Advanced gas phase combustion models: validation for biogases by means of LES and experiments as well as application to biomass furnaces

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Abstract

The increasing power of computers allows advanced combustion models to be used in CFD simulations for engineering applications like biomass furnaces. Such models are especially valuable because of their ability to predict chemical radicals as well as kinetically limited processes like NOx formation, thus improving the overall prediction quality of CFD simulations. At the same time an evaluation of the accuracy of such models is difficult due to the strong coupling between chemistry and turbulence in turbulent reacting flows. This paper presents results of the step-wise validation of the Eddy Dissipation Concept (EDC) in combination with the reduced reaction mechanism for methane combustion ARM 19.

Computationally expensive Large Eddy Simulations (LES) of the Sandia D flame were carried out in order to minimise the influence of turbulence modelling on the numerical results. A comparison of LES results with experimental data justified the choice of the reduced reaction mechanism. Once validated, the reduced chemical mechanism was combined with the EDC and applied to simulations of the Sandia D flame and the Sandia CO/H2/N2 flame B chosen as approximations of biomass combustion gases. A good agreement between numerical and experimental data was achieved. Furthermore, sensitivity analyses were carried out with various combinations of turbulence models, combustion models and reaction mechanisms of different complexity in order to evaluate the individual influence of every model input on the overall results.

All findings of the present study concerning the accuracy and limitations of EDC are considered in the ongoing research on the modelling of combustion processes in biomass furnaces. The validated model proved to be a valuable tool for improved combustion prediction.

Keywords

CFD combustion modelling, LES, Eddy Dissipation Concept, Laminar Flamelet Model, biomass furnace

1 Introduction

A large variety of turbulent combustion models of different complexity levels exist; some of them are now available in the commercial CFD codes. CFD-aided design and optimisation of engineering applications like biomass furnaces are usually based on simpler combustion models in combination with global reaction mechanisms, e.g. the Eddy Dissipation Model.
EDM) [14, 15], mainly due to the limiting factor of calculation time. The increasing efficiency of computers and numerical methods is now making the application of advanced combustion models and more detailed reaction mechanisms ever more attractive. Such models are especially valuable because of their ability to more accurately predict chemical radicals as well as slow chemistry processes like NO\textsubscript{x} formation, thus improving the overall quality of the combustion simulation. An evaluation of the accuracy of such models is difficult because the chemistry and turbulence in turbulent reacting flows are strongly coupled and because the overall accuracy of the numerical prediction of turbulent reactive flows is very sensitive to the prediction of the turbulent flow field.

Large Eddy Simulations (LES) considerably improve the prediction accuracy of turbulent flow compared to the Reynolds Averaged Navier Stokes (RANS) simulations. Since in LES the largest part of the turbulent energy cascade is resolved, LES can be applied for fundamental investigations of turbulent flows. New numerical techniques like ISAT (In-Situ-Adaptive-Tabulation) allow for the tabulation of reaction kinetics and therefore also for the integration of complex reaction kinetics in LES.

This paper presents results of the step-wise validation of the Eddy Dissipation Concept (EDC) for RANS in combination with a reduced reaction mechanism for methane combustion ARM 19 with a view to their application to biomass combustion systems. As a first step, the mechanism was evaluated by means of LES of Sandia Flame D, [1]. Applying the same mechanism, 2D RANS simulations of this flame were carried out with different turbulence models and turbulent combustion models in order to investigate the influence of turbulence and combustion modelling on the overall simulation results. Subsequently, 2D simulations of experimentally studied flame Sandia CO/H\textsubscript{2}/N\textsubscript{2} B [2] were performed with different combustion models and reaction mechanisms of different complexity, ranging from global to detailed, in order to investigate the sensitivity of the numerical results to different combustion models and reaction mechanisms.

2 Models applied

All simulations performed within the present work were carried out using the commercial CFD solver FLUENT® 6. Two general approaches for turbulence modelling, RANS and LES, were followed. Various RANS turbulence models (\(k-\varepsilon\) models and the Reynolds Stress Model) as well as different combustion models (Eddy Dissipation Concept, Eddy Dissipation Model and Steady Laminar Flamelet Model) were applied. A brief description of the turbulence and combustion models employed is given in the following. For a more detailed explanation see [5]. The reaction mechanisms used for numerical investigations will be referenced in the respective chapters.

