It was adapted to reproduce the exact formulation of the chemical

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production rate of a single Arrhenius-reaction in a neuron. The trainable degrees of freedom of the network correspond now exactly to the Arrhenius constants. The basic structure is shown schematically in Fig. 7.

The mixture concentrations and the temperature as well as the stoichiometric coefficients of the simulated reaction serve as input values for a network node. The output is the exact chemical source term. The main disadvantage of this approach is that the stoichiometric coefficients for each response neuron have to be given, i.e. a simplified reaction mechanism has to be guessed. The major advantage is that the trained weighting functions correspond now directly to the Arrhenius constants and can therefore be easily adopted into any CFD method.

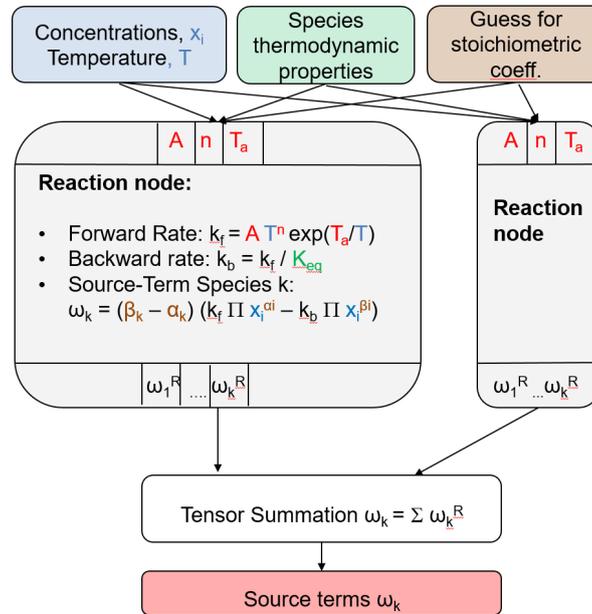
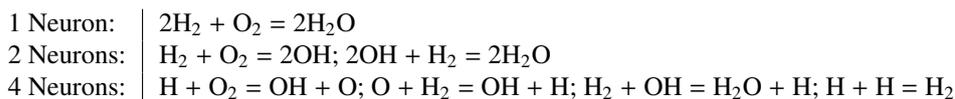


Figure 7: Structure of neural Arrhenius nodes

The hydrogen/oxygen ignition in a stoichiometric, isobaric reactor at starting conditions of 1200K and 200kPa was considered as an application example. Neural networks with 1, 2 and 4 nodes (reactions) were used. The 8-species, 19-reactions Jachimowski mechanism³ was used as a reference and to create the training data.

The specified stoichiometric coefficients of the networks with 1, 2 and 4 nodes correspond to the following global reactions:



Optimization was performed for the Arrhenius constants and the activation energies of the individual reactions. The set of stoichiometric constants was kept constant.

Results for the time histories of the mass fraction of water vapor and temperature for optimized neural networks with 1, 2 and 4 Arrhenius-neurons are shown in Fig. 8. In general, the training data could be well reproduced with the given global reaction mechanisms. The approach further avoids unphysical drift in the equilibrium state and imposes physical consistency. A higher number of neurons results in an improved accuracy of the predictions. The main deficiencies are the exact reproduction of the ignition delay and the thermodynamic state at equilibrium which both are affected by the reduced number of species and the resulting absence of radicals.

It was observed, that the objective function of the optimizer had an extremely large effect on the quality of the results. In the example, logarithmic mean error squares were used. Furthermore, when using 3 Arrhenius constants (A , n and T_a), ambiguous results arise where different combinations of n and T_a resulted in a similar reduction of the optimization target function.

Due to the adapted mathematical structure, the stiffness of the problem was directly mapped into the network nodes which, in general, led to an extremely difficult and tedious optimization process. For networks with more than 4 reaction nodes no optimum of the weighting factors could be found. Hence, the applicability of this method appears to be limited to a very small number of reactions.

