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2D-CFD Simulation of a Syngas Burner with Experimental Validation

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Abstract: Biomass-derived syngas is a promising alternative to fossil fuels for various applications, including internal combustion engines for electricity generation and direct combustion for thermal energy. However, numerical modeling of syngas burners is still scarcely addressed in literature compared to more common fuels, posing challenges for the design of high-efficiency combustors with low pollutant emissions. This study presents a two-dimensional computational fluid dynamics (CFD) simulation of a syngas burner, validated against experimental data. The syngas adopted in the combustion tests is produced using a small-scale gasifier prototype fueled by wood pellets. At first, the syngas is premixed with air, then it moves in a cylindrical burner where the key parameters are monitored, including syngas and air volume flow rates, temperature, and syngas composition. Additionally, an emission analyzer is used to measure O_2, CO, NO, and NO_2, concentrations in the exhaust gases. Given the axial symmetry of the problem, a two-dimensional model is developed to save the computational effort. The simulation results are compared to the experimental measurements including burner temperature and emissions. Despite the simplicity and the reduced effort compared to high-fidelity simulations, the 2D model proves to be able to properly predict both temperature inside the burner and emissions at the exhaust. Therefore, it turns out to be a valuable tool to guide the design of syngas burners.

Keywords: Biomass; CFD; Combustion; Emissions; Syngas

1 Introduction

Small-scale gasification systems are gaining more and more interest in the scientific community [1], due to the possibility to exploit residual biomasses in rural areas in which there is abundance of such resources. Through small-scale gasification systems, it is possible to obtain a fuel gas from solid biomass that can be used for electrical and thermal energy generation. Gasification is a thermochemical process that occurs under sub-stoichiometric (oxygen-limited) conditions, enabling the conversion of carbonaceous materials into a mixture of valuable products such as fuel gases or chemical intermediates for further synthesis. Considering an average composition, syngas is made of combustible gases (40%), such as CO, CH_4 and H_2, and non-combustible gases (60%) like N_2 and CO_2 [2]. Among the biomass-to-electricity conversion technologies, gasification is considered the most efficient, offering higher energy conversion efficiency and significantly lower pollutant emissions, particularly nitrogen oxides (NO_x) and sulfur oxides (SO_x), compared to conventional direct combustion [1].

Focusing on the production of thermal energy by syngas, premixed combustion is a promising mode as fuel and oxidizer are perfectly mixed before entering the burner combustion chamber. This favors the mitigation of emissions such as NO_x and unburnt hydrocarbons. However, turbulent premixed combustion modelling in gas burners is not free of difficulties. It is necessary to consider aspects such as radiative heat transfer, turbulence-flame interaction, emission modelling and exact mixture composition, as they can lead to misleading predictions of gas temperature and emissions in the burnt gases. For instance, Bidi et al. [3] studied the effects of radiative models on numerical simulations of methane-air premixed combustion, concluding that the results with radiation model are in much better agreement with the measurements and the effect of radiation can influence both temperature and emissions. As for the turbulence-flame interaction, Halouane and Dehbi [4] studied premixed hydrogen combustion using two different

closure models, namely Eddy Dissipation Concept (EDC) and Turbulent Flame Closure (TFC). Thanks to validation against experimental data, both models proves to be able to reasonably well predict combustion for all the cases studied in the paper. However, the authors show that higher accuracy comes only at the expense higher computational cost. Regarding the emissions modelling, detailed-chemistry-based approaches are more and more diffused in order to obtain accurate estimations. In this kind of studies, detailed chemistry can be solved both online and offline. In the former case, during the CFD simulation, each cell is considered as a reactor where chemical kinetics is solved to provide source terms to the scalar transport equations [5]. In the latter case, chemistry is tabulated (and, then, tables are exploited in the CFD simulation) or it is solved a posteriori in reactors, such as in references [6–8]. These studies use methane as fuel and conduct transient numerical simulations combined with the use of idealized reactors to decouple NO_x prediction from CFD modeling. Such decoupled approach is found to predict reasonably well NO_x emissions. Finally, literature demonstrates the importance of the gas composition. Uncertainties can lead to inaccuracies of the simulation results, especially in terms of emissions. For instance, Wang et al. [9, 10] investigated the effect that some additional reactants have on the emissions of a syngas combustor. In fact, it is likely to have impurities in the syngas as a consequence of the formation process from biomass. The results clearly indicate that, for example, the presence of ammonia in the syngas composition can significantly change the NO_x level in the combustion process [11].