2.1 LES

In LES the time-dependent governing equations of the turbulent reactive flow are spatially filtered, whereas in FLUENT the finite-volume discretisation itself provides the filter width. In other words, if the length and time scales are fully resolved, the LES is equivalent to a DNS (Direct Numerical Simulation). The unknown sub-grid-scale (SGS) stress tensor in the filtered momentum equation is modelled with the Smagorinsky approximation, whereas the Smagorinsky constant of the SGS eddy viscosity was evaluated dynamically. In general, any of the chemical source-terms closures developed for RANS can be applied to the reacting-flow LES, when appropriately modified [7]. In the present work, the Laminar Chemistry (LC)
model for LES was used, validated in [8] on two experimental flames. In the LC model filtered species and temperature transport equations are solved using an assumed shape filtered mass density function. Here, uniform scalars are assumed at scales smaller than the grid, i.e. SGS fluctuations of species concentrations and temperature are ignored.

2.2 RANS

In the RANS approach of a turbulent reactive flow, FLUENT solves density-averaged (Favre-averaged) instead of time-averaged (Reynolds-averaged) transport equations for mass and momentum. Depending on the mathematical formulation of the combustion model, additional density-averaged transport equations are solved.

2.2.1 Turbulence models

The closure of the momentum equations is given by a turbulence model. In the present work two turbulent viscosity based models (Standard \( k-\varepsilon \) and Realisable \( k-\varepsilon \) models) as well as the Reynolds Stress Model (RSM) were applied. The latter accounts for the anisotropic nature of the turbulence, as the equations for all six components, \( \overline{u_i u_j} \), of the Reynolds stress tensor are solved, together with an equation for the dissipation rate of turbulent kinetic energy, \( \varepsilon \). The Standard \( k-\varepsilon \) and Realisable \( k-\varepsilon \) models rely on the isotropic eddy viscosity hypothesis. In this case, the Reynolds stresses are formulated in terms of the turbulent kinetic energy, \( k \), the mean velocity gradients and the eddy viscosity, \( \mu_T \), which is in turn determined as

\[
\mu_T = \rho C_\mu \frac{k^2}{\varepsilon},
\]

with density \( \rho \), Favre-averaged \( k \) and \( \varepsilon \) and model constant \( C_\mu \). Transport equations for the turbulent kinetic energy and the dissipation rate of the turbulent kinetic energy are formulated and solved. Contrary to the Standard \( k-\varepsilon \) Model, \( C_\mu \) is no longer constant in the Realisable \( k-\varepsilon \) Model and is expressed as a function of the main strain and rotation rates in order to satisfy the Schwarz inequality. Moreover, the formulation of the transport equation for the dissipation rate differs in these two models. An important advantage of the Realisable \( k-\varepsilon \) Model over the Standard \( k-\varepsilon \) Model is a more accurate prediction of the spreading rate of round jets.

2.2.2 Combustion models

The Eddy Dissipation Concept (EDC) [9] is an advancement of the Eddy Dissipation Model (EDM) by Magnussen and Hjertager [11]. Both models are applicable to premixed, non-premixed and partially premixed combustion and are formulated for the generalised \( N \) species description of the chemistry, closing reaction rates which appear as source terms, \( R_i \), in the conservation equations for chemical species \( i \):

\[
\nabla (\rho \overline{u_i Y_i}) = \left( \rho D_{i,m} + \frac{\mu_T}{Sc_T} \right) \nabla Y_i + R_i.
\]

Here, \( D_{i,m} \) is the diffusion coefficient for species \( i \) and \( Sc_T \) is the turbulent Schmidt number, taken equal to 0.7.

The EDM calculates the reaction rate as the lowest (limiting) value of mixing rates proportional to the break-up of fuel, oxygen and product eddies as well as a kinetic rate
without taking the influence of turbulent fluctuations into account. This model is reasonably accurate for most industrial applications and numerically robust, but cannot account for strong coupling between turbulence and reaction kinetics.

In the EDC the reaction rate is modelled by an empirical expression based on the assumption that the reactions take place mainly in the smallest length scales of the turbulent energy cascade, called fine structures, which are of the order of the Kolmogorov length scale in one or two dimensions. The volume fraction of the fine structure regions is calculated as

$$\gamma^* = \left( \frac{3C_{D1}}{4C_{D2}} \right)^{3/4} \left( \frac{\nu^* \varepsilon}{k^*} \right)^{3/4},$$

with the model constants $C_{D1} = 0.134$ and $C_{D2} = 0.5$, the Favre-averaged values of $k$ and $\varepsilon$ of the mean flow, and the kinematic viscosity $\nu^*$ in the fine structures.

