

## NUMERICAL SIMULATION OF O<sub>2</sub>/CO<sub>2</sub> COMBUSTION IN DECOMPOSITION FURNACE

by

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*The cement industry has become the second largest source of CO<sub>2</sub> and NO<sub>x</sub> emissions after the power industry, it is imperative to reduce CO<sub>2</sub> and NO<sub>x</sub> emissions. O<sub>2</sub>/CO<sub>2</sub> combustion technology can achieve CO<sub>2</sub> enrichment and NO<sub>x</sub> reduction. As a result, its application possibilities are bright. In this article, a TTF-type decomposition furnace serves as the research object for a CFD simulation. In addition, the effects of pulverized coal combined O<sub>2</sub>/N<sub>2</sub> and pulverized coal mixed O<sub>2</sub>/CO<sub>2</sub> combustion on the velocity field, temperature field, material component, and NO<sub>x</sub> concentration distribution in the furnace are investigated concerning the changes of kinetic parameters of CaCO<sub>3</sub> decomposition under different working conditions. Compared with the O<sub>2</sub>/N<sub>2</sub> atmosphere, the temperature distribution in the high temperature zone of the decomposition furnace is more uniform under the O<sub>2</sub>/CO<sub>2</sub> atmosphere. The temperature range is reduced in the area of extremely high temperatures. The NO<sub>x</sub> concentration at the decomposition furnace exit is reduced by 37%. The high concentration of CO<sub>2</sub> at the output can be recycled and reused to reduce the greenhouse effect effectively. In addition, the high CO<sub>2</sub> partial pressure increases the exit temperature by 111 K, doubles the O<sub>2</sub> concentration, but decreases the raw meal decomposition rate from 95.9-82.2%. The process parameters must be improved to adapt to the O<sub>2</sub>/CO<sub>2</sub> combustion technology.*

**Key words:** O<sub>2</sub>/CO<sub>2</sub> combustion, CO<sub>2</sub> emission reduction, numerical simulation

### Introduction

With the rapid growth of global energy demand, the use of fossil fuels has led to an increase in CO<sub>2</sub> emissions and a worsening of the greenhouse effect. Therefore, the reduction of CO<sub>2</sub> emissions has become an important research field. As the second largest source of CO<sub>2</sub> emission after the electric power industry [1], the cement industry has great potential to reduce CO<sub>2</sub> emissions. The most promising development technology to achieve CO<sub>2</sub> emission reduction in the cement industry is CO<sub>2</sub> capture technology. In order to achieve CO<sub>2</sub> capture, CO<sub>2</sub> must be separated directly from the flue gas, and the difficulty and cost of standard capture technology are significant. Therefore, O<sub>2</sub>/CO<sub>2</sub> combustion technology was born and has attracted more and more attention [2, 3].

Cement kiln O<sub>2</sub>/CO<sub>2</sub> combustion technology is to mix high purity O<sub>2</sub> (>95%) with circulating flue gas and passes it into the decomposition furnace and rotary kiln for combustion so that pulverized coal combustion is burned in the O<sub>2</sub>/CO<sub>2</sub> atmosphere. After multiple enrichment, the CO<sub>2</sub> gas in the kiln tail has high purity and can be directly recycled, stored, and utilized. Also, CO<sub>2</sub> has higher heat and mass transfer characteristics than N<sub>2</sub>, which can

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improve the thermal efficiency of cement kiln equipment. At the same time, replacing N<sub>2</sub> with CO<sub>2</sub> can significantly reduce the amount of thermodynamic NO<sub>x</sub> generation [4], and the O<sub>2</sub>/CO<sub>2</sub> combustion technology used in cement kiln does not affect the clinker strength [5].

Many scholars have compared the fuel combustion situation in the O<sub>2</sub>/CO<sub>2</sub> atmosphere and the O<sub>2</sub>/N<sub>2</sub> atmosphere, tested the overall performance [6, 7] and the flame stability [8, 9], and conducted the numerical simulation of the flame structure [10, 11]. The result shows that flame propagation and oxygen diffusion are slower in O<sub>2</sub>/CO<sub>2</sub> atmosphere regardless of fuel type. Suda *et al.* [12] pointed out that the main reason is that the volumetric specific heat capacity of CO<sub>2</sub> is higher than that of N<sub>2</sub>. For pulverized coal, Debo *et al.* [13] found through experimental research that the ignition temperature and burnout temperature of pulverized coal in the O<sub>2</sub>/N<sub>2</sub> atmosphere are lower than that in the O<sub>2</sub>/CO<sub>2</sub> atmosphere. Zhang *et al.* [14] studied the combustion of pulverized coal in the O<sub>2</sub>/CO<sub>2</sub> atmosphere boiler and found that the ignition time of pulverized coal in the O<sub>2</sub>/CO<sub>2</sub> atmosphere would be delayed.

Currently, the application of O<sub>2</sub>/CO<sub>2</sub> combustion technology in cement kilns mainly remains in the theoretical analysis of technical and economic feasibility [15, 16], as well as small-scale and pilot studies [17]. With the increasing maturity and accuracy of computer numerical simulation technology, the decomposition furnace simulation study can be conducted in O<sub>2</sub>/CO<sub>2</sub> atmosphere using CFD simulation technology [18]. Francisco *et al.* [19] and Mario and Bakken [20] verified that modern kiln burners are suitable for oxygen fuel combustion without additional modification by experimental and numerical simulation methods, respectively. In the decomposition furnace, Xu *et al.* [21] conducted a numerical simulation study on the combustion of pulverized coal in the decomposition furnace under the O<sub>2</sub>/CO<sub>2</sub> atmosphere. They found that the combustion rate of pulverized coal and the decomposition rate of raw meal in the decomposition furnace under the O<sub>2</sub>/CO<sub>2</sub> atmosphere was reduced. Zhang *et al.* [22] found that the O<sub>2</sub>/CO<sub>2</sub> combustion technology can significantly reduce the outlet NO<sub>x</sub> and does not affect the normal work of the decomposition furnace through a numerical simulation study of O<sub>2</sub>/CO<sub>2</sub> combustion in the cement decomposition furnace. However, the aforementioned simulation study on the combustion of O<sub>2</sub>/CO<sub>2</sub> in the decomposition furnace needs to include the consideration of the changes in the kinetic parameters of CaCO<sub>3</sub> decomposition after substituting N<sub>2</sub> with CO<sub>2</sub>. It cannot support the application of this technology in the cement decomposition furnace. An experimental study by Tian *et al.* [23] showed that compared with O<sub>2</sub>/N<sub>2</sub> atmosphere, the decomposition reaction time of CaCO<sub>3</sub> in the O<sub>2</sub>/CO<sub>2</sub> atmosphere was prolonged, while the decomposition rate decreased. In addition, the activation energy and pre-exponential factor were greatly improved. Therefore, to further promote the application of O<sub>2</sub>/CO<sub>2</sub> combustion technology in the decomposition furnace, the effects of the changes concerning the kinetic parameters of CaCO<sub>3</sub> decomposition in the O<sub>2</sub>/CO<sub>2</sub> atmosphere should be further explored.

