THE CFD SIMULATION OF REACTIVE FLOW IN PARALLEL FLOW REGENERATIVE SHAFT KILNS USING POROUS MEDIA MODEL

by

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Understanding the flow pattern of the gas jets in packed beds can have considerable significance in improving reactor design and process optimization. This study researches the fuel diffusion in the radial direction and the flame length in a packed bed of a parallel flow regenerative shaft kiln. This kiln is characterized that the fuel is injected vertically in the packed bed using a lot of lances in the cross-section while the combustion air is distributed continuously. Such a large, packed bed has to be approximated as a porous media. This assumption is used to model the reactive flow in the kilns. Using a box with 700 spheres of 52 mm spheres in body-centered cube arrangement the local concentrations of injected nitrogen in air-flow were measured. The measured values match approximately with those calculated with the porous media model. The studied parameters are the number of burners and burner arrangements. The radial mixing of fuel and air in a packed bed is relatively bad. Therefore, a lot of burners are needed for better temperature homogenization in the cross-section.

Key words: *CFD, shaft kilns, porous media, burner arrangement, burner number, flame length*

Introduction

Due to its importance, the calcination process of limestone in shaft kilns has been often simulated. The heat and mass transfer and the pressure drop in a packed bed can be calculated very well. These equations are given for example in [1]. Here, also the mechanism and the modeling of the limestone decomposition are explained. Hai Do *et al.* [2] simulated the limestone calcination process in the parallel flow regenerative (PFR) kiln with a resolved lumpy particle model. The influence of a lot of parameters like stone size, energy consumption, throughput, *etc.* was discussed. However, the main assumptions must be used, that temperature distribution in the cross-section was perfect, and that the flame length and combustion behavior must be predicted. Krause *et al.* [3] and Bluhm-Drenhaus *et al.* [4] researched the calcination process in a PFR kiln with coupled 3-D DEM-CFD simulation. However, the packed bed must be simplified as a porous medium and only a small section of kiln could be considered because of limited computational time.

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Authors in [5-10] modeled some other types of shaft kilns. The simplifications have always been made, that the fuel distribution in the cross-section is homogeneous and the length of the combustion zone is predicted. In Hai Do and Specht [11] it is shown based on measurements that the radial temperature differences in the packed bed near the burner system can be more than 200 K. Consequently, for further optimization of the kiln process the combustion behavior and the length of the flame in a packed bed must be known.

The flow in the gap between the particles of a packed bed was researched in [12-15]. All studies were focused on the contact point treatment, *e.g.* as gap, bridge, *etc.*, and thus on optimizing the mesh. It was shown, that because of limited computational time, the number of particles must be lower than 1000. Therewith it is not possible to simulate the flow in a packed bed of a kiln. As a consequence, the packed bed of a shaft kiln has to be treated as a porous medium.

Authors in *e.g.* [16, 17] is described how to calculate reactive flows in a porous medium. The requirement is always a strongly isotropic flow. This is the case if the pores are in the µm- and mm-range. However, in the packed bed of lumpy stones, the pores are in cm-range. Therefore, the CFD calculations have to be validated with experiments. Filkoski *et al.* [18] showed that preheating of air for combustion and for drying of raw material has significant annual energy savings and a relatively short simple payback period on the investment. In Mohammadpour [19] the injection of fuel and air in a cross-flow to a packed bed was investigated. This is the case for counter flow single (CFS) kilns shown left in fig. 1. It was shown, that the particle diameter and the ratio of combustion air (cross-flow) and cooling air (vertical flow) are the main influencing parameters. The porosity is of low influence for values lower than 0.6. This study will be continued here for the PFR kiln with the axial lance system in parallel flow.

