



Article Modeling of a Blast Furnace with Both CFD and Thermodynamics Principles

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Abstract: In this paper, we revisit a turbulent mixing of gas and air in a gas burner with computational fluid dynamics (CFD) models. The quality of such a turbulent mixture is based on temperature, pressure, and velocity distributions as well as the distributions of different molecules, turbulent kinetic energy, and turbulent dissipation rate. In order to identify a precise combination of a gas and air mixture in a gas burner, which directly influences the quality of the combustion flame and reduces the amount of carbon monoxide (*CO*) emission in flue gases, thermodynamic principles are utilized based on the balancing ratio of molecular weights and the balancing ratio of mass flows between gas and air. Moreover, input parameters, such as volume flow rates, pressure, mass ratio, temperature, turbulent kinetic energy, and turbulent dissipation rate, are judiciously chosen with proper boundary conditions for both axisymmetric two-dimensional and three-dimensional models. It is confirmed that the effectiveness of gas and air mixture and combustion depends on the gas burner model, more specifically, on the sizes and locations of gas and air inlets and outlets as well as operation conditions.

Keywords: combustion; computational fluid dynamics; meshing; turbulence; gas burner; mass transfer; heat transfer

1. Background and Objectives

A gas burner is a device in which the chemical energy of a gas mixture is converted into thermal energy through combustion [1]. The released thermal energy is used in industries as a source of heat and to further initiate and sustain a continuous chemical reaction [2]. For a combustion to take place, fuel, oxygen, and heat must be provided. In this case, fuel is supplied from the gas or methane, and oxygen is provided through the abundant supply of air with nearly 20% oxygen and 80% nitrogen by the ratio of numbers of molecules or partial pressures. In practice, gas burners can be divided into three categories based on the gauge pressure of a gas that enters the burners through the gas inlet: namely, low-pressure gas burners with a gauge pressure up to 5 kPa, medium-pressure gas burners with a gauge pressure above 300 kPa [3]. Furthermore, gas burners can also be characterized as three types based on the processes through which gas is mixed with air: namely, gas burners without premixing of gas and air, with a partial premixing, and with a complete premixing [3]. The air that enters a burner can be either cold or pre-heated. Air enters a gas burner by a gauge pressure created within multiple air inlets.

In this paper, we analyze a medium-pressure gas burner that is typically used in blast furnaces for the production of magnesia clinker and aim to provide some validation of the operating conditions and comments on further improvements. A magnesite material is decomposed in the combustion chamber of a blast furnace for the initiation of a chemical reaction that leads to the decomposition of magnesite [4]. Therefore, the quality of flame and combustion efficiency are very important in the decomposition process of magnesite material into magnesia clinker. The operation related information provided by the Computer Control Technology (CCT) company in Slovak Republic, a European Union (EU)



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Copyright: © 2022 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). member, as listed in Table 1, indicates a high concentration of carbon monoxide (*CO*) in flue gases of the blast furnace. The other objective and impetus of this research is certainly related to the desire for a continuous reduction in substances of detriment to the global environment.

Table 1. Measured carbon monoxide (*CO*) concentration in ppm within flue gases of the blast furnace provided by CCT company.

Date	Time	CO (ppm)
16 September 2015	9:14	3658
	9:30	2256
	10:24	1550
18 September 2015	10:17	2145
	10:44	2247
	11:29	2147
22 September 2015	10:15	3028
	10:44	2876
	10:57	2481

The measurements in Table 1 show a high parts per million (ppm) of carbon monoxide (*CO*) in flue gases of the blast furnace in question, which suggests an incomplete combustion commonly induced by an insufficient supply of oxygen (O_2) or air. The average measured *CO* amount is approximately 2500 ppm, which is significantly higher than the norm set by the European Union (EU) on industrial emissions, namely, a *CO* amount below 81.1 ppm [5]. If companies operating with such blast furnaces do not satisfy these EU limits, they will have to pay a fine. In the worst scenario, they may have to shut down their operations. A high ppm of carbon monoxide (*CO*) is directly linked to inefficient or incomplete combustion [6]. In this paper, we would like to employ thermodynamic principles to identify the optimal mixing ratio between gas and air and validate the current operation conditions. In this study, the gas is assumed to be mainly methane (*CH*₄). When methane in gaseous phase is combusted with oxygen (O_2), which is commonly provided with the air supply, an exothermic reaction is triggered. Thus, following Hess's law, which states that the enthalpy change of an overall reaction is the same no matter what path it takes, at room temperature, 27 °C or 300 K, the complete combustion reaction of gas and air is simply described as

$$CH_4(gas) + 2O_2(gas) = CO_2(gas) + 2H_2O(liquid) + 890.3 \text{ kJ}.$$
 (1)

Note that in the reaction stipulated in Equation (1) and all other reactions in this paper, the coefficient before the chemical species stands for the number of molecules measured in mol. In this reaction, we use the standard molar enthalpy of formation around 27 °C or 300 K. Moreover, the formation enthalpies for methane (CH_4) in gaseous form, water (H_2O) in liquid form, carbon dioxide (CO_2) in gaseous form, and oxygen (O_2) in gaseous form are -74.81 kJ/mol, -285.8 kJ/mol, -393.5 kJ/mol, and 0 kJ/mol, respectively. Thus, by balancing both sides of the reaction as stipulated in Equation (1), we can confirm that 1 mol of methane combines with 2 mol of oxygen which requires roughly 8 mol of nitrogen in the air, or strictly speaking, an oxygen and nitrogen gas mixture, if the proportionalities based on numbers of molecules between oxygen and nitrogen molecules in the air are assumed to be 20% and 80%, respectively, the complete combustion will produce the thermal energy or heat at the amount of 890.3 kJ. However, in practice, the perfect proportionality may not happen at all time and in all places. Therefore, partial methane oxidation must also be studied and understood [7]. In general, at room temperature, or 300 K, we have the following intermediate stages for methane oxidation

$$2CH_4(gas) + O_2(gas) = 2CO(gas) + 4H_2(gas) + 71.4 \text{ kJ};$$
(2)

$$CH_4(gas) + CO_2(gas) = 2CO(gas) + 2H_2(gas) - 247.3 \text{ kJ};$$
(3)

$$CH_4(gas) + H_2O(liquid) = CO(gas) + 3H_2(gas) - 250.1 \text{ kJ};$$
(4)

$$2CO(gas) + O_2(gas) = 2CO_2(gas) + 564.0 \text{ kJ};$$
(5)

$$CO_2(gas) + H_2(gas) = CO(gas) + H_2O(liquid) + 2.8 \text{ kJ}.$$
 (6)