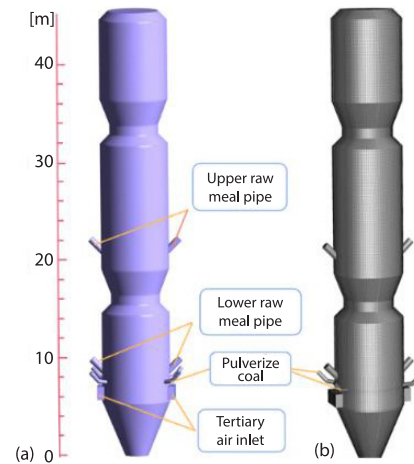
This research is based on the CFD numerical simulation approach and the widely used commercial software FLUENT based on verifying the pulverized coal coupled air combustion model and referring to the variations of the kinetic decomposition parameters of calcium carbonate in an O<sub>2</sub>/CO<sub>2</sub> atmosphere. The effect of pulverized coal coupling O<sub>2</sub>/CO<sub>2</sub> combustion technology in decomposition furnaces was analyzed and compared, providing theoretical support for promoting O<sub>2</sub>/CO<sub>2</sub> combustion technology in decomposition furnaces.

## Geometric model and boundary condition

### Model introduction

This research uses a CFD numerical simulation analysis based on the actual 3500 tonne per day cement decomposition furnace operating at a cement plant. The decomposition

furnace model is TTF type, it contains two shrinkage regions and three spray regions, which provides the benefits of a powerful reflux impact and longer spray times, the high temperature zone in the middle of the combustion zone can be created by the feeding method of separating the upper and lower feeding points, which can significantly improve the combustion speed of pulverized coal. Figure 1 illustrates the geometric model. The height of the body of the decomposition furnace is 45.68 meters, while the effective interior diameter is 3.5 meters. It consists of the vertebral body, the primary combustion chamber, the middle portion, the top portion of the decomposition furnace, and the shrinkage port. The tertiary air duct is distributed symmetrically on both sides of the bottom of the main combustion chamber, and the four pulverized coal tubes are distributed uniformly above the tertiary air duct. The raw meal is decomposed in a graded manner. The raw meal feeding points are located above the pulverized coal burner and in the center of the decomposition furnace, with two in each tier and four in total. The flue gas created in the cement rotary kiln enters the decomposition furnace from the bottom of the lower vertebral body and escapes through the higher outlet.



**Figure 1. The TTF decomposition furnace structure and mesh**

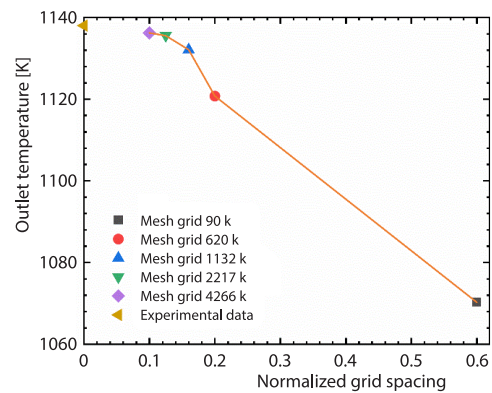
The ANSYS ICEM was used to generate the structured hexahedral grid, and some regions were encrypted to improve simulation accuracy. The total number of created grids was 2217 k. The resulting grid was dense, and no bad grids were produced. The minimal orthogonal quality was 0.72, and the minimum Angle was 45°, satisfying the conditions for calculation precision and calculation time.

*Mesh independence*

To explore the influence of the number of grids on the simulation results. The outlet temperature of the decomposition furnace in a typical air atmosphere was selected as the research parameter for grid independence verification. The setting of these meshes is listed in tab. 1. We compared the grid number with the decomposition furnace outlet temperature, and the comparison results are shown in fig. 2, when the grid number exceeds 1132 k, the temperature at the decomposition furnace outlet changes

**Table 1. Parameter setting of grid refinement study**

Grid group	Normalized grid spacing	Outlet temperature	Element number
1	0.6	1070.28	90 k
2	0.2	1120.76	620 k
3	0.16	1132.09	1132 k
4	0.125	1135.54	2217 k
5	0.1	1136.23	4266 k



**Figure 2. Comparison of outlet temperature among different densities of grid mesh**

minimally, and the error with the measured value is within a reasonable range. Thus the grid number 2217 k is selected for this simulation study.

