Numerical Simulations of the Temperature and Velocity Fields in a Plasma-Arc System and Equilibrium Calculations of Steam Injected for Syngas Recovery from POPs

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ABSTRACT

A direct current (DC) experimental facility of 30 kW with plasma-arc technology was set up to study the pyrolysis process in the laboratory. The temperature and velocity fields make a great impact on the transfer and reaction among the molecules, and so determining the destruction efficiency. It's difficult to directly measure the temperature of the arc region, therefore numerical simulation becomes a substitute method. According to the dimension of this facility, a magnetohydrodynamic model is used to simulate the temperature and velocity fields. The section drawings clearly exhibit the phenomenon of cathode jet and cathode spot. Furthermore, the treatment of Persistent Organic Pollutants (POPs) agents in a steam-plasma system for syngas recovery has been simulated. Based on the principle of Gibbs free energy minimum, the equilibrium product distribution versus steam content and temperature is calculated. Amount of syngas increases with the increase of temperature, the process acts as energy transformation - electrical energy is finally restored in the syngas. At the ideal temperature of POPs treatment, the energy recovered (Q_{re}) and the energy input (Q_{in}) both increase with the increase of steam content, but Q_{in} subtracted from Q_{re} gets to maximum while the molar ratio of oxygen to carbon (O/C) is near 1. The results show that the plasma-arc technology is an environmentally friendly and economically feasible for the disposal of POPs.

INTRODUCTION

POPs, a kind of toxic chemical substances that persist in the environment and bio-accumulate in living organisms, can result in human cancer, deformity and genetic mutation; through the grasshopper effect, they can be transported to the area away from the emission source and cause global spread of pollution. The Stockholm Convention on Persistent Organic Pollutants was adopted on May 22 2001 and signed by more than 90 countries including China, and had united these countries working towards the total eradication of these POPs. The convention which entered into force on May 17 2004 requested that nine kinds of POPs pesticides should be destroyed within a decade, polychlorinated biphenyls (PCBs) in the electrical equipments must be eliminated before 2025 while the most feasible and environmentally friendly technology and practice must be adopted to reduce the discharge of by-products of POPs such as dioxin and furan. But DDT, hexachlorobenzene and mirex are still being produced and used in China; PCBs totaled more than 10,000 tonnes is not treated and disposed of in a rational coordinated framework. POPs by-products involves many industrial sectors and cannot be easily reduced.

Incineration is not an effective solution for treating chloride compounds because dioxins and furans, produced by incomplete oxidation, remain in the off-gases as thermally persistent species. Thermal plasma reactors offer the following unique advantages for the destruction of POPs: (1) the steep thermal gradients in the reactor permit species exiting it to be quenched at very fast rates so allowing the attainment of meta-stable states and non-equilibrium compositions, thereby minimizing the reformation of POPs; (2) the volume of off-gas produced is much smaller than that by conventional combustion processes and so is easier and less expensive to manage; (3) The high energy density and temperature associated with thermal plasmas, and the correspondingly fast reaction time, offer the potential for a large capacity with a small reactor. The combination of above characteristics allows plasma technology to be a feasible method for destruction of POPs. [1-3]

Several studies have been conducted to determine whether thermal plasma processes can be used for the gasification of carbonaceous wastes to reduce their weight and volume, and to produce syngas (hydrogen + carbon monoxide + hydrocarbon fractions). A plasma system using graphite electrodes was used to investigate the gasification of carbonaceous wastes. The test was carried out using two different experimental conditions: argon plasma and argon/steam plasma which was generated by adding steam to argon plasma. The results showed a larger weight reduction in the case of steam plasma than in the case of the argon plasma. It is concluded that the gasification of carbon by thermal plasma with steam is very effective for the disposal of carbonaceous wastes into syngas. [4-6]

NUMERICAL SIMULATION

Temperature and Velocity Fields in a Plasma-Arc System

In the previous studies, the magneto hydrodynamic approach is normally introduced to simulate the small arc region, but it is difficult to be applied in the reaction region for the waste treatment. In this paper with the software of FLUENT, numerical simulation of the 30 kW DC plasma-arc reactor (fig.1) is made to predict the temperature and velocity fields. The simulation region includes the arc region and the reaction region.

