



CFD SIMULATION OF REACTIVE FLOW IN COUNTER FLOW SHAFT KILNS USING POROUS MEDIA MODEL

Kamyar Mohammadpour* Ali Chitsazan, Eckehard Specht

Institute of Fluid Dynamics and Thermodynamics, Otto von Guericke University, Magdeburg, Germany

ABSTRACT

The length of flame and behavior of the flame and homogenization in temperature distribution play the main roles to obtain a better quality of lime. Performing experiments in a real lime shaft kiln plant are quite complicated. A lime shaft kiln normally has a large geometry, including a height of 15 meters and a diameter of 3 meters, and is filled with large stones moving in a vertical direction. In most cases, the measuring instruments are damaged. Due to these difficulties, modeling of physical and chemical processes is required for having a better understanding of the process and optimizing the parameters. The current study attempts to demonstrate the viability of using computational fluid dynamics (CFD) as a design tool for such packed beds by visualizing the flow structure in the reacting zone. The porous media model (PMM) introduced as a method of simulations of Counter Flow Single (CFS) shaft kilns. The simulation result validates by experiment-packed bed measurements. The main objective of this research study is to illustrate the key parameters affecting the flame length such as the kiln diameter, number of burners and particle diameter in counter flow shaft kilns. Results showed that when the kiln diameter increased from 1m up to 4m, the flame length is decreased by about 0.8m. When the number of burners is increased by three times, the flame length is decreased by about 0.8m. When the particle diameter increased from 20mm up to 150mm (by approximately seven times), the flame length increased by about 0.8m.

Keywords: *Counter Flow Shaft kiln, Porous Media Model, Flame Length, Kiln Diameter, Number of Burners, Particle Size*

1. INTRODUCTION

Radial cross-flow injection in Kiln has been in considerable studies for the last many years. Although many conclusions have been reported and all capable contributions were taken into account for a better understanding of the phenomena. There are still very few studies carried out in the field of chemical and thermal industrial applications. The evaluation of the parameters of mixing such as the mixture fraction and the equilibrium mixture fraction is done accurately taking into consideration the mixing conditions details (Tao et al., 2002; Nield and Bejan, 2005). A more flourishing aspect related to big-scale industrial problems was analyzed (Salari et al., 2008)

Reactors with Packed bed type with jet injections are extensively used in various industrial applications, such as counter flow single (CFS) shaft kilns and parallel regenerative flow (PFR) shaft kilns. The uniform distribution of fuel gas determines the quality of final products from Kiln (Dixon and Nijemeisland, 2001). Several parameters on an industrial scale in kilns are involved in direct impact on design such as: Jet injection, types of jet, number of jets, Momentum flux ratio and penetration depth, kiln diameter, the volumetric flow ratio of flue gas, various other factors which were not experimentally viable to calculate (Smith and Ranade, 2003). In the modern era of technology, Computational fluid dynamics (CFD) emerges as a vital tool for synchronizing the big scale problems. It allows researchers and scientist to after math predict and design the desired fluid dynamics in geometrically complicated equipment such as packed reactors (Muppidi and Krishnan, 2006).

The CFD simulations of the structure of the shaft kiln with jet injections are done in experimental sample scales. There are two different

types of models referred to by the term CFD simulation in the field of packed-bed modeling (Salari et al., 2007; Smith and Ranade, 2003). Mainly all processes inside the Kiln in porous particles are fractionated into two as represented by source or sink terms in the conservation equations and are corrected for volume fraction and particle transport limitations (Xu, 2009; Xu et al., 2005). In the current study, the bed is treated as an effective porous medium (Nield and Bejan, 2005). The mathematics simulation model of limestone calcination in shaft kilns shows reasonable accuracy (Krause et al., 2017) with measurements. The fuel gas is introduced at the upper side of the burning zone, where the material can absorb most of the heat released by combustion (Hallak, 2016).

The effect of the particle diameter and the operation process on the gas temperature distribution is done by Matlab program code. The influence of the fuel type on the calcination process is accurately outlined on the ground of industrial measurements (HaiDo et al., 2011).

This model is widely used in chemical reactors and shaft kilns consisting of a solid catalyst and a packed column filled with solid particles to achieve a large interfacial area. The temperature homogenization of reactive and non-reactive flows after radial jet injections in a confined cross-flow is done in a packed bed (Nirmolo, 2007; Nirmolo et al., 2008).

The results of the CFD porous media model and experiment measurement in parallel injection flow in packed bed compared as well. The results show more accuracy between CFD and experiment data when the suitable turbulence model and percent of turbulence intensity are chosen (Mohammadpour et al., 2017). The comparison between the discrete particle model and porous media model shows the best fitting between two CFD models and experiment results (Alkhalaf and Specht, 2017; Alkhalaf et al., 2018).

* Corresponding author. Email: kamyar_m.pour@yahoo.de

The simulations of counter flow shaft kilns (CFS) ($H=8\text{m}$, $D=2\text{-}4\text{m}$) are almost not possible by the Discrete Particle Model (DPM). Hence, a new CFD simulation method would be more valuable. The porous media model includes a less number of nodes and it requires shorter computational times when compared to the Discrete Particle Model (DPM). The CFD consideration of cross-flow mixing in the structured packed bed and validation shows the porous media model decreases the number of nodes and computational time (Mohammadpour, 2019).

