Optimal artificial neural networks
and tabulation methods for chemistry representation
in LES of a bluff-body swirl-stabilized flame

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Abstract

Large-eddy simulations (LES) of the Sydney bluff-body swirl-stabilized methane–hydrogen flame are performed, employing two chemistry representation methods, namely a conventional structured tabulation technique and artificial neural networks (ANNs). A generalized method for the generation of optimal artificial networks (OANNs) has been proposed by Ihme et al. [M. Ihme, A.L. Marsden, H. Pitsch, Neural Comput. 20 (2) (2008) 573–601]. This method is, for the first time, applied in LES of turbulent reactive flows, guaranteeing an optimal chemistry representation with error control, which was previously not possible. The network performance with respect to accuracy, data retrieval time, and storage requirements is compared with the structured tabulation of increasing resolution, and effects of long-time error accumulation on the statistical results during a numerical simulation are discussed. Using the optimization algorithm, it is demonstrated that ANN accuracies can be achieved which are comparable with structured tables of moderate to fine resolution. Furthermore, it is shown that for a comparable number of synaptic weights, the network fitness increases with increasing number of hidden layers. Compared to the tabulation technique, data retrieval from the network is computationally more expensive; however, the additional overhead associated with the ANN evaluation remains acceptable in LES applications. Results for flow field statistics and scalar quantities which are obtained from LES are in good agreement with experimental data, and possible reasons for the differences between computed and measured temperature profiles near the bluff-body are discussed. The difference in the velocity statistics between simulations employing structured table and network representation are small, and deviations in the CO\textsubscript{2} profiles on the fuel-rich side of the flame are mainly attributed to the sensitivity of CO\textsubscript{2} with respect to changes in progress variable.

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1. Introduction

Numerical predictions of turbulent reactive flows often involve fuels that are described by chemical mechanisms comprising hundreds of
species and thousands of elementary chemical reactions. The direct integration of such detailed chemical mechanisms in unsteady three-dimensional flows is currently limited by available computational resources [1].

In situ adaptive tabulation (ISAT) [2] and solution mapping using piecewise polynomial approximation (PRISM) [3] are examples for methods, in which only the accessed thermochemical state space is computed during the simulation and stored in a table for further reuse, resulting in a considerable reduction of the computational time.

An alternative approach to the direct integration of the detailed chemical system is the parameterization of the thermochemical quantities in terms of a reduced set of reaction coordinates. Examples are the intrinsic low-dimensional manifold (ILDM) model [4], and flamelet-based combustion models, such as the laminar flamelet model for the description of non-premixed flames [5,6] or the flamelet-generated manifolds (FGM) [7] and the flame prolongation of ILDM (FPI) method [8] for the representation of premixed and partially premixed flames.

In these models, the accessible thermochemical state space is precomputed and is typically stored in a structured table as function of the reduced set of reaction coordinates. In a numerical simulation, additional transport equations for these reaction coordinates are then solved and the corresponding thermochemical composition is retrieved from the table by interpolation. In order to facilitate a fast data retrieval, structured tables with equidistant grid spacing in all coordinate directions are often employed.

Since the chemical reaction rates and radical distributions are typically confined to a narrow region in composition space around the stoichiometric condition, such structured tables require a rather fine resolution, resulting in large storage requirements, which constrains the number of independent reaction coordinates typically to less than five.

Artificial neural networks (ANNs), methods employing self-similarity solutions [9], or re-modeling [10] are attractive alternatives to tabulation techniques for the representation of chemical systems. ANNs have been applied for chemistry approximation by different groups [11–14]. Important advantages of ANNs over tabulation methods are their cost-effective and smooth function representation and modest memory requirements, since only the architecture and the synaptic weights of the network must be stored. However, a major drawback of ANN applications is that the optimization process based on different network architectures can result in both, rather similar as well as vastly different function approximations. Their accuracy is reflected by the so-called network fitness and depends on different parameters, such as the number of layers and neurons, the neural transfer functions, the network connectivity, and the size of the training set. The selection of a particular network architecture with near-optimal fitness is therefore non-trivial and often arbitrary. To overcome this limitation, a methodology for the generation of optimal artificial neural networks (OANNs) with local error control has recently been developed by Ihme et al. [15]. This method employs a generalized mixed variable pattern search algorithm and identifies this network architecture which results in the lowest approximation error.