Compared to the existing literature, this study develops a two-dimensional, steady-state combustion model able to properly predict emissions and temperature profile in a syngas burner thanks to detailed modeling of turbulence-flame interaction, radiative heat transfer, gas composition and emissions formation via detailed chemistry.

2 Materials and Methods

In this section, both the experimental and the numerical setups are presented.

2.1 Experimental Setup

Gasification experiments are conducted using a laboratory-scale prototype named the "Femto Gasifier" (Figure 1), designed and constructed at the University of Modena and Reggio Emilia [12]. The system is developed to enable preliminary testing of various biomass feedstocks. It features an Imbert-type downdraft reactor and it is optimized for tests requiring limited quantities of biomass. The gasifier is operated under positive pressure conditions, with the air blower placed upstream of the reactor. A dedicated sampling port enables the collection and analysis of syngas. The tests are conducted outdoors. Wood pellets are adopted as feedstock and the produced syngas is subsequently combusted in a flare (Figure 2).

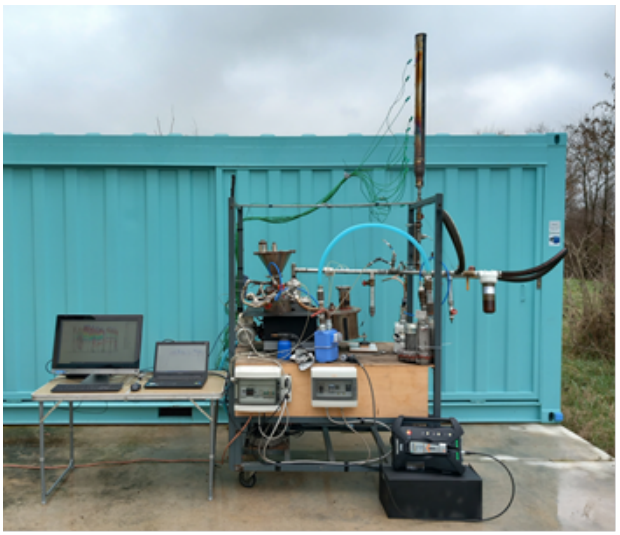

Figure 1. Femto Gasifier during a test

Two devices are employed for the cleaning of the syngas produced by the gasifier. The first, located immediately downstream of the reactor, is a cyclone separator, used to remove the majority of particulate matter from the syngas stream. The second is a filter equipped with a nylon net cartridge. It is important to note that no system is specifically included for the removal of ammonia (NH_3). Therefore, traces of this compound are expected to be present in the syngas, as it is commonly found in gases derived from lignocellulosic biomass [13].

In order to evaluate the results of the test, several instruments are used. In particular, the volume flow rates of air and syngas are measured using two volumetric flow meters.

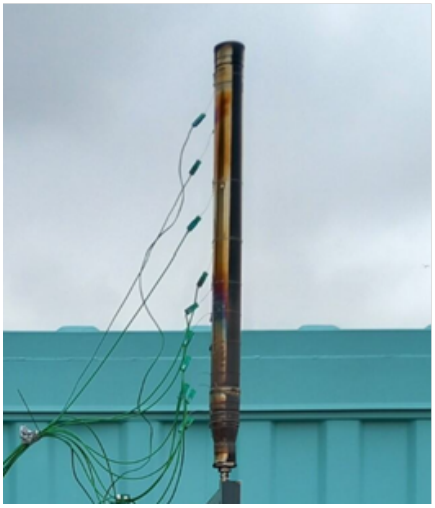

Figure 2. Flare equipped with thermocouples

Gas samples are analyzed using a Pollution MicroGC GCX micro gas chromatograph, to obtain the gas composition. The instrument is calibrated for the main non-condensable gas species including H_2, O_2, N_2, CO, CO_2, and CH_4.

