Impact of hydrogen admixture on interacting premixed flames in domestic boilers

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Abstract. The injection of hydrogen into the natural gas network can contribute to the large-scale integration of renewables, as hydrogen can be easily produced through electrolysis from wind or solar energy. However, the addition of hydrogen to natural gas influences fuel properties, asking for the assessment of the safe and efficient operation of existing end-user equipment, such as domestic burners and boilers. In this work, 3-dimensional resolved numerical simulations based on Computational Fluid Dynamics are carried out to shed light on the effect of H2 addition on the combustion process occurring in condensing boilers equipped with perforated cylindrical burners. To this purpose, multi-hole geometries emulating a portion of a perforated burner are analyzed. Since the burner holes are positioned very close to each other, the interaction of the adjacent laminar premixed flames is observed to occur with influence on the flow and thermo-chemical fields which differ from those of a single premixed flame. The addition of hydrogen was found to lead to an anticipation of the reaction zone, although the general features observed with the G222 gas (23% H2, 77% CH4) were alike those of the G20 gas (100% CH4).

1. Introduction

A key role for decarbonization is played by the integration of power-to-gas with the natural gas grid in order to face the problem of storing and transporting overproduction of energy from renewables at times of excess. In particular, hydrogen can be produced in a very sustainable manner through electrolysis employing wind or solar energy as a power source and water [1]. However, adding hydrogen to natural gas influences gas properties, leading to significant challenges for the safe and efficient operation of existing end-user equipment, such as domestic burners and boilers. Even though maximum hydrogen fractions, up to 20% are foreseen for domestic applications, there is little proof of the adequate performance of such systems when adding hydrogen [2].

Domestic condensing boilers are usually equipped with cylindrical or flat perforated burners that inject a premixed mixture into the combustion chamber. The major feature of such burners is to provide a short-length flame and uniform temperature [2]. The existing literature concerns mainly experimental investigations aimed at determining the burner performance in different operating conditions. Lee et al. [3] analyzed experimentally flame stability, NOx and CO emissions from a perforated cylindrical burner fed with methane, observing that the optimal equivalence ratio is 0.70 < φ < 0.75. These results were confirmed by Najarnikoo et al. [4] who observed a stable blue flame to be ensured by equivalence ratios 0.70 < φ < 0.73. Schiro et al. [5] investigated experimentally the performance of cylindrical premixed burners coupled to a very common domestic premixed boiler setup, with special attention to metal fiber application on the burner surface. Very recently Soltanian et al. [6] applied chemiluminescence to a multi-hole cylindrical burner with the aim to investigate OH* and CO2* emissions, which are directly related to the heat release rate. They suggested that the heat transfer rate was maximized with an equivalence ratio φ ≈ 0.82. Ding et al. [7] showed that OH* chemiluminescence signals could be used for sensing the equivalence ratio in a domestic boiler also in the case of variable fuel composition, including H2 admixtures. Burbano et al. [8] analyzed the effects of hydrogen addition to methane on the flame structure and CO emissions in atmospheric burners.

Further and significant insight into the combustion process, allowing to better comprehend the experimental evidence, may be gained from resolved numerical simulations, based on the application of Computational Fluid Dynamics (CFD) techniques, which have grown...
considerably in the last decades along with the rapid development of computational power. So far CFD has been applied to condensing boilers mainly to address the problem of gas distribution and mixing upstream of the burner and only a few works have dealt with the simulation of the combustion process. Zhao et al. [9] and Zhang et al. [10] presented two different studies to optimize geometry parameters of a premixed cylindrical burner using CFD in order to reduce NOx and CO emissions. Hassan et al. [11] developed a two-dimensional CFD model based on partially premixed and equilibrium chemistry calculations to simulate the combustion process taking place in the combustion chamber of a domestic boiler equipped with a perforated cylindrical burner. Recently, Hinrichs et al. [12] carried out numerical simulations with detailed chemistry to shed light on the main pathways to pollutant emissions, i.e., NOXs and CO, which is in a condensing boiler. Their model was limited to a single-hole of a perforated cylindrical burner. The CO concentration in the cooled exhaust gas was observed to be significantly larger than the chemical equilibrium one because of the rapid quenching, triggered by the fast depletion of OH radicals, of CO oxidation reactions. The present work is aimed at carrying out resolved CFD simulations to analyze flame interactions in multi-hole geometries emulating a portion of burners, which are fitted in a domestic condensing boiler. In such burners the holes are usually positioned very close to each other and hence flame interactions may arise, thus affecting the resulting fluid-dynamic and thermo-chemical fields. The effect of hydrogen addition to natural gas on the multi-hole flame is then analyzed by feeding the G222 gas (23% H₂, 77% CH₄) and comparing results with the conventional G20 gas (100% CH₄).