The length of flame and behavior of the flame and homogenization in temperature distribution play the main roles to obtain a better quality of lime. The combustion behavior is influenced by various parameters such as particle diameter, the velocity of fuel, air-fuel ratio, lance diameter, air velocity, and the number of burners. Performing experiments in a real lime shaft kiln plant are quite complicated. A lime shaft kiln normally has a large geometry, including a height of 15 meters and a diameter of 3 meters, and is filled with large stones moving in a vertical direction. In most cases, the measuring instruments are damaged. Due to these difficulties, modeling of physical and chemical processes is required for having a better understanding of the process and optimizing the parameters. The simulation techniques using Computational Fluid Dynamics (CFD) modeling are particularly beneficial for systems such as shaft kilns. CFD models are increasingly used in the field of combustion, especially for simulating a non-premixed diffusion flame within lime shaft kilns. Hence, the packed bed has to be approximated as a porous medium to model the reactive flow in the kilns. Before that, experimental validation is conducted in the Institute of Fluid Dynamics and Thermodynamics, Otto von Guericke University, Magdeburg, Germany utilizing a section of a packed bed. The scope of this research is to investigate the influence of kiln diameter, number of burners and particle diameter on the flame length in counter flow shaft kilns using a porous media model. The simulation results deliver new information about the processes inside the kiln not available so far. For example, the simulation provides detailed and spatially resolved data like gas velocity, temperature, fuel distribution in various heights and direction. The results of this research can have considerable significance in improving reactor design and combustion process optimization.

2. OPERATING PRINCIPLE OF A CFS-KILN

Figure 1 depicts a counter flow single lime shaft kiln (CFS) used to produce lime from limestone (Niold and Bejan, 2005; Krause et al., 2017). A single shaft kiln is a vertical shaft where limestone is charged at the top of the kiln and quicklime is discharged at the bottom. To calcine the limestone, the heat is generated by fuel combustion where fuel is introduced with air using burner lance systems radially from outside at different heights in the kiln. Additionally, the air is blown at the discharge of the kiln to cool the product in a counter-current manner. The limestone is preheated by the combustion gases in a counter-current mode to about 800 C before it reaches the burning zone. In this zone, the limestone is heated to a temperature between 900 C and 1500 C, which is sufficiently high to liberate carbon dioxide (CO_2) and obtain the derived lime.

In CFS kilns, the fuel jet must burn in the vertical direction. As a consequence, the required thermal energy was introduced through radially-arranged burners situated at one or more burner levels. Fuel and combustion air was distributed evenly throughout the CFS kiln using a defined number of burners arranged at the burner levels. The CFS kiln considered here has a total height of 10 m and a diameter of 2 m. The fuel which is used is natural gas. The specific energy consumption is $E=3.8 \text{ MJ/kg}_{\text{lime}}$. The specific kiln throughput is 200 t/d.

The kiln's specific fuel input was calculated by Eq. (1) when the fuel lower heating value was $37,000 \text{ kJ/m}^3_{\text{fuel}}$ and heat consumption value was $3800 \text{ kJ/kg}_{\text{lime}}$:

$$ECFS=(\text{Heat Consumption})/(\text{Lower Heating Value})=0.1 \quad (1)$$

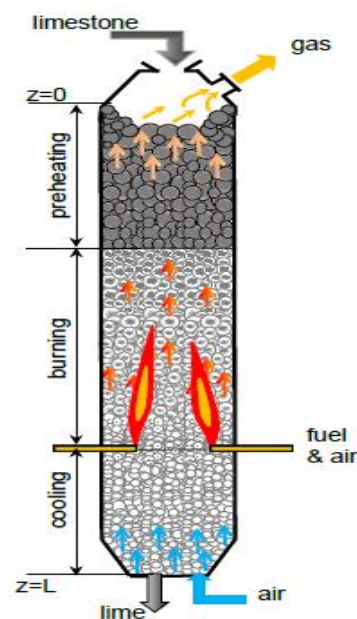


Figure 1: Schematic of Counter Flow Single lime Shaft Kiln (CFS)

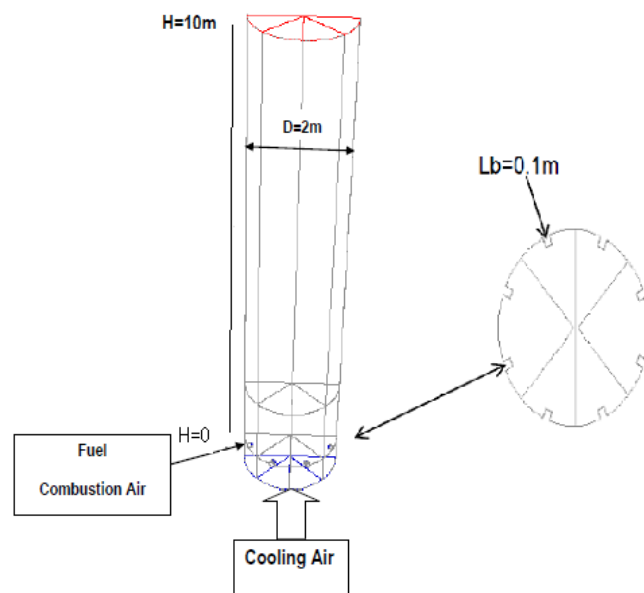


Figure 2: Structure and dimension of CFS kiln and injections

The fuel flow rate was calculated using Eq. (2) when the lime mass flow rate was 200 tons per day.