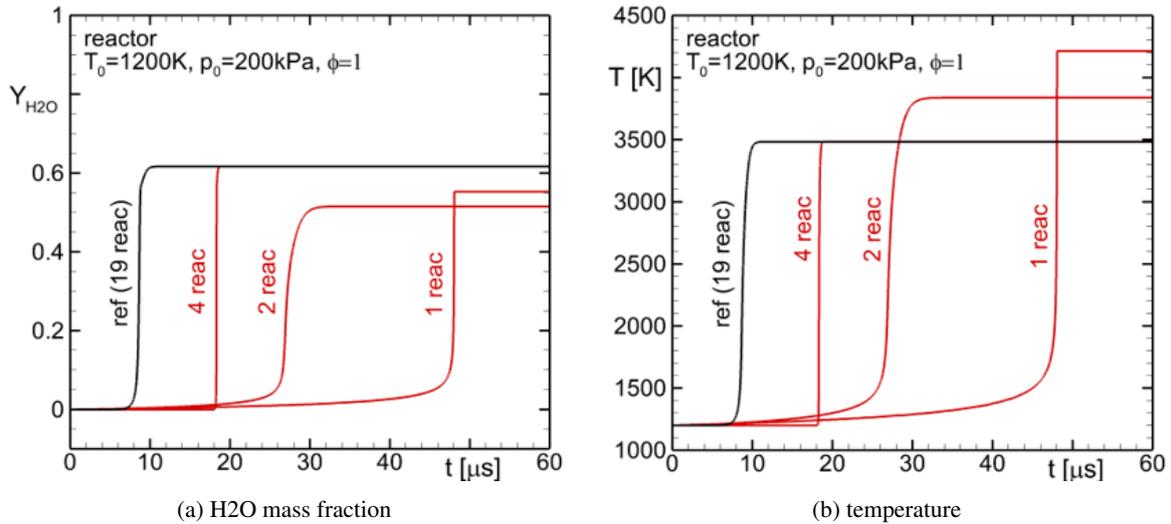


Figure 8: Results of networks with exact Arrhenius-neurons

4.4 Summary of predictive capabilities and properties of classical neural networks

The experience gained from different neural network structures studied so far can be summarized as follows:

1. The estimation of the chemical source term based on the application of a neural network works approximately.
2. By adapting the mathematical structure, a considerable reduction of the degrees of freedom is possible while maintaining the accuracy.
3. Nevertheless, the achieved accuracy is not sufficient for robust practical application. Further, physical consistency (e.g. equilibrium states) is not trivial to enforce.
4. Implementing the exact source term calculation in a neural network structure provides promising and consistent results for simplified global kinetic mechanisms. However, this approach is limited to mechanisms with a low number of reactions and involves a tedious and error-prone optimization process.

5. Neural networks for the prediction of reaction rates

5.1 Motivation

The various approaches pursued so far for the direct prediction of the chemical source terms based on the local mixture composition and the thermodynamic state could not be developed to a robust and physically consistent application-ready status. The reason is primarily the large mathematical stiffness of the underlying problem. For a fundamental improvement, the reduction of the stiffness and a change in the mathematical properties of the system to be replaced by neural networks appears to be required. This is accomplished by predicting reaction rates rather than chemical source terms by neural networks and then using these rates in the algebraic formulation of the law of mass action. Since reaction rates are always positive, logarithmization and scaling are possible in a considerable more straightforward manner.

To improve the accuracy of this method, the optimized reaction rates are allowed to be arbitrary functions of temperature and pressure. For application in CFD-solvers, this requires a only minor additional infrastructure for the treatment of tabulated rates. The direct implementation of neural network predictions into the solver is not required which facilitates the practical application of this approach.

5.2 Mathematical formulation

The reaction rates of a given mechanism can be calculated directly via the pseudo-inverse matrix of the concentration terms of the law of mass action. This requires the knowledge of the source terms and the mechanism under consideration (products and reactants of the reactions with their stoichiometric coefficients). Hence, the present approach will optimize the reaction rates of a prescribed global mechanisms to reproduce reference source terms for a given mixture state.

This results in a considerable reduction of the mathematical stiffness which is achieved from the separation of the law of mass action and the reaction rates. All summation terms disappear in the resulting formulation for the reaction rates, hence, logarithmization is possible.

