Research Paper

Numerical Simulation of Cement Kiln Combined with Thermal Plasma for SF₆ Pyrolysis

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Abstract

Although SF₆ gas has been used as insulation in electric power and transmission equipment, it is a very harmful greenhouse gas. SF₆ can be injected inside the cement kiln, for pyrolysis and safe conversion, during cement production. As the temperature distribution inside a kiln is not uniform, the pyrolysis and conversion efficiency of SF₆ are low. In this study, a kiln reactor combined with thermal plasma torches was applied to develop a high pyrolysis rate for SF₆. A numerical analysis was conducted to investigate the variation of heat flow that thermal plasma causes inside the cement kiln. The simulations were conducted for kilns that did and did not include a thermal plasma torch. The results showed that the average temperature inside the kiln with thermal plasma was relatively low due to the gas-mixing effect of the latter; however, the peripheral temperature was stabilized. In addition, the temperature of the near kiln inlet increased. As a result, it is expected that the internal temperature of a kiln combined with thermal plasma technology will become uniform due to the gas-mixing effect of thermal plasma, and the SF₆ pyrolysis efficiency will increase as the temperature of the local region rises.

Keywords: SF₆, Decomposition and conversion, Numerical analysis, Cement kiln, Thermal plasma

1. Introduction

Sulfur hexafluoride (SF₆) has been widely used as a typical insulating gas in electric power distribution and transmission equipment. It is a chemically stable perfluorocarbon compound containing the fluorine element. It is also a considerably harmful greenhouse gas, which have a long lifetime in the atmosphere and a high global warming potential of 23,900 (CO₂ = 1) [1-5]. SF₆ must be treated to be converted into environmentally safe compounds as emission amounts are increasing with industry growth [6,7].

SF₆ can be injected inside the cement kiln, for pyrolysis and safe conversion, during the cement production process. It is theoretically pyrolyzed above 2000 K [8]; therefore, a cement kiln with a temperature of around 2000 K is a suitable environment for SF₆ pyrolysis [9-11]. Additionally, kilns contain a large amount of calcium oxide (CaO), which is an effective reactant for converting pyrolyzed SF₆ radicals into

fluorite (CaF₂) [12,13]. CaO is produced by the decarboxylation of calcium carbonate (CaCO₃), which is the main ingredient in cement. Therefore, SF₆ can be converted to a safe material, without affecting the cement production process, by the reaction between CaO and SF₆.

As the temperature inside a kiln is not uniformly distributed according to the internal space, however, pyrolysis and conversion efficiency are low [11-13]. Therefore, it is necessary to develop a technique by which to effectively maximize its disposal and energy efficiency.

The thermal plasma technique provides a region of high temperature, of over several thousand Kelvin, to enable SF₆ pyrolysis [14]. It also provides advantages such as a rapid reaction time and the presence of abundant reactive species [15-17].

This work investigated the use of a cement kiln combined with a thermal plasma torch as an efficient disposal technique for high-capacity SF₆. Thermal plasma offers an additional heat source and improves the SF₆ pyrolysis process. A numerical analysis was

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performed to investigate variation of the heat flow inside the cement kiln by thermal plasma. In this work, the simulations were carried out for kilns combined with and without a thermal plasma torch.

II. Experimental details

A. Simulation of thermal plasma

- Model description

A DC nontransferred thermal plasma torch was used as an additional heat source for decomposing SF_6 [18,19]. The thermal plasma characteristics inside the torch were simulated using the DC plasma torch in unstructured grid system code [20,21], which is a self-developed magnetohydrodynamic code [22–25]. In the present study, two-dimensional (2-D) numerical modeling of thermal plasma was carried out under usual assumptions [25–29]. The nontransferred arc plasma was assumed to be quasi-neutral, steady, optically thin, and at local thermodynamic equilibrium under atmospheric pressure [29]. The gravitational force was considered negligible compared to the Lorentz force [30]. As the plasma flow can be modeled in a manner similar to a fluid, the hydrodynamic movements were described using the Navier-Stokes equations in terms of cylindrical coordinates (r , θ , z) [31]. The plasma flow inside the torch were described using the equations of the conservation of mass (Eq. (1)), momentum (axial component, Eq. (2); radial component, Eq. (3); azimuthal component, Eq. (4)), and energy (Eq. (5)), as given below:

$$\frac{\partial}{\partial z}(\rho u) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r v) = 0 \quad (1)$$