Fig.1 30kw DC Plasma-Arc Reactor

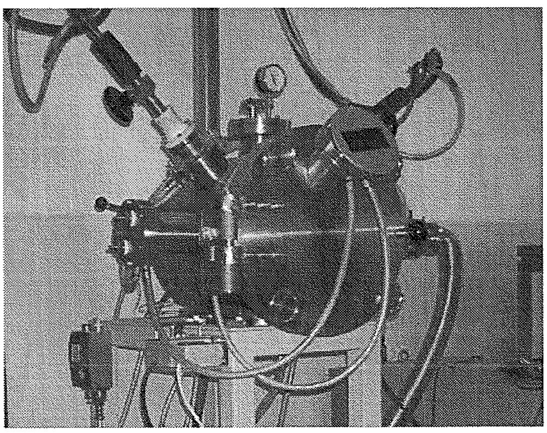
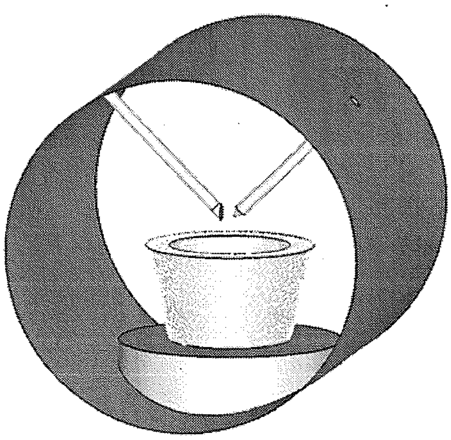


Fig.2 Simplified Simulation Region



The momentum sources are respectively

$$X : j_y B_z - j_z B_y$$
$$Y : j_x B_z - j_z B_x$$
$$Z : j_x B_y - j_y B_x$$

The energy source is

$$\frac{j_x^2 + j_y^2 + j_z^2}{\sigma} + \frac{5}{2}\frac{k}{e}\left(\frac{j_x}{C_p}\frac{\partial h}{\partial x} + \frac{j_y}{C_p}\frac{\partial h}{\partial y} + \frac{j_z}{C_p}\frac{\partial h}{\partial z}\right)$$

The electric potential equation is

$$\nabla \cdot (\sigma \nabla V) = 0$$

The magnetic equation is

$$-\nabla^2 \vec{B} = -\mu[(\frac{\vec{j}}{\sigma}) \times \nabla \sigma]$$

Where j is the electric current density; B is magnetic field induced intensity; σ is electric conductivity; C_p is heat capacity under constant pressure; h is enthalpy; μ is magnetic permeability of vacuum.

Fig3. Velocity Vector Field Near the Crucible

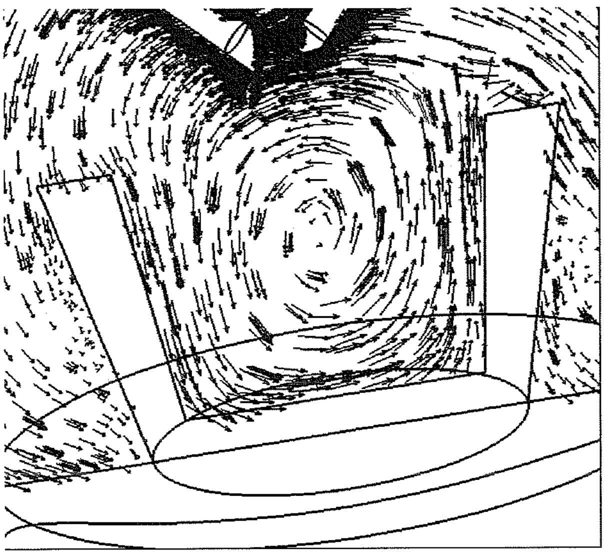
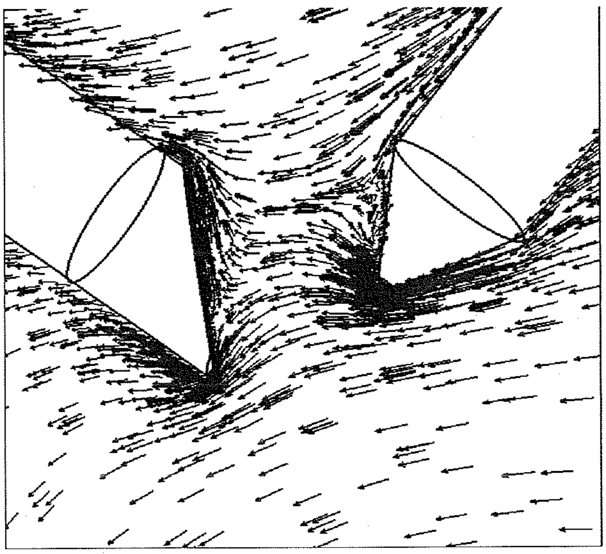


Fig4. Velocity Vector Field Near the Electrodes



The maximum of velocity gets to 200 m/s near the electrodes, and the maximum of temperature exceeds 20000 K in arc region. Fig.4 and Fig. 6 respectively exhibit the phenomenon of cathode jet and cathode spot.