### Boundary conditions

The boundary conditions necessary for the calculation are set according to the collected data in the test conditions, and the velocity inlet boundary conditions are utilized for both the flue gas inlet and the tertiary air inlet. The flue gas inlet velocity is 36 m/s, and the tertiary air inlet velocity is 31 m/s. The decomposition furnace outlet boundary condition is pressure outlet, and the pressure value is  $-1250$  Pa. Raw meal and pulverized coal are both imported mass-flow inlets. The Ultimate analysis and proximate analysis of pulverized coal are depicted in tab. 2. In contrast, the composition analysis of raw meals is illustrated in tab. 3, and the mass-flow and average temperature of coal powder and calcium carbonate inlet are depicted in tab. 4. The decomposition furnace is divided into several regions, and the corresponding wall surface temperature is set with the measured temperatures of the various areas. The other positions of the furnace body are selected as the wall surface, and the boundary condition of the wall surface is set as the constant temperature boundary.

**Table 2. Proximate and ultimate analyses of pulverized coal**

Ultimate analysis					Proximate analysis				$Q_{gr.ad}$ [MJkg <sup>-1</sup> ]
$C_{ad}$	$H_{ad}$	$O_{ad}$	$N_{ad}$	$S_{ad}$	$FC_{ad}$	$V_{ad}$	$A_{ad}$	$M_{ad}$	
60.5	4.03	18.34	1.04	0.26	53.49	30.68	11.69	4.14	26.9

**Table 3. Raw meal compositions [%]**

Loss*	SiO <sub>2</sub>	Al <sub>2</sub> O <sub>3</sub>	Fe <sub>2</sub> O <sub>3</sub>	CaO	MgO
36.74	12.56	3.69	2.22	43.41	1.38

\* Loss represents the burning loss of raw meal, characterize the percentage of gaseous products (such as H<sub>2</sub>O, CO<sub>2</sub>, etc.) and organic matter content in the total amount of raw meal.

**Table 4. Mass-flow and temperature of coal and CaCO<sub>3</sub>**

Parameter	Coal	CaCO <sub>3</sub>	
		Upper	Lower
Mass-flow [kgs <sup>-1</sup> ]	0.95	20	14.6
Temperature [K]	331	1043	1043

This study compares the O<sub>2</sub>/CO<sub>2</sub> atmosphere with the O<sub>2</sub>/N<sub>2</sub> atmosphere to better understand the combustion changes of the decomposition furnace under the O<sub>2</sub>/CO<sub>2</sub> atmosphere. Compared with the O<sub>2</sub>/N<sub>2</sub> atmosphere, only the tertiary air, coal supply air, and N<sub>2</sub> in the flue gas inlet in the standard air atmosphere are replaced by CO<sub>2</sub> in the O<sub>2</sub>/CO<sub>2</sub> atmosphere, and the other boundary conditions remain unchanged. Under an O<sub>2</sub>/N<sub>2</sub> atmosphere, each component's volume concentration in the tertiary air and pulverized coal inlet gas is 21% O<sub>2</sub> and 79% N<sub>2</sub>. Each component's volume concentration in the flue gas inlet gas is 12.7% CO<sub>2</sub>, 2.8% O<sub>2</sub>, 0.1% CO, and 84.4% N<sub>2</sub>. Under an O<sub>2</sub>/CO<sub>2</sub> atmosphere, each component's volume concentration in the tertiary air and pulverized coal inlet gas is 21% O<sub>2</sub> and 79% CO<sub>2</sub>. In comparison, each component's volume concentration in the flue gas inlet gas is 97.1% CO<sub>2</sub>, 2.8% O<sub>2</sub>, and 0.1% CO.

## Model selection and numerical solution method

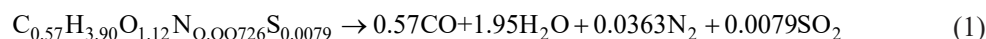
### *Turbulence governing equation*

The gas-phase turbulence model adopted the Realizable  $k-\varepsilon$  [24] model, which is suitable for the decomposition furnace.

### *Discrete phase model*

The discrete phase model model was utilized to solve the particle phase's motion trajectory in the decomposition furnace. The pulverized coal particles were assumed to be spherical, and the particle size was determined using the Rosin-Rammler distribution. The maximum particle size of coal dust is 90  $\mu\text{m}$ , the minimum particle size is 50  $\mu\text{m}$ , and the average particle size is 60  $\mu\text{m}$ . The effect of turbulence on particles is considered. A particle phase random orbit model is established to track the discrete phase, and 23000 coal powder particles are tracked.

In the decomposition furnace, the finite-rate/eddy-dissipation model in the species transport model was utilized for the combustion of pulverized coal and the decomposition of calcium carbonate. The explosion of pulverized coal typically occurs in two-stages: volatile separation and explosion have been assumed to appear first in the coal-combustion process, followed by the eruption of char. The two competing rates model was used for volatile combustion. When the volatile combustion is complete, the remaining coke is reacted, and the reaction rate is controlled by the kinetic/diffusion model chosen. The pulverized coal oxidation reaction is:



For the raw meal decomposition study of the decomposition furnace, the raw meal is approximately regarded as CaCO<sub>3</sub>, and the species transport model is utilized to simulate the decomposition process. The decomposition reaction of CaCO<sub>3</sub>:



In an O<sub>2</sub>/CO<sub>2</sub> atmosphere, the kinetic parameters of CaCO<sub>3</sub> decay differ from those in an O<sub>2</sub>/N<sub>2</sub> atmosphere. Due to the sluggish diffusion speed of CO<sub>2</sub> created by the decomposition of CaCO<sub>3</sub> at high partial pressures of CO<sub>2</sub>, which hinders other decomposition reactions and the decay of CaCO<sub>3</sub>, its pre-exponential factor and activation energy are enhanced proportionally. Table 5 summarizes the kinetic parameters from eqs. (1)-(3).