The objective of the present work is the application of OANNs in combustion simulations and a detailed performance analysis of OANNs with respect to accuracy, data retrieval time, and storage requirements in direct comparison with conventional tabulation methods.

The methane–hydrogen/air flame SMH1 from the Sydney bluff-body swirl-stabilized burner configuration [16–19] is used as geometric configuration for the LES to investigate the effect of the long-time error accumulation during the simulation on the statistical results.

The remainder of this article is organized as follows. The mathematical formulation and the combustion model are summarized in the next section, and the two techniques for the chemistry representation are described in Section 3. The performance of both methods with respect to accuracy, memory requirements, and computational time for both the tabulation method and OANNs is compared and discussed in Section 4. Computational results from three large-eddy simulations of the SMH1 flame are presented in Section 6, and the paper finishes with conclusions.

2. Mathematical formulation and combustion model

In LES of turbulent reactive flows, the Favre-filtered form of the Navier–Stokes equations are solved. Favre-filtered quantities are denoted by a tilde, and an overbar refers to volume-filtered quantities. The residual stress tensor, appearing as unclosed term in the momentum equations, is modeled by a dynamic Smagorinsky model [20,21]. In addition to the residual stresses, the filtered density is also unknown and is dependent on temperature and species distribution in the flame. Therefore, a combustion model is employed which relates the density and all other thermochemical quantities to a reduced set of reaction coordinates.

In the present work, the flamelet/progress variable (FPV) approach [22,23] is used for the prediction of the turbulent reactive flow field. The model is based on the steady laminar flamelet equations [5,6], in which all thermochemical quantities are parameterized by the mixture fraction \( Z \).
and the scalar dissipation rate $\gamma_Z$. However, for reasons which are outlined in Refs. [22] and [23], in the FPV model the scalar dissipation rate is replaced by a reaction progress variable $C$. This reactive scalar corresponds to a linear combination of major product mass fractions, and is here defined as $C = Y_{CO_2} + Y_{CO} + Y_{H_2O} + Y_{H_2}$. With this, all thermochemical quantities, denoted by $\phi$, can then be written as $\phi = \mathcal{F}_\phi(Z, C)$, where $\mathcal{F}$ denotes the FPV chemistry library, and $\phi$ is obtained by employing a presumed PDF approach, in which the joint PDF of $Z$ and $C$ is modeled by a beta distribution for the mixture fraction and a mixture fraction-conditioned Dirac function for the progress variable [22]. The Favre-filtered form of all thermochemical quantities can then be written as $\tilde{\phi} = \tilde{\mathcal{F}}_\phi(Z, \tilde{\phi}, \mathcal{C})$. The choice of the PDF closure model was motivated by the following reasons. First, it was shown in previous studies that this closure model accurately predicts the turbulence/chemistry interaction for stably burning flames [24], and it was reported that extinction and reignition effects may not be of significance in this flame [16,25]. Second, the primary focus of this work is on the chemistry representation rather than on the combustion modeling. However, it is important to point out that a major advantage of OANNs is their applicability to higher-dimensional chemistry representations. This is particularly relevant when more complex turbulence/chemistry interactions are modeled requiring more than three parameters.

In addition to the solution of the Favre-filtered Navier–Stokes equations, the FPV model requires also the solution of the Favre-filtered conservation equations for mixture fraction, progress variable, and residual mixture fraction variance, which is denoted by $Z^\varphi$. More details are given in Ref. [26] and are here omitted for brevity.