In fact, by combining the information for the reaction equation in Equation (1), we can easily identify, with some linear algebra manipulations, that the molar formation enthalpy for carbon monoxide (*CO*) in gaseous form, around 27 °C or 300 K, is -110.5 kJ/mol. It is also confirmed that like oxygen (O_2) in gaseous form, around 27 °C or 300 K, the molar formation enthalpy for hydrogen (H_2) is zero. Notice however, according to Hess's Law, the reaction stipulated in Equation (1) still represents the complete combustion of methane and oxygen with perfect proportionality [8]. In fact, high reaction temperatures above 750 °C are normally required for such complete conversion of methane to carbon dioxide and water [9,10]. Consequently, we can modify the relevant reactions to those at 1000 K [11],

$$CH_4(gas) + 2O_2(gas) = CO_2(gas) + 2H_2O(gas) + 800.0 \text{ kJ};$$
(7)

$$2CH_4(gas) + O_2(gas) = 2CO(gas) + 4H_2(gas) + 45.2 \text{ kJ};$$
(8)

$$2H_2(gas) + O_2(gas) = 2H_2O(gas) + 496.0 \text{ kJ};$$
(9)

$$CO_2(gas) + H_2(gas) = CO(gas) + H_2O(gas) - 34.5 \text{ kJ}.$$
 (10)

Furthermore, we also have three reactions which can eventually produce soot, a solid form of carbon (*C*):

$$2CO(gas) = CO_2(gas) + C(solid) + 171.0 \text{ kJ};$$
(11)

$$CH_4(gas) = 2H_2(gas) + C(solid) - 89.9 \text{ kJ};$$
 (12)

$$CO(gas) + H_2(gas) = H_2O(gas) + C(solid) + 136.0 \text{ kJ}.$$
 (13)

In this paper, we would like to provide the field engineers who deal with the combustion of methane with a better or perhaps more comprehensive understanding of the related combustion reactions at different stages and temperatures. In Refs. [9–11], the water is commonly listed as a liquid for a temperature of around 300 K and as a gas for a temperature of around 1000 K. We hope that these listed details along with specific heats for exothermic or endothermic reactions at two different temperatures will provide our readers with a more complete view of both complete and incomplete methane combustion. Furthermore, as depicted in Equation (1), when the proportionality of methane (gas) and oxygen (air) is not ideal, more importantly, the vapor content within the air, measured by relative humidity or absolute humidity, the air and gas mixture does not yield a complete combustion, and instead an incomplete combustion reaction of gas and air is produced. Assume ideal gas conditions hold for both methane and air, stated as follows:

$$pV = nR_uT, (14)$$

$$pv = RT, (15)$$

where *v* is the specific volume also defined as the reciprocal of the density ρ , *V* is the total volume, *p* is the total pressure, *T* is the temperature, *R_u* is the universal gas constant, and *R* is the gas constant defined as *R_u*/*M* with *M* and *n* as the molar mass and the number of molecules in mol for the gas in question.

It is clear based on Equations (14) and (15) that the mass of the gas in question is calculated as m = Mn or m = V/v. Thus, with the same pressure and temperature, typically, 1 m³ of CH_4 requires 2 m³ of O_2 , which is equivalent to the same proportionality of 1 mol of CH_4 to 2 mol of O_2 , which can be provided by 10 mol of air with the addition of 8 mol of N_2 . The generated heat for the reaction with mol as the unit for the amount of molecules is stipulated in Equation (1) or (7). From the information obtain from CCT company, under the ambient pressure 101 kPa and room temperature 300 K, 280 m³/h of gas and 3000 m³/h of air are typically used for the analyzed blast furnace for the production of magnesia clinker, which, according to Equation (14), correspond to 11,338.3 mol/h of gas and 121,481.8 mol/h of air, respectively. Again, 121,481.8 mol/h of the air supply corresponds to 24,296.4 mol/h of the oxygen (O_2) supply, which is roughly two times the gas supply as required in the reaction stated in Equation (1).

2. Key Balance Ratios

In order to achieve a high efficiency of combustion, we need to compare a molecular weight balancing ratio of gas and air to a mass flow balancing ratio of gas and air [1,12]. In this paper, for simplicity, we assume that air is composed of approximately 80% of nitrogen (N_2) and 20% of oxygen (O_2), which yields an equivalent molar mass 28.8 kg/kmol. Therefore, within 10 mol of air we have about 2 mol oxygen (O_2) and 8 mol nitrogen (N_2) [12]. The combustion stipulated in Equation (1) requires 2 mol of oxygen (O_2) and 1 mol of methane (CH_4). The molecular masses for air, oxygen and methane are given as follows:

$$M_{CH_4} = 16 \text{ g/mol} \text{ or } \text{kg/kmol},$$

 $M_{O_2} = 32 \text{ g/mol} \text{ or } \text{kg/kmol},$
 $M_{N_2} = 28 \text{ g/mol} \text{ or } \text{kg/kmol},$
 $M_{air} = 28.8 \text{ g/mol} \text{ or } \text{kg/kmol}.$

Within the air, the mass balancing ratio of oxygen and nitrogen based on a simple 20% and 80% ratio for partial pressure or number of molecules or mol numbers is calculated as follows:

Balancing ratio =
$$\frac{0.2M_{O_2}}{0.2M_{O_2} + 0.8M_{N_2}} \times 100 = \frac{0.2 \times 32}{0.2 \times 32 + 0.8 \times 28} \times 100 = 22.22\%.$$

Thus, as recommended by the reaction stipulated in Equation (1), one mol of gas or methane (CH_4) will react with two mol of oxygen (O_2) which have eight mol of nitrogen (N_2) in the air supply and will have a mass balance ratio between the gas and the air supply

Balancing ratio =
$$\frac{M_{CH_4}}{2M_{O_2} + 8M_{N_2}} \times 100 = \frac{16}{2 \times 32 + 8 \times 28} \times 100 = 5.56\%.$$
 (16)

Finally, the mass balancing ratio of gas and gas and air mixture based on a simple one to ten mol or one to ten volume mixing at the same temperature and pressure is then calculated as

Balancing ratio =
$$\frac{M_{CH_4}}{M_{CH_4} + 10M_{air}} \times 100 = \frac{16}{16 + 288} \times 100 = 5.263\%$$

Note that although the gas and air can be supplied into the burner at different pressure and temperature. Once mixed within the chamber, at all spatial locations, it is reasonable to assume the same pressure and same temperature conditions. Hence, the mass balance ratio calculated in Equation (16) is an important reference for complete combustion. This ratio will be compared to the actual balancing ratio of mass flow of gas and air in a different section utilizing the following spatial statistical equations over any cross-sectional area *A*:

$$\bar{c} = \frac{\int_{A} c dA}{\int_{A} dA},$$

$$\bar{\sigma}_{c}^{2} = \frac{\int_{A} (\frac{c-\bar{c}}{\bar{c}})^{2} dA}{\int_{A} dA},$$

$$\bar{\sigma}_{cu}^{2} = \frac{\int_{A} (\frac{c-\bar{c}}{\bar{c}})^{2} u dA}{\int_{A} u dA};$$
(17)

where *c* stands for the time-average concentration of a chemical species, \bar{c} represents the spatial arithmetic mean concentration of a chemical species, $\bar{\sigma}_c$ refers to the spatial concentration standard deviation, and $\bar{\sigma}_{cu}$ is the flow concentration standard deviation.