The calcination process for lime quality and energy consumption has always to be optimized. The combustion behavior and thus, the heat release determines the calcination rate. 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. However, all of these have not been adequately investigated for design purposes in the literature. Measurements of temperature and concentration are not possible, because of the movement of the bed, no measuring devices can be stuck through the wall and centered in the bed. The influence of design parameters can only be researched using CFD. 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 utilizing a section of a packed bed. The experiments were done in the Institute of Fluid Dynamics and Thermodynamics, Otto von Guericke University, Magdeburg, Germany. The studied parameters are the number of burners and burner arrangements. Results of this research can have a considerable significance in improving the reactor design and process optimization.

Design principle of lime shaft kilns

A large variety of lime shaft kiln designs is used for centuries around the world. The two most essential shaft kilns are: CFS shaft kiln and PFR shaft kilns.

Lime burning is a high temperature process where the reactive materials are packed in a vertical shaft. Heat is required for the calcination of the limestone:

$$CaCO_3 + \text{heat} \rightarrow CaO + CO_2 \tag{1}$$

Due to gravity force, these materials move downward to pass three process zones before reaching the final product quality. The fuel is injected from burners either at the radial direction (CFS) or axial direction (PFR). The CFS shaft kiln is used for hard burnt lime and the PFR for soft burnt lime [20].

Figure 1(a) shows a CFS shaft kiln. Limestone is charged at the top of the kiln and quicklime is discharged at the bottom. The heat for calcination of the limestone is generated by fuel combustion. The fuel is introduced with air through a burner lance system from outside at different heights. These lances are placed in the lower region of the kiln. Additionally, the air is blown in at the discharge of the kiln to cool the product in a counter-current manner. The total gas flows in counter current to the stones.

The combustion gases preheat the limestone at about 800 °C before reaching the burning zone. In this zone, the limestone is heated up to a temperature of about 1500 °C, which is sufficiently high to liberate CO_2, and obtain the wanted lime quality.

Figure 1(b) shows a PFR shaft kiln. Two vertical shafts are connected through a crossover channel. The fuel is injected through lances which are placed vertically in the packed bed. The fuel injection level is for this type of kiln in the upper region of the shaft. The main features of a twin PFR kiln are:

– Parallel flow of stone and combustion gases in the burning shaft of the kiln. Therefore, the stone temperatures remain below about 1200 °C, which leads to a soft burnt lime.
– Regenerative preheating of the packed bed in the non-burning shaft, which leads to low flue gas temperatures and there with low energy consumption.
– Counterf low of lime and air in the cooling zone.

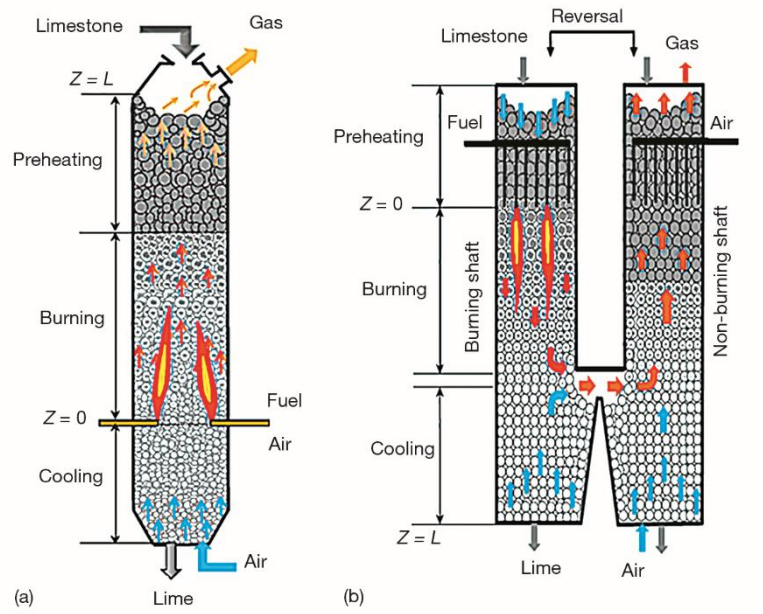

Figure 1. Schematic design of a CFS (a) and a PFR lime shaft kiln (b) [21, 22]
(*for color image see journal web site*)

The combustion gas flows downward with the stones. At the end of the burning zone, it flows through the cross-over channel to the non-burning shaft. Here, the gas flows

upwards in counter-current mode to the stones to preheat them. The heat transfer is therefore a transient process. As a consequence, after a reversal period of about 15 minutes, the fuel is injected into the other shaft, fig. 1(b), and the combustion gas flows through the cross-over channel in the left shaft and leaves the kiln again at the top.