In Figure 2, the flare is shown. It is possible to notice 11 Type-K thermocouples used to estimate the temperature profile along the axis of the burner. Most of the thermocouples are placed in the initial portion of the combustion chamber, to accurately capture the temperature variations associated with the initial flame development.

In addition, emissions are measured at the burner outlet. The analysis is carried out using the "Testo Model 350" analyzer. This is a portable analyzer equipped with a probe that allows for the sampling of the exhaust gas, which are then analyzed using integrated sensors.

2.2 Numerical Setup

This section focuses on the presentation of the 2D-CFD model, whose geometry is visible in Figure 3. One the most critical aspects of the model is represented by the boundary conditions, especially those at the inlet. In fact, in order to speed up the combustion simulations, the 2D domain starts just before the combustion chamber. Therefore, mixing simulation is not considered. Moreover, it would not be possible to simulate mixing in a 2D framework, as the experimental apparatus is such that the disposition of syngas and air pipes is not axisymmetric. Therefore, it is necessary to simulate the mixing process separately in a 3D framework, so that level of mixing before the combustion chamber as well as flow field can be estimated to generate boundary conditions for the 2D domain.

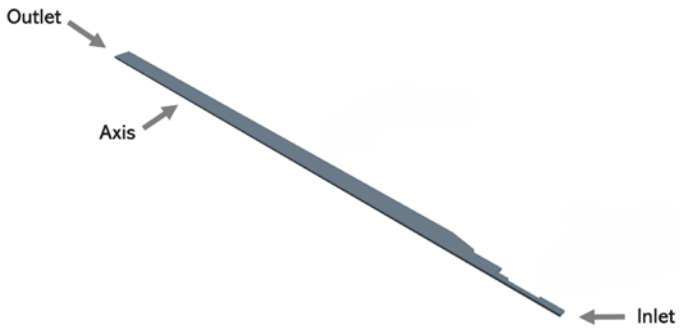

Figure 3. 2D geometrical domain

In the light of this, also a 3D-CFD model is developed. The geometry includes a vertical pipe (where mixing occurs) receiving syngas and air from two lateral smaller pipes. On the top, the geometrical domain ends after the combustion chamber starts. Therefore, it includes also part of the 2D domain. In particular, the outlet is placed just after the small steel grid located at the combustion chamber inlet and used to enhance flame stabilization. A section of the grid is visible in Figure 4. The geometry is discretized through a trimmer mesh with characteristic size of 1 mm. In order to consider the presence of the grid, a local refinement with characteristic size reduced to 0.125 mm is operated. Lastly, for a proper simulation of the gradients close to the walls, 6 prism layers are used, to guarantee a

"Low-Reynolds" approach. The total number of cells is roughly 3 M. In terms of physics, the number of models is limited, as the problem consists only in a steady-state cold flow simulation. A multi-component gas is considered. Turbulence is modelled by the Realizable k-ε model. Regarding the boundary types, the two inlet sections of air and syngas are "Mass Flow Inlet" boundaries, while the outlet section is a "Pressure Outlet". For the two inlets, mass fractions are specified, according to the compositions of air and syngas. Both boundary and initial conditions are derived from the experiments.

Once the numerical setup of the 3D model is clarified, the attention can be focused on the 2D framework. It is important to point out that both 2D and 3D models are built within STAR-CCM+ 2210 [14], licensed by SIEMENS DISW. As visible in Figure 3, the 2D-CFD model includes pressure reducer, steel grid and the entire combustion chamber. First of all, the adoption of a 2D approach is possible thanks to the geometry of the domain. De facto, it roughly coincides with the portion of flare visible in Figure 2, thus it is evidently axisymmetric.