### 3. Chemistry representation

The thermochemical state space is obtained from the solution of the steady laminar flamelet equations. More than 80 flamelets along the complete S-shaped curve are computed and used for the compilation of the structured tables and for the generation of the OANNs, which are later used in the LES application.

In the LES computation, information about the filtered quantities of density $\rho$, chemical source term for the progress variable $\bar{\omega}_C$, kinematic viscosity $\bar{v}$, and molecular diffusivity $\bar{z}$ are required. In addition, for the computation of statistical properties of the flame structure, the filtered temperature $\bar{\Theta}$, and mass fractions of $CO_2$ and $H_2O$ are also obtained from the state relation. In order to increase the resolution in the direction of the mixture fraction variance, the unmixedness $\tilde{S} = Z^\varphi / (\bar{Z}(1 - \bar{Z}))$ is introduced and all thermochemical quantities, which are of importance for the numerical simulation, are then parameterized as

$$\phi = \tilde{\mathcal{F}}_\phi(Z, \tilde{S}, \mathcal{C})$$

and $\phi = (\bar{\rho}, \bar{\omega}_C, \bar{v}, \bar{z}, \bar{\Theta}, \bar{Y}_{CO_2}, \bar{Y}_{H_2O})^T$. This information is made accessible during the simulation through a structured table or OANNs. Both chemistry representation methods are explained next.

#### 3.1. Tabulation method

In the following, all Favre-averaged thermochemical quantities are stored in a structured table as function of the three scalars $\bar{Z}$, $\bar{S}$, and $\mathcal{C}$. The table, in the following denoted by $\mathcal{F}_Z$, uses an equidistant grid spacing in $\bar{Z}$ and $\mathcal{C}$ directions, respectively, and a geometric growth law is used for the discretization in the $\bar{S}$ direction. A bisection method is employed as search algorithm in all directions, and a tri-linear interpolation is used to compute values between the grid points.

In the following, four structured tables with increasing resolution are generated. After the performance of these tables is assessed in a direct comparison with OANNs, two of these tables are employed in LES to investigate the effect of the long-time error accumulation on the statistical results.

#### 3.2. Optimal artificial neural networks

An ANN is a computational model for storing and retrieving knowledge, which is acquired during a learning process. The architecture of an ANN can be characterized by an arrangement of layers and neurons, nodal connectivity, and nodal transfer functions. In the following, the class of multilayer perceptrons (MLPs) is considered. An example of such an MLP-network is shown in Fig. 1, having three input and one output channels, and $N_L = 3$ hidden layers with 2, 3, and 1 neurons in each layer, respectively. The number of neurons in each hidden layer is denoted by $N_N$. The connectivity between the neurons can

![Fig. 1. Architecture of a multilayer perceptron.](image_url)
be represented by the underlying directed graph $G$. The output $y_j$ of each neuron $i$ is computed according to $y_j = \psi_j\left(\sum w_{ij} x_i\right)$, where $x_i$ is the $i$th input signal and $w_{ij}$ is the corresponding synaptic weight. These weights are adjusted during a training process using a Levenberg–Marquardt algorithm. In the following the neuron in the last hidden layer employs a linear transfer function with $\psi(s) = s$, and sigmoidal transfer functions are used for all other neurons.

For specified network connectivity and transfer functions, the fitness of a particular ANN architecture $J(\mathcal{A})$ is dependent on $N_L$, $N_N$, and the approximated thermochemical quantity $\bar{\phi}$. The network fitness is in the following quantified by the cost function:

$$J(\mathcal{A}) = \log_{10} \left[ \left( \frac{1}{N_s} \sum_{j=1}^{N_s} (\bar{\phi}_j - \bar{\phi}^*_j)^2 \right)^{1/2} \right]$$

where $N_s$ is the number of test samples and $\bar{\phi}^*_j$ is the $j$th sample value. In order to allow for an objective comparison among different networks, the cost function is normalized.