$$\rho u \frac{\partial u}{\partial z} + \rho v \frac{\partial u}{\partial r} = -\frac{\partial P}{\partial z} + j_r B_\theta - \left[\frac{1}{r} \frac{\partial}{\partial r}(r \tau_{rz}) + \frac{\partial \tau_{zz}}{\partial z} \right] \quad (2)$$

$$\begin{aligned} \rho u \frac{\partial v}{\partial z} + \rho v \frac{\partial v}{\partial r} = \\ -\frac{\partial P}{\partial r} - j_z B_\theta - \left[\frac{1}{r} \frac{\partial}{\partial r}(r \tau_{rr}) - \frac{\tau_{\theta\theta}}{r} + \frac{\partial \tau_{rz}}{\partial z} \right] + \frac{\rho v_\theta^2}{r} \end{aligned} \quad (3)$$

$$\rho u \frac{\partial v_\theta}{\partial z} + \rho v \frac{\partial v_\theta}{\partial r} = -\left[\frac{1}{r^2} \frac{\partial}{\partial r}(r^2 \tau_{r\theta}) + \frac{\partial \tau_{z\theta}}{\partial z} \right] - \frac{\rho v v_\theta}{r} \quad (4)$$

$$\begin{aligned} \rho u \frac{\partial h}{\partial z} + \rho v \frac{\partial h}{\partial r} = \frac{j_z^2 + j_r^2}{\sigma} - S_R + \frac{5k_B}{2e} \left(\frac{j_z}{c_p} \frac{\partial h}{\partial z} + \frac{j_r}{c_p} \frac{\partial h}{\partial r} \right) \\ + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{k}{c_p} \frac{\partial h}{\partial r} \right) + \frac{\partial}{\partial z} \left(\frac{k}{c_p} \frac{\partial h}{\partial z} \right) + v \frac{\partial P}{\partial r} + u \frac{\partial P}{\partial z} \end{aligned} \quad (5)$$

where h is the specific enthalpy, k is thermal conductivity, c_p is the specific heat at constant pressure, and S_R is the radiation loss by the optically thin plasma assumption. The electromagnetic properties, such as magnetic field and current density, are important for numerically analyzing the discharge phenomena. In the 2-D simulation, the current density $\vec{j}$ satisfied the current continuity equation, $\vec{\nabla} \cdot \vec{j} = 0$. The current continuity equation can be written in terms of electric potential ϕ , as shown in Eq. (6) [32], and it was employed to determine the electromagnetic fields in the arc.

$$\begin{aligned} j_r = -\sigma \frac{\partial \phi}{\partial r}, j_z = -\sigma \frac{\partial \phi}{\partial z} \quad \text{and} \\ \frac{\partial}{\partial z} \left(\sigma \frac{\partial \phi}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(\sigma r \frac{\partial \phi}{\partial r} \right) = 0 \end{aligned} \quad (6)$$

As a thermal plasma jet has turbulent flow, the k - ϵ model was used to include the thermal plasma jet is turbulent flow characteristics [21,25,32,33].

- Boundary conditions and simulation results

The computational domain for simulation of the thermal plasma torch are shown in Fig. 1. For the 2-D modeling of the torch, the plasma forming gas inlet, torch outlet, cathode wall, anode wall, and plasma fluid zone for free space plasma were designated as the boundary conditions. A numerical simulation of the thermal plasma jet was performed to investigate the arc discharging, flow, and electrical characteristics

Figure 1. (Color online) Simulation domain and grid system of a thermal plasma torch.

Table I. Operating condition of DC nontransferred thermal plasma torch.

Data	Working gas (N ₂) (L/min)	Current (A)	Arc voltage (V)	Power (kW)
Measured	110.0	110.0	215.0	23.65
Calculated			215.9	23.75

Figure 2. (Color online) Profiles of (a) temperature and (b) axial and radial velocity according to radial direction at the torch exit.

inside the torch. The operating conditions of the plasma torch are given in Table I. N₂ was used as the plasma-forming gas with a flow rate of 110 L/min. The actual plasma input power, 23.65 kW, was provided with the arc current, 110 A. A comparison of the measured and calculated power is also presented in Table I. The calculated input power was 23.75 kW and the measured input power was 23.65 kW. This shows a small difference of 0.004 %, which proves the reliability of the calculation results. Figure 2 shows the temperature and velocity profiles according to the radial direction at the torch exit. As in Fig. 2(a), it was confirmed that the temperature of the thermal plasma jet core was 5000 K or more at the torch exit. Considering that SF₆ is pyrolyzed as 99.99999 %

around 4000 K, it is expected that SF₆ passing through a high-temperature region is completely pyrolyzed. Figure 2(b) shows the profiles of the axial and radial velocity at the torch exit. The extracted temperature and velocity values at the torch exit were used as the ‘plasma inlet’ boundary conditions for the kiln simulation.