The time scale $\tau^*$ over which species are assumed to react in fine structures is modelled as

$$\tau^* = \left( \frac{C_{D2}}{3} \right)^{1/2} \left( \frac{\nu^*}{\varepsilon} \right)^{1/2}.$$

In FLUENT the fine scales are treated as constant pressure plug flow reactors, with initial conditions taken as the current species concentrations, $Y_i$, and temperature, $T$, in the cell. In the reactors, the reactions proceed over time $\tau^*$. An integration of the reaction rates over the residence time in the fine structures via a time-stepping method can then be used for the calculation of the fine structure values, namely species concentrations in the fine structures, $Y_i^*$ and temperatures, $T^*$, which can considerably differ from the locally averaged values. The source term in the species equation for species $i$ is modelled by

$$R_i = \frac{\rho \gamma^*}{\tau^*} \left[ \gamma^* \left( Y_i - Y_i^* \right) \right].$$

The ISAT (In-Situ Adaptive Tabulation) algorithm by Pope is applied in FLUENT for the tabulation of the chemical state space (species concentrations, temperature, pressure) during the CFD simulation, resulting in speed-up factors of up to 100 per iteration. The interpolation error tolerance strongly determines the accuracy of the simulation results and the time needed for the generation of the ISAT table.

In the Steady Laminar Flamelet (SLF) approach, equations for the Favre-averaged mixture fraction, $f$:

$$\nabla(p^* f) = \nabla \left( \frac{\mu_f}{\sigma_f} \nabla f \right),$$

and the variance of mixture fraction, $f^2$:

$$\nabla(p^* f^2) = \nabla \left( \frac{\mu_f}{\sigma_f} \nabla f^2 \right) + C_g \mu_f (\nabla f)^2 - C_d \rho \frac{\varepsilon}{k} f^2,$$

are solved instead of species transport equations (2). The values for the constants $\sigma_f$, $C_g$, and $C_d$ in the equations (6) and (7) are 0.85, 2.86 and 2.0, respectively. Under assumption of fast chemistry, the turbulent flame brush is modelled as an ensemble of distinct thin steady
laminar flames, called flamelets, which are geometrically represented by a counter-flow burner configuration. The species mass fractions and temperature along the axis of the laminar counter-flow flame can be transformed from physical space to mixture fraction space and under several simplifying assumptions, in particular equal diffusivities of the species considered, uniquely described by the mixture fraction and the scalar dissipation rate. For the specified values of the scalar dissipation rate, which quantify the departure from the chemical equilibrium, the flamelets are calculated and the profiles of species mass fractions and temperature are stored as a function of mixture fraction and scalar dissipation. Using presumed probability density functions (PDF) for the (presumed) statistically independent mixture fraction ($\beta$-function) and the scalar dissipation rate ($\delta$-function), the chemistry is linked to the turbulence and the pre-PDF table is generated a priori in terms of the mixture fraction, the mixture fraction variance and the scalar dissipation rate. Thus, time-consuming computations of the full chemistry at run-time are avoided and the mass fractions of the species and the gas temperature are retrieved from the pre-PDF table.

Despite the enormous advantage in the reduction of calculation time, there is a serious limitation concerning the application of SLF to engineering problems. SLF is limited to a few progress variables, which are insufficient for the description of complex combustion situations in biomass grate furnaces. On the contrary, EDC and EDM can be employed for such applications without restrictions.

3 Discussion of Results

The results from the validation of the EDC based on LES and 2D RANS simulations of the well-known Sandia D flame and the 2D RANS simulation of a simple syngas flame (Sandia CO/H$_2$/N$_2$ flame B) are presented. Moreover, results from comprehensive sensitivity analyses based on simulations of these flames using various turbulence models, combustion models and reaction mechanisms are presented and discussed. The prediction of NO$_x$ formation is beyond the scope of the present work, therefore no results regarding this issue have been included.

3.1 Sandia Flame D

The experimentally investigated piloted flame Sandia D [1, 17] is a widely accepted validation case for turbulent combustion modelling. The burner, consisting of a main round jet and a concentric pilot, is placed in a wind tunnel. The main jet is a mixture of methane with oxygen in a volume ratio of 25% to 75%. A lean burnt fuel/air mixture was applied as a pilot for the purpose of flame stabilisation.