In the following, the number of layers and neurons per non-linear layers are considered to be free parameters, and we wish to find this combination of $N_L$ and $N_N$ which results in the optimal network with the lowest cost function. For the generation of such an optimal ANN, a generalized pattern search (GPS) methods is used [15, 27]. This derivative-free optimization method generates a sequence of iterates, whose cost function is non-increasing [27]. All points at which the cost function is evaluated are restricted to lie on a mesh. The algorithm proceeds in two stages: a search and a poll step. The search step allows for a mesh-restricted local and global exploration of the parameter space. In this step, a finite number of search points is evaluated with the objective of identifying a region with a reduced cost function. In order to reduce the computational cost of the algorithm, the search step can be supplemented by a surrogate function, such as Kriging approximation. In the case of an unsuccessful search step, a poll step in a discrete neighborhood of the current best point with the lowest cost function is executed. If all poll steps are unsuccessful, the mesh is refined, and a new iteration, starting with a search step, is performed. Although the GPS method is very robust, this algorithm does not guarantee that the solution is a global minimum. The limit point of the sequence of iterations, however, corresponds to a local optimal solution, which is defined with respect to a set of neighbors. More details on the algorithm and its application to ANNs in the presence of categorical variables such as neural transfer functions or nodal connectivities can be found in Ref. [15].

4. Performance analysis

The accuracy, memory requirements, and computational costs associated with the table interpolation and the network evaluation are addressed in this section.

Since $N_L$ and $N_N$ are input parameters to the optimization algorithm, the sensitivity of these parameters on the network fitness is analyzed first. For this, three different network optimizations are performed, having 6, 4, 3 hidden layers and 8, 12, 16 neurons per non-linear hidden layer, respectively. This results in a comparable number of synaptic weights for all three optimization cases. In order to reduce the statistical error [15], five runs with different initializations and different test samples were performed for each of the three networks. Results of the study are summarized in Fig. 2. The open symbols show the mean values of the cost function computed from all five network candidates of a particular network structure, and the error bars show the standard deviation. From this figure it can be concluded that the network fitness increases with increasing number of hidden layers. This result is different from the findings by Flemming et al. [14], where it was argued that a network with two non-linear layers results in the best fitness characteristics, and further increase in the number of layers would only increase the computational cost with only minimal improvements in the fitness. In fact, the results of Fig. 2 show that the approximation error can be improved by as much as a factor of four when five instead of two non-linear hidden layers are used.

In the following, each thermochemical quantity is represented by one network, whose architecture is obtained from the GPS optimization. Based on the findings of the previous paragraph, the maximum size of the network is restricted to five hidden layers, in which the last layer contains only one linear neuron. The maximum number of neurons in the remaining four layers is set to eight, having a sigmoidal transfer function. The connectivity matrix is kept constant, corresponding to a fully-connected feed-forward network. The training set used for adjusting the synaptic weights consists of 50,000 samples, and all $N_s = 1.2 \times 10^6$ flamelet data samples are used to evaluate

Fig. 2. Sensitivity of the number of hidden layers and neurons per layer on the network fitness.
Note that a reduction of the table size by a factor of two can be achieved by storing the data in single precision format.

The ratio of the time required to retrieve information from the network and the structured table is shown in Fig. 3. The averaged time to evaluate all test samples is denoted by $\tau$ with subscripts $\mathcal{A}$ and $\mathcal{F}$ referring to the ANN and tabulation, respectively. Compared to the $400 \times 50 \times 400$ table, the network evaluation is more than three times slower. Note, however, that in the LES application, the table retrieval of all thermochemical quantities amounts to less than three percent of the overall computational time, so that the additional overhead associated with the network evaluation remains acceptable.

Finally, the effect of the table interpolation and ANN representation on the temporal spectra for temperature and chemical source term are analyzed. For this, temporal signals at different locations in the flame for $Z$, $S$, and $C$ are collected from the LES of a bluff-body swirl-stabilized flame, which is described in the next section. From these time series, the chemical source term is evaluated from the table and from the OANN. The corresponding spectra were computed and are shown as function of frequency $f$ in Fig. 4. It is interesting to point out that all spectra obtained with the table interpolation converge with increasing table resolution to the ANN spectra in the mid- and high-frequency range. This suggests that a smoother flow field solution can be obtained by employing an OANN approximation, which may also result in faster convergence and more robust simulations.