Needless to say, the mixing uniformity is measured in terms of two relative standard deviations $\bar{\sigma}_c$ and $\bar{\sigma}_{cu}$ of the concentration c with respect to the arithmetic mean \bar{c} . In the simulation, we compute \bar{c} , $\bar{\sigma}_c$, and $\bar{\sigma}_{cu}$ near the end of the burner. Moreover, we also recognize that the integrals $\int_A udA$ and $\int_A cudA$ are directly related to the volume flow rates and tracer concentration through mass balances. Denoting \dot{V}_1 and \dot{V}_2 as the flow rates of the streams with tracer concentrations c_1 and c_2 , respectively, from the mass conservation laws, we obtain

$$\int_{A} u dA = \dot{V}_{1} + \dot{V}_{2},$$
$$\int_{A} c u dA = c_{1} \dot{V}_{1} + c_{2} \dot{V}_{2}$$

which will be used to validate the computational results.

Similarly, assume the ideal gas law holds with the same pressure and temperature, in this case, based on the reaction stated in Equation (5), 2 m³ of *CO* requires 1 m³ of O_2 which is equivalent to the same proportionality of 2 mol of *CO* to 1 mol of O_2 . More specifically, according to Equation (14), under the ideal gas situation, 2 m³ of *CO* at room temperature, 27 °C or 300 K, with the pressure equal to that of the atmospheric pressure $p_0 = 101$ kPa contains about 81.0 mol carbon monoxide (*CO*) molecules, which, based on the exothermic reaction depicted in Equation (5), generates 22.84 MJ heat after the complete conversion of carbon monoxide (*CO*) into carbon dioxide (*CO*₂) [13]. Particular attention will be focused on the volume fraction of air and methane for different models of gas burners and different input parameters of gas and air [3]. Notice that in this exothermic reaction, the heat from the reaction will elevate the enthalpy of the surrounding environment and the substances from the combination of *CO* and O_2 , namely, CO_2 . In practice, due to incomplete combustion, carbon monoxide is formed, and the heat generated in the burning of the residual *CO* per hour is calculated as

$$\dot{Q} = \frac{CO(\text{ppm})}{1,000,000} (\dot{V}_g + \dot{V}_a) \cdot Q_{CO} = \frac{2500}{1,000,000} \frac{1}{2} \times (280 + 3000) \times 22.84 = 93.644 \text{ MJ/h},$$

where *CO* (ppm) stands for the parts per million (ppm) of *CO* measured in flue gases, in this case 2500, \dot{V}_g and \dot{V}_a represent the operation flow rate with the unit m³/h for gas and air, respectively, and Q_{CO} is the heat in MJ/m³ produced in the burning of *CO* under the same ambient pressure and room temperature, which in this case is 22.84 MJ per 2 m³ of *CO*.

It is very important to burn CO in order to achieve complete combustion. However, based on the provided information from the industry, it is obvious that in the blast furnace in question, there is not enough oxygen to burn CO and, therefore, there is a high CO concentration, measured in parts per million (ppm) in flue gases. To reiterate, the measured carbon monoxide (CO) amount in ppm within flue gases is approximately 2500 and under the ambient pressure 101 kPa and room temperature 300 K the heat generated in the burning of carbon monoxide (CO) is 11.42 MJ/m^3 , thus with $280 \text{ m}^3/\text{h}$ of gas and $3000 \text{ m}^3/\text{h}$ of air, the heat generated in the burning of the residual carbon monoxide (CO) is around 93.644 MJ/h. Moreover, under the same ambient pressure and room temperature, the volume proportionality is the same as the proportionality of molecules measured in mol. Thus, following the 20% and 80% proportionality of oxygen and nitrogen molecules within air, 3000 m³/h air volume flow rate indeed provides 600 m³/h oxygen supply which is needed to completely react or combust with roughly $300 \text{ m}^3/\text{h}$ gas or methane. In practice, 11 units of air and 1 unit of gas are used to propagate combustion [12] with some excessive oxygen to compensate for localized incomplete combustion and the byproduct carbon monoxide.

The outdated design of a gas burner that is typically used in blast furnaces for a production of magnesia clinker is the main cause of the combustion problems. The typical burner, as depicted in Figure 1, does not provide adequate space to mix gas with air. In fact, in this type of compact blast furnaces with transverse mixing, natural convection as discussed in Ref. [14] is not significant. Moreover, the flame is kindled at the gas outlet and immediately gets in touch with the mineral material. Based on the information provided by the CCT company, the proposed concentric blast furnace in this study has one gas inlet and two air inlets as depicted in Figure 2 and uses similar input parameters as listed in Table 2.

Gas

Air

Volume flow rate m ³ /h	1.5	50
Temperature K	288	293
Gauge pressure kPa	251	7
gas inlet		gas outlet air outlet

 Table 2. Operation parameters for the analyzed blast furnace with one typical gas burner.

Figure 1. A typical gas burner model for a production of magnesia.



Figure 2. Mesh details for the center gas inlet and boundary conditions in three-dimensional ADINA model.

Assume the ideal gas law holds for both air and gas. The specific volume for gas v_g and air v_a are calculated as, based on the gas pressure p_g and the air pressure p_a and other information listed on Table 2,

$$v_{g} = \frac{R_{g}T_{g}}{p_{g}} = 0.42476 \text{ m}^{3}/\text{kg},$$

$$v_{a} = \frac{R_{a}T_{a}}{n_{a}} = 0.78318 \text{ m}^{3}/\text{kg};$$
(18)

along with the density for gas ρ_g and ρ_a

$$\rho_g = \frac{p_g}{R_g T_g} = 2.35430 \text{ kg/m}^3,$$

$$\rho_a = \frac{p_a}{R_a T_a} = 1.27685 \text{ kg/m}^3.$$
(19)

For the two air inlet model shown in Figure 2, the volume flow rate for gas \dot{V}_g is 1.5 m³/h and the volume flow rate for air \dot{V}_a is 50 m³/h. Therefore, the operation weight or mass balance for the ADINA model with two air inlets as depicted in Figure 2 is evaluated as

Balancing ratio =
$$\frac{\rho_g V_g}{\rho_a \dot{V}_a} \times 100 = \frac{2.35430 \times 1.5}{1.27685 \times 50} \times 100 = 5.53\%.$$

This balance ratio matches with the requirement for the complete combustion calculated with thermodynamics principles.