B. Simulation of cement kiln

- Model description

A rotary kiln involves rotation of a cylindrical kiln to convert raw material to cement clinkers, however rotation of the kiln was disregarded in this study [34]. The steady state continuity, momentum, and energy equations were employed to solve the flow field. The renormalization group (RNG) k - ϵ model, derived from the Navier-Stokes equations using the RNG method, was used to model the turbulence [35]. The SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm was used to couple the pressure and velocity. For gas phase radiation, the radiation was modeled with a P-1 radiation model of Fluent [36]. The discrete phase model was employed to calculate the trajectories of the coal particle. The process of coal combustion was computed using the eddy dissipation model.

- Gas phase model

The equations of continuity and momentum are shown in Eqs. (7) and (8) below:

$$\frac{\partial}{\partial x_i}(\rho u_i) = S_{p,g} \quad (7)$$

$$\frac{\partial}{\partial x_i}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i + F_i + S_{p,g} \quad (8)$$

The source term $S_{p,g}$ in Eq. (8) is caused by the interaction between combustion particles and gas. The transport equations for the RNG k - ϵ turbulence model are defined as:

$$\frac{\partial}{\partial x_i}(\rho k u_i) = -\frac{\partial}{\partial x_j} \left(\alpha_k \mu_{eff} \frac{\partial k}{\partial x_j} \right) + G_k + G_b - \rho \epsilon \quad (9)$$

$$\begin{aligned} \frac{\partial}{\partial x_i}(\rho \epsilon u_i) = & -\frac{\partial}{\partial x_j} \left(\alpha_\epsilon \mu_{eff} \frac{\partial \epsilon}{\partial x_j} \right) + C_1 \frac{\epsilon}{k} (G_k + C_3 G_b) \\ & - C_2 \rho \frac{\epsilon^2}{k} - R_\epsilon \end{aligned} \quad (10)$$

The parameters G_k and G_b in Eqs. (9) and (10) are the kinetic energies generated due to the mean velocity gradients and buoyancy, respectively.

The energy equation is given in Eq. (11) as follows:

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\vec{v}(\rho E + P)) = \nabla \cdot (k_{eff} \nabla T - \sum_j h_j \vec{j}_j + (\vec{\tau}_{eff} \cdot \vec{v})) + S_h \quad (11)$$

The terms on the right side of the energy equation are expressions of the energy transfer. The term S_h includes the radiation and combustion heat transfer rates.

In this study, the radiation was modeled as the P-1 model, which is in charge of the radiation exchange between coal particles and gas.

$$-\nabla \cdot \vec{q}_r = aG - 4an^2\sigma T^4 \quad (12)$$

In Eq. (12), a is the absorption coefficient, G is the incident radiation, n is the refractive index of the medium, and σ is the Stefan-Boltzmann constant; $-\nabla \cdot \vec{q}_r$ represents the term of radiation flux, which can be replaced by the energy equation to account for a heat source as result of radiation.

- Particle description

The motion of the coal particle was calculated using the Lagrangian frame [37,38]. The corresponding Lagrangian equation for particle tracking is as follows:

$$\frac{d\mu_p}{dt} = F_D(\mu - \mu_p) + \frac{g_x(\rho_p - \rho)}{\rho_p} + F_x \quad (13)$$

where μ and μ_p are the gas and particle velocities, respectively; $F_D(\mu - \mu_p)$ is the drag force per unit particle mass; $g_x(\rho_p - \rho)/\rho_p$ is the gravitational force; F_x represents the additional force.

Combustion processes of coal are first treated as devolatilizing. The coal particles are heated by the energy from the gas. After, the coal particles begin to devolatilize. The single-rate model was employed to solve the rate of devolatilization, assuming that the rate of devolatilization was defined using the one-step Arrhenius scheme and depends on the residual volatiles of the particles [39].

$$-\frac{dm_p}{dt} = k[m_p - (1 - f_{x,0})(1 - f_{y,0})m_{p,0}] \quad (14)$$

In Eq. (14), m_p and $m_{p,0}$ are the mass and initial mass of the particles, respectively; $f_{x,0}$ and $f_{y,0}$ are the mass fractions of volatiles initially present in the particle and the evaporating material, respectively. The kinetic rate k is represented by:

$$k = Ae^{-(E/RT)} \quad (15)$$

where A is the pre-exponential factor, and E is the activation energy.