Table 1
Architecture of the OANNs identified from the GPS algorithm for all thermochemical species which are relevant for the LES application

<table>
<thead>
<tr>
<th>Species</th>
<th>ANN architecture</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\overline{p}$</td>
<td>4-8-4-4-1</td>
</tr>
<tr>
<td>$\overline{\omega}_C$</td>
<td>6-4-8-4-1</td>
</tr>
<tr>
<td>$\overline{v}$</td>
<td>7-8-8-1</td>
</tr>
<tr>
<td>$\overline{z}$</td>
<td>8-8-8-1</td>
</tr>
<tr>
<td>$\Theta$</td>
<td>8-4-7-8-1</td>
</tr>
<tr>
<td>$\overline{Y}_{CO_2}$</td>
<td>4-8-8-4-1</td>
</tr>
<tr>
<td>$\overline{Y}_{H_2O}$</td>
<td>3-8-8-8-1</td>
</tr>
</tbody>
</table>

The connectivity corresponds to a fully-connected feed-forward network with sigmoidal transfer functions for all non-linear neurons.

Table 2
Comparison of memory requirements and network fitness between tabulation method with increasing resolution and OANNs

<table>
<thead>
<tr>
<th>Table size</th>
<th>Memory (MB)</th>
<th>Cost function</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\overline{p}$</td>
<td>$\overline{\omega}_C$</td>
<td>$\overline{v}$</td>
</tr>
<tr>
<td>100 $\times$ 13 $\times$ 100</td>
<td>7</td>
<td>-1.544</td>
</tr>
<tr>
<td>200 $\times$ 25 $\times$ 200</td>
<td>53</td>
<td>-1.858</td>
</tr>
<tr>
<td>400 $\times$ 50 $\times$ 400</td>
<td>427</td>
<td>-2.553</td>
</tr>
<tr>
<td>800 $\times$ 100 $\times$ 800</td>
<td>3417</td>
<td>-2.553</td>
</tr>
<tr>
<td>ANN</td>
<td>0.1</td>
<td>-2.478</td>
</tr>
</tbody>
</table>

Note that a reduction of the table size by a factor of two can be achieved by storing the data in single precision format.

![Fig. 3. Ratio between the time required to retrieve information from the network, $\tau_{\mathcal{A}}$, and the table, $\tau_{\mathcal{F}}$.](image-url)
5. Experimental configuration and numerical setup

The SMH1 flame from a series of bluff-body swirl-stabilized flame experiments is used to analyze the effects due to errors in the table interpolation and in the ANN approximation on the statistical flow field quantities in the context of an LES application.

The burner configuration of this well-characterized flame consists of a central fuel nozzle of 3.6 mm diameter which is surrounded by a bluff body with $D_{\text{ref}} = 50$ mm diameter. Swirling air at an axial bulk velocity of $U_s = 42.8$ m/s is supplied through an annulus of 10 mm width. The burner is surrounded by a coflowing air stream with an axial velocity of $U_e = 20$ m/s. The fuel consists of a methane/hydrogen mixture in a volumetric ratio of 1:1. The bulk exit velocity of the fuel stream is $U_J = 140.8$ m/s. The geometric swirl number for this configuration is $S_g = 0.32$. The turbulent flow field of this flame series was measured by Kalt et al. [16] and Al-Abdeli and Masri [17], species measurements were performed by Kalt et al. [16] and Masri et al. [18], and all experimental results are available from Ref. [19].