3. Turbulent Modeling with Heat Transfer and Mass Transfer

CFD is a powerful tool which can be used to model turbulent fluid flows along with heat transfer and mass transfer. In practice, a comparison of balancing ratios of molecular weights and mass flow rates between gas and air is employed to estimate a suitable input parameters [12]. Generally, in the best case, these balancing ratios should be identical everywhere in the gas burner outlet where the combustion takes place [12]. Significant deviations might suggestion specific changes for operational conditions or even geometrical alteration need to be made. In this paper, we utilize both Solidworks Flow Simulation and ADINA to simulate an interaction of turbulent gas and air flows in the gas burner. It is essential to set up boundary conditions correctly in order to obtain reliable and meaningful results [15]. In general, we have three sets of boundary conditions, namely, turbulent fluid flow, heat transfer, and mass transfer, which are required for inlets, wall, and outlets as

depicted in Figure 2. In this study, we use the $k - \epsilon$ model to simulate flow characteristics for turbulence flow conditions [15].

Unlike the purely analytical study of the mixing jet trajectory documented in Ref. [16], CFD tools on heat transfer and mass transfer were introduced in the study of various transverse and concentric mixing arrangements [15]. We consider here the turbulent flow of a homogeneous, viscous, incompressible fluid with constant properties. The gas or methane is considered a different chemical species. By representing the fluctuating parts in the eddy viscosity v_t , turbulent kinetic turbulent kinetic energy k, and turbulent dissipation rate ϵ , we obtain the following governing equations from the mass and momentum conservation equations [17,18]:

$$\frac{\partial v_i}{\partial x_i} = 0$$

$$\frac{\partial v_i}{\partial t} + v_j \frac{\partial v_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[(\nu + \nu_t) \frac{\partial v_i}{\partial x_j} \right]$$
(20)

where ρ , v, v_t , v_i , and p stand for fluid mass density, kinematic viscosity, eddy viscosity, time-average fluid flow velocity in direction x_i , and time-average pressure, respectively.

Furthermore, for the standard k- ϵ turbulent model, we have two additional equations:

$$\frac{\partial k}{\partial t} + v_j \frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + \nu_t \Phi - \frac{k}{\bar{T}}$$

$$\frac{\partial \epsilon}{\partial t} + v_j \frac{\partial \epsilon}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] + a_1 \frac{1}{\bar{T}} \nu_t \Phi - a_2 \frac{\epsilon}{\bar{T}}$$
(21)

where a_1, a_2, σ_k , and σ_{ϵ} are designated constants; Φ denotes the inner product of the velocity strain tensor $2e_{ij}e_{ij}$ with $e_{ij} = \frac{1}{2}(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i})$; and the turbulent time scale \bar{T} and viscosity v_t are expressed as

$$\bar{T} = \frac{k}{\epsilon} + \sqrt{\frac{\nu}{\epsilon}}$$
(22)

$$\nu_t = c_\mu k \bar{T} \tag{23}$$

with a constant c_u .

In addition to the mass and momentum conservation equations with the $k - \epsilon$ turbulent model, we employ the following tracer conservation equation to model the mass transfer phenomena in the turbulent flow,

$$\frac{\partial c}{\partial t} + v_j \frac{\partial c}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\frac{\nu}{Sc} + \frac{\nu_t}{\sigma_c} \right) \frac{\partial c}{\partial x_j} \right]$$
(24)

where *c*, *Sc*, and σ_c are the time-average concentration of a chemical species, the Schmidt number, defined as the ratio between the kinematic viscosity ν and the mass diffusivity *D*, and a selected constant.

Finally, the energy equation with temperature as the primary unknown within the burner

$$\frac{\partial T}{\partial t} + v_j \frac{\partial T}{\partial x_j} = \frac{\partial}{\partial x_j} \left[(\frac{\nu}{Pr} + \frac{\nu_t}{\sigma_d}) \frac{\partial T}{\partial x_j} \right] + q_s$$
(25)

where *T*, *Pr*, σ_c , and q_s are the time-averaged temperature, Prandtl number defined as the ratio between the kinematic viscosity ν and the thermal diffusivity α , a selected constant, and a heat source commonly from a reaction.

In this study, for the turbulent mixing model with gas and air, we assume the mass density $\rho = 1.2 \text{ kg/m}^3$ and the kinematic viscosity $\nu = 1.48 \times 10^{-5} \text{ m}^2/\text{s}$. Furthermore, the thermal conductivity *k* is 0.026 W/mK, and the specific heat for constant pressure c_p is 1004 J/kgK. Hence, thermal diffusivity α , defined as a ratio between the thermal conductivity *k* and the product of the density ρ , and the specific heat for constant pressure c_p can be calculated as

$$\alpha = rac{k}{
ho c_p} = 2.158 imes 10^{-5} \mathrm{m}^2 \mathrm{/s}.$$

The governing Equations (20), (21), (24) and (25) are implemented in the ADINA-F program. Moreover, the turbulent related diffusivities for heat transfer and mass transfer, namely, $\frac{v}{S_c} + \frac{v_t}{\sigma_c}$ and $\frac{v}{Pr} + \frac{v_t}{\sigma_d}$, respectively, as functions of spatial locations are incorporated in the user-supplied subroutine provided by the ADINA software. In this work, we select $a_1 = 1.44$, $a_2 = 1.92$, $\sigma_k = 1.0$, $\sigma_c = 1.3$, $c_\mu = 0.09$, Sc = 0.9 which corresponds to the mass diffusivity $D = 2.20 \times 10^{-5} \text{m}^2/\text{s}$, Pr = 0.927 which corresponds to the thermal diffusivity $\alpha = 2.158 \times 10^{-5} \text{m}^2/\text{s}$, $\sigma_c = 0.9$, and $\sigma_d = 0.9$. Furthermore, if we use the reaction equation at 1000 K and roughly ambient pressure, for the exothermic reaction in Equation (7), we have the volume for 1 kmol gas or methane as 82.3 m³, consequently, the heat generated per volume Q_s is calculated as 9.72 MJ/m³. According to Ref. [19], for a diameter of 23 mm reaction vessel, we have the reaction speed documented in Table 3. Employing the regression method presented in Ref. [20], for a circular reaction vessel with a diameter of 23 mm, we have an approximation of the reaction rate r (mm/s) with respect to the pressure p (torr or mmHg) at a relatively low temperature 620 °C or 893 K

$$r = C_1 p^{C_2},$$

where the constants C_1 and C_2 are evaluated, according to the experimental data presented in Table 3, as 3.3267×10^{-7} and 2.7462, respectively.

Table 3. Reaction rate with a cross-sectional diameter 23 mm.