**Table 5. Kinetic parameters of the reactions**

Reactant	$A$	$E$ [Jkmol <sup>-1</sup> ]	Reaction orders
Volatile	$2.119 \cdot 10^{11}$	$2.027 \cdot 10^8$	$[\text{volatile}]^{0.2}[\text{O}_2]^{1.3}$
CO	$2.239 \cdot 10^{12}$	$1.7 \cdot 10^8$	$[\text{CO}]^1[\text{O}_2]^{0.25}$
O <sub>2</sub> /N <sub>2</sub> CaCO <sub>3</sub>	$1.0 \cdot 10^9$	$1.95 \cdot 10^8$	CO <sub>2</sub> dominant
O <sub>2</sub> /CO <sub>2</sub> CaCO <sub>3</sub>	$3.16 \cdot 10^{31}$	$7.801 \cdot 10^8$	CO <sub>2</sub> dominant

### *The NO<sub>x</sub> generating model*

The NO<sub>x</sub> generation is also an essential generation of understanding pulverized coal combustion. In general, the burst of pulverized coal produces three types of NO<sub>x</sub>: thermal NO<sub>x</sub>, fuel NO<sub>x</sub>, and prompt NO<sub>x</sub>. Due to the minimal fraction of prompt NO<sub>x</sub> in the pulverized coal combustion process, only thermal NO<sub>x</sub> and fuel NO<sub>x</sub> are discussed in this paper. The software

Fluent uses post-processing to calculate NO<sub>x</sub> so that NO<sub>x</sub> generation is influenced by the combustion calculation results [25]. The main reactions of thermal NO<sub>x</sub>:

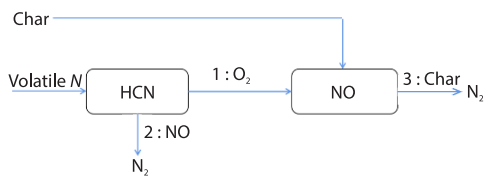


Figure 3. Fuel NO<sub>x</sub> formation path

With a complex generation mechanism, fuel NO<sub>x</sub> accounts for a significant share of the total NO<sub>x</sub>. Figure 3 shows the generation of fuel NO<sub>x</sub> [26]. It is hypothesized that N in the fuel is distributed between volatiles and coke, that N in volatiles is converted to NO via the reaction intermediate HCN, and that some unreacted

HCN is employed as a reducing agent to convert NO to N<sub>2</sub>. N in a coke can be restored immediately to NO.

#### Radiation model

The P1 radiation model is utilized to calculate the radiation heat transfer between the particle and gas phases. The P1 model is ideal for calculating the heat transfer between the gas and particles in a decomposition furnace due to its small calculation volume and rapid calculation speed. The gas phase absorption coefficient is calculated using the WSGGM model. The parameters used for traditional WSGGM must be changed in the O<sub>2</sub>/CO<sub>2</sub> atmosphere due to the high CO<sub>2</sub> partial pressure to accurately replicate the O<sub>2</sub>/CO<sub>2</sub> combustion gas radiation [27, 28].

#### Numerical solution

The finite volume method is used to discretize the continuous phase control equation. The calculation process adopts the SIMPLE algorithm of pressure and velocity coupling. The discrete format pressure is selected as PRESTO! The others use a second-order upwind discrete format. Using TDMA iterative solution, the continuity and energy equation residuals are less than 10<sup>-6</sup>, and the rest of the residual is less than 10<sup>-3</sup> as convergence criteria. For the coupling of the continuous phase and particle phase, Solving the constant phase first and then adding a discrete phase is adopted for the coupling of the continuous phase and particle phase.

### Numerical simulation results analysis

#### Verification of the numerical simulation results

In order to verify the reliability of the simulation results, we compared the measured data with the main parameters of the decomposition furnace outlet under the O<sub>2</sub>/N<sub>2</sub> conditions. As shown in tab. 6, within 5% are the relative errors of the decomposition furnace outlet temperature and the raw meal decomposition rate under the actual O<sub>2</sub>/N<sub>2</sub> conditions, indicating that the selected numerical model is reliable. Shown in fig. 4 are the gas phase composition and measured values at the outlet of the decomposition furnace under O<sub>2</sub>/N<sub>2</sub> working con-

Table 6. Comparison of simulation and measured values

Parameter	O <sub>2</sub> /N <sub>2</sub>	Measured values
Outlet temperature	1132 K	1154 K
Raw meal decomposition rate	95.9%	92.3%

ditions, in which the simulated value of each gas concentration at the outlet of the decomposition furnace is close to the measured value. It indicates that the simulation results meet the requirements of the actual working condition.

### Velocity distribution

As shown in figs. 5(a) and 5(b), a good symmetry is observed among the velocity distribution in the decomposition furnace under the two working conditions. Further, the presence of a reflux zone in the bottom vertebral body and the middle part of the decomposition furnace is beneficial to prolong the residence time of the pulverized coal in the furnace and to mix with the raw meal thoroughly. At the same time, the velocity of the air-flow through the shrinking mouth of the decomposition furnace increases remarkably and produces the three ejection effects. Therefore, the heat exchange between the material and the air-flow is strengthened. It is favorable to improve the burning rate of pulverized coal. In addition, by comparison, the velocity distributions under the two working conditions were the same. Meanwhile, the difference between the two is primarily reflected in the size of the reflux area. The main reason is the variation of the pulverized coal combustion and the decomposition of raw meals under the O<sub>2</sub>/CO<sub>2</sub> atmosphere.

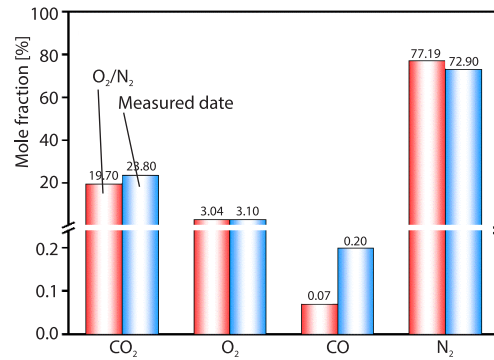


Figure 4. Comparison of simulation and field test at the outlet gas phase composition