An important factor in a shaft kiln is the burner system. The number of burners and arrangements determine the fuel distribution in the cross-section. Moreover, temperature homogenization leads to better lime product quality [20].

Computation details and grid generation

The CFD calculations are conducted using ANSYS FLUENT [23]. Figure 2 shows the scale of the used PFR kiln and the mesh generation. Because of the limited computational time of 3-D reactive flows, a small kiln diameter of 2 m was used. However, this diameter is sufficient to research the influence of all parameters. The packed bed height of 8 m is a typical height for the burning zone. The simulation of the real flow between the particles requires an exceptionally fine mesh, which results in a too high computational time. Consequently, the packed bed has to be approximated as a porous medium. This assumption is used to model the reactive flow in the kilns.

The Ergun equation is used to calculate the pressure drop in the packed bed [19]:

$$\frac{\Delta P}{L} = 150\frac{(1-\phi)^2}{\phi^3}\frac{\mu U}{d_\mathrm{p}^2} + 1.75\frac{1-\phi}{\phi^3}\frac{\rho U^2}{d_\mathrm{p}} = \frac{1}{\alpha}\frac{\mu U}{d_\mathrm{p}^2} + \frac{1}{2c_2}\frac{\rho U^2}{d_\mathrm{p}} \tag{2}$$

where d_p [mm] is the mean particle diameter, ϕ [–] – the porosity, μ [kgm^{-1}s^{-1}] – the viscosity, and U [ms^{-1}] – the velocity. The permeability and inertial loss coefficient in each component direction can be identified as:

$$\alpha = \frac{d_\mathrm{p}^2\phi^3}{150(1-\phi)^2}, \quad C_2 = \frac{3.5(1-\phi)}{d_\mathrm{p}\phi^3} \tag{3}$$

Both coefficients must be calculated with porosity and particle diameter.

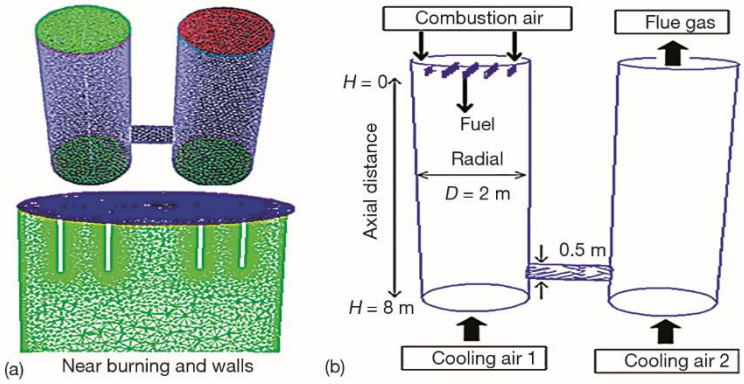

Figure 2. Computational domain and grid of a PFR shaft kiln; (a) mesh-grid generation and (b) structure and geometry (*for color image see journal web site*)

The combustion air and fuel enter the burning zone with uniform velocity and temperature. In a firing system of shaft kilns, the air and the fuel are injected into the kiln by two separate flows without being premixed. Therefore, the combustion in shaft kilns is non-premixed. The non-premixed model approach couple's intermediate species prediction, dissociation effects, and rigorous turbulence chemistry. 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. For research about turbulence reactive flow, a non-premixed model must be used. In lime shaft kilns, the chemical kinetics are rapid so that the flow is near chemical equilibrium.