Total pressure (torr or mmHg)	50	100	150	200
Reaction rate (mm/s)	0.015	0.105	0.345	0.64

As depicted in Figure 3, the reaction rate for methane at the temperature 620 °C and ambient pressure (760 torr or mmHg) can be estimated as 1.1268×10^{-5} m³/s, which is a product of the cross-sectional area of the container and the reaction rate in mm/s, depicted in Figure 3. Hence, the rate of heat generated in this reaction q_s as 109.51 W/m³. The modification of these constants based on the experimental validation and sensitivity analyses will be conducted and reported in a different study. Notice here the gas or methane supply is measured by volume flow rate \dot{V}_g evaluated as follows

$$\dot{V}_g = \frac{\pi}{4} u_{ig} d_{ig}^2 = 0.00041667 \text{ m}^3/\text{s} = 1.5 \text{ m}^3/\text{h},$$

where the average velocity for the gas inlet u_{ig} and the gas inlet diameter are 5.3052 m/s and 10 mm, respectively.



Figure 3. Methane reaction rate as a function of pressure.

We must note the subtle difference between the rate of heat generation per volume q_s which is based on the combustion rate at a given pressure and the rate of thermal energy \dot{Q} calculated based on the volume flow rate as well as the heat generated in the exothermic reaction at a given temperature, say 1000 K

$$\dot{Q} = 800 \text{ kJ/mol} \times \frac{(101,000 + 251,000) \text{ Pa}}{8.314 \text{ J/molK} \times 1000 \text{ K}} \times 1.5 \times \frac{1000}{288} \text{ m}^3/\text{h} = 176.41 \text{ MJ/h}.$$

Notice here that we have used the ideal gas law for the conversion of volume flow rates at different temperature and pressure according to the following equation:

$$\frac{P_1 V_1}{T_1} = \frac{P_2 V_2}{T_2},$$

where P_1 , V_1 , and T_1 stand for pressure, volume, and temperature, respectively, at the operation conditions, and P_2 , V_2 , and T_2 stand for pressure, volume, and temperature, respectively, at the standard conditions for the chemical reaction.

In general, the heat transfer equation is based on the energy conservation. In the future, similar to Ref. [21], entropy or free energy conservation equations can also be added in addition to the turbulent modeling with heat transfer and mass transfer equations as presented in this work. Furthermore, unlike liquid water, air is very much compressible as a fluid. For ideal and adiabatic air in reversible thermodynamic processes, namely, isentropic conditions, we commonly have

$$p = C \rho^{\gamma}$$

where γ is the so-called heat capacity ratio defined as the ratio between the specific heat for constant pressure c_p and the specific heat for constant volume c_v , p is the absolute pressure or total pressure, and C is a constant.

For most of the diatomic gas, the heat capacity ratio γ is 1.4. With the ideal gas law expressed as

 $p = \rho RT$,

it is clear that the bulk modulus β defined as $\rho \frac{dp}{d\rho}$, or $-v \frac{dp}{dv}$, with the specific volume v as the reciprocal of the density ρ , can also be expressed as

$$\beta = \rho \frac{dp}{d\rho} = \rho c^2 = \rho \gamma RT_{\mu}$$

where the sound speed for the air *c* can also be expressed as $\sqrt{\gamma RT}$.

Therefore, the incompressible fluid model can also be modified with the nearly incompressible or slightly compressible model by replacing the continuity equation in Equation (20) with the following, as presented in Ref. [22]

$$\frac{\partial v_i}{\partial x_i} + \frac{\dot{p}}{\beta} = 0$$

For the air at room temperature, around 300 K, at the atmospheric pressure 101 kPa, the density ρ can be calculated as

$$\rho = \frac{p}{RT} = \frac{101,000 \times 28.8}{8314 \times 300} = 1.1662 \text{ kg/m}^3,$$

and the sound speed *c* is evaluated as

$$c = \sqrt{\gamma RT} = 348.204 \text{ m/s}.$$

Consequently the bulk modulus β can be evaluated as follows

$$\beta = \rho c^2 = 141.4 \times 10^5$$
 Pa.

In this simulation, consider the insignificant change of temperature and pressure, we use the fluid density $\rho = 1.2 \text{ kg/m}^3$ with the corresponding bulk modulus $\beta = 150 \text{ kPa}$. With such a low bulk modulus, we expect to have an appreciable volume flow rate change between the inlets and the outlet, especially for computational models with low mesh densities.

A gas burner design can also have a fair significant impact on the effectiveness of gas and air mixing. From the locations of gas and air inlets to the specific flow rates, many design considerations as well as operation conditions need to be carefully analyzed in order to achieve a thorough turbulent mixing within the gas burner and generate a balanced and complete combustion process in the combustion chamber. One of the gas burners, provided by CCT company, uses transverse pipes to mix gas with air as shown in Figure 1. In essence, an air injector is introduced from the side, whereas the gas inlet is situated at the center of the gas burner. In this type of gas burner, the air and gas do not have enough space to mix within the gas burner. Therefore, gas is injected directly into the combustion chamber and immediately gets in touch with the mineral material. This gas burner design tends to have an excessive amount of unburned CO accumulated in flue gases over time. In order to improve the combustion efficiency, we consider a gas burner model with sufficient room for concentric mixing. As studied and documented in Ref. [15], concentric pipes have been found to be more effective in turbulent mixing than transverse pipes as demonstrated in Figure 4. In the proposed concentric mixer, a gas injector is inserted in between two air injectors as shown in Figure 2. We use this concentric model to simulate the turbulent mixing of gas and air with ADINA. We employ the similar length and width of a gas burner which provide the same operation conditions as those currently used in industry. As illustrated in Figure 2, boundary conditions for heat transfer and mass transfer are prescribed. Within the wall, the convective heat transfer conditions with the coefficient $h_c = 0.2 \text{ W/m}^2\text{K}$ are used along with the zero mass flux conditions. Notice that to simplify the CFD turbulent model, we also imply that the gas and air have similar densities. As depicted in Figure 2, the inlet velocity for air u_{ia} is 22.1049 m/s with the diameter of the two

air inlet $d_{ia} = 20$ mm; whereas the velocity for the gas inlet u_{ig} , namely, the center inlet, is 5.3052 m/s with the diameter $d_{ig} = 10$ mm. Hence, the volume flow rate of gas or methane into the burner \dot{V}_g is calculated as $\pi u_{ig} d_{ig}^2/4 = 0.00041667 \text{ m}^3/\text{s}$, or 1.5 m³/h; whereas the total volume flow rate of air into the burner \dot{V}_a is calculated as $n\pi u_{ia} d_{ia}^2/4 = 0.013889 \text{ m}^3/\text{s}$, or 50 m³/h, where the number of the air inlet *n* is 2 for the ADINA model as depicted in Figure 2.