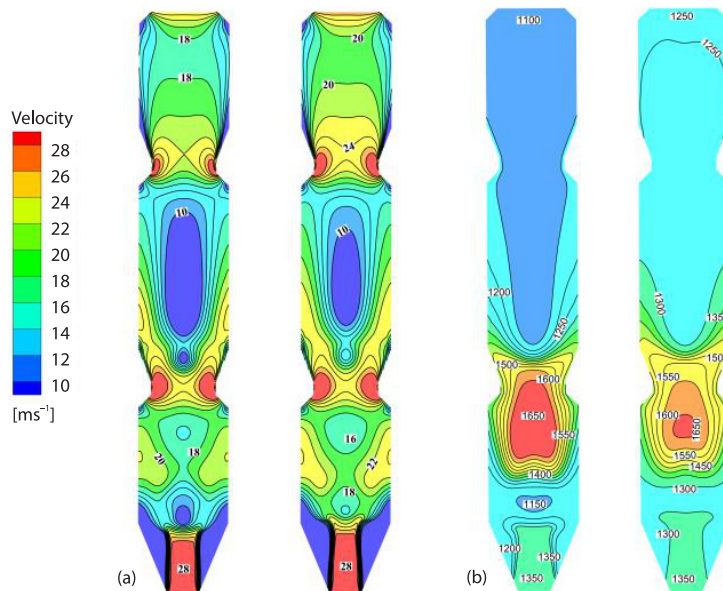


Figure 5. Velocity contours and temperature contours under O<sub>2</sub>/N<sub>2</sub> and O<sub>2</sub>/CO<sub>2</sub> atmosphere; (a) velocity contours and (b) temperature contours

### Temperature distribution

According to the temperature cloud map in figs. 5(c) and 5(d), the decomposition furnace temperature increases and then decreases from the bottom to the top in both conditions. In the first section of the main body, the pulverized coal under high temperature cracking combustion released a large amount of heat and produced a local high temperature area. In the second section main body, as the heat release rate of pulverized coal combustion decreases,  $CaCO_3$  decomposes and absorbs heat in a large amount. The temperature in the furnace gradually dropped with a *V*-shaped distribution. When it reached the outlet of the decomposition furnace, the temperature gradually tended to be stable. In addition, by comparing the temperature cloud maps of the two working conditions, it can be seen that the high temperature region in the upper part of the lower raw meal tube in the  $O_2/CO_2$  atmosphere is reduced compared with  $O_2/N_2$  atmosphere. To describe this phenomenon more clearly, we selected the cross-section cloud images at 11 m, 12 m, and 13 m of the primary combustion zone of the decomposition furnace for comparison, as shown in fig. 6. Line A represents the  $O_2/N_2$  atmosphere, and Line B stands for the  $O_2/CO_2$  atmosphere. The comparison shows that at the same position in the main combustion area, the high temperature area of the  $O_2/CO_2$  atmosphere is significantly reduced, and the temperature distribution is more uniform. The main reason is that the combustion capacity of pulverized coal deteriorates under the  $O_2/CO_2$  atmosphere. At the same time, the  $CO_2$  molecules are more radiant and have a more uniform temperature distribution compared with the  $N_2$  molecule. It can also be seen from the temperature cloud map in figs. 5(c) and 5(d) that the temperature keeps increasing from the upper raw meal tube to the outlet of the decomposition furnace under the  $O_2/CO_2$  atmosphere compared with the  $O_2/N_2$  atmosphere, mainly because of the high concentration of  $CO_2$  in the stove under  $O_2/CO_2$  atmosphere inhibits the decomposition of  $CaCO_3$ . It results in a decrease in the total heat absorbed by the deterioration of the raw meal and an increase in the temperature in the furnace.

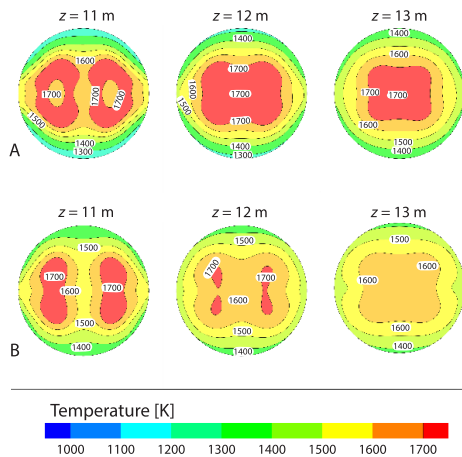


Figure 6. The decomposition furnace z section 11 m, 12 m, and 13 m temperature contour

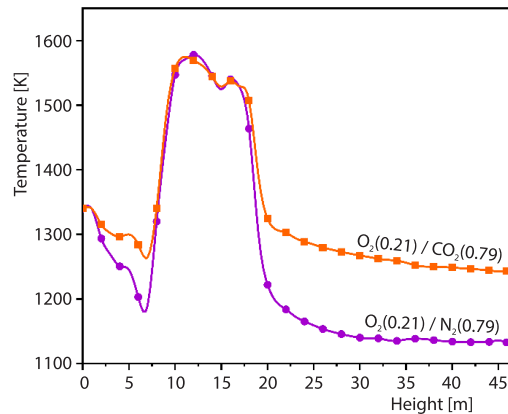


Figure 7. The average cross-sectional temperature along the decomposition furnace

The average temperature of the decomposition furnace section is shown in fig. 7. The temperature in the  $O_2/CO_2$  atmosphere, except the central combustion zone, is higher than  $O_2/N_2$  atmosphere because the high  $CO_2$  partial pressure suppresses the decomposition of  $CaCO_3$ . The average temperature of the outlet section of the decomposition furnace is 1243 K, which is 111 K more elevated than 1132 K in the  $O_2/N_2$  atmosphere.