In this work, methane is used as fuel to provide heat for calcination. The CH_4 is injected through lances into the packed bed. The two-step CH_4/air combustion model was applied. The combustion gas contains CO_2 and H_2O, and, from the air, O_2 and N_2. The components can be calculated from the molecular balances. The unburnt components CO and H_2 are the second step of the combustion of CH_4:

$$CH_4 + \frac{3}{2}O_2 \rightarrow CO + 2H_2O, \quad CO + \frac{1}{2}O_2 \rightarrow CO_2 \tag{4}$$

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 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 [23]. All the convergence criteria are set to below 10^{-3}. These cut-off values for convergence are used for all elements in the model, temperature, densities, pressures, flow, velocities, and the mean mixture fraction. This method is advised by the user guide and also used in other CFD combustion simulation research [23].

Figure 3 shows the flame length, L_f [m], related to the cell number for PFR kilns. The mesh cells vary from 500000 to 3200000. For all cells, less than 2911000, the flame length varies. Therefore 2911500 cells have been selected, which gives 616573 nodes and 79890 faces.

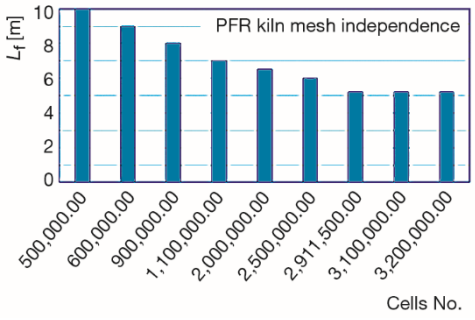

Figure 3. Mesh independence study for a flame length

Result and discussion

Experimental validation

Experiments were done to validate the CFD simulation. The experimental set-up is shown in fig. 4. A box with the dimensions of 600 mm in length, 364 mm in width, and 600 mm in height was used as a shaft. Ceramic spheres with a diameter of 52 mm were filled in as a packed bed. Two different gases were injected into the packed bed. Air was injected from a blower into the packed bed from the bottom through a perforated plate with 66 holes. The diameter of the air holes was 20 mm. This perforated plate causes an even distribution of

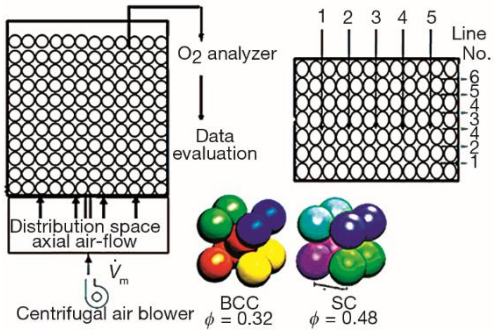

Figure 4. Experimental set-up
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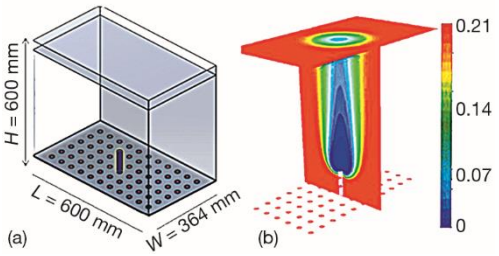

Figure 5. Dimensions and position of injections and contour of oxygen; (a) parallel flow injection and (b) O_2 mole fraction contour
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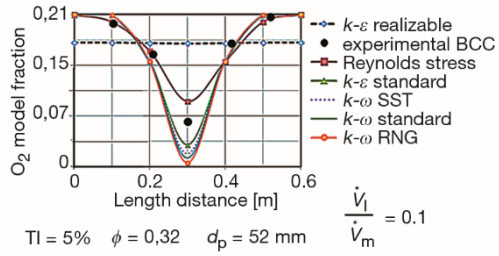