To obtain an expression for the reaction rates, we start with the law of mass action where the chemical source term of a species, s , is obtained by summation over all reactions, r :

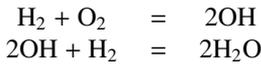
$$\dot{\omega}^s = \sum_r (n_{b/r}^s - n_{f/r}^s) \underbrace{\left[\prod_i X_i^{n_{f/r}^i} - \frac{1}{K_{eq}} \prod_i X_i^{n_{b/r}^i} \right]}_{\Pi_r} k_{f/r} \quad (6)$$

here, n are the stoichiometric coefficients, X the molar concentrations, K_{eq} the equilibrium constant and k_f reaction rates. The subscripts f and b refer the the forward and backward direction of a reaction.

The separation of the forward rate, k_f , enables the expression of the source terms in matrix form. The elements of the matrix are a function of molar concentration and temperature. The terms Π_i are defined in the bracket in equation 6:

$$\underbrace{\begin{pmatrix} \dot{\omega}^1 \\ \dot{\omega}^2 \\ \vdots \\ \dot{\omega}^{N_s} \end{pmatrix}}_{\underline{\dot{\omega}}} = \underbrace{\begin{bmatrix} (n_{b/1}^1 - n_{f/1}^1) \Pi_1 & (n_{b/2}^1 - n_{f/2}^1) \Pi_2 & \dots & (n_{b/N_r}^1 - n_{f/N_r}^1) \Pi_{N_r} \\ (n_{b/1}^2 - n_{f/1}^2) \Pi_1 & (n_{b/2}^2 - n_{f/2}^2) \Pi_2 & \dots & (n_{b/N_r}^2 - n_{f/N_r}^2) \Pi_{N_r} \\ \vdots & \vdots & \ddots & \vdots \\ (n_{b/1}^{N_s} - n_{f/1}^{N_s}) \Pi_1 & (n_{b/2}^{N_s} - n_{f/2}^{N_s}) \Pi_2 & \dots & (n_{b/N_r}^{N_s} - n_{f/N_r}^{N_s}) \Pi_{N_r} \end{bmatrix}}_{\underline{M}^{[N_k, N_\omega]}(X_i, T)} \underbrace{\begin{pmatrix} k_{f/1} \\ k_{f/2} \\ \vdots \\ k_{f/N_r} \end{pmatrix}}_{\underline{k}} \quad (7)$$

A simple example to illustrate the approach from equations 6 and 7 is given below for a 2-step combustion mechanism of hydrogen and oxygen:



The matrix form with separated reaction rates and concentration terms from the law of mass action reads:

$$\begin{pmatrix} \dot{\omega}^{H_2} \\ \dot{\omega}^{O_2} \\ \dot{\omega}^{OH} \\ \dot{\omega}^{H_2O} \end{pmatrix} = \begin{bmatrix} -\Pi_1 & -\Pi_2 \\ -\Pi_1 & 0 \\ 2\Pi_1 & -2\Pi_2 \\ 0 & 2\Pi_2 \end{bmatrix} \begin{pmatrix} k_{f/1} \\ k_{f/2} \end{pmatrix} \quad (8)$$

with the matrix elements:

$$\begin{aligned} \Pi_1 &= X_{H_2} X_{O_2} - \frac{1}{K_{EQ}} X_{OH}^2 \\ \Pi_2 &= X_{OH}^2 X_{H_2} - \frac{1}{K_{EQ}} X_{H_2O}^2 \end{aligned} \quad (9)$$

The main result of equation 7 is that the source terms can be expressed as the product of the matrix \underline{M} (dimensions: number of reactions x number of species) and the vector of reaction rates. This reads in short notation:

$$\underline{\dot{\omega}} = \underline{M}(X_i, T) \underline{k} \quad (10)$$

If the number of reactions (N_r) is less than or equal to the number of species (N_s), \underline{M} can be uniquely inverted and leads to an expression for \underline{k} as a function of the source terms. With the pseudo inverse \underline{M}^+ we get:

$$\underline{k} = \underline{M}^+(X_i, T) \underline{\dot{\omega}} \quad (11)$$

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(\underline{M}^+ is the pseudo-inverse for $N_r < N_s$ and the exact inverse for $N_r = N_s$)