After the released volatile of the particle is completely burned, combustion of the char begins. To describe char burning, the kinetic/diffusion-limited rate model was used, as given in Eq. (16), which assumed that the surface reaction rate is determined by either kinetics or the diffusion rate [40].

$$\frac{dm_p}{dt} = -A_p p_{ox} \frac{D_0 R}{D_0 + R} \quad (16)$$

where A_p is the surface area of the particle, p_{ox} is the partial pressure of oxidant species in the gas, and R is the kinetic rate, as shown in Eq. (17).

$$R = Ce^{-(E/RT_p)} \quad (17)$$

where C is the kinetic-limited rate pre-exponential factor, and E is the reaction activation energy.

- Boundary conditions

In this study, a numerical analysis was conducted to examine variation of the heat flow inside the cement kiln by thermal plasma. For the two cases, simulations were conducted of the kiln combined with and without thermal plasma. The simulation domain and three-dimensional grid system for the numerical modeling of the cement kiln is shown in Fig. 3. The kiln length and diameter were 94 and 5.36 m, respectively. Coal along with coal carrier air, primary air, and central air were injected through the burner, and secondary air was entered around the burner. The diameter of the burner was 0.72 m. The boundary conditions of the kiln imposed primary and secondary velocity inlet, pressure outlet, and no-slip wall, respectively. The flow rate and boundary conditions for kiln

Figure 3. (Color online) Three-dimensional simulation domain and grid system for modeling cement kiln.

Table II. Flow rate and boundary conditions for kiln operation.

Boundary condition	Inlet velocity (m/s)	Temperature (K)
Flow rate of primary air	89.99	300
Flow rate of coal / coal feeding	38.00 / 4.17 (kg/s)	300
Flow rate of central air	1.447	300
Flow rate of secondary air	7.559	1300

[a]

[b]

Figure 4. (Color online) Illustration of inlet boundary of cement kiln (a) without thermal plasma and (b) with thermal plasma.

operation are detailed in Table II. The simulation domains of the two cases are compared in Fig. 4. It can be clearly seen from Fig. 4(b) that three thermal plasma torches were installed at the center of the

Figure 5. (Color online) Thermodynamic equilibrium composition of 1 mol SF₆ according to temperature.

burner. The distance between each torch was 0.0571 m and the diameter of the plasma torch was 0.011 m; the same for all three.

III. Results and discussion

A. Thermodynamic equilibrium calculation of SF₆ pyrolysis

Calculating the chemical equilibrium composition predicts the thermodynamic properties including decomposition temperature and recombination of SF₆. The thermodynamic equilibrium composition was calculated for the temperature range of 300–6000 K under atmospheric pressure to estimate the decomposition temperature of SF₆. The calculation was achieved using HSC chemistry version 9 (Outotec), which is designed for chemical reactions and equilibria calculations of mixed gas. The thermodynamic equilibrium composition of 1 mol SF₆ in the given temperature range under atmospheric pressure is shown in Fig. 5. As a result, it was confirmed that SF₆ began to dissociate into SF₅, SF₄, SF₃, SF₂, SF, and F₂ at 1300 K, and completely dissociated into S and F atoms at over 4000 K. CaF₂ was produced by the reaction of pyrolyzed SF₆ and CaO according to the following chemical reaction inside the kiln:

To predict the re-decomposition temperature of CaF₂, the thermodynamic equilibrium composition of CaF₂ was calculated for the temperature range 300–6000 K under atmospheric pressure. The result is presented in Fig. 6. CaF₂ began to pyrolyze at temperatures above 3000 K, indicating the possibility that CaF₂ can

Figure 6. (Color online) Thermodynamic equilibrium composition of 1 mol CaF_2 according to temperature.

Figure 7. (Color online) Temperature distribution inside cement kiln; (a) entire simulation region of kiln and (b) enlarged region near the inlet boundary of kiln up to 15 m.

be pyrolyzed when it is mixed with high-temperature thermal plasma, of several thousand Kelvin or more. Therefore, it is necessary to simulate the temperature distribution inside the kiln combined with the thermal plasma torch, which provides a region of high temperature over 10,000 K to prevent re-decomposition.