### The CO and CO<sub>2</sub> distribution

From the results in figs. 8(a) and 8(b), the decomposition furnaces CO are divided into two parts. One is the small amount of CO carried by the kiln tail flue gas itself, which forms a small area in the inlet. The second is the CO produced by incomplete combustion of pulverized coal in the primary combustion zone, including a reduction zone with higher concentration. Under the action of tertiary air, the previously mentioned two react quickly with oxygen. They are converted into CO<sub>2</sub>, resulting in the continuous upward consumption of CO with the air-flow until the CO at the outlet of the decomposition furnace is wholly consumed. Compared with the two working conditions, the maximum local concentration of CO in the O<sub>2</sub>/N<sub>2</sub> atmosphere is 0.31%, and CO in O<sub>2</sub>/CO<sub>2</sub> atmosphere is 0.4%. It indicates that the pulverized coal is almost completely burned. In the O<sub>2</sub>/CO<sub>2</sub> atmosphere, the CO content in the flue gas inlet and the main combustion area has increased. It is consistent with the results of Tan *et al.* [29] on a 0.3 MW vertical combustor research facility. The main reason is that the high concentration of CO<sub>2</sub> can inhibit the synthesis of CO and reduce the conversion rate of CO, thus improving its content.

As seen from figs. 8(c) and 8(d), the CO<sub>2</sub> entering from the bottom flue gas inlet of the decomposition furnace under the O<sub>2</sub>/N<sub>2</sub> atmosphere gradually increases along the decomposition furnace from bottom to top, with a slight decrease in the concentration at the tertiary air position. The main reason is that the added attention of air is diluted. And in the primary combustion area, the CO<sub>2</sub> concentration gradually increases due to the combustion of pulverized coal and the release of CO<sub>2</sub> from the decomposition of calcium carbonate. Specifically, the enriched CO<sub>2</sub> concentration at the outlet of the decomposition furnace was 19.7%. Besides, in the O<sub>2</sub>/CO<sub>2</sub> atmosphere, the CO<sub>2</sub> concentration at the bottom flue gas inlet was as high as 97.1%. It dramatically changes the distribution of CO<sub>2</sub> concentration. At the tertiary air location, the CO<sub>2</sub> concentration is diluted and reduced due to the addition of an O<sub>2</sub>/CO<sub>2</sub> atmosphere. In addition, two low concentration zones are created due to the inhibition of CaCO<sub>3</sub> decomposition by the high CO<sub>2</sub> atmosphere near the upper and lower raw metal pipes. Two V-shaped areas also appear in the corresponding fig. 9. After that, the CO<sub>2</sub> concentration was gradually enriched and stabilized, reaching 75.4% at the outlet of the decomposition furnace.

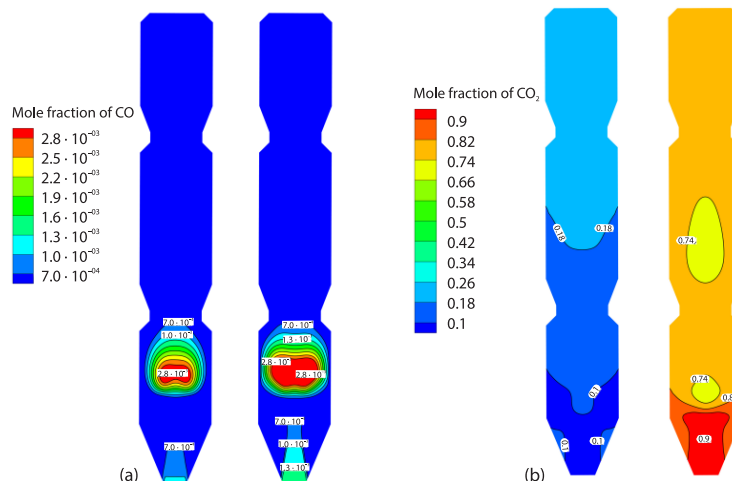


Figure 8. The CO and CO<sub>2</sub> mole fraction distributions under O<sub>2</sub>/N<sub>2</sub> and O<sub>2</sub>/CO<sub>2</sub> atmosphere; (a) CO mole fraction and (b) CO<sub>2</sub> mole fraction

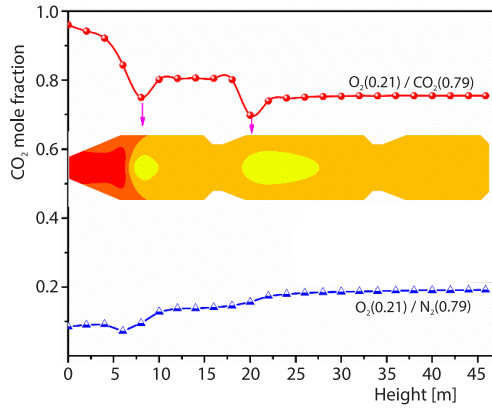


Figure 9. Average cross-sectional CO<sub>2</sub> mole fraction along the decomposition furnace

*The CaCO<sub>3</sub> and CaO distribution*

According to figs. 10(a) and 10(b), combined with fig. 11, the trends of CaCO<sub>3</sub> concentration in the two working conditions are relatively consistent. In both cases, the height direction is first rising, then falling, followed by rising, and finally falling again. The two elevated positions correspond to the raw meal entrance, and the second peak of the curve is higher because of the more extensive feed of the upper raw meal. First, after entering the decomposition furnace, CaCO<sub>3</sub> decomposes rapidly due to the high temperature environment generated by the pulverized coal combustion. It has been entirely spoiled by the time it reaches the entrance of the upper raw meal. Subsequently,

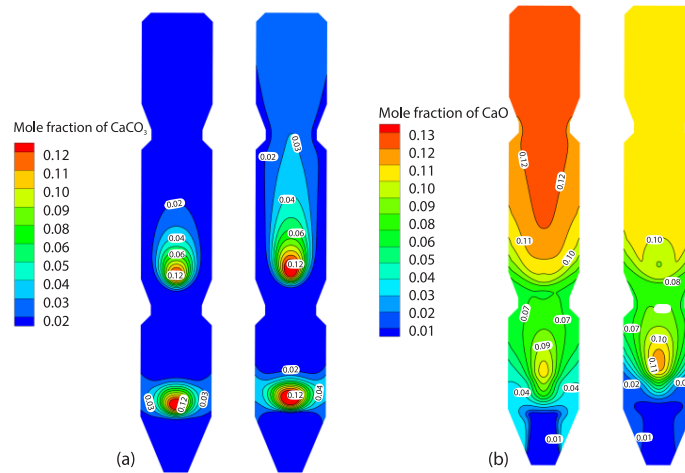


Figure 10. The CaCO<sub>3</sub> and CaO mole fraction distributions under O<sub>2</sub>/N<sub>2</sub> and O<sub>2</sub>/CO<sub>2</sub> atmosphere; (a) CaCO<sub>3</sub> mole fraction and (b) CaO mole fraction