Figure 4. Mass ratio of transverse pipe mixers with various injection angles and various concentric mixers [15].

For the center inlet, according to Refs. [5,23,24], we select the turbulent intensity k_i for this smooth inlet pipe with a straight axis as 0.02472, which is virtually an average of two approximations, namely, $k_i = 0.055Re^{-0.0407}$ and $k_i = 0.0227Re^{-0.1}$, with the Reynolds number $Re = u_{ig}d_{ig}/\nu = 3584.57$. Thus, the turbulent kinetic energy k of the center inlet with the diameter $d_{ig} = 10$ mm and the inlet velocity $u_{ig} = 5.3052$ m/s is estimated as

$$k = 1.5(k_i u_{i\sigma})^2 = 0.02579 \text{ m}^2/\text{s}^2$$

and the rate of energy dissipation ϵ is estimated as

$$\epsilon = \frac{k^{3/2}}{0.3d_{ig}} = 1.3805 \text{ m}^2/\text{s}^3.$$

Likewise, for the two air inlets with a different velocity based on balancing ratio of volume flow rates, according to Refs. [5,23,24], we select the turbulent intensity k_i for this smooth inlet pipe with a straight axis as 0.02213, which is virtually an average of two approximations, namely, $k_i = 0.055Re^{-0.0407}$ and $k_i = 0.0227Re^{-0.1}$, with the Reynolds number $Re = u_{ia}d_{ia}/v = 29.871 \times 10^3$. Thus, the turbulent kinetic energy k of the two air inlets with the diameter $d_{ia} = 2$ mm and the inlet velocity $u_{ia} = 22.105$ m/s can be estimated as

$$k = 1.5(k_i u_{ia})^2 = 0.35894 \text{ m}^2/\text{s}^2$$
,

and the rate of energy dissipation ϵ is estimated as

$$\epsilon = \frac{k^{3/2}}{0.3d_{ia}} = 35.842 \text{ m}^2/\text{s}^3.$$

As shown in Figure 5, in the ADINA-F transient analysis for the turbulent mixing with heat transfer and mass transfer for the newly proposed concentric gas burner, velocity vector (**v**), pressure (*p*), turbulent kinetic energy (*k*), turbulent dissipation rate (*e*), and mass concentration (*c*) have converged simultaneously. In general, boundary conditions need to be set up very precisely in order to obtain correct results from CFD analysis. In this case, the boundary conditions are defined on both gas and air inlets, on the wall, and on the gas burner's outlet. In the three-dimensional Solidworks Flow Simulation model shown in Figure 6, the gas inlet boundary conditions correspond to volume flow rate at 0.001959 m³/s, temperature at 288 K, and total pressure at 352 kPa as listed in Table 2. Using the correlation estimated in the previous section, the air inlet boundary conditions volume flow rate at 0.0340 m³/s for each of the two air inlets, temperature at 293 K, and total pressure at 108 kPa. For the three-dimensional ADINA model, the gas inlet boundary conditions are the volume flow rate at 0.00041667 m³/s, temperature at 288 K, and total

pressure at 352 kPa as listed in Table 2. Using the correlation estimated in the previous section, the comparable air inlet boundary conditions volume flow rate at 0.006944 m³/s for each of the two air inlets, temperature at 293 K, and total pressure at 108 kPa. Note that in both ADINA and Solidworks models, the ratio between volumetric flow rates of gas and air are very much close to the balancing ratio identified with thermodynamics principles. For the wall's boundary conditions, we assume that the wall has no-slip conditions, which means that when the fluid gets in touch with the wall, its velocity is 0 if the wall is stationary [25]. The wall is assumed to have no roughness with ideal reflection. Additionally, the wall is $0.2 \text{ W/m}^2 K$. The gas burner's outlet boundary condition is just a constant pressure, which is 101 kPa at the temperature of 293 K. This type of a boundary condition is used when the pressure is known and the flow distribution is unknown [26].

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TIC=	0	0.950-04	0.01E-05	0.250-05	0.200-02	0.14E-05	54754	0.01E-00	247	0.200+01	54756	0.700-00	247	0.200+01
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ITE=	4	0.79E-03	0.40E-04	0.65E-03	0.51E-02	0.12E-03	89043	0.24E-08	247	0.20E+01	89043	0.24E-08	247	0.20E+01
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Figure 5. ADINA convergence ratios for velocity vector, pressure, temperature, turbulent kinetic energy, turbulent dissipation rate, and mass concentration.



Figure 6. Three-dimensional Solidworks Flow Simulation model of a gas burner with multiple outlet openings.

As depicted in Figure 6, two options are considered in the Solidworks Flow Simulation, namely, the outlet with 7 and 10 openings with diameter 6 mm and 5 mm, respectively. Notice that the total opening cross-sectional area stays roughly the same due to the following approximation,

$$7\pi\frac{6^2}{4}\simeq 10\pi\frac{5^2}{4}$$

Similarly, in the comparable three-dimensional ADINA simulations, the gas burner outlet can be set with five circular exits, each of which has a diameter of 7.0711 mm with a collective area very close to that of Solidworks Flow Simulation outlets. In the ADINA simulation, for better visual of the mixture of gas and air, the outlets have an axial extension of 10 mm. The centers of these outlets have the respective coordinates (16, 16), (-16, 16),(-16, -16), (16, -16), and (0, 0) in mm. Finally, in order to further validate the simulation results, we also employ an equivalent two-dimensional axisymmetric flow model with comparable volume flow rates for gas and air inlets and mixture outlet as depicted in Figure 7. The mesh densities around both internal and external walls of the gas inlet are slightly higher than the interiors. Furthermore, at the tip of the gas inlet, a z-cut plane at z = -0.12 m, very much visible in Figure 7, a refined mesh density is employed to resolve the jet turning and mixing issues around the gas inlet tip within the burner. In this two-dimensional axisymmetric flow model, the total air and gas volume flow rates are maintained to be the same as in the comparable three-dimensional model. Thus, the velocity, turbulent kinetic energy, and turbulent dissipation rate to the gas inlet stay the same, whereas the velocity u, turbulent kinetic energy k, and turbulent dissipation rate ϵ as boundary and initial conditions for the air inlet, which has an annulus shape between the radius 0.02 m and 0.04 m, are modified as follows:

$$u = \frac{2\pi d_{ia}^2 u_{ia}}{4\pi (0.04^2 - 0.02^2)} = 3.6841 \text{ m/sec},$$



where d_{ia} and u_{ia} represent the diameter and the average flow velocity of the air inlet in the three-dimensional ADINA simulation model, in this case 2 mm and 22.105 m/s, respectively.

Figure 7. Mesh details for two-dimensional ADINA axisymmetric turbulent flow model with heat transfer and mass transfer.