The Sandia D flame was predicted numerically by means of 3D LES and 2D RANS within the present work. In both cases, the computational domain extended from 5 main jet diameters behind the nozzle exit plane to 100 main jet diameters in the axial direction and 50 main jet diameters in the radial direction. The same unstructured grid (193,968 hexahedral cells) with cell clustering near the nozzle and jet shear layers as described in [8] was applied in LES. A structured grid of 8,450 cells with local refinement close to the nozzle and to the symmetry axis was generated for the 2D RANS simulations. Burner geometry data as well as boundary conditions applied for the simulations correspond to those of measurements, [1] and are given in Table 1.

Since the influence of radiation in the present test case was small, the radiation effects were neglected and not accounted for in the calculations.
The reaction progress in turbulent combustion is strongly dependent on both reaction kinetics and turbulence properties. Since LES allows for a considerably improved prediction of turbulent flows compared to conventional RANS simulations, the reaction mechanism ARM 19 was validated by means of LES. Usually, reduced mechanisms are validated against detailed ones by means of ideal reactor calculations under certain conditions of interest. The application of LES for this purpose gives the opportunity to investigate the mechanism under real flame conditions.

Table 1: Burner geometry data and boundary conditions for Sandia flame D

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jet mixture CH4/air</td>
<td>25/75</td>
<td>Vol%</td>
</tr>
<tr>
<td>Pilot mixture composition</td>
<td>[1]</td>
<td></td>
</tr>
<tr>
<td>Main jet inner diameter</td>
<td>7.2 mm</td>
<td></td>
</tr>
<tr>
<td>Pilot annulus inner diameter</td>
<td>7.7 mm</td>
<td></td>
</tr>
<tr>
<td>Pilot annulus outer diameter</td>
<td>18.9 mm</td>
<td></td>
</tr>
<tr>
<td>Jet bulk velocity</td>
<td>49.6 m/s</td>
<td></td>
</tr>
<tr>
<td>Pilot bulk velocity</td>
<td>11.4 m/s</td>
<td></td>
</tr>
<tr>
<td>Air coflow bulk velocity</td>
<td>0.9 m/s</td>
<td></td>
</tr>
<tr>
<td>Jet exit temperature</td>
<td>294 K</td>
<td></td>
</tr>
<tr>
<td>Pilot exit temperature</td>
<td>1,880 K</td>
<td></td>
</tr>
<tr>
<td>Co-flow temperature</td>
<td>291 K</td>
<td></td>
</tr>
</tbody>
</table>

The results of LES reported in [8], which were obtained for the 19 species ARM chemical mechanism [18], were compared to the results of LES performed within the present work with the 9 species ARM chemical mechanism [12] and measurement data. Both mechanisms are reductions of the GRI-Mech 2.11 under steady-state species assumptions. ARM 19 is a more general reaction mechanism for methane oxidation, performing well in a wide range of combustion conditions, whereas ARM 9 was optimised for the description of methane oxidation under fuel-lean premixed combustion conditions.

Fig. 1 shows the comparison of LES results with experimental data for the flame temperature and the mass concentrations of CO and OH along the centreline of the flame. The present LES using the ARM 9 reaction mechanism is based on the same numerical method as in [8]. The unsteady statistics, i.e. mean and RMS values, resulting from both LES are averaged over four flow-through times. The flow-through time equals the average time that a particle injected at the main jet nozzle exit needs to leave the computational domain.

The axial location of the peak temperature is captured very well with both mechanisms, as can be seen in Fig. 1a. The spreading rate of the main jet is slightly over-predicted in the case of ARM 9, leading to the shift in the simulated temperature profile. The influence of the reaction kinetics on the simulation results becomes visible by the prediction of the mean CO concentrations (see Fig. 1b). In the case of ARM 9, they are clearly over-predicted at the location around the temperature peak, which correspond to (near) stoichiometric conditions. The mean CO concentrations obtained with ARM 19 are in perfect agreement with the measurements. Fig. 1c shows the simulated mean OH concentrations. For both mechanisms, the OH peak is associated with the corresponding maximum of the mean temperature predicted. Again, the results obtained with ARM 19 agreed better with the experimental data than those achieved with ARM 9.
Due to the obvious superiority of the ARM 19 this mechanism was applied in the further numerical investigations based on 2D RANS simulations. The results of these simulations obtained with different combinations of turbulence and combustion models are shown in Fig. 2 in comparison with experimental data. All RANS results presented are grid independent.
Two different models were applied for the description of the turbulence-chemistry interaction, namely the Eddy Dissipation Concept (EDC) and the Steady Laminar Flamelet (SLF) Model. Furthermore, for each combustion model, the influence of turbulence modelling on the overall results was investigated using the RSM and the Realisable $k$-$\varepsilon$ Model. Additionally, a simulation based on the EDC in combination with the Standard $k$-$\varepsilon$ Model was carried out. Here, the constant $C_{1\varepsilon}$ of the $\varepsilon$-equation was changed from 1.44 (the standard value) to 1.6. This is a standard correction proposed for this model in order to achieve an improvement in the prediction of the jet spreading rate [13].