$$\dot{V}_{\text{Fuel}} = ECFS \dot{M}_{\text{lime}} = 0.1 \times 200 = 0.24 \text{ m}^3 / \text{s} \quad (2)$$

The fuel velocity depends on the burner diameter and the number of burners. The fuel velocity was calculated using Eq. (3).

$$\dot{V}_{\text{Fuel}} = \frac{n\pi}{4} d^2 U_f = \frac{8 \times 3.14}{4} \times 0.0025 U_f = 0.24 \rightarrow U_f = 15.28 \text{ m/s} \quad (3)$$

The amount of air was calculated using Eq. (4) as shown below:

$$\dot{V}_{air} = \lambda \dot{V}_{fuel} = 1.3 \times 9.5 \times 0.24 = 2.964 \text{ m}^3/\text{s} \quad (4)$$

The amount of cooling air depends on the mass flow of lime and is calculated using Eq. (5).

$$\dot{M}_{air} C_{p,air} = \dot{M}_{lime} C_{p,lime} \quad (5)$$

$$\dot{M}_{cooling\ air} = \frac{C_{p,lime}}{C_{p,air}} \dot{M}_{lime} = 1.8 \times \frac{0.9}{1.15} = 1.4 \text{ m}^3/\text{s} \quad (6)$$

Therefore, the minimum value of cooling air is always 1.4 m³/s and the rest value from 3 m³/s is 1.6 m³/s. This amount of air was injected from combustion air burners. The dimensions and specification details of radial flow injection are summarized in Table 1.

Table 1: Specification and details of injections and flow.

Fuel volume flow	Fuel velocity	Air Volume flow total	Combustion Air volume flow Maximum	Cooling Air Volume flow Minimum
\dot{V}_{Fuel}	U_{Fuel}	\dot{V}_{air}	\dot{V}_j	$\dot{V}_m = \dot{V}_{Cooling\ air}$
$\frac{\text{m}^3}{\text{s}}$	$\frac{\text{m}}{\text{s}}$	$\frac{\text{m}^3}{\text{s}}$	$\frac{\text{m}^3}{\text{s}}$	$\frac{\text{m}^3}{\text{s}}$
0.24	15.2	3	1.6	1.4

3. SIMULATION METHOD

3.1 Porous Media Model (PMM)

The porous medium is a body composed of a solid matrix and a void space that can be filled with one or more fluids. In a multiphase system, the void space is filled by two or more fluids that are immiscible with each other. A distinct boundary is maintained between them, which provides the derivation of mathematical methods for fluid flow in porous media. Additionally, some assumptions, as well as restrictions, are placed upon the geometry of the porous medium. An assumption is required in the framework of the volume fraction concept. It refers to the porous solid, which models a controlled space. The pores there are filled with a gas or a liquid. Moreover, it is also assumed that all pores are statistically distributed (Nield and Bejan, 2005).

3.2 Using the Ergun equation for a Packed Bed

Considering the modeling of a packed bed, the appropriate constants can be derived by using the Ergun equation. It provides to obtain a semi-empirical correlation applied for many kinds of packing:

$$\frac{\Delta P}{L} = 150 \cdot \frac{(1 - \phi)^2}{\phi^3} \cdot \frac{\mu \cdot U}{d_p^2} + 1.75 \cdot \frac{1 - \phi}{\phi^3} \cdot \frac{\rho \cdot U^2}{d_p} \quad (7)$$

$$= \frac{1}{\alpha} \cdot \frac{\mu U}{d_p^2} + \frac{1}{2 \cdot c_2} \cdot \frac{\rho U^2}{d_p}$$

Where d_p [mm] is the mean particle diameter, ϕ [-] is the porosity, μ [Kg/(m.s)] is the viscosity and U [m/s] is the velocity. The permeability and inertial loss coefficient in each component direction can be identified as:

$$\alpha = \frac{d_p^2 \times \phi^3}{150 \times (1 - \phi)^2} \quad C_2 = \frac{3.5 \times (1 - \phi)}{d_p \times \phi^3} \quad (8)$$

As seen from Equation (7), both coefficients are determined by the pack bed geometry and the particle diameter (Xu, 2009; Nield and Bejan, 2005).

3.3 CFD Model Description

The combustion air and fuel enter the burning zone with uniform velocity and temperature. The combustion in shaft kilns is non-premixed. The non-premixed model is based on the Probability Density Function (PDF). The PDF method is used for fast turbulent mixing processes with the finite rate formulation. In lime shaft kilns, the chemical kinetics are rapid so that the flow is near chemical equilibrium. Methane is used as fuel to provide heat for calcination. The two-step methane/air combustion model was applied. All the computational work was carried out using the commercial software ANSYS Fluent 14. The fluent solver uses a finite volume procedure, which converts the governing differential equation presented into algebraic form, together with the SIMPLE (Semi Implicit Method for Pressure Linked Equations) algorithm to solve these equations numerically. The discretization algorithm is standard for pressure, and the first-order upwind for momentum, the SIMPLE scheme, has been employed for pressure-velocity coupling. All the convergence criteria are set to below 10⁻³.

Mesh generation is an important part of the CFD approach, particularly for complex geometries such as packed beds. The accuracy of the simulation is strongly affected by the mesh structure. Therefore, the mesh study has been performed to find a proper mesh density that balances between fines enough grids for acceptable accuracy and computing time. The tetrahedral prism layer mesh and number of nodes with 0.33 million was applied. To reach more accuracy, the wall function less than 30 with 1.5 million cells was applied. (see Table 2).