B. Simulation results for cement kiln

Figure 7 presents the temperature distribution inside the cement kiln. Figure 7(a) shows the temperature distribution inside the kiln on the x -plane ($y = 0$ m). Meanwhile, Fig. 7(b) shows the temperature distribution inside the kiln without thermal plasma near the inlet boundary of the kiln. The maximum temperature of the gas inside the kiln was 2321 K, and the temperature was relatively high at the region of coal burning. A region of low temperature up to 5 m was confirmed to have formed as a result of the primary air and central air injected at 300 K. The average temperature of the gas was approximately 1500 K. Considering that the pyrolysis temperature of SF_6 is

Figure 8. (Color online) Temperature distribution inside cement kiln combined with thermal plasma; (a) entire simulation region of kiln and (b) enlarged region near the inlet boundary of kiln up to 15 m.

approximately 2000–3000 K, it was predicted that SF_6 will not be completely pyrolyzed only by the temperature of the kiln. Hence, thermal plasma was used as a heat source to increase the pyrolysis rate of SF_6 . The kiln combined with thermal plasma was numerically analyzed, and the change of thermal flow inside the kiln was examined.

C. Simulation results for cement kiln combined with thermal plasma

Figure 8(a) shows the temperature distribution inside the cement kiln combined with thermal plasma on the x -plane ($y = 0$ m). Figure 8(b) shows the temperature distribution inside the kiln combined with thermal plasma near the inlet boundary of the kiln. Comparing the temperature distribution inside the kiln near the inlet boundary for both cases, it was confirmed that the temperature is relatively low at the coal burning region for the kiln combined with thermal plasma. In addition, the low-temperature region formed up to 7 m in length.

A comparison of the velocity vector field near the inlet boundary of the kiln is shown in Fig. 9; (a) shows the vector field inside the kiln without thermal plasma, and (b) shows the vector field inside the kiln combined with thermal plasma. As in Fig. 9(b), the air which entered through the burner was observed to be quickly drawn to the center. Figure 10(a) shows the mole fraction of CO_2 inside the kiln, and Fig. 10(b) shows the case-applied thermal plasma. Figure 10(b) confirms that the concentration of CO_2 remarkably decreased and rapidly diffused to the periphery. Due to the rapid mixing of the air by thermal plasma, the reaction between the gas was accelerated, and it was

Figure 9. (Color online) Velocity field of flow inside cement kiln (a) without thermal plasma and (b) with thermal plasma.

Figure 10. (Color online) Mole fraction distribution of CO₂ inside cement kiln (a) without thermal plasma and (b) with thermal plasma.

predicted that coal burning occurred rapidly. The temperature profiles according to the radial direction at the points 10, 15, and 20 m along the central axis of the kiln are shown in Fig. 11. As the distance from the kiln inlet increases, it can be seen that the temperature changes inside the kiln combined with thermal plasma were less than those of the original kiln (without thermal plasma). The temperature inside the kiln was confirmed to become uniform as the high-temperature gas diffused to the surroundings rather than forming the local high-temperature region. The temperature distribution near the inlet boundary of the kiln for the two cases are compared in Figs. 12(a) and 12(b). It can be seen clearly from Fig. 12(b) that a high-temperature region of approximately 4000 K or

Figure 11. (Color online) A comparison of temperature profiles of the kiln without thermal plasma and the kiln combined with thermal plasma along the central axis according to radial direction.

Figure 12. (Color online) Temperature distribution inside cement kiln near the kiln inlet region (a) without thermal plasma and (b) with thermal plasma.

more was locally formed up to 0.5 m as applied thermal plasma. It is expected that SF₆ injected from the burner will be mixed in the high-temperature region and sufficiently pyrolyzed.

IV. Conclusions

In this study, a numerical analysis was carried out to investigate variation of the heat flow inside a cement kiln by thermal plasma for the high-capacity pyrolysis of SF₆. As a result of the thermodynamic equilibrium calculations, SF₆ dissociates at a temperature range of ~1300–2000 K and completely pyrolyzes to each element at 4000 K. From the simulation results, it was confirmed that the average temperature of gas inside the kiln was approximately 1500 K. Therefore, it is predicted that SF₆ will not completely decompose by only the temperature of the kiln. The average temperature inside the kiln combined with thermal

plasma was analyzed to be relatively low due to the gas-mixing effect of the thermal plasma; however, the peripheral temperature was stabilized. In addition, it was confirmed that the temperature near the inlet boundary of the kiln increased due to the injected thermal plasma. It is expected that the high-temperature region formed locally by thermal plasma will increase the pyrolysis rate of SF_6 . As a result, the internal temperature of the kiln combined with thermal plasma should become uniform due to the gas-mixing effect of thermal plasma, and the pyrolysis rate of SF_6 and the pyrolysis process efficiency increase as the temperature of the local region rises.

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