2. Numerical model

Preliminary, 1-D freely propagating flames simulated using OPENSMOKE-SUITE [13] with GRI3.0 mechanism, including 53 reactive chemical species and 325 elementary reactions, in order to analyze the flame structure. Subsequently, a 3-D model with CFD was developed to gain insight into the effect of geometrical configuration on the interaction between the flames.

2.1. Physical model

3-D simulations of lean hydrogen-methane-air laminar premixed flames were performed using the GRI-Mech 3.0 [14] kinetic mechanism. The conservation equations for mass, momentum, energy, and transport equations for the mass fractions of chemical species were solved in steady-state conditions:

$$\nabla \cdot (\rho v) = 0 \quad (1)$$
$$\nabla \cdot (\rho vv) = \nabla p + \nabla \cdot (\tau) \quad (2)$$
$$\nabla \cdot (\rho (vE + p)) = \nabla \cdot (k_{eff} \nabla T) + S_h \quad (3)$$
$$\nabla \cdot (\rho vY_i) = -\rho D_i \nabla^2 Y_i + R_i \quad (4)$$

where \( v \) is the velocity, \( \tau \) is the stress tensor, \( S_h \) is the energy source term, including the contribution of radiation, \( Y_i \) is the mass fraction of the \( i \)-th species and \( k_{eff} \) is the effective thermal conductivity. \( R_i \) is the net rate of production or destruction of the \( i \)-th chemical species by chemical reaction (described later in this section). \( D_i \) is the molecular diffusion coefficient of the \( i \)-th chemical species in the mixture. Binary diffusion coefficients are firstly calculated following the kinetic theory and a modification of the Chapman–Enskog formula; then \( D_i \) is obtained by applying the Wilke’s mixing rule. Radiation is taken into account with the P1 model [15, 16] using the weighted-sum-of-gray-gases model with coefficients from Smith [17] to estimate spectral properties.

2.2. Computational domain

The multi-hole geometry is shown in Fig. 1 and consists of four holes having a diameter \( D \) placed at the vertices of an \( R \times 1.1R \) rectangle. In order to investigate the effect of flame interaction, the distance between the holes was varied by using different \( R/D \) ratios thus leading to the three geometries in Table 1.

| Domain | \( R \times 1.1R \) | \( N_{cell} \) |
|--------|------------------|-------------|
| \( R1 \) | 250x1.5Dx1.65D | 1.5D-1.65D | 56000 |
| \( R2 \) | 250x1.75Dx1.9D | 1.75Dx1.9D | 64000 |
| \( R3 \) | 250x2.2Dx2.2D | 2x2.2D | 73000 |

The 3-D geometries and corresponding grids were created using ANSYS-ICEM. The symmetries of the burner suggest that a quarter of the hole can be considered; however, in order to better study the flame interaction, four quarters of holes were used as depicted in Fig. 1. The computational grids were generated by ensuring \( \sim 8 \) points within the flame thickness, estimated from the 1-D simulation of the freely propagating flame. The thermal flame thickness is calculated using the temperature profile across the flame front [18]:

$$l_T = \frac{(T_h - T_w)}{\left(\frac{\partial T}{\partial z}\right)_{max}}$$
where $T_b$ and $T_u$ are the burnt and unburnt temperature respectively, while $(\partial T/\partial z)_{\text{max}}$, representing the temperature gradient.