Table 2: CFS Kiln Structure and Mesh Generation



In Figure 3 a discussion about mesh independent study for the flame in packed bed is presented. It shows the length of flame related to the cell number. It can be seen that the mesh number varied from 50000 to around 1900, 000, where the coarse mesh is associated with a large variation on

the length of the flame. Moreover, the figure demonstrates that, increasing mesh more than 1,500,000 cells lead to a relative constant in the length of the flame. Consequently, to minimize the computational time and an optimum number of cells with high accuracy, the mesh with 1,500,000 cells has been selected to carry out all the cases of non-premixed simulation of CFS shaft kiln.

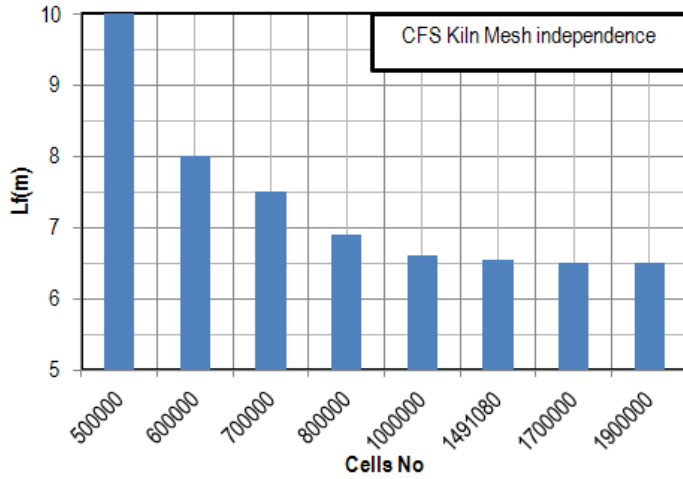


Figure 3: Mesh independence study for the length of the flame

4. EXPERIMENT VALIDATION

The CFD Turbulence model is valid by experiment packed bed measurement. In this case, nitrogen was injected from bundles to the experiment-packed bed at a pressure of 7 bars. The flow rate was fixed at 25 m³/hr for all the cases. The pressure was adjusted by a ball valve, and the flow rate was adjusted using a rotameter. After that, the air was injected from a blower into a packed bed through air holes. The experiment measurement was performed for volume ratio $V_j/V_m=0.1$ (Mohammadpour et al., 2017; Alkhalaf et al., 2018). When the exact flow rate of air and nitrogen was supplied, the mole fraction of O₂ was measured with the help of a gas analyzer. The height of measurement was 459 mm from the bottom and it had 104, 208, 312, 416, and 520 mm distance from walls (5 points) (Figure 4).

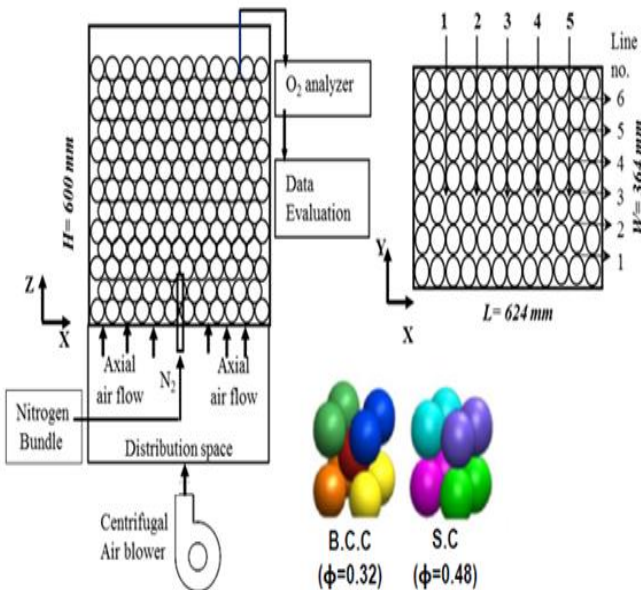


Figure 4: Schematic of the experiment packed bed measurement

The contours of oxygen are shown in Figure 5. In this case, different types of turbulence models were simulated when the porosity was $\phi=0.32$. As shown in Figure 6, the SST K- ω shows more accuracy with the experiment result.