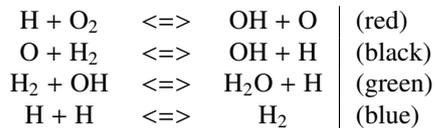
The entire algorithm for the expression and optimization of simplified reaction mechanisms is summarized as follows:

1. Creating training data: set of chemical source terms for given mixture state and composition.
2. Specification of a simplified reaction mechanism.
3. Setting up the matrix M for the equations of the simplified mechanism.
4. Calculation of the reference reaction rates of the simplified mechanism by multiplying the pseudo-inverse of M with the source terms of the original mechanism (training data)
5. Use of small neural networks (typically 2 layers with 3 nodes each) to represent the data for k .
6. Use of the optimized tabulated reaction rate data in the CFD solver.

5.3 Example results for a H_2/O_2 reactor

The method from section 5.2 is to be demonstrated using the optimization of a global 4-step mechanism for the calculation of the ignition behavior in an isobaric H_2/O_2 reactor.

Given global mechanism (the colors correspond to the line colors in Fig. 9):



Training data were obtained from two reference calculations using a Jachimowski mechanism (8 species - 19 reactions). The initial values in the reactor were:

equivalence ratio	temperature	pressure
1.0	1100K	200kPa
0.8	1400K	200kPa

The training data obtained from equation 10 for the 4 reactions given above are shown as symbols in figure 9. The optimized reaction rates were generated by using simple neural networks (2 layers of 3 nodes each) for interpolation and smoothing of the training data and are shown as lines in the figure ("AI-Interpolation").

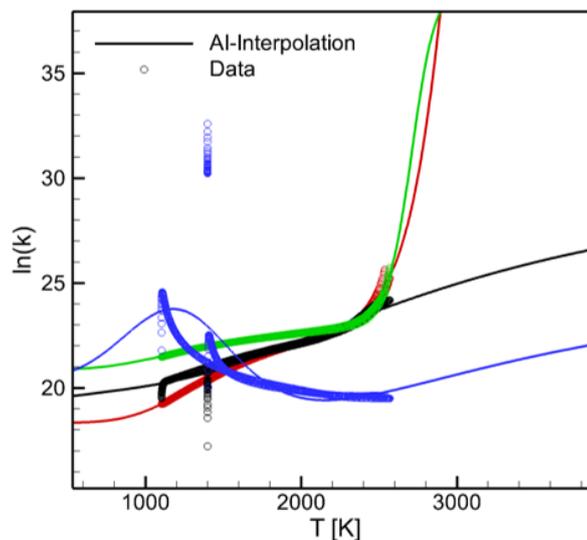


Figure 9: Reaction rates of the global H_2/O_2 mechanism

Results for applying the optimized global 4-step mechanism are shown in figure 10. The red line corresponds to the reference solution of the detailed mechanism, the blue line represents the result of the optimized global mechanism.

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The agreement to the reference data is also good for areas of application outside of the data range which was used for training. Both the ignition delay time and the equilibrium state are reproduced correctly. The approach to use neural networks to optimize reaction rates rather than predict source terms effectively avoids inconsistent results such as the equilibrium drift observed in the previous sections.

Another advantage of the approach presented here is that the results for optimized global mechanisms can be used directly in CFD solvers without major changes of the infrastructure. An example result with a comparison between a TAU and a CANTERA calculation (equivalence ratio of 0.8 and starting temperature of 1200K, isochoric reactor) is given in Fig. 11.

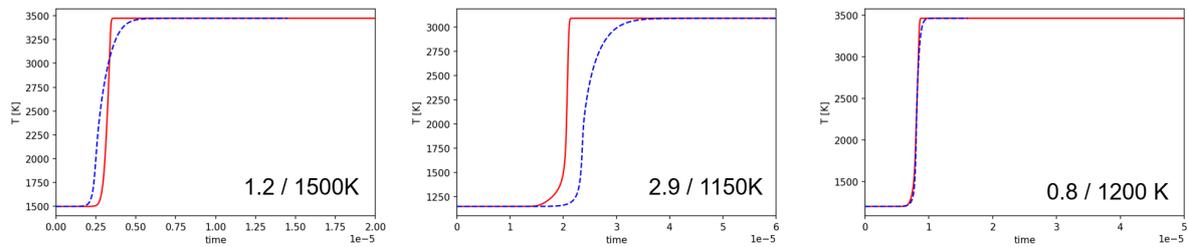


Figure 10: Results obtained with the optimized 4-step mechanism (labels denote the initial equivalence ratio and reactor temperature)