To discretize the 2D domain, a characteristic size of 0.5 mm is used, while two prism layers are applied near the walls. To account for the presence of the steel grid, a local mesh refinement is performed, similarly to the 3D case, with a reduced size of 0.125 mm. The total number of cells obtained using these parameters is roughly 200 k, leading to a great advantage compared to a 3D approach. In Figure 4, a portion of the resulting mesh is shown. In particular, the refinement in correspondence of the grid is shown.

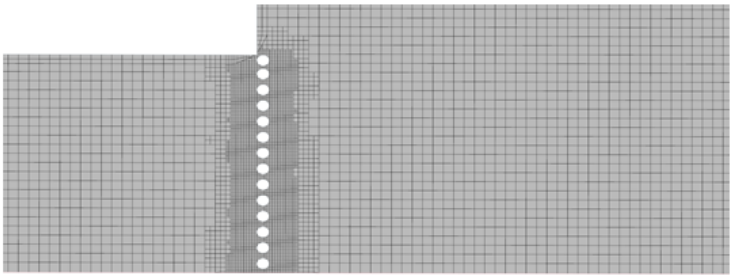

Figure 4. 2D mesh

Compared to the 3D model, the physical setup is similar. The flow is still a multi-component ideal gas, with turbulence modeled by the Realizable k-ε. The main difference is related to the presence of combustion in the 2D framework, which has to be considered. The approach here adopted for combustion modeling is based on Complex Chemistry (CC, also known as detailed chemistry) and Eddy Dissipation Closure (EDC) models (CC+EDC). The CC model is suitable for introducing detailed chemical information into CFD simulations. The adopted chemical reaction scheme is the GRI-Mech 2.11 [15], which includes 49 species and 279 reactions. To evaluate the effect of turbulence on combustion, the Complex Chemistry model is coupled with a turbulence–chemistry interaction model. In this work, the Eddy Dissipation Concept model [16–18] is adopted to account for the interaction between chemical kinetics and turbulent flow.

Radiation models are included to consider the effect of radiative heat transfer. The inclusion of radiation significantly improves the accuracy of the numerical temperature profiles. In this study, the Participating Media Radiation model is used [14]. Then, the combination of Gray Thermal Radiation model and Weighted Sum of Gray Gases Method [19–21] is exploited for the calculation of the absorption coefficient k. Such a combination is commonly adopted in simulations involving air–fuel combustion processes. In this approach, gases are modeled as gray bodies characterized by absorption coefficient κ and absorptivity α. The relationship between these two quantities is described by the Bouguer-Lambert law, expressed by Eq. (1).

$$\alpha = 1 - e^{-ks} \tag{1}$$

where, the parameter s is called Optical Path Length (OPL).

Interestingly, in order to improve the agreement between numerical and experimental outcomes, both EDC and WSGG models undergo calibration. The EDC model accounts for the effect of turbulence on combustion by modifying the source term in the chemical species transport equations. In particular, the source term is multiplied by a scalar function f [14] including two empirical constants: the "fine structure length constant" Cl and the "fine structure time constant". At the end of the calibration process, it is found that the optimal value of Cl is 1.3, while the default value is 2.1377. In particular, reducing Cl slows down the production/consumption rates of the scalars, resulting in increased unburned species at the exhaust.

Moving to the calibration of the WSGG model, in this case the parameter of interest is OPL. The value can range from the size of a single cell to the size of the entire domain, depending on the optical depth of the region where combustion occurs. Reducing OPL results in a decrease of the temperature profile values. This adjustment enables

the solver to better capture the thermal radiation absorption process by the gas-phase molecules. In this case, the optimal value of OPL resulting from the calibration process is 12.5 mm.

Compared to the 3D model which is set to adiabatic (as no reaction occurs in the mixing region), in the 2D framework the convective heat transfer is considered. Hence, the walls are characterized by a pair of heat transfer coefficient and reference temperature to mimic convection with the external ambient and the thickness of the flare is considered by means of a thermal resistance.

Regarding the inlet boundary, it is a "Velocity Inlet". The boundary conditions in terms of velocity, turbulent kinetic energy, turbulent dissipation rate and temperature are derived from the 3D model. In particular, the profiles are obtained by averaging in the azimuthal direction the relevant quantities over a horizontal section plane corresponding to the inlet of the 2D model.