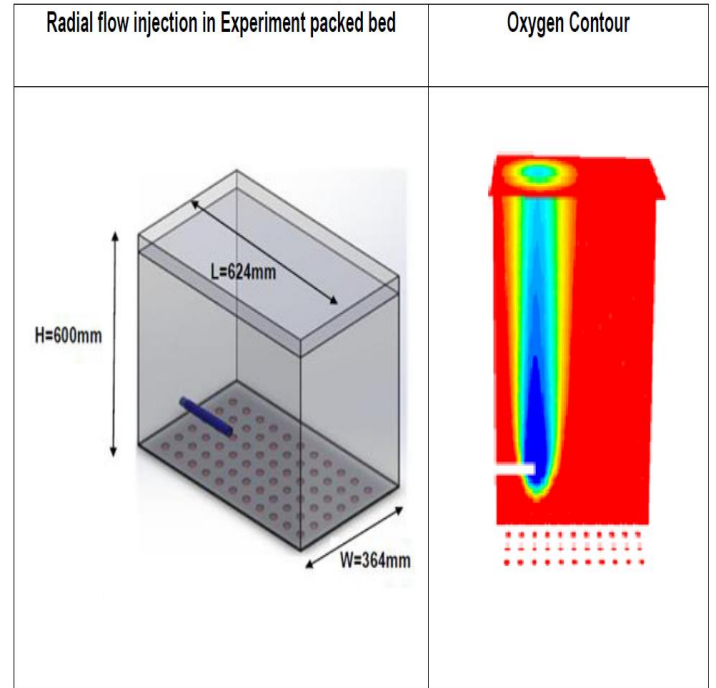


Figure 5: Packed bed dimension and contour of oxygen

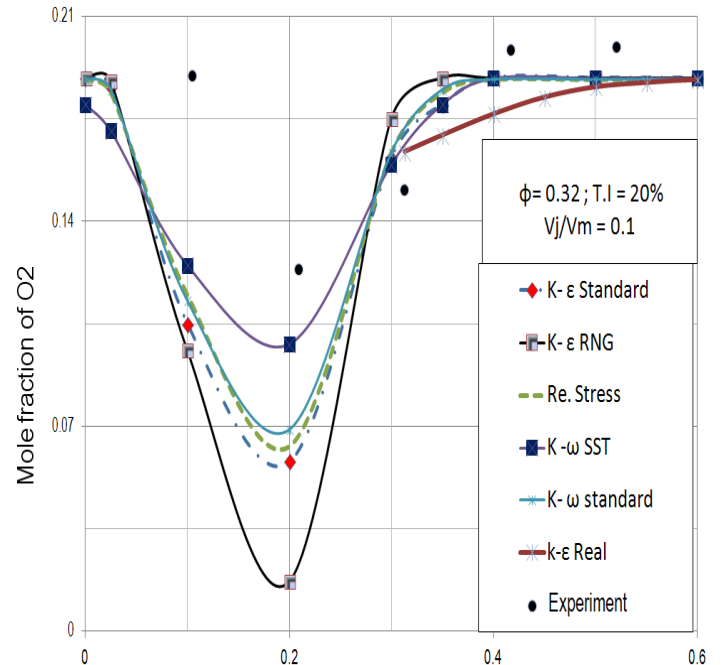


Figure 6: Conclusion of simulation and Experiment validation

The CFD simulation introduced the PMM method. Thus, the PMM method can be used as a CFD simulation model for CFS shaft kilns. As mentioned in the introduction, the advantage of PMM is that it can be used in the simulation of kilns with real a dimension of about 10 m in height without limitation in the number of nodes and computational times.

5. RESULTS AND DISCUSSIONS

5.1 Definition of Flame Length (L_f)

As it's shown in Figure 7, Methane is reduced to zero at a distance of about 4 m from burners, while CO reaches zero at a distance of approximately 6 m. The flame length is the position where the CO fraction has fallen to zero. This is shown in Figure 8.

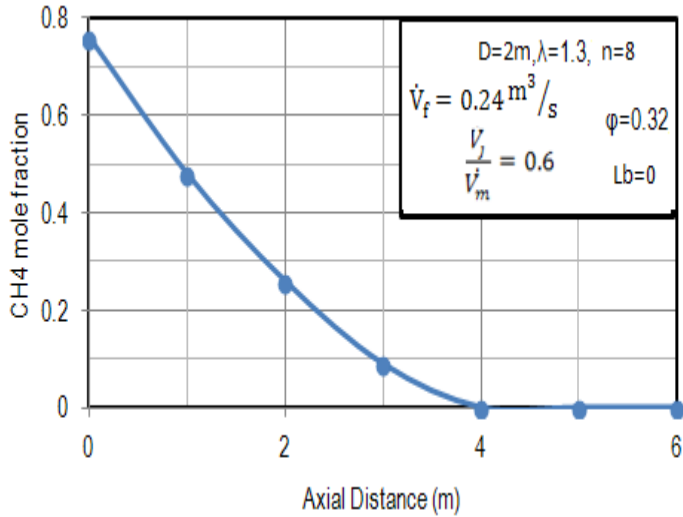


Figure 7: Axial CH4 profile

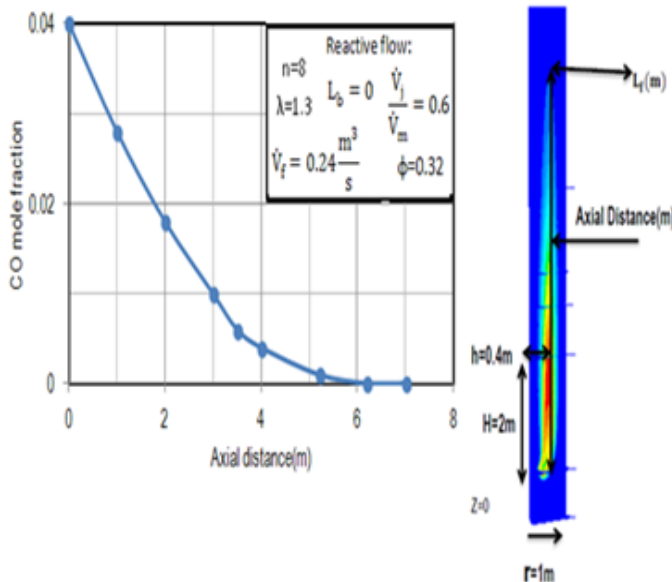


Figure 8: Axial CO profile (definition of flame length)

Fuel profile is shown at different heights in Figure 9. The maximum value of fuel is always in the distance of 0.4 m from walls. The higher the distance from the burners is, the less the amount of the fuel would be.