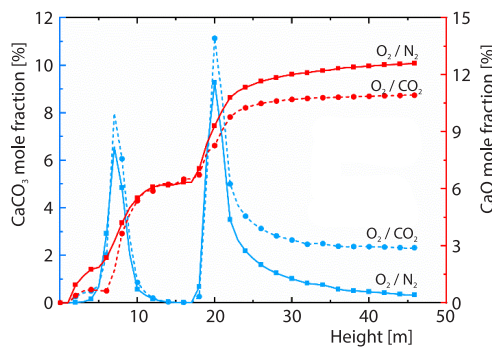


Figure 11. Average cross-sectional CaCO<sub>3</sub> and CaO mole fraction along the decomposition furnace

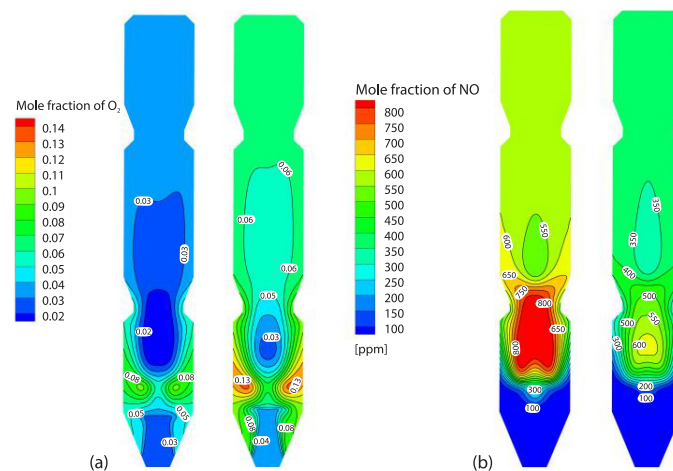
after feeding the raw meal into the upper raw meal pipe, the CaCO<sub>3</sub> mole material fraction climbs up rapidly, decreases after decomposition, and stabilizes. Comparing the two working conditions, the CaCO<sub>3</sub> concentration peak of the upper and lower raw meal pipes in the O<sub>2</sub>/CO<sub>2</sub> atmosphere is higher than that of the O<sub>2</sub>/N<sub>2</sub> atmosphere. The main reason is that the O<sub>2</sub>/CO<sub>2</sub> atmosphere suppresses CaCO<sub>3</sub> decomposition some extent, and the added CaCO<sub>3</sub> is not decomposed in time. This results in a large local CaCO<sub>3</sub> concentration in the O<sub>2</sub>/CO<sub>2</sub> atmo-

sphere. In addition the peak value, the variation of CaCO<sub>3</sub> concentration at 0-6 m and 8-20 m of the decomposition furnace are similar under the two working conditions. At 20 m from the outlet, the CaCO<sub>3</sub> concentration in O<sub>2</sub>/CO<sub>2</sub> atmosphere is higher than that in O<sub>2</sub>/N<sub>2</sub> atmosphere. The main reason is that not only is temperature dependent is the decomposition, but also subject to the partial pressure of CO<sub>2</sub>. In the case of the dominant role of temperature in the main combustion zone, CaCO<sub>3</sub> can decompose entirely in both atmospheres at a suitable temperature. However, after the main combustion zone, the temperature of the decomposition furnace decreases due to the addition of raw meal in the upper raw pipe, and the partial pressure of CO<sub>2</sub> plays a dominant role in the decomposition of CaCO<sub>3</sub>. The high partial pressure of CO<sub>2</sub> in the O<sub>2</sub>/CO<sub>2</sub> atmosphere is not conducive to the further decomposition of CaCO<sub>3</sub>. This eventually leads to higher concentrations of CaCO<sub>3</sub> in the O<sub>2</sub>/CO<sub>2</sub> atmosphere than in the normal air atmosphere after the main combustion zone. The calculated mass-flow rates of CaCO<sub>3</sub> at the outlet of O<sub>2</sub>/N<sub>2</sub> and O<sub>2</sub>/CO<sub>2</sub> are 2.9 kgs and 12.3 kgs., respectively, the corresponding decomposition rates are 95.9% and 82.1%. Compared with the O<sub>2</sub>/N<sub>2</sub> atmosphere, the decomposition rate of CaCO<sub>3</sub> under the O<sub>2</sub>/CO<sub>2</sub> atmosphere can be improved by optimizing the process parameters.

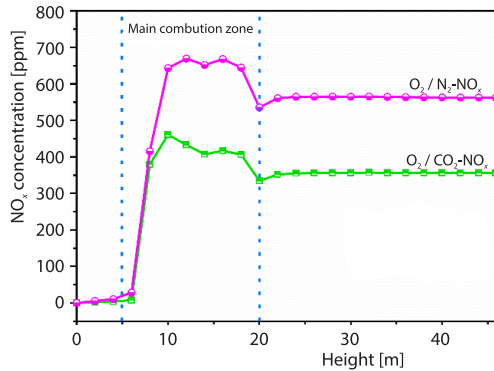
According to the results of figs. 10(c) and 10(d), combined with fig. 11, the trend of CaO concentration is just opposite to that of CaCO<sub>3</sub>, showing a gradual enrichment from bottom to top. When the concentration of CaCO<sub>3</sub> attention near the upper and lower raw meal tubes decreases-significantly, the growth rate of CaO is the fastest. As the decomposition rate of CaCO<sub>3</sub> in the upper furnace body drops, the growth rate of CaO becomes smaller and stabilizes at the outlet of the decomposition furnace. Compared with the two working conditions, it can be found that the enriched CaO content at the decomposition furnace outlet is reduced in the O<sub>2</sub>/CO<sub>2</sub> atmosphere, down from 12.6% in the typical air atmosphere to 10.9%.