Lastly, the inlet mass fractions refer to the air-syngas mixture. As it will be shown in the results, the 3D simulation reveals a very effective mixing between air and syngas. Therefore, a homogeneous mixture is imposed at the velocity inlet.

The outlet section is defined as a "Pressure Outlet", where ambient pressure is imposed as the outlet discharges into the environment.

3 Results

In this section the results of the experiments are shown at first. Then, the numerical results are presented, from both 3D and 2D models.

3.1 Experimental Results

The results obtained from gasification and subsequent combustion test are in terms of syngas composition, volume flow rate, emissions and temperature profile.

The operating point analyzed in this study is identified as a stable working condition of the burner.

The experimentally measured volume flow rates of air and syngas are shown in Table 1.

Table 1. Volume flow rates of air and syngas

Q_a [L/s]	Q_{syn} [L/s]
0.93	0.626

To evaluate the syngas composition, samples are analyzed. However, it is interesting to note that, due to the adopted gas analyzer, it is not possible to evaluate the presence of ammonia. This component is usually present in syngas from woody biomass and it strongly affects NO_x emissions. In order to consider the presence of ammonia for the simulations, a concentration of NH3 is added to the gas composition given by the chromatograph. The adopted NH3 concentration relies on typical values found in literature [13]. The mass fractions of the different components, without addition of ammonia, are summarized in Table 2, while the results considering NH3 are presented in Table 3.

Table 2. Syngas mass fractions without NH_3

H_2	N_2	CH_4	CO	CO_2
0.008	0.5157	0.0155	0.1663	0.2945

Table 3. Syngas mass fractions with NH_3

H_2	N_2	CH_4	CO	CO_2	NH_3
0.008	0.5153	0.0155	0.1664	0.2945	0.0002

Another result comes from the combustion test, which provides the temperature profile along the axis of the flare. In Table 4, it is possible to see the temperatures resulting from the measurements, each one presented with its standard deviation.

The last result is related to the emissions measured at the burner outlet. Similarly to temperature, measurements are performed once the burner reaches a steady-state condition. Exhaust gases are sampled, for the analysis, by a copper tube that allows to place the probe at the flare outlet. The results are reported, in Table 5, in ppm for CO and NO_x, and volume fraction for CO_2 and O_2. Each result is reported along with the standard deviation.

Table 4. Thermocouple measurements

Thermocouples	Temperature [K]	Standard Deviation [K]
TC1	1292	± 14
TC2	1137	± 8
TC3	1069	± 19
TC4	1100	± 11
TC5	1038	± 7
TC6	1001	± 10
TC7	964	± 7
TC8	882	± 18
TC9	856	± 6
TC10	842	± 5
TC11	725	± 10

Table 5. Measurement of emissions

PPM NO_x	PPM CO	%CO_2	%O_2
181 ± 4	51.3 ± 3	16.6 ± 0.2	3.9 ± 0.2

3.2 Numerical Results

Since the main goal of the 3D model is to evaluate the mixing of air and syngas, the 3D results presented in the following focus on this aspect. In this regard, Figure 5 and Figure 6 show mass fractions of CH_4 and N_2 on a horizontal section plane corresponding to the inlet of the 2D domain. It is possible to evaluate the mixing by means of the mass fraction homogeneity of the most relevant components.

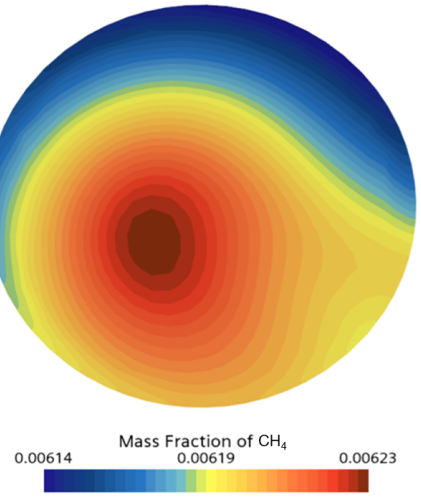

Figure 5. Mass fraction of CH_4

The results show minimal (not to say negligible) variation of the concentrations of the scalars on the section plane. This indicates that the mixing obtained in the system is effective. So, on the one hand, it is possible to adopt a two-dimensional axisymmetric model for the combustion analysis. On the other hand, for the 2D simulations, it is reasonable to introduce in the computational domain a perfectly premixed mixture.