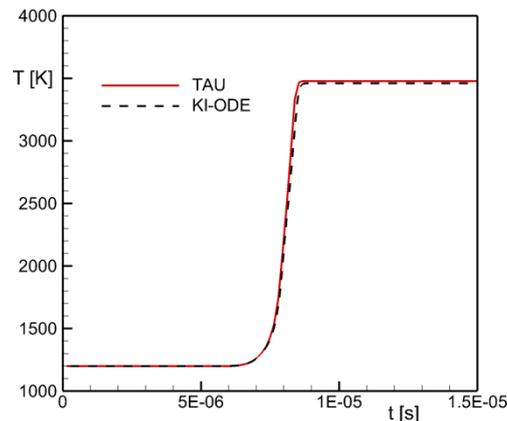


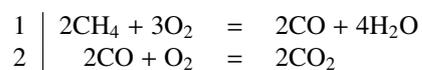
Figure 11: Comparison of the direct solution of the reactor ODE system and the implementation in the TAU CFD solver

6. Benchmark application: Simplification of a complex methane-oxygen combustion mechanism

Finally, a lifted CH_4/O_2 flame will be considered as a benchmark application for the process presented in the previous section. For the reference solution and to create the training data, the 66 reactions - 19 species - Mechanism by Slavinskaya et al. used.⁹ The mechanism is validated for a pressure range between 1-60bar, an equivalence ratio of 1-2 and a temperature range of 900-1800K.

The goal is to emulate the lifted flame structure of a CH_4/O_2 single injector element with an optimized 2-step mechanism. The reactions were adapted from the Westbrook Dryer scheme.¹⁰

The reactions of the global 2-step mechanism are:



The training data were obtained from the analysis of an isobaric reactor at a starting temperature of 1400K, a pressure of 1bar and an equivalence ratio of 1. Zero reaction rates in the low temperature limit were enforced to improve the physical consistency of the final mechanism below the temperature range of the training data. Small neural networks

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(2 layers with 5 nodes each) were then used to fit the reaction rates of the global scheme to the reference rates obtained from equation 11. The optimized reaction rates of the 2-step mechanism and the comparison to the training data in the reactor test case are shown in Fig. 12.