Figure 10 shows the radial profile of the superficial velocity at different heights. At the position of the maximum temperature, the velocity has the highest value too. The longer the distance from the burner level is, the higher the velocity would be. At the radial distance of 0.25 m from the walls, the velocity drops continuously to the value of zero at the walls. The velocity profile after the distance of 2 m from burners shows the same trend. There is no major change in the velocity profile after 2 m distance from burners.

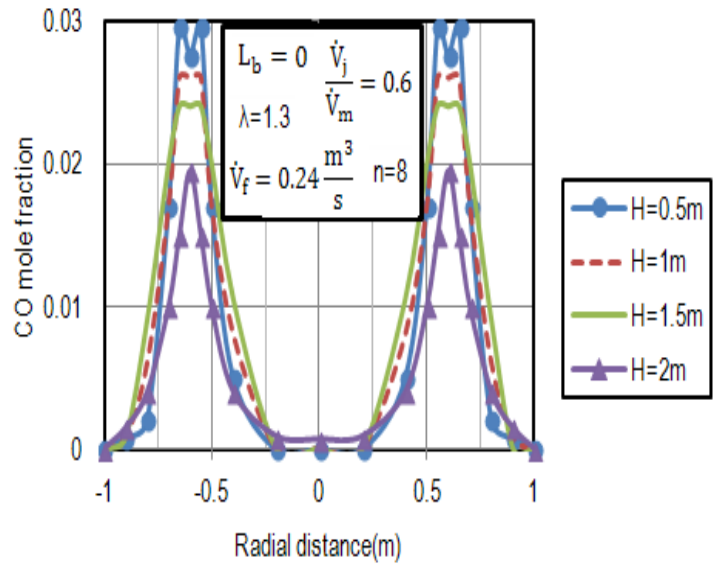


Figure 9: Fuel profile at different heights.

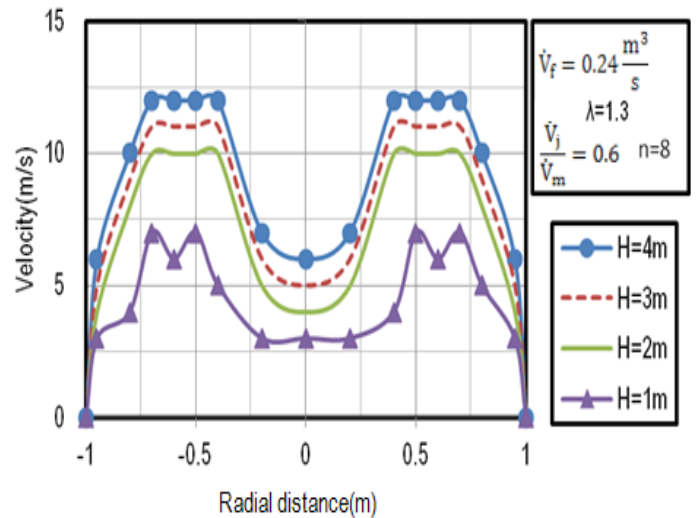


Figure 10: Velocity profile at different heights.

The mass flow rate is the product of velocity and density. The density and velocity profile is shown in Figure 11. The mass rate after 2 m is more even.

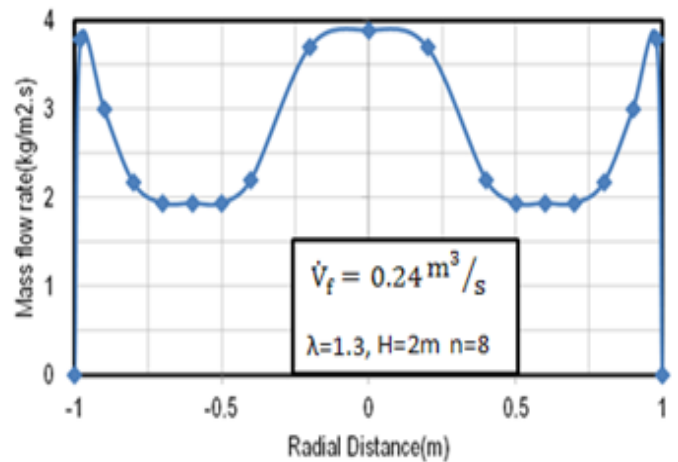


Figure 11: Mass flow rate in the radial direction when H=2 m.

The radial temperature profile is shown in Figure 12 at different heights. The penetration depth is 0.5 m from walls which are 0.4 m from burner depth. The maximum temperature is after the height of 3m from burners. The maximum temperature then decreases, and the temperature in the core and near walls increases. Homogenization starts after the height of 3 m from burners.