A reasonable qualitative prediction of the flame was achieved for all model combinations. But looking into details, in contrast to LES, none of the model combinations applied in RANS simulations came even close to a quantitatively good agreement between numerical results and measurement data. As can be seen from Fig. 2a, the temperature peak predicted with both RSM and the Realisable $k$-$\varepsilon$ Model, independent of the combustion model used, is shifted towards the burner. Furthermore, the application of the SLF led to an over-prediction of the temperature peak, whilst the application of EDC resulted in slightly too high peak temperatures. The underestimation of the stoichiometric flame length with both combustion models was caused by an over-prediction of the spreading of the main jet by both RSM and the Realisable $k$-$\varepsilon$ Model. The tuning of the model constant in the Standard $k$-$\varepsilon$ Model resulted

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**Figure 2:** Axial profiles of temperature (a), turbulent kinetic energy (b), CO mass concentration (c) and OH mass concentration (d)

Explanations: exp…experimental data from [1]; SLF…Steady Laminar Flamelet; EDC…Eddy Dissipation Concept; RSM…Reynolds Stress Model; RKE…Realisable $k$-$\varepsilon$ Model; SKE…Standard $k$-$\varepsilon$ Model
in a better prediction of the temperature slope up to its peak, which is clearly overestimated. An increase of the production term in the $\varepsilon$-equation by means of constant tuning led to a considerable decrease of the turbulent kinetic energy (see Fig. 2b). Consequently, this simulation showed very poor agreement between the turbulent kinetic energy predicted and experimental data.

Fig. 2c shows a comparison of the predicted CO concentrations with measurements. The CO concentration peaks calculated with EDC are slightly higher than the experimental values, whereas the maxima predicted with the SLF are more than twice as high. Contrary to the results obtained for CO concentrations, the OH concentrations calculated with the SLF agreed well with the measurements (see Fig. 2d). The application of the EDC resulted in a distinct overestimation of the radical, most probably caused by the overestimation of the temperature in this case. The differences between the results of the species field obtained with different turbulence models (with exception of the Standard k-\varepsilon Model) were small for both combustion models applied.

3.2 Sandia CO/H$_2$/N$_2$ jet flame B

The Sandia CO/H$_2$/N$_2$ B flame investigated experimentally in [2, 6] is a non-piloted jet flame. The fuel composition of the jet is 40% CO, 30 H$_2$ and 30% N$_2$, by volume. The burner is placed in a low velocity air co-flow.

This flame was chosen for the purpose of validation due to the following reasons. The syngas used as a fuel in experiments has a composition close to that of the flue gas in a biomass furnace. Furthermore, the flow field pattern investigated experimentally reflects the real situation in those regions of the furnace which are affected by incoming streams of recirculated flue gas and secondary air.

The Sandia CO/H$_2$/N$_2$ flame B was predicted numerically by means of 2D RANS simulations within the present work. The RANS investigations of the Sandia flame D clearly showed that the application of RSM led to no significant improvement compared to results obtained with the Realisable k-\varepsilon Model, which in turn outperforms the Standard k-\varepsilon Model. Since RSM requires more iteration steps to converge as well as more CPU time per iteration than the Realisable k-\varepsilon Model all further simulations were carried out with the Realisable k-\varepsilon Model. The computational domain extended 100 main jet diameters in the axial and 50 main jet diameters in the radial direction. In contrast to the Sandia D flame, the profiles for the velocity and turbulence variables based on measurement data were applied at the nozzle exit plane as jet inlet boundary conditions. The burner geometry data and boundary conditions applied for the simulations correspond to those of measurements, [2] and are given below.