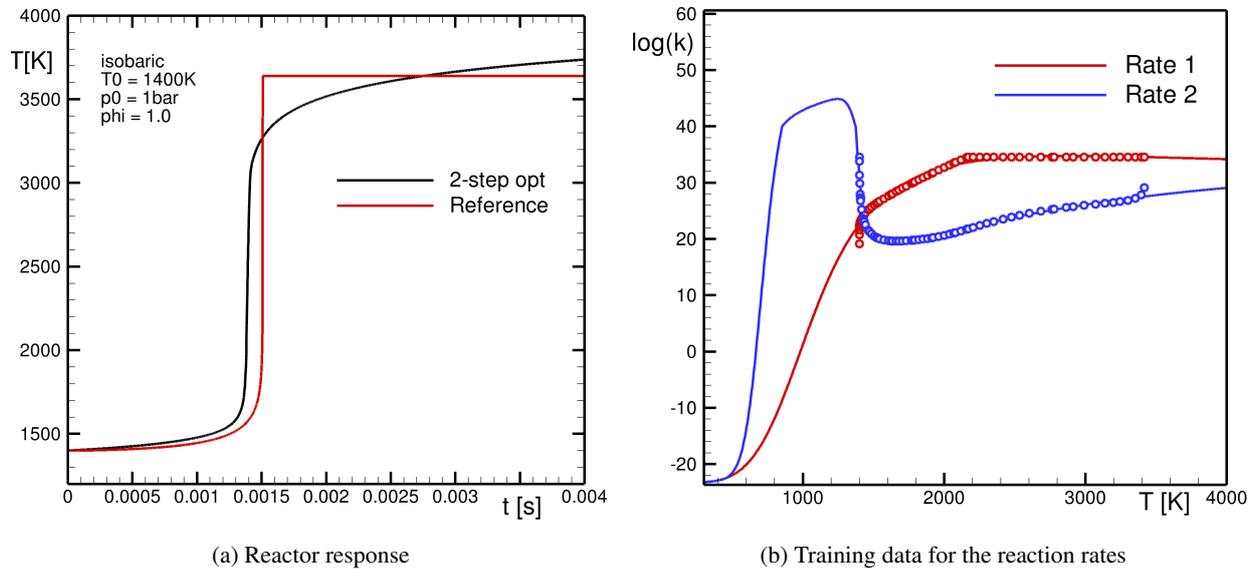


Figure 12: Neural network based simplification of the CH_4/O_2 mechanism

Benchmark calculations were carried out with the DLR flow solver TAU⁸ for both the optimized and the original 2-step mechanism. An isolated CH_4 injector with a diameter of 20cm was considered in an oxygen co-flow under the following conditions:

central	CH_4	$p = 1\text{bar}$, $T = 1300\text{K}$, $u = 1000\text{m/s}$
annular	O_2	$p = 1\text{bar}$, $T = 1400\text{K}$, $u = 2000\text{m/s}$

The flow conditions and geometrical dimensions of the testcase were arbitrarily chosen to obtain a lifted flame. The results are summarized in the figures 13 to 15. The figures show that the optimized mechanism can simulate the ignition delay with high accuracy. A significant improvement in the results compared to the original mechanism can also be observed for the flame structure (sections in figure 15).

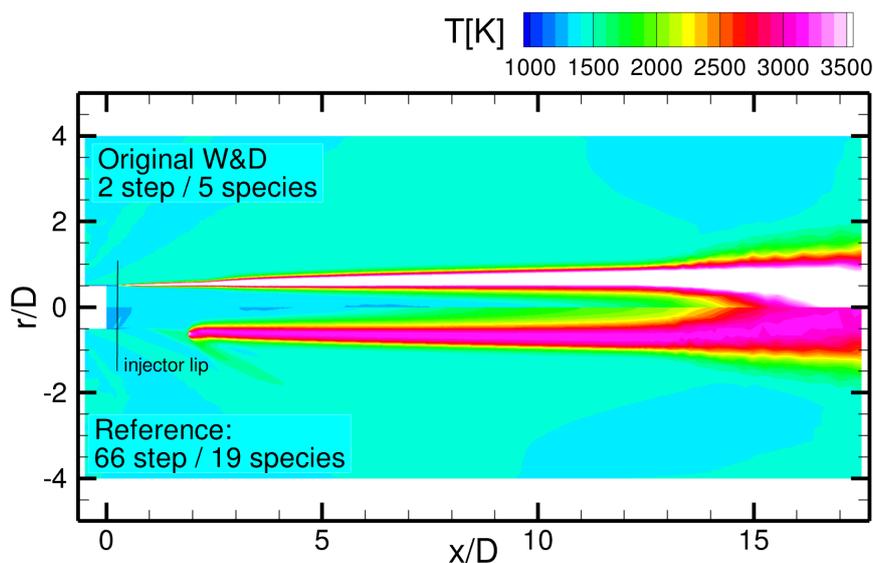


Figure 13: Comparison between the reference 66-step and the original 2-step mechanism