The Favre-filtered transport equations for mass, momentum, mixture fraction, progress variable, and residual mixture fraction variance are solved in cylindrical coordinates [22]. The computational domain is $5D_{\text{ref}} \times 3D_{\text{ref}} \times 2\pi$ in axial, radial, and circumferential directions, respectively. The radial direction is discretized by 230 unevenly spaced grid points concentrated in the shear layer region surrounding the fuel jet and swirling annulus. The grid in axial direction uses 192 points and is stretched in downstream direction while the circumferential direction is equally spaced and uses 64 points. The turbulent inflow profiles for the fuel nozzle and annulus are computed from a separate pipe flow simulation by enforcing the bulk axial and azimuthal velocity reported in the experiment. The GRI 2.11 mechanism [28] is used for the description of the chemistry.

6. Results

In this section, results from three LES computations employing two structured tabulations with different resolutions and OANNs for the chemistry representation are presented. Statistical data are collected over four flow-through-times. For reference, the azimuthal and temporal averaged quantity of a scalar $\phi$ is denoted by $\langle \phi \rangle$, and the resolved scalar variance is indicated by $\langle \phi^2 \rangle$.

6.1. Velocity field

Radial profiles of axial and azimuthal velocity components at four axial locations are shown in Figs. 5 and 6. All three numerical simulations are in overall good agreement with experimental data up to the neck region of the flame, corresponding to $L_N \approx 1.4D_{\text{ref}}$. Downstream of this location, the decay rate of the fuel jet stream is under-predicted. The computational results suggest that the contraction of the swirling stream is slightly under-predicted up to $L_N$ and over-predicted downstream of this location. Azimuthal velocity profiles are presented in Fig. 6, and good agreement between experiment and simulations is evident for the mean velocity in the region up to the end of the recirculation zone. Further downstream, all three simulations over-predict the strength of the axial vortex.
A comparison of the statistical flow field results shows that both methods for the chemistry representation yield very similar results, and differences are only apparent in the region close to the centerline. Interestingly, the increasing table resolution has only a marginal effect on the statistical velocity profiles.

6.2. Scalar fields

Radial profiles of the mean mixture fraction are shown in Fig. 7. Both, simulations and experiments predict a region of homogeneous mixture directly behind the bluff body. The location of stoichiometry is aligned with the inner shear layer of the swirling stream. Since the value of the stoichiometric mixture fraction is $Z_{st} = 0.042$, accurate prediction of the shear layer is crucial for the determination of species and temperature distributions. Even though all three simulations slightly over-predict the spreading rate of $\langle Z \rangle$, the computed axial decay rates are in excellent agreement with the experiments.

The computed instantaneous and averaged temperature fields are presented in Fig. 8, where the solid line corresponds to the location of stoichiometric mixture. The instantaneous temperature contours show a wide range of turbulent scales and some entrainment of fresh air into the flame zone at the end of the recirculation bubble. It is speculated that regions of low flame temperature at different locations in the neck region of the flame provide some evidence for local extinction and reignition, however, this was not further investigated here. Up to $L_N$, the averaged temperature field shows strong heat release in a narrow zone on the fuel-rich side of the stoichiometric surface, and the width of this zone increases with increasing downstream distance.

Mixture fraction-conditioned results for temperature and mass fractions of CO$_2$ and H$_2$O are shown in Fig. 9. All computations over-predict the conditional data at $x/D_{ref} = 0.2$ around $Z_{st}$, which corresponds to the location in the inner shear layer of the swirling stream, and a possible explanation for the discrepancy is provided in the next paragraph. The predictions for temperature and water mass fraction are in excellent agreement with experimental data at further downstream locations. While all simulations are in good agreement for temperature and H$_2$O, the simulation with the OANN representation deviates from the table simulation for CO$_2$ on the fuel-rich side of the flame. In a data analysis it was found that this discrepancy can be attributed to the following two reasons. First, results from simulations employing OANNs and the conventional tabulation technique showed some small differences in the statistical results for the progress variable, which are

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**Fig. 6.** Comparison of measured and calculated mean and resolved rms statistics of azimuthal velocity at different axial locations in the Sydney SMH1 flame.

**Fig. 7.** Comparison of measured and calculated mean and resolved rms statistics of mixture fraction at different axial locations in the Sydney SMH1 flame.