Fig. 5 Temperature Field In the Whole Region

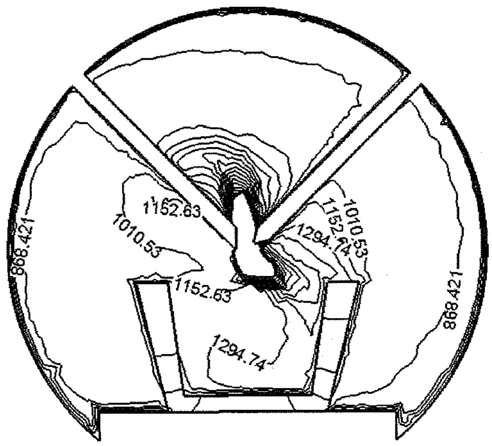
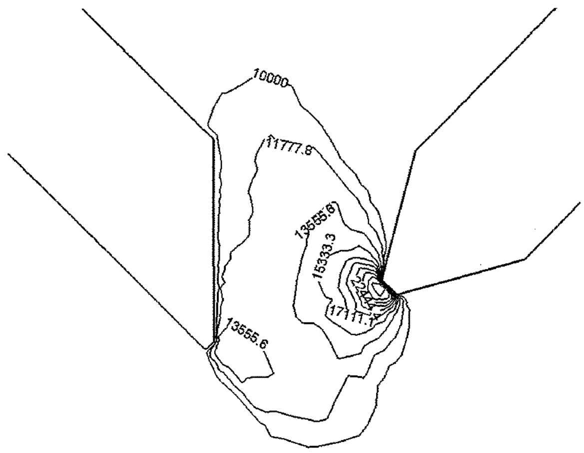


Fig. 6 Temperature Field Near the Electrodes



Steam Injected for Syngas Recovery from Chlorobenzene

The average temperature is considerably high and temperature gravity leads to intense thermal convection in the plasma reactor that the reaction gets to the equilibrium state in a short time, so the numerical simulation results will accord properly with practice. The twelve kinds of POPs listed firstly in the "Stockholm Convention" are all chlorinated aromatic hydrocarbon compounds, so pure chlorobenzene (C_6H_5Cl) is selected as the agent. In this section, the feeding amount of C_6H_5Cl is 1 mol and steam content (α) which is the ratio of quality of steam to C_6H_5Cl. α is from 0.1 to 0.6 and average temperature in the reaction area is from 800 K to 1800 K.

Fig.7 Pyrolysis of C_6H_5Cl in Argon Atmosphere (α=0)

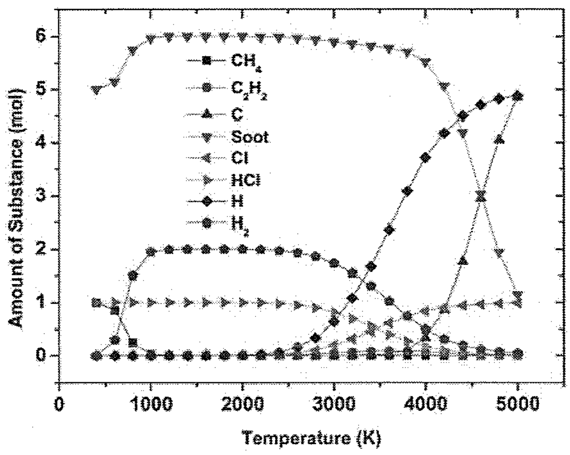


Fig.8 Amount Change of Products with Temperature

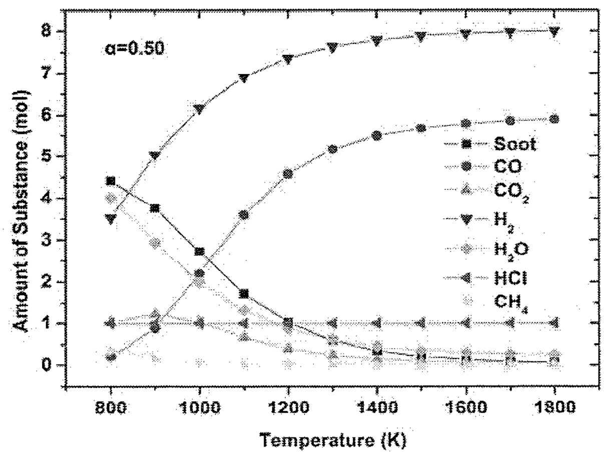


Figure 7 shows that, a lot of soot which is hard to collect and utilize appears in the pyrolysis product of C_6H_5Cl in reductive atmosphere as α=0. As shown in figure 8, with the increase of temperature from 800 K to 1800 K, amount of CO and H_2 increases while that of soot and steam decreases.