Hence, we have the new Reynolds number for the air inlet Re = 0.02u/v = 4978.6, we select the turbulent intensity k_i for this smooth inlet pipe with a straight axis as 0.02429, which is virtually an average of two approximations, namely, $k_i = 0.055Re^{-0.0407}$ and $k_i = 0.0227Re^{-0.1}$. Thus, the turbulent kinetic energy k of the center inlet with the diameter $d_{ia} = 0.02$ m and the inlet velocity u = 3.6841 m/s is estimated as

$$k = 1.5(k_i u)^2 = 0.012014 \text{ m}^2/\text{s}^2$$
,

and the rate of energy dissipation ϵ is estimated as

$$\epsilon = \frac{k^{3/2}}{0.3 \times 0.02} = 0.21947 \,\mathrm{m}^2/\mathrm{s}^3.$$

With these sets of turbulent approximations, it is easy to verify that as the inlet flow velocity approaches zero, which corresponds to a low Reynolds number, both turbulent kinetic energy and turbulent dissipation rate will approach zero, which matches with the physical understanding of the nature of turbulence. With respect to the outlet, all five circular outlets with a diameter of 7.071 mm are merged into one single annulus outlet between a radius 0.02 m and 0.04 m, which will produce the same outlet cross-sectional area as five outlets in three-dimensional ADINA simulation and seven or ten outlets in threedimensional Solidworks Flow Simulation. The advantages of adopting a two-dimensional axisymmetric flow model, as depicted in Figures 7 and 8, with comparable heat transfer and mass transfer conditions are the speed and efficiency of computation, which provide us with more detailed evaluations of different design options and operation conditions. To reiterate, as presented in this paper, the balancing ratio of molecular weights of gas and air is 5.53%, which is very close to the operation conditions provided by CCT company. In all flow rates for gas and air, balancing ratios calculated with thermodynamics principles and comparable with input parameters given by CCT company are employed for all ADINA and Solidworks Flow Simulation models [12].



Figure 8. ADINA modeling results for two-dimensional axisymmetric turbulent flow model with heat transfer and mass transfer.

4. Simulation Results and Further Discussions

In ADINA three-dimensional turbulent modeling with heat transfer and mass transfer, as confirmed in Figures 9 and 10, after 25 time steps with the time step size $\Delta t = 0.01$ s, the turbulent flow is fully developed and has reached the steady solution. In fact, assuming the density difference is ignored, the exit flow cross-sectional area A is computed as 6.63746×10^{-3} m², by combining with the average axial flow velocity $u_0 = 2.04263$ m/s, we clearly reproduced the total volume flow rate which is close to that of the inlets, namely, $50 + 1.5 = 51.5 \text{ m}^3/\text{h}$. The final exit volume flow rate is around 48.809 m³/h, with an appreciable amount of volume difference, which is expected due to the introduction of the methane at the colder temperature, as shown in Table 2, and the fact that the gas is much more compressible than water as a fluid. Moreover, the average turbulent kinetic energy and turbulent dissipation rate at the z-cut surface with z = -0.5 m which is very near the exit of the gas burner are $8.2769 \times 10^{-2} \text{ m}^2/\text{s}^2$ and $3.6249 \text{ m}^2/\text{s}^3$, respectively. In comparison with the initial and entrance turbulent conditions of air and gas inlets, much of the turbulent kinetic energy is dissipated in the mixing process. as a result, as one of the good mixing indicators, both turbulent kinetic energy and dissipation rate are greatly reduced at the exit of the gas burner. Of course, the temperature distribution depicted in Figure 9 also reflects the physical reality that is a relatively warm air stream with the surrounding temperature, which is assumed to be 20 °C, will elevate the relatively cool temperature of the gas (methane) which is assumed to be 15 °C. In addition, in comparison with the outlet with smaller holes as shown in Figure 8, the pressure within the burner without smaller holes in its outlet, as shown in Figure 9, tends to be much smaller and close to the atmospheric pressure. Furthermore, the averaged concentration of the gas (methane) and the corresponding relative standard deviation as defined in Equation (17) near the

exit are calculated as 1.22833×10^{-3} and 0.0532303, respectively. Although the average concentration of the gas does not provide any realistic sense due to the key assumption of this CFD turbulent simulation with heat transfer and mass transfer, which is the same mean density assumption, as shown in Figure 9, the small relative standard deviation suggests that the newly proposed concentric gas burner does provide enough space for mixing before ignition and combustion. This conclusion is also verified with the so-called variance and standard deviation, in this case, 4.27508×10^{-9} and 6.53841×10^{-5} . Finally, the appreciable difference between the volume flow rates at the inlets and outlets also suggests that as we continue to increase the operation flow rates, we must consider the full-fledged compressible aerodynamics within the gas burner, which will be a different subject for a completely new research direction.



Figure 9. ADINA modeling results for three-dimensional turbulent flow model with heat transfer and mass transfer.



Figure 10. Average velocity at the flow exit around 0.5 m from the inlets in ADINA modeling as a function of time.

As previously stated, we used a concentric model in order to achieve a concentric turbulent mixing of gas and air in which a gas injector is inserted into a gas burner, and air injectors are located above and below a gas injector. We used Solidworks Flow Simulation software to study the design model as depicted in Figure 6, and to simulate velocity and volume fraction of gas and air in order to observe the turbulent mixing of gas and air. Similar boundary conditions were set for gas and air inlets, the wall, and for the gas burner's outlets. First, we examined the velocity distribution, which is an important factor in observing a turbulent mixing. We wanted to examine gas and air flows, and observe how they interact with each other. However, the simulation as showed in Figure 11 includes a swirling of air in the area where air enters the gas burner, which is an undesirable effect. It means that the air does not flow into the burner continuously, and is swirled before it mixes with gas. Gas flows into the burner at a different velocity and flow rate and causes the air to swirl. The swirling would be more effective in the region where gas and air interact with each other. In order to prevent the air swirling before it mixes with the gas, we have altered the design of the gas burner. We have a diffuser-like expansion to provide more mixing space for air and gas mixture. Additionally shown in Figure 11, in this improved model on the right, the air does not swirl in the region where the gas enters the burner. Instead, the expansion enhanced the turbulent mixing through the gas burner. In addition, for the three-dimensional Solidworks Flow Simulation model, we also analyzed the velocity at the burner's outlet. According to Ref. [27], the velocity at the gas burner's outlet for the gas burners with low combustion speed should be less than 40 m/s. As depicted in Figure 12, we obtained the converged velocity at outlets after sufficient number of iterations as the air and gas flow through the gas burner with 10 circular openings each of which has a 5 mm diameter or 7 circular openings each of which has a 6 mm in diameter. In general, these small openings tend to increase the pressure of the incoming mixed fluid, and therefore, the exit velocity. As shown in Figure 12, the exit velocity at the outlet with ten 5 mm diameter circular openings exceeds 50 m/s which is beyond the maximum velocity required for this type of gas burners [27]. By altering the outlet with seven 6 mm diameter circular openings, Solidworks Flow Simulation also confirms that the velocity of the air and gas mixture drops below 40 m/s, as shown in Figure 12, which satisfies the required design limit for this type of gas burners. The Solidworks Flow Simulation results also allow us to study the volume fraction of gas and air. As expected, the volume fraction of air is very much dominant through the gas burner as demonstrated in Figures 9 and 13. On the other hand, the volume fraction of gas decreases as the air and gas flow through the gas burner, which suggests further mixing. Finally, combustion occurs only during specific volume fraction ranges of gas and air. Furthermore, the combustion propagates when the gas and air mixture contains $5\sim15\%$ of gas [28]. Figure 14 shows the volume fraction of air and gas, respectively. The volume fraction of air at the gas burner's outlet converges to the value of 0.95, whereas the volume fraction of gas converges to the value of 0.05, as depicted in Figure 14. The volume fraction of gas 0.05 does represent 5% of gas in the gas and air mixture at the burner's outlet which is sufficient to start combustion [28].