**Fig. 8.** Instantaneous and averaged temperature fields of the Sydney SMH1 flame, computed with ANN chemistry representation. The solid line shows the location of stoichiometric mixture fraction with $Z_{st} = 0.042$. 
mainly due to differences in the data retrieval methods for the evaluation of the chemical source term. The second reason is that CO$_2$ exhibits a strong sensitivity to variations in the progress variable at fuel-rich conditions and large value for the progress variable. Therefore, the small over-prediction of $e_C$ in the simulation employing OANNs result in the under-prediction of CO$_2$ which is shown in Fig. 9. In summary, the differences in the conditional data for CO$_2$ are not attributed to poor network fitness but rather to the strong sensitivity of CO$_2$ with respect to progress variable and small differences in $e_C$ between simulations employing OANNs and conventional tabulation techniques.

In order to investigate the reason for the discrepancies at $x/D_{ref} = 0.2$ and the associated rapid heat release in the inner shear layer of the swirling stream, a mesh refinement study and a sensitivity analysis of the FPV combustion model was conducted. In this study it was found that the temperature profiles are only weakly sensitive to an increasing numerical resolution in the inner shear layer region of the swirling stream. Also, the reduction of the scalar dissipation rate around $Z_{st}$, due to the recirculation zone behind the bluff body does not significantly affect the flame structure at the first measurement location. The effect of the residual scale model was assessed by analyzing flamelet profiles at $x/D_{ref} = 0.2$, and it was found that a significant increase in $Z^{u2}$ would be required to match the experimental data. Although a transport equation for $Z^{u2}$ was solved, it is believed that modeling errors alone cannot be made responsible for this discrepancy.

In the current simulation, an adiabatic combustion model is used and wall heat loss effects are not considered. Therefore, the flame is attached to the edge of the bluff-body. However, it is speculated that wall heat losses around this edge lead to flame quenching and lift-off, and a possible formation of a triple flame. In order to substantiate this hypothesis, a separate simulation was performed, in which the chemical source term in the transport equation for $C$ was set to zero up to $x = 0.15D_{ref}$. Although more sophisticated models can be employed to consider heat loss effects [29], this admittedly simplistic model provides valuable information on the sensitivity of the simulation results to potential wall heat losses. Temperature profiles obtained from this simulation are compared with the adiabatic simulation and experimental data in Fig. 10. This figure shows that the consideration of non-adiabatic effects leads to a reduction of the peak temperature in the shear layer, and provides some evidence that an improved prediction of the flame base may require the consideration of wall heat loss effects.

7. Conclusions

Large-eddy simulations of the Sydney bluff-body swirl-stabilized SMH1 flame were performed, using a flamelet/progress variable model. This model employs a chemistry representation method, in which all thermochemical quantities are parameterized in terms of three statistical scalar quantities. For the chemistry representation, a conventional tabulation technique and an approximation method using OANNs were employed.

The main objective of this work was the thorough analysis and comparison of both chemistry representation methods in terms of accuracy, memory requirements, computational costs, as well as the effects of long-time error accumulation on the results during a numerical simulation. The following conclusions can be drawn:

- By employing a network optimization method, a specific ANN architecture for each of the thermochemical quantities can be identified.
with comparable or better accuracy than conventional structured tables; however, at considerably lower storage requirements.

- For networks with similar number of synaptic weights, it was shown that the fitness of the OANNs increases with increasing number of hidden layers.
- Compared to the tabulation method, data retrieval from the network can take as much as five times longer. Since the efficient table retrieval of all thermochemical quantities in an LES application amounts typically to less than three percent of the overall computational time, the additional overhead remains acceptable.
- The computed velocity and scalar statistics are in good agreement with experimental data. It is speculated that the over-prediction of temperature and species distributions close to the bluff-body is attributed to wall heat loss effects and some numerical evidence for this hypothesis is provided.

The code for the generation of optimal artificial neural networks is available from the first author.

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