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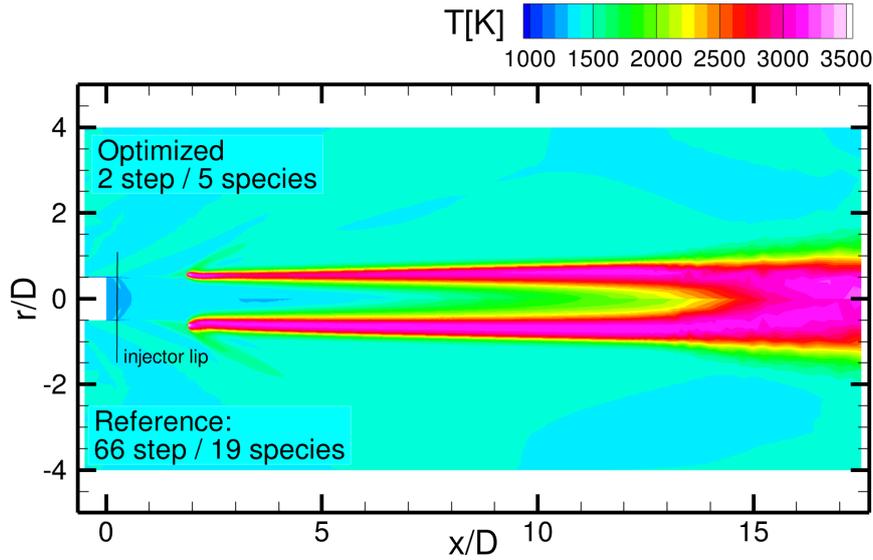
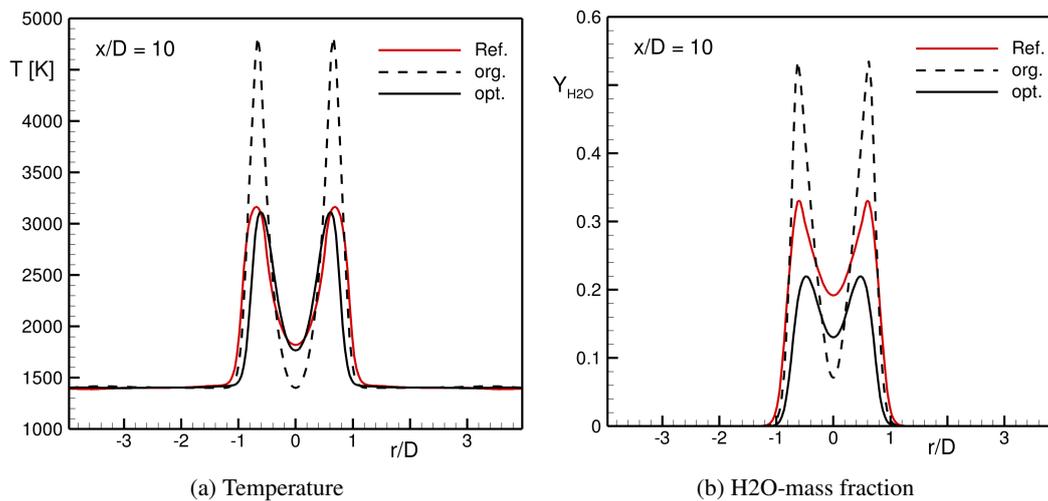


Figure 14: Comparison between the reference 66-step and the optimized 2-step mechanism

Figure 15: Cuts at an axial location of $x/D = 10.0$ (Ref: 66-step, org: original 2-step and opt: optimized 2-step)

7. Summary

Significant results from the evaluation of the different approaches to use neural networks for the treatment of reacting flows in CFD solvers are:

1. In principle, neural networks are found to be able to predict the chemical source terms (formation rates of the mixture components involved) from the local mixture composition and the thermodynamic state.
2. The most important problem is the large mathematical stiffness of the problem. Formation rates vary over many orders of magnitude and can take positive and negative values.
3. Despite the overall good accuracy, there are problems in the exact prediction of vanishingly small source terms. This leads to drift phenomena in the equilibrium composition and erroneous predictions of ignition delay.
4. The problem of stiffness could be partially solved by adapted mathematical structures of the neural network. In particular, robust results could be achieved with the "Arrhenius nodes" (see section 4.3). However, in this case the rigidity has been shifted to the training process of the neural network, so that the optimization of a unique

parameter set is extremely complex. It was often not possible to find a converged optimum for the weighting factors in the network.

5. Promising results could be achieved by using neural networks to optimize reaction rates instead of directly estimating the chemical source term. Reaction rates do not take on negative values which enables the analysis and optimization in logarithmic space. Only minor modifications in CFD solvers are required to use the resulting tabulated rate functions (k as a function of temperature and potentially also other state variables). The main disadvantages of this approach are the restriction of the maximum number of chemical reactions to the number of species involved and the need to prescribe a simplified reaction mechanism.

8. Acknowledgments

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