Figure 11. Gas and air velocity profiles in Solidworks Flow Simulation.



Figure 12. Velocity distributions with 7 openings each of which has a diameter of 6 mm (**b**) and 10 openings each of which has a diameter of 5 mm (**a**) in Solidworks Flow Simulation.



Figure 13. Volume fraction spatial distributions of gas and air in Solidworks Flow Simulation.



Figure 14. Volume fraction of air, converging to 0.95 (**left**) and volume fraction of methane, converging to 0.05 (**right**) in Solidworks Flow Simulation.

5. Conclusions

In this paper, we demonstrated that the combustion within the burner can be improved using thermodynamics and computational fluid dynamics (CFD). It is important to correctly set up input parameters such as mass flow rate, pressure, turbulent kinetic energy, turbulent dissipation rate, and temperature. Additionally, the selection of mass flow ratio has to be based on the thermodynamic principles with a specific molecular weight ratio for a complete combustion in order to achieve a high efficiency of burning. Our calculations also confirmed that the initial input parameters used in an actual industrial gas burner analyzed in this work could be further optimized, and the gas burner design itself could be improved. In order to obtain balanced ratios in the gas burner, it is very important that gas and air are fully mixed before the combustion, which will take place at the outlets. For a high combustion efficiency, swirling and other turbulent mixing behaviors of fluid flows must occur in the region with no stationary circulation zones. In the concentric model that we propose in this paper, air mixes with gas immediately near the entrances and inlets. The mixture spatial uniformity measured by the variance and standard deviation over the cross-sectional area near the outlet has confirmed the improvements. Additionally, the measured volume fraction of gas (0.05) and air (0.95) at the gas burner's outlet will be sufficient to start and to propagate combustion. The velocity at the gas burner's outlet, with seven 6 mm diameter circular openings is within 40 m/s required for the category of gas burners suitable for the production of magnesia clinker [27]. We believe that the improved design of a gas burner as well as proper selections of operation conditions, such as volume flow rates based on CFD simulations and thermodynamic principles, will finally help to identify suitable input parameters for individual gas burners and solve the problem with an excessive amount of carbon monoxide (*CO*) in flue gases.

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Nomenclature

ν	fluid kinematic viscosity in m ² /s;
β	fluid bulk modulus in kPa;
с	sound speed within fluid, gas or air, in m/s;
ν_t	turbulent eddy viscosity in m ² /s;
k	turbulent kinetic energy in m^2/s^2 ;
ϵ	turbulent dissipation rate in m^2/s^3 ;
D	mass diffusivity in m^2/s ;
k	thermal conductivity in W/mK;
ρ	fluid, gas or air, density in kg/m ³ ;
C _p	specific heat for constant pressure in kJ/kgK;
c_v	specific heat for constant volume in kJ/kgK;
γ	heat capacity ratio defined as $\frac{c_p}{c_{v_i}}$;
α	thermal diffusivity defined as $\frac{k}{\rho c_p}$ in m ² /s;
С	time-average concentration of a chemical species;
Ē	spatial arithmetic mean concentration of a chemical species;
$\bar{\sigma}_c$	spatial concentration standard deviation of a chemical species;
$\bar{\sigma}_{cu}$	flow concentration standard deviation of a chemical species;
Ī	turbulent time scale in s;
Va	air volume flow rate in m^3/s or m^3/h ;
\dot{V}_{g}	gas volume flow rate in m^3/s or m^3/h ;
v_i	time-average fluid flow velocity in direction x_i in m/s;
u _o	velocity of a mixture in a burner's outlet in m/s;

Α	cross-sectional area of inlet for gas or air in m ² ;
u_{ig}	velocity of an inlet for gas in a burner in m/s;
u_{ia}	velocity of an inlet for air in a burner in m/s ;
d_{ig}	size of a burner gas inlet diameter in m;
d_{ia}	size of a burner air inlet diameter in m;
k_i	turbulent intensity k_i ;
v_g	specific volume for gas in m ³ /kg;
v_a	specific volume for air in m ³ /kg;
$ ho_g$	density for gas in kg/m ³ ;
$ ho_a$	density for air in kg/m^3 ;
p_g	total pressure for gas in kPa;
pa	total pressure for air in kPa;
p_o	ambient pressure in kPa;
T_a	air temperature in K;
T_g	gas temperature in K;
Т	time-averaged temperature in K;
R_a	gas constant for air in kJ/kgK;
R_g	gas constant for methane in kJ/kgK;
Re	Reynolds number of gas or air defined as $\frac{ud}{v}$;
Sc	Schmidt number of gas or air defined as $\frac{v}{D}$;
Pr	Prandtl number of gas or air defined as $\frac{v}{\alpha}$;
Q_s	heat generated from a reaction in J/m^3 ;
Ż	rate of heat based on volume flow rate in MJ/h;
q_s	rate of heat generated from a reaction in a unit volume in W/m^3 ;
Qсо	rate of heat generated for the burning of carbon monoxide (CO) in MJ/s;
Qco	heat generated for the burning of carbon monoxide (CO) in MJ/m^3 ;
CO (ppm)	carbon monoxide (CO) measured in flue gases in parts per million (ppm);
e _{ij}	velocity strain tensor $\frac{1}{2}(\frac{\partial v_i}{\partial x_i} + \frac{\partial v_j}{\partial x_i})$ in 1/s;
Φ	inner product of velocity strain tensor $2e_{ij}e_{ij}$ in $1/s^2$;
r	reaction rate at specific pressure in mm/s; and
h _c	convective heat transfer coefficient in W/m^2K .

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