### The O<sub>2</sub> and NO<sub>x</sub> distribution

According to figs. 12(a) and 12(b), under the O<sub>2</sub>/N<sub>2</sub> atmosphere, the O<sub>2</sub> carried by the tertiary air has the highest concentration in the decomposition furnace primary combustion area was about 8~14%. Due to the decisive vortex flow action of tertiary air, the high concentration of O<sub>2</sub> region is distributed in the near-wall area of the tertiary air. In contrast, the central area



**Figure 12. The O<sub>2</sub> mole fraction distributions and NO<sub>x</sub> contours under O<sub>2</sub>/N<sub>2</sub> and O<sub>2</sub>/CO<sub>2</sub> atmosphere; (a) O<sub>2</sub> mole fraction and (b) NO<sub>x</sub> contours**



**Figure 13. Average cross-sectional NO concentration along the decomposition furnace**

O<sub>2</sub>/CO<sub>2</sub> atmosphere increased to 6.05% at the outlet of the decomposition furnace, which is twice as high as in the O<sub>2</sub>/N<sub>2</sub> atmosphere.

As can be seen from figs. 12(c) and 12(d), the NO<sub>x</sub> content in the primary combustion area increases rapidly under the O<sub>2</sub>/N<sub>2</sub> atmosphere. It forms a high concentration NO<sub>x</sub> area corresponding to the high temperature area in fig. 13. The local maximum NO<sub>x</sub> concentration can reach 670 ppm (equivalent to 738 mg/m<sup>3</sup>), primarily due to the rapid generation of thermal NO<sub>x</sub> and fuel NO<sub>x</sub> in the main combustion area. In the vicinity of the upper raw meal tube, the decomposition furnace temperature is reduced due to the addition of many raw meals. Also, the NO<sub>x</sub> content decreases to a certain extent until it stabilizes at the decomposition furnace outlet with a value of about 562 ppm (equivalent to 619 mg/m<sup>3</sup>). Under the O<sub>2</sub>/CO<sub>2</sub> atmosphere, there is almost no thermal NO<sub>x</sub> generation because no N<sub>2</sub> is introduced. At the same time, the high concentration of NO<sub>x</sub> in the primary combustion zone is significantly reduced because the high CO<sub>2</sub> atmosphere increases the mass fraction of CO in the decomposition furnace. Reducing CO has an inhibitory effect on the generation of fuel NO<sub>x</sub>. After the gradual dilution of the updraft, the concentration of NO<sub>x</sub> at the outlet of the decomposition furnace is stabilized at 355 ppm (equivalent to 391 mg/m<sup>3</sup>). Remarkably, compared with the O<sub>2</sub>/N<sub>2</sub> atmosphere, the NO<sub>x</sub> at the outlet of the decomposition furnace is reduced by 37%.

## Conclusions

For the TTF decomposition furnace, the coal powder combustion and calcium carbonate decomposition under O<sub>2</sub>/N<sub>2</sub> and O<sub>2</sub>/CO<sub>2</sub> atmosphere were investigated and compared, and the mechanism was studied, are as follows.

- The results show that a high CO<sub>2</sub> atmosphere dramatically influences the kinetic parameters of CaCO<sub>3</sub> decomposition with a corresponding increase in pre-exponential factor and activation energy compared with O<sub>2</sub>/N<sub>2</sub> combustion-supporting mode. As a result, the outlet temperature of the decomposition furnace in the O<sub>2</sub>/CO<sub>2</sub> atmosphere was increased by 111 K, and the oxygen content was doubled. At the same time, the decomposition rate of raw meals in the decomposition furnace decreased from 95.9-82.1% under the O<sub>2</sub>/CO<sub>2</sub> atmosphere. Given this, optimizing the process parameters to improve the decomposition rate of CaCO<sub>3</sub> under the O<sub>2</sub>/CO<sub>2</sub> atmosphere is necessary.
- Under the O<sub>2</sub>/CO<sub>2</sub> atmosphere, the velocity field in the furnace did not change significantly. Meanwhile, with the strong radiation capacity of CO<sub>2</sub> molecules, the temperature distribu-

concentration is negligible. With the combustion of pulverized coal, O<sub>2</sub> is rapidly consumed, and the concentration gradually decreases. Concentration at the outlet of the decomposition furnace was only 3.04%, which is consistent with the measured value. Compared with the O<sub>2</sub> concentration in O<sub>2</sub>/CO<sub>2</sub> atmosphere, the O<sub>2</sub> content in the primary combustion region in the O<sub>2</sub>/CO<sub>2</sub> atmosphere was about 9~17%. It is mainly because the high CO<sub>2</sub> concentration in O<sub>2</sub>/CO<sub>2</sub> atmosphere deteriorates the combustibility of pulverized coal and reduces the O<sub>2</sub> consumption. Under this influence, along the direction of furnace height, the O<sub>2</sub> concentration of the whole decomposition furnace in the

tion in the high temperature zone in the furnace was more uniform, and the range of the high temperature area was narrowed. It is beneficial to improve the clinker strength and reduce the fume volume. In addition, the high concentration of CO<sub>2</sub> at the outlet can be recovered and collected, which is conducive to the reduction of CO<sub>2</sub> emission.

- The high CO<sub>2</sub> partial pressure significantly reduced the thermal NO<sub>x</sub> in the decomposition furnace. Compared with the O<sub>2</sub>/N<sub>2</sub> atmosphere, the high concentration of NO<sub>x</sub> area was significantly reduced in the primary combustion area under the O<sub>2</sub>/CO<sub>2</sub> atmosphere, and the concentration of NO<sub>x</sub> at the decomposition furnace was reduced from 619-391 mg/m<sup>3</sup>. The NO<sub>x</sub> at the outlet of the decomposition furnace was decreased by 37%.

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