### 2.3. Boundary conditions

Velocity inlet was set at the bottom side of the holes, through which air-fuel mixture enters with a uniform velocity $v = 1.5$ m/s and temperature, $T_u = 300$ K, ensuring a fully laminar flow. The mixture composition corresponds to an equivalence ratio $\phi = 0.8$ for both the G20 and G222 fuels. At the exit of the domain, a pressure outlet boundary is prescribed. The conduction heat exchange between the burner and the gas mixture is considered to set the wall temperature between the holes higher than the inlet condition ($T_w = 750$ K). All other sides of the domain are prescribed with symmetry boundary conditions. The burner wall temperature was estimated experimental data available for this type of burner.

### 2.4. Solution methodology

The above set of equations was solved with the pressure-based coupled algorithm available in ANSYS-FLUENT 19.2 [19] using a central differencing scheme for diffusion terms and a second-order upwind scheme for convection terms. Chemistry integration was carried out using the direct integration method. The fuel-oxidizer mixture is ignited by patching a region near to the inlet by setting a high temperature (2500 K). At convergence, normalized residuals did not change with iterations and were all below $10^{-6}$.

### 3. Results

Figure 2 shows the temperature, CH$_4$, O$_2$, and OH mole fractions along the flame axis for the G20 gas as computed by the 1-D and 3-D simulations, the latter being carried out for different distances between the burner holes. The same analysis is shown in Fig. 3 in the case of hydrogen addition, i.e., for the G222 gas. We can observe a different behavior in the temperature profile between the 1-D and 3-D simulations, as in the latter simulations the temperature in the fresh zone is influenced by the heat exchange with the wall corresponding to the burner plate. Moreover, the downstream temperature is found to diminish with increasing the distance between the holes, i.e., $R$. Major species as CH$_4$ and O$_2$ mole fractions, indicated a good agreement between 1-D and 3-D predictions and literature [20], thus confirming also the accuracy of the reacting module available in the CFD code. Conversely, the OH concentration highlights significant differences between the freely propagating flame and the 3-D model; moreover, the OH levels appear to be different for the three $R$ values, thus indicating that the distance between the burner holes affects the reaction region. The strongest reaction zone, which is denoted by the highest

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**Fig. 1.** Sketch of the (a) burner portion, (b) computational domain, and (c) grid.

**Fig. 2.** Profiles along the hole axis of (a) Temperature, CH$_4$, O$_2$ and (b) OH mole fractions predicted by 1-D (solid lines) and 3-D (dashed lines) models. G20 gas.
values of the OH flame marker, occurs for the smallest R values, i.e., for the closest flames.

Figure 4 illustrates the temperature field in the longitudinal plane crossing the axes of two adjacent holes in the case of methane (i.e., G20 gas) and for the three different R values. The downstream temperature decreases with increasing the hole-to-hole distance; this is because the surface area of the burner plate increases, thus resulting in a higher overall heat transfer rate from the gas to the burner plate. The temperature profiles along the axis of the hole show the same trend, although with a different slope in the reaction zone (see Fig. 4). In particular, the flame front moves downstream with increasing the hole-to-hole distance. The velocity field is reported in Fig. 5 for the same G20 gas.

The velocity values are normalized with respect to the laminar flame speed $S_L$, calculated from the 1-D freely propagating flame simulations. The velocity distribution indicates the presence of two velocity peaks along the hole axis. The first peak may be explained by the gas acceleration due to the mixture heat up; this first peak takes place at $Z = 1D$ independently on the hole-to-hole distance. The second velocity peak occurs just downstream of the flame front thus its position increases from $Z = 2.1D$ to $Z = 2.3D$ when increasing R from $R = 1.5D$ to $R = 2.0D$, i.e., from the R1 to R3 case. Actually, this second peak is well visible for the smallest hole-to-hole distance, while it can be scarcely discerned for the largest R value, i.e., for the R3 case. Indeed the second velocity peak can be ascribed to flame interactions; when the hole-to-hole distance is limited, the velocity field is disturbed by the heat transfer associated with the presence of the adjacent reacting jets resulting in a further acceleration of the flow.

The distribution of OH mole fraction is reported in Fig. 6. Firstly we can observe that maximum OH concentration occurs for the lowest hole-to-hole distance, indicating the strongest reaction zone. Secondly, we can notice how the OH distribution moves closer to the burner plate by increasing the hole-to-hole distance. In particular, the wavy shape of the OH concentration is more pronounced with increasing the R value, thus approaching a single premixed flame behavior. In the case of hydrogen addition, i.e., G222 gas, we observe the downstream temperature to decrease with increasing R in agreement with the features of the G20 case. Fig. 7a compares the temperature profile...
Fig. 6. Distribution of OH mole fraction in the longitudinal plane crossing the axes of two adjacent holes for (a) $R = 1.5D$, (b) $R = 1.65D$, (c) $R = 2.0D$ and (d) temperature profiles along the hole axis. G20 gas.