**Table 2: Burner geometry data and boundary conditions for Sandia CO/H$_2$/N$_2$ flame B**

<table>
<thead>
<tr>
<th></th>
<th>value</th>
<th>unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>jet mixture CO/H$_2$/N$_2$</td>
<td>40/30/30</td>
<td>Vol%</td>
</tr>
<tr>
<td>nozzle inner diameter</td>
<td>7.72</td>
<td>mm</td>
</tr>
<tr>
<td>nozzle outer diameter</td>
<td>9.46</td>
<td>mm</td>
</tr>
<tr>
<td>jet inlet velocity</td>
<td>profile from [2]</td>
<td>m/s</td>
</tr>
<tr>
<td>air coflow bulk velocity</td>
<td>0.7</td>
<td>m/s</td>
</tr>
<tr>
<td>jet exit temperature</td>
<td>292</td>
<td>K</td>
</tr>
<tr>
<td>co-flow temperature</td>
<td>290</td>
<td>K</td>
</tr>
</tbody>
</table>
As mentioned in [3], experimental convenience (in this case absence of a pilot) may cause numerical problems. During experiments the flame appeared to be fully attached to the nozzle. The tiny recirculation zone that stabilised the flame in reality could not be predicted numerically. In all 2D simulations performed with the EDC (independent of the reaction mechanism applied), the flame was piloted artificially by means of a small fluid zone, the temperature of which was fixed to a certain value. This zone was attached to the nozzle and acted as an ignitor.

![Graphs showing axial profiles of temperature, turbulent kinetic energy, CO mass concentration, and OH mass concentration](image)

**Figure 3:** Axial profiles of temperature (a), turbulent kinetic energy (b), CO mass concentration (c) and OH mass concentration (d)

Explanations: exp… experimental data from [2]; SLF… Steady Laminar Flamelet; EDC… Eddy Dissipation Concept; EDM… Eddy Dissipation Model; Amag… Magnussen constant of the Eddy Dissipation Model, values used Amag = 4 and Amag = 0.6

In addition to the validation case Sandia D flame, the influence of the choice of the combustion model on the numerical prediction of the Sandia CO/H₂/N₂ flame B was studied and evaluated by a comparison with experimental data (Fig. 3). All RANS results presented are grid independent. Again, the radiation was neglected due to the minor influence it has in the present configuration. The simulations based on the EDC and the SLF were carried out with the ARM 19 reaction mechanism. Additionally, the calculations also included results obtained in [15] for the same flame using the Eddy Dissipation Model (EDM) in combination with a global 3-step methane mechanism by Brink [4] for two different values of the empirical Magnussen constant $A_{mag}$ ($A_{mag} = 0.6$ and $A_{mag} = 4$). The constant, which determines...
The mixing rate in the EDM (i.e., the reaction rate under assumption that the combustion process is mainly mixing-limited) is not universally valid. Normally, the originally proposed value $A_{\text{mag}} = 4$, is too high for the present application, [15]. The second value of the empirical constant, $A_{\text{mag}} = 0.6$, is found to be best suitable for the combustion simulation of biomass grate furnaces [16]

A qualitatively good prediction of the flame was common to all combustion models applied. Again, an over-prediction of the jet spreading rate resulted in a shift of the temperature peak towards the burner, independent of the combustion model used (see Fig. 3a). Both EDC and SLF captured the peak value very well, whereas in the case of EDM a reduction of the highly overestimated peak temperature (obtained with $A_{\text{mag}} = 4$) was achieved by a modification of the empirical constant ($A_{\text{mag}} = 0.6$). Combustion modelling has no significant impact on the prediction of the turbulent flow field, as can be seen on curves of the turbulent kinetic energy depicted in Fig. 3b. The same can be stated for the prediction of the concentration of CO (see Fig. 3c), whereas in the case of EDM a slight improvement was achieved by tuning of the model constant. Since the global mechanism by Brink does not include any radicals, Fig. 3d shows OH concentrations predicted only by EDC and SLF in combination with ARM 19. Similar to the results obtained for the Sandia D flame, EDC over-predicts the value and location of the OH concentration peak. Although in the case of SLF the concentration peak is also shifted towards the burner, the peak value of OH concentration is only slightly underestimated.

Fig. 4 shows the results of the investigations concerning the influence of the reaction mechanism on the accuracy of the numerical prediction. For this purpose four reaction mechanisms were chosen and combined with the EDC: a global one (Brink, 7 species, no radicals), the reduced ARM 9 and ARM 19 mechanisms and a detailed reaction mechanism. The last one is based on Kilpinnen 92 [10] - a detailed mechanism developed for description of NOx chemistry in biomass combustion systems. In the present work all nitrogen-containing species, except N2, are removed from the kinetics, resulting in a mechanism for 32 species described with 153 reactions.