Moving to the combustion results of the 2D model, they are proposed in terms of temperature profile along the burner axis and emissions at the outlet. In the following, the results of different cases will be presented. “Base” case does not include ammonia in the composition of the syngas and both EDC and radiative heat transfer models are not adopted. In particular, neglecting EDC means that turbulence-flame interaction is neglected. The second case is referred to as “EDC”, since the EDC model is introduced (with Cl already calibrated). “EDC+Rad” case includes EDC and radiative models (both properly calibrated, thus also OPL is set to the optimal value). Lastly, “NH3” case represents the final model, namely the one characterized by the best setup, in which also the presence of ammonia in the initial composition of the syngas is considered.

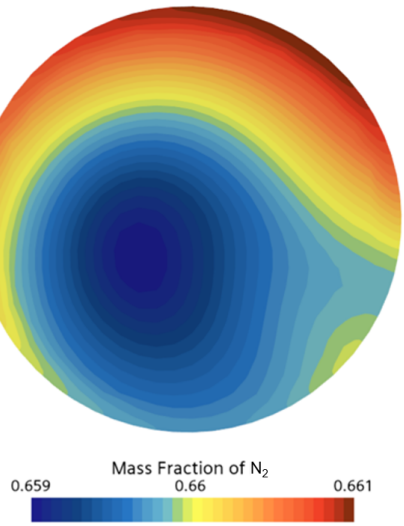

Figure 6. Mass fraction of N_2

In order to evaluate the temperature profile in the simulation, probes are inserted in the model in correspondence of the flare axis, where the thermocouples are placed. As for the emissions, since they are experimentally measured in a precise point of the domain, a single probe point is used to evaluate the ppm of CO and NO_x and the volume fractions of O_2 and CO_2.

In Figure 7, it is possible to see the temperature profiles obtained in the different cases, while Figure 8 and Figure 9 summarize the results relative to the emissions at the burner outlet. Starting from the temperature profiles, it is possible to notice that an acceptable agreement is obtained only introducing radiation in the model. As for the emissions, all the investigated setups are able to return correct concentrations of O_2 and CO_2 at the exhaust. The main differences among the cases deal with CO and NO_x. Only introducing the EDC (i.e. considering the turbulence-flame interaction) it is possible to improve the CO prediction. Finally, the concentration of ammonia has to be necessarily introduced in the gas composition, otherwise there is no way to obtain a concentration of NO_x at the exhaust that is close to the experimental counterpart.

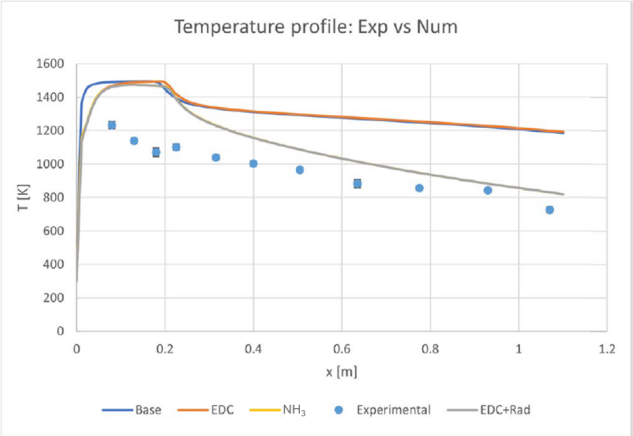

Figure 7. Temperature profile: Experimental vs numerical

4 Conclusions

In this work, a 2D-CFD model for the simulation of combustion in a syngas burner is developed. It includes accurate modeling of turbulence-flame interaction, radiative heat transfer, gas composition and emissions formation via detailed chemistry. The model is validated against experimental data in terms of temperature and emissions. Overall, a good agreement is obtained between CFD and experimental outcomes in terms of both gas temperature and main emissions, namely CO and NO_x. Minor discrepancies can be noticed for the temperature estimation and they can be ascribed to the radiation model, which requires further calibration.