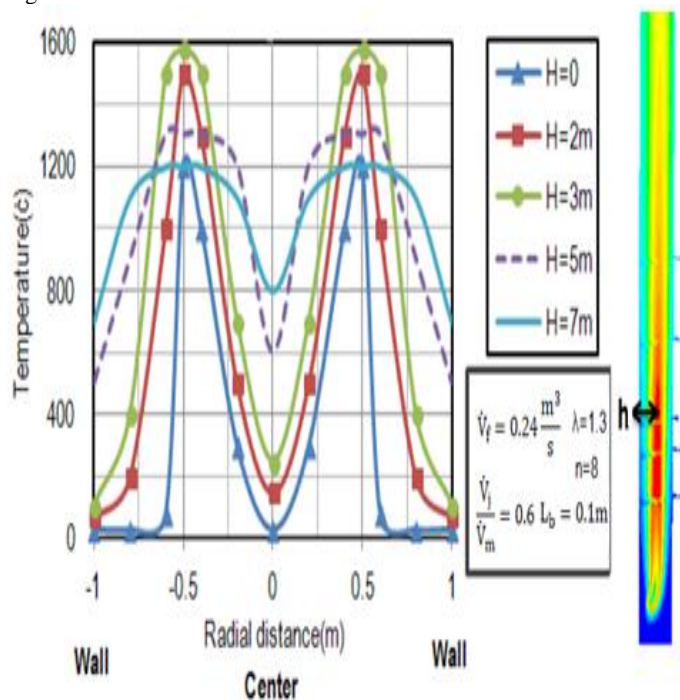


Figure 12: Temperature profile at different heights

The CO contours are shown at various heights and in the radial direction in Figure 13. The length of the flame is calculated in case the number of burners is $n=8$ and at about $L_f=6.5$ m.

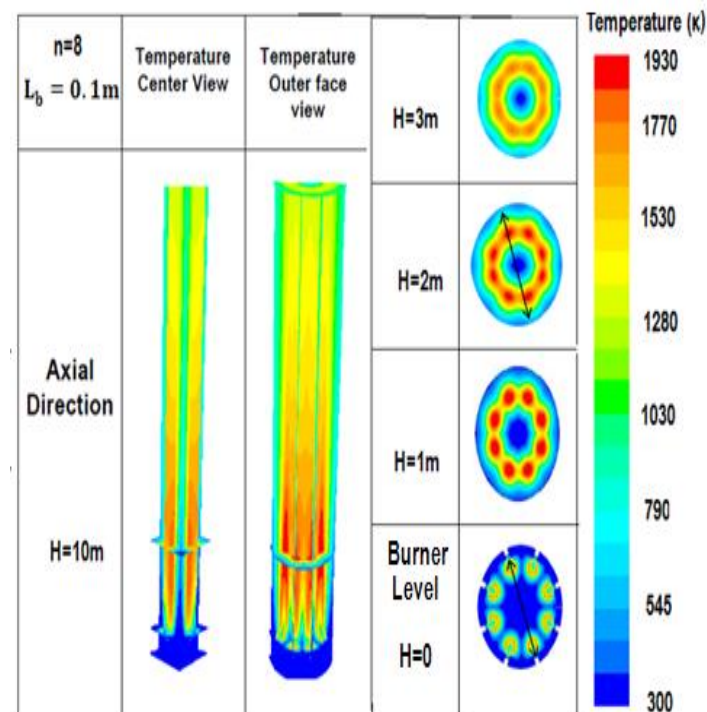


Figure13: Temperature contours in radial and axial directions.

It can be seen in Figure 13, the temperature in the core is minimum. However the temperature in circumferential distance relatively homogenous.

The CO contours are shown at various heights and in radial direction in Figure 14. The length of the flame is calculated in case the number of burners is $n=8$ and at about $L_f=6.5$ m.

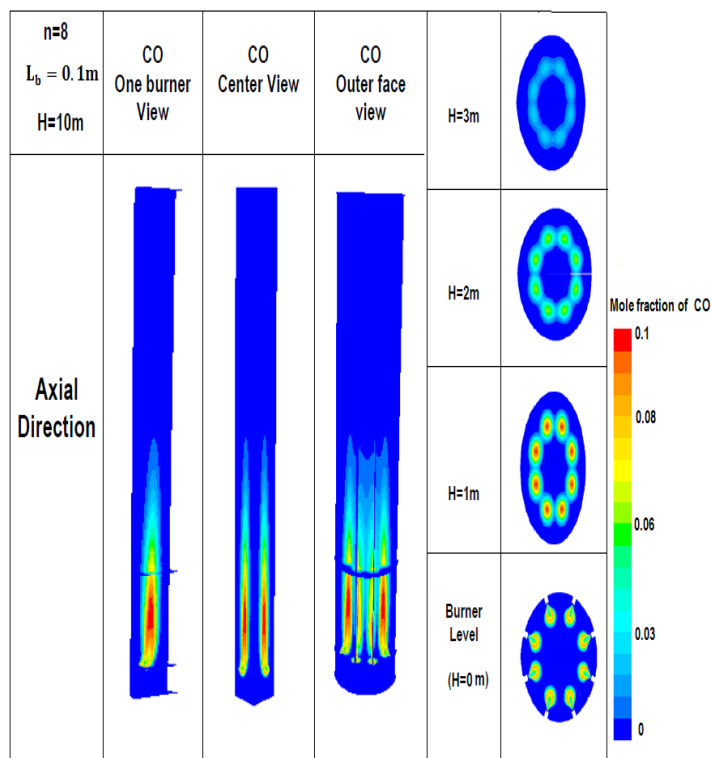


Figure 14: CO contours in different directions ($\frac{V_f}{V_m} = 0.6$).

5.2 Influence of Kiln Diameter on Flame Length

Table 3 shows the influence of the various kiln diameters ($D=1-4$ m) on the flame length. The mass flow of limestone fixed at 200 ton/day. For this aim, the fuel and air volume flows were kept constant. When the kiln diameter increased from 1m up to 4m, the flame length is decreased by about 0.8m.