The simulations performed with different reaction mechanisms led to similar results, which showed the same deviations from the measurements, with some exceptions for the simulation carried out with the global reaction mechanism. The application of the detailed mechanism resulted in the lowering of the peak temperature value towards the measured value (Fig. 4a) when compared to the results obtained with the reduced mechanisms. The peak temperature is slightly overestimated with both reduced mechanisms ARM 9 and ARM 19, whereas the maximum temperature obtained with the global mechanism is slightly under-predicted. The differences in the prediction of the turbulent kinetic energy obtained with detailed and both reduced mechanisms are very small, except for the maximum value (Fig. 4b). Compared to the results of the simulations with detailed and reduced chemistry, the global mechanism showed some differences in the prediction of both temperature and the turbulent kinetic energy in the high temperature region of the flame. These are connected through the model formulation, as the species source term is expressed in terms of turbulence quantities. Moreover, the heat capacity of the gas mixture and, consequently, its temperature is influenced by the absence of the radicals in the global mechanism. Based on the results obtained for the species field (see Fig. 4c for CO and Fig. 4d for OH concentrations), it can be stated that an improvement in the description of the chemistry has no considerable impact on the calculation results in this case. The prediction of the OH concentrations in the case of the ARM 9 mechanism represents an exception. Contrary to the other mechanisms applied,
ARM 9 led to a second OH concentration peak. It is worth noting that a more detailed description of the chemistry causes a considerable increase in calculation time. The time needed for the generation of the ISAT table and the number of species transport equations that need to be solved increases with the number of species considered.

As expected, the application of the global mechanism in combination with EDC led only to a slight increase in calculation time and no improvement in the numerical prediction, when compared to the simulation performed with the EDM, in which the model constant was modified (Fig. 3, 4). Here it should be noted that reasonably good results obtained with EDM rely on the artificial damping of the mixing-limited reaction rate by tuning of the model constant. Such a measure is justified in the present validation case, where the turbulent mixing overwhelms the impact of the kinetics. Generally, the combustion process taking place in a furnace is not mixing-limited throughout. Kinetically dominated processes like NO\textsubscript{x} formation and slow CO burnout in quenched flames can be predicted only with models which account for the detailed description of the chemistry.

**Figure 4:** Axial profiles of temperature (a), turbulent kinetic energy (b), CO mass concentration (c) and OH mass concentration (d)

Explanations: exp…experimental data from [2]; arm19…numerical results obtained with ARM 19 reaction mechanism; arm9…numerical results obtained with ARM 9 reaction mechanism; Kilp92…numerical results obtained with truncated Kilpinen 92 reaction mechanism; global…numerical results obtained with global reaction mechanism by Brink
4 Summary and conclusions

The paper presents a comprehensive evaluation of the accuracy of the advanced combustion models provided within the commercial CFD code FLUENT with special attention to the restrictions concerning their application to the simulation of turbulent reactive flow in industrial biomass furnaces. Since the reaction progress in turbulent combustion is strongly dependent both on reaction kinetics and turbulence properties, the combination of the EDC combustion model, Realisable $k-\varepsilon$ Model and ARM 19 chemistry mechanism was validated in a step-wise approach.

By means of LES of the benchmark flame Sandia D, the reduced mechanism ARM 19 was validated by comparison with the results of a LES performed with the ARM 9 mechanism as well as measurement data. As LES is by far more accurate than the RANS approach in the prediction of turbulent flows, the influence of turbulence modelling errors on the overall combustion results were minimised. Therefore, LES provided a valuable insight into the performance of the reaction kinetics under real flame conditions.

The ARM 19 mechanism was applied in 2D RANS simulations of the same flame, focusing on the investigation of the influence of the choice of the turbulence model (Standard $k-\varepsilon$ Model, Realisable $k-\varepsilon$ Model, RSM) and the combustion model (EDC, SLF) on the overall prediction accuracy. The simulation results were in good agreement with the experimental data only in qualitative terms, independent of the combination of the models chosen. It was obvious that the accuracy of the numerical results was more strongly affected by turbulence modelling. The application of the computationally more expensive RSM led to no significant improvement compared to the Realisable $k-\varepsilon$ Model, which in turn outperforms the Standard $k-\varepsilon$ Model. The Realisable $k-\varepsilon$ Model was thus chosen for all further investigations.