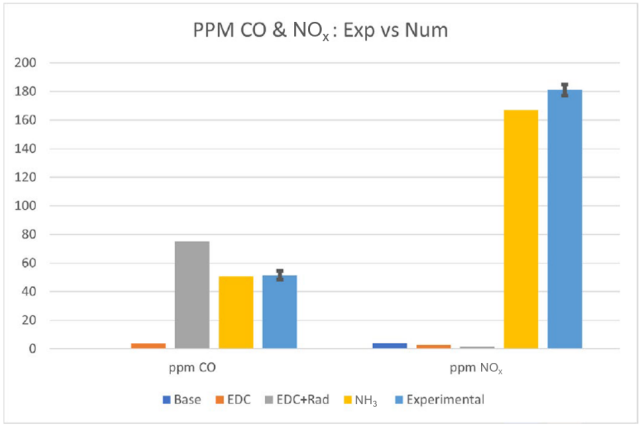

Figure 8. CO abd NO_x emissions: Experimental vs numerical

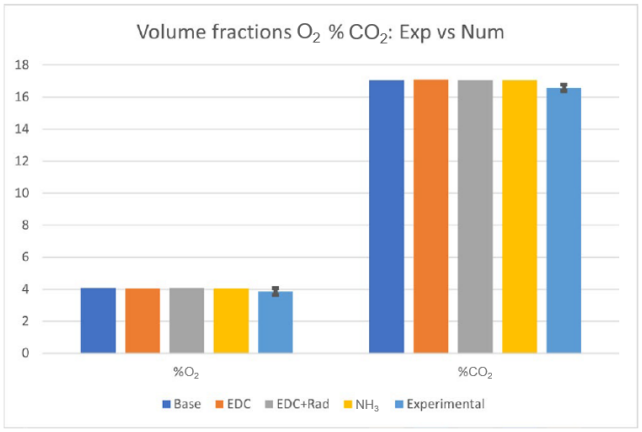

Figure 9. Numerical-experimental comparison O_2 and CO_2 emissions

On the experimental side, future developments will include the implementation of an adequate gas cleaning system to remove ammonia from the produced syngas. Once ammonia is effectively removed, NO_x emissions can be significantly reduced, as confirmed by numerical results. On the numerical side, the modelling approach will be refined by further tuning of the radiation and other combustion models will be tested to improve the predictive capabilities of the numerical framework.

As shown in the study, the 2D-CFD numerical model demonstrates good accuracy in predicting both temperature and emissions, while maintaining a low computational cost. Therefore, it can be a very effective tool for the design of high efficiency burners. In turn, this is crucial to properly exploit the syngas potential as energy source, for the sustainable development of rural areas where biomass is readily available.

Acknowledgment

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Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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Nomenclature

CFD	Computational Fluid Dynamics
3D	Three Dimensional
2D	Two Dimensional
CC	Complex Chemistry
EDC	Eddy Dissipation Concept Weighted Sum of Gray Gases
WSGG	
NO_x	Nitrogen Oxide
SO_x	Sulfur Oxide
CO	Carbon Monoxide
CH_4	Methane
H_2	Hydrogen
N_2	Nitrogen
CO_2	Carbon Dioxide
TFC	Turbulent Flame speed Closure
CRN	Chemical Reactor Network
NH_3	Ammonia
O_2	Oxygen
TC	Thermocouple
ppm	Parts Per Million
BC	Boundary Condition
IC	Initial Condition
k	Absorption coefficient
OPL	Optical Path Length [mm]
TKE	Turbulent Kinetic Energy [J/kg]
TDR	Turbulent Dissipation Rate [m^2/s^3]

Greek symbols

α	Absorptivity, dimensionless

Subscripts

a	air
syn	syngas