Table 3: Influence of kiln diameter on flame length

$n=24$ $V_f=0.24\text{m}^3/\text{s}$	$D=1\text{m}$	$D=2\text{m}$	$D=4\text{m}$
$L_f(\text{m})$	6.1	5.7	5.3

5.3 Influence of Number of Burners on Flame Length

Next, the influence of several burners on the flame length will be discussed. For this aim, the fuel and air volume flow and burner diameter were kept constant. Less fuel injected from more number of burners covered more area in the radial direction. Hence, the higher the number of burners is, the shorter the flame would be. This causes better

homogenization in radial directions. As a consequence, when the number of burners is increased by three times, the flame length is decreased by about 0.8m. The calculation of the length of the flame is provided in Table 4.

Table 4: Influence of the number of the burner on length of the flame

$D=2m, \phi=0.32$	n	8	16	24
$d_f=50\text{ mm}$ $L_b = 0.1m$	$L_f(m)$	6.5	6	5.7

The CO contours in axial and radial directions are shown in Figures 15. The flame is shorter when 24 burners are used compared to 8 burners. However, the more the number of burners is, the deeper the penetration depth becomes. It can be seen that the CO distribution in the circumferential direction is relatively homogeneous after a 2m distance from the burners.

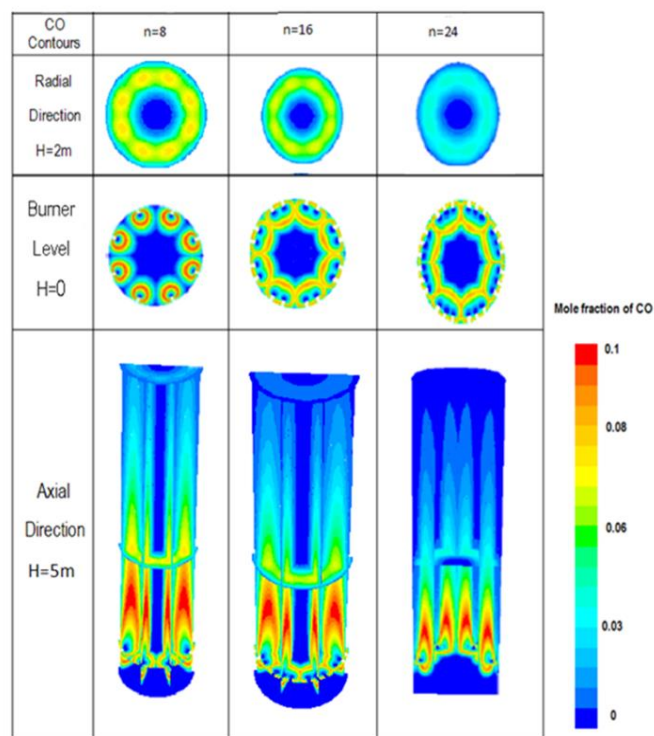


Figure 15: Influence of number of burners on the flame length

5.4 Influence of Particle Diameter on Flame Length

Table 6 shows the influence of particle diameters on the flame length. For this aim, all the other operating parameters were kept constant. It can be seen that bigger particle diameters lead to a longer flame length. When the particle diameter increased from 20mm up to 150mm (by approximately seven times), the flame length increased by about 0.8m.

Table 6: Influence of particle size on length of the flame.

n=8	$D_p=100mm$	$D_p=50mm$	$D_p=20mm$
$L_f(m)$	6.5	6.3	6.1

6. CONCLUSIONS

The current research study describes the development of a simulation approach for the reactive zone a CFS-Kiln. The simulation focus on the combustion gas flow field. In this case, the method of porous media model PMM introduced. The $k-\omega$ SST Turbulence model shows more accuracy with the experiment measurements. Therefore, the PMM replaced to discrete particle model (DPM). The PMM model simulation presented delivers new information about the processes inside the kiln not available so far. For example, the simulation provides detailed and spatially resolved data like gas velocity, temperature, fuel distribution in various heights and direction. These parameters cannot be provided by measurements. These results may help to optimize the kiln design, performance and operational modes in terms of high temperature distribution and energy efficiency.

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NOMENCLATURES

A	Area (m^2)
D_p	Particle diameter (mm)
D	Kiln diameter (m)
D_h	Hydraulic diameter (m)
d_L	Burner diameter (m)
H	Height (m)
h/r	Penetration depth (-)
L	length (m)
L_f	Length of flame (m)
L_b	Burner depth (m)
n	Number of burners (-)
T.I	Turbulence Intensity (-)
U_j	Injection velocity (m/s)
U_m	Main air velocity (m/s)
\dot{V}_{fuel}	Fuel volume flow (m^3/s)
\dot{V}_j	Combustion air volume flow (m^3/s)
\dot{V}_m	Cooling air volume flow (m^3/s)
Y^+	near-wall region (-)
Δp	Pressure drop (pa)

Greek Symbols

ϕ	Porosity (-)
λ	Excess air number (-)
μ	Dynamic viscosity (kg/m.s)
ρ	Density (kg/m^3)
ω	Specific turbulence dissipation rate (1/s)
ϵ	Turbulent dissipation rate (m^2/s^3)
k	Turbulent kinetic energy (m^2/s^2)

Abbreviations

CFD	Computational Fluid Dynamics
CFS	Contour Flow Single Shaft Kiln
DPM	Discrete particle model
PFR	Parallel Flow Regenerative Shaft Kiln
PMM	Porous Media Model
BCC	Body Center Cubic
SC	Simple Cubic

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