2D RANS simulations of a syngas flame (Sandia CO/H$_2$/N$_2$ B), which represents a good approximation of flue gases from solid biomass combustion, were carried out with two combustion models (EDC and SLF) in combination with ARM 19 chemistry. The results were compared to experimental data and numerical data from a simulation with a simpler EDM model, in which a global reaction mechanism was used and a modelling constant was tuned. Again, the shortcomings of turbulence modelling concerning the prediction of round jet spreading reduced the sensitivity to the combustion model applied. The simulation results of the EDC and the SLF were relatively similar. Although the application of SLF resulted in shorter computation times and a better prediction of OH concentrations, the EDC was selected for further investigation due to the restrictions of the SLF regarding the description of the combustion situation in a biomass grate furnace. Furthermore, the results achieved with EDM deviated slightly more significantly from the measurement results, but could be improved by strong tuning of a modelling constant. This model, however, cannot handle processes with a strong kinetic influence. Additionally, the case-dependent tuning of the modelling constants may lead to a shift of the combustion situation and even to unrealistic results in some cases, e.g. NO$_x$ prediction and slow CO oxidation.

Furthermore, the influence of the description of the reaction kinetics on the prediction of turbulent reactive flows by EDC was studied by means of the simulation of the syngas flame. The results achieved with two reduced mechanisms (ARM 9 and ARM 19) and a detailed reaction mechanism (Kilpinen 92 without nitrogen-containing species) were similar and also showed the same deviations from the measurement data. The results obtained with a global reaction mechanism showed slightly larger deviations from the experimental data, but were
relatively good from a qualitative perspective. This points out once again that the influence of
the reaction kinetics and the model for turbulence-chemistry interaction on the prediction of
mixing-limited combustion problems (the present validation case) is almost negligible. On the
other hand, the description of kinetically limited processes, e.g. NO\textsubscript{x} formation and slow CO
oxidation in cold boiler regions, requires more detailed reaction mechanisms than global ones
involving radicals, which can be meaningfully handled in CFD simulations only by applying
more sophisticated combustion models.

Due to its more general formulation compared to the SLF, the EDC proved to be the best
option and a valuable tool for the improved prediction of combustion processes in engineering
applications. Moreover, the EDC represents an important basis for the modelling of NO\textsubscript{x}
formation due to its capability to account for the interaction of turbulence and reaction
kinetics in a more detailed way (prediction of radicals) than the simpler EDM. Since the EDC
is strongly dependent on the prediction of turbulence properties, an advancement in
turbulence modelling is expected to improve the accuracy of the EDC. All findings of the
present study concerning the accuracy and limitations of EDC form a valuable basis for the
ongoing research activities concerning the modelling of combustion processes in biomass
grate furnaces.

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Nomenclature

\begin{align*}
C_d & \quad \text{constant in equation of mixture fraction} \\
& \quad \text{variance [-]} \\
C_{D1} & \quad \text{constant of the EDC model [-]} \\
C_{D2} & \quad \text{constant of the EDC model [-]} \\
C_g & \quad \text{constant in equation of mixture fraction} \\
& \quad \text{variance [-]} \\
C_\mu & \quad \text{constant in equation for eddy viscosity [-]} \\
D_{i,m} & \quad \text{diffusion coefficient for species } i [\text{m}^2/\text{s}] \\
f & \quad \text{mixture fraction [-]} \\
f' & \quad \text{variance of mixture fraction [-]} \\
k & \quad \text{turbulent kinetic energy [m}^2/\text{s}^2] \\
R & \quad \text{source term in species equation [kg/m}^3\text{s}] \\
S_{T} & \quad \text{turbulent Schmidt number [-]} \\
T' & \quad \text{temperature in fine structures [K]} \\
\nu & \quad \text{velocity [m/s]} \\
Y & \quad \text{species mass concentration [-]} \\
Y' & \quad \text{species mass concentration in fine structures [-]} \\
\gamma' & \quad \text{volume fraction of fine structures [-]} \\
\varepsilon & \quad \text{dissipation rate of turbulent kinetic energy} \\
& \quad [\text{m}^2/\text{s}^3] \\
\mu_r & \quad \text{eddy viscosity [Pa s]} \\
\nu' & \quad \text{kinematic viscosity of fine structures [m}^2/\text{s}] \\
\rho & \quad \text{density [kg/m}^3] \\
\sigma_T & \quad \text{constant in equation of mixture fraction} \\
& \quad \text{variance [-]} \\
\tau' & \quad \text{time scale of fine structures [s]}
\end{align*}
References