Figure 6. Oxygen profile for different turbulence models and measured values (BCC arrangement)
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air in the packed bed. Nitrogen coming from bundles was injected into the packed bed using a lance with a diameter of 20 mm. The lance was fixed in the middle of the packed bed from the bottom, that the nitrogen flows parallel with the air. The nitrogen flow rate was fixed at $\dot{V}_j$ = 25 m^3 per hours for all the cases. A ball valve adjusted the pressure, and the air volumetric flow rate was measured by using a flow meter. Firstly, the air-flow rate was adjusted by the valve and was fixed $\dot{V}_m$ = 250 m^3 per hours. When the exact flow rate of air and nitrogen was supplied, the mole fraction of O_2 was measured with the help of a gas analyzer with an accuracy of ±0.2 and a response time of 45 seconds. Therefore, a little bit of gas was sucked off with a small lance. In simple cube (SC) arrangement the lance could be stuck into the bed between the spheres in vertical and horizontal directions as shown in fig. 4 on the right side. In body centered cube (BCC) arrangement the lance could only be stuck in the bed between the spheres in horizontal directions.

Figure 5 shows the positions of the lance in the perforated plate and the calculated contours of oxygen. The spheres were arranged in BCC and SC as shown in fig. 4. The BCC has a porosity of 0.32 and SC has a porosity of 0.48.

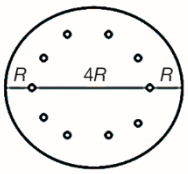
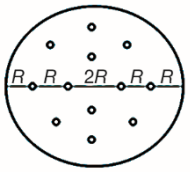
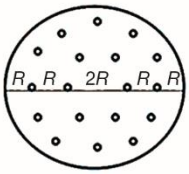
Figure 6 shows the measured oxygen concentrations as big points for the case that the ratio of the injected nitrogen to the blown-in air is 0.1 for the BCC arrangement. At the length distance of 0.3 m, where the nitrogen is injected (position of lance), the O_2 has its lowest concentration. This figure also includes the calculated profiles. The parameter is the turbulence model. The turbulence intensity (TI) is fixed at 5%. The k-ε standard turbulence gives the best fitting with the measured values. In all cases, the calculated concentrations at the injection position are a little lower than the measured ones. For the SC arrangement, the calculated and measured profiles do not match, which is not shown here. The reason is the channeling of the flow in the packed bed. Therefore, the flow is more anisotropic and not strongly isotropic, which is the requirement for a porous medium [15]. Therefore, this research is performed based on BCC arrangement and porosity of 0.32. In Alkhalat and Specht [15] it is shown that the measured concentrations match perfectly with the calculated values using the particle resolved model, which means calculations of the real flow between the gaps of the spheres. From these results, it can be concluded that the flow mixing in a packed bed of stones cannot

be perfectly calculated using the porous media model (PMM), but with sufficient accuracy. Therefore, it is postulated that also the reactive flow in a packed bed of stones can be approximately calculated using the PMM. However, as a consequence of [12-15], the packed bed of a shaft kiln has to be treated as a porous medium.

Influence of burner arrangement

Various arrangements for the burners are possible. As presented in tab. 1, three principal arrangements were studied to discuss the influence on the flame length. The first arrangement includes ten burners placed only in an outer ring. In the second arrangement, the burners are placed in two rings, eight burners in the outer ring and four burners in the inner ring. In the third arrangement, again, two rings are used, but twelve burners are placed in the outer ring and six burners in the inner ring. The distance between the burners is R = 0.33 m, and the distance up to the cross-over channel is 6 m, which is a typical length for the burning zone in PFR kilns. The diameter of the shaft is 2 m, and the fuel amount is 0.13 m^3/s.

Table 1. Three types of burner arrangement

Number of burners	n = 10	n = 12	n = 18
Principle arrangement R = 0.33 m			

The burner diameter, d_f [mm], is kept constant at d_f = 50 mm. The excess air number λ [–] is kept constant at λ = 1.3. Table 2 shows the used data.