Table 2: Thermal flame thickness estimated from 1-D and 3-D simulations.

|       | 1-D | 3-D $R1$ | 3-D $R2$ | 3-D $R3$ |
|-------|-----|----------|----------|----------|
| G20   | 0.664D | 0.497D | 0.792D | 0.854D |
| G222  | 0.605D | 0.512D | 0.845D | 0.890D |

Table 3: Outlet CO value in ppm for all cases.

|       | 3-D $R1$ | 3-D $R2$ | 3-D $R3$ |
|-------|----------|----------|----------|
| G20   | 887      | 485      | 259      |
| G222  | 694      | 383      | 146      |

along the hole axis obtained for the three configurations with G20 and G222 gas. We can notice that $H_2$ addition leads to an anticipation of the temperature rise due to the high reactivity of hydrogen. However, it is worth noting that the G222 gas contains a limited amount of hydrogen, which represents 23% by volume of the fuel corresponding to 3.6% by weight. The 1-D simulations pointed out a small difference in the laminar flame speed which was estimated to be 0.27 m/s and 0.35 m/s for the G20 and G222 gas, respectively, in agreement with the other works [21, 22]. Figure 7b shows the velocity profiles along the hole axis for both G20 and G222 gas. Also in the case of $H_2$ addition, two velocity peaks can be identified, the second one being more evident for the $R1$ case as imputed to flame interaction. The OH concentration, in Fig. 7d, confirms the shift of OH peak towards the burner for the G222 gas due to the hydrogen reactivity. In order to better highlight the effect of $H_2$ addition, the distribution of the radical, i.e., HCO, is shown in Fig. 8 for the two gases in the three configurations. Injecting $H_2$ leads to a shift of HCO towards the burner and a small increase (slightly visible in the contours) of the width of the HCO region. Augmenting hole-to-hole distance causes both a lowering of the radical concentration and an increase in the width of the HCO region. These effects are confirmed in Fig. 7c that shows the HCO concentration along the hole axis. We can also notice a shift in the profile due to the hydrogen addition when comparing the G222 to the G20 gas. This funding is in agreement with the values of flame thermal thickness, which were estimated from temperature profiles. Such values are reported in Table 2 for all configurations and two mixtures. For sake of comparison, the thermal thickness for the freely propagating flame is also shown. In the 1-D model the flame thermal thickness value decreases...
when adding hydrogen, while the opposite behavior was observed for all 3-D simulations, this unusual behavior can be attributed to the flame interaction (especially for the RI case) and the heat flux exchanged between the flame and the burner plate. Table 3 shows the value of CO at the outlet for all simulations. The addition of hydrogen leads to a reduction of the CO values, in agreement with the literature [8]. We can notice the CO concentration to decrease with increasing the hole-to-hole distance for both G20 and G222 gases. It is worth noting that the above values are generally much higher than those of condensing boilers as the present numerical model does not take into account the quenching due to the presence of the heat exchanger.

4. Conclusion

A 3-D model was developed to investigate laminar premixed flames positioned very close to each other to emulate portions of perforated burners of condensing boilers. For small hole-to-hole distance, the flow field was found to be different from that of a single laminar premixed flame because of flame interactions. In particular, the flame interaction leads to a velocity peak downstream of the reaction region. The OH flame marker and the distribution of the HCO radical indicated a stronger and thinner reaction region for smaller hole-to-hole distances. Consistently, the flame thermal thickness was found to augment with increasing the distance between the burner holes. Hydrogen addition leads to a shift towards the burner of the reaction region, although the behavior of the G20 and G222 gases was rather similar. This can be explained by the relatively low hydrogen content in the inlet mixture, especially considering the premixed flame configuration. Further work will be needed to include in the numerical model the effect of the heat exchanger to predict the influence of H2 addition on both CO and NO emissions.

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