Table 2. Used data for n = 10-18

CH_4 volume flow [m^3s^{-1}]	Burner diameter, d_f, [mm]	Fuel velocity, U_f, [ms^{-1}] n = 10	Fuel velocity, U_f, [ms^{-1}] n = 12
0.13	50	6.6	5.6
Combustion air volume flow [m^3s^{-1}]	Combustion air velocity [ms^{-1}]	Kiln diameter D [m]	Fuel velocity, U_f, [ms^{-1}] n = 18
1.6	0.5	2	3.7

Figure 7 shows twelve burners placed on the outer ring and six burners on the inner ring. It can be seen that the mole fraction of CO at the wall and in the core is very less and the CO mole fraction in the circumferential distance is relatively homogeneous for different heights, H [m].

Figure 8 shows the CO mole fraction profiles in the radial direction along the line given in tab. 1 of those three arrangements after a height of 3 m. No fuel reaches the wall and very little reaches the core. That is the reason for the low temperature at these positions. The homogenization is better in the cross-section for the higher number of burners. From this figure, it can be concluded that the minimum number of burners, n, must be 18.

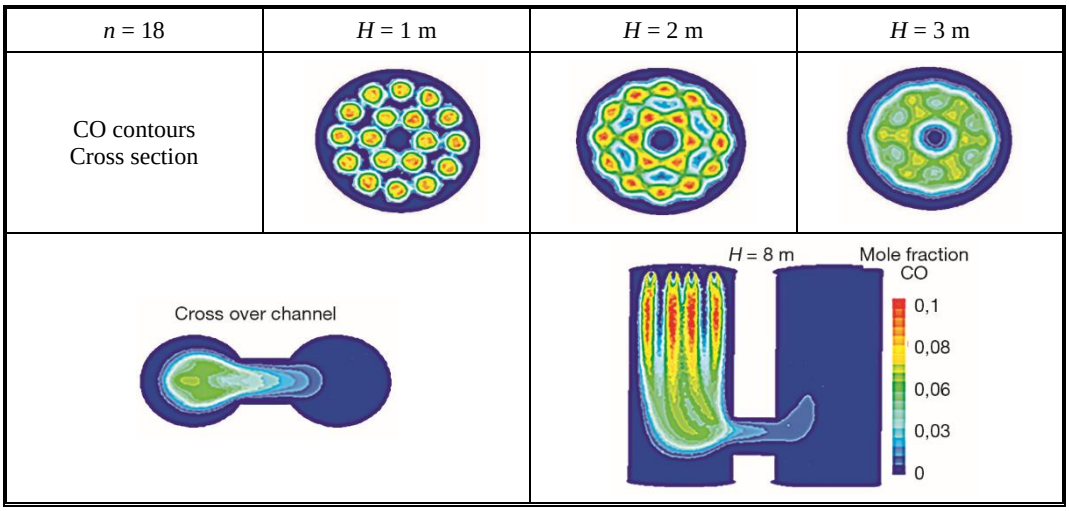


Figure 7. Contours of CO when *n* = 18 (*for color image see journal web site*)

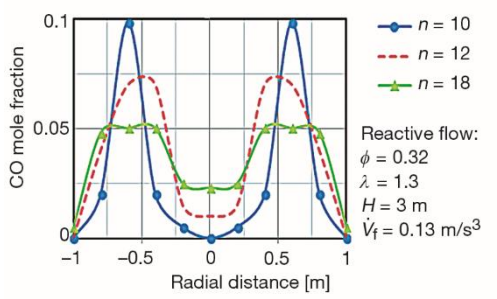


Figure 8. The CO profiles in cross-section at *H* = 3 m

Conclusions

The research study demonstrates that PMM is a proper approach to simulate the reactive flow in the packed bed of a shaft kiln. The *k-ε* turbulence model shows the best accuracy with the experimental measurements. The flow in the packed bed can only be researched using CFD with the PMM model, because of the high temperature and the movement of the bed. The number of burners and arrangements determine the fuel distribution in the cross-section. The diffusion of the fuel in the radial direction is very bad in a packed bed and the homogenization is better in the cross-section for the higher number of burners. Results of this research can have considerable significance in improving reactor design and process optimization.

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