Increase of temperature makes the occurrence of the reaction below, $C(S)+H_2O \rightarrow CO+H_2$. Steam injected reacts with hot soot that amount of syngas which has high caloric value is enhanced. The process acts as energy storage - electrical energy is transformed to plasma energy and then stored in the produced syngas. Amount of HCl doesn't change with temperature and chlorine exists only in HCl. Between 1400 K and 1800 K, amount of main products keeps invariable basically.

Figure 9 shows that the amount change of equilibrium products with α when average temperature is 1600 K which is an ideal treatment temperature. Amount of HCl doesn't change with α. With the increase of α from 0.1 to 0.5, amount of CO and H_2 increases while that of soot decreases and steam which reacts completely does not exist in the product. With the increase of α from 0.5 to 0.6, amount of CO decreases while that of CO_2, H_2 and steam, which does not react, increases. When α is near 0.5, steam injected produces relatively large amount of syngas, inhibits the formation of soot in the product and doesn't cause energy waste with no excessive steam.

Fig. 9 Amount change of products with α

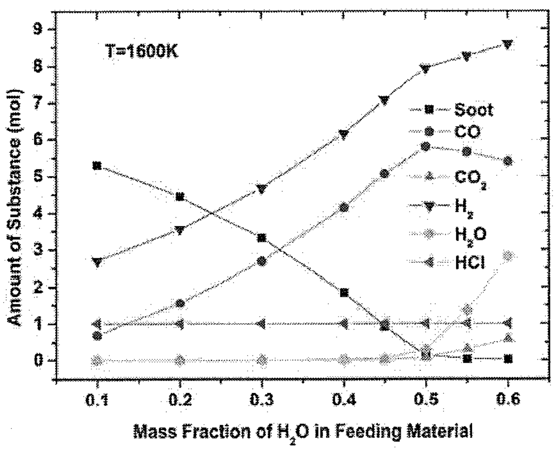
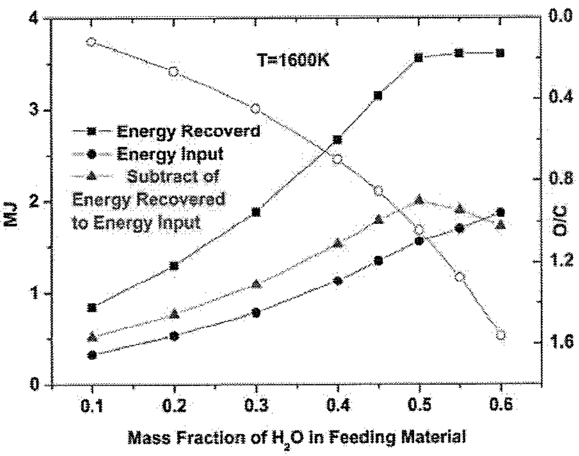


Fig. 10 Amount change of Q_{in}, Q_{re} and Q_{sub} with α



The reaction in the reactor is

$$C_6H_5Cl + mH_2O \rightarrow n_1C(S) + n_2CO + n_3CO_2 + n_4H_2 + n_5H_2O + n_6HCl + Q_0$$

where amount of reactants and resultants are respectively 1, m, n_1, n_2, n_3, n_4, n_5, n_6 mol; the heat release of reaction (Q_0) is obtained through enthalpy of formation of reactants and resultants at the state when temperature is 298.15K and pressure is 1 atm; Δh_f^i is sensible enthalpy of each resultant at1600 K.

The energy input (Q_{in}) is

$$Q_{in} = \sum_{i=1}^{6}\left(\Delta h_f^i \times n_i\right) - Q_0$$

at the equilibrium state.

$$CO+\frac{1}{2}O_2 \rightarrow CO_2+282.964 \ \ kJ/mol$$

$$H_2+\frac{1}{2}O_2 \rightarrow H_2O+241.826 \ \ kJ/mol$$

CO and H_2 have high caloric value, so syngas in the off-gas can be incinerated for energy recovery.

The energy recovered (Q_{re}) is

$$Q_{re} = n_2 \times 282.964 + n_4 \times 241.826 \ \ kJ/mol$$

As shown in Figure 10, when α increases from 0.1 to 0.6, Q_{in} and Q_{re} both increase but the maximum of Q_{sub} (Q_{in} subtracted from Q_{re}) appears in the range where α is between 0.45 and 0.55 while the molar ratio of O/C is near 1.

Steam Injected for Syngas Recovery from Trichlorobiphenyl

PCBs are a kind of POPs listed in the "Stockholm Convention". The most commonly observed health effects in people exposed to large amounts of PCBs are skin conditions such as acne and rashes. Research on exposed workers has shown changes in blood and urine that may indicate liver damage. PCB exposures in the general population are not likely to result in skin and liver effects. Most of the studies of health effects of PCBs in the general population examined children of mothers who were exposed to PCBs. Animals that ate food containing large amounts of PCBs for short periods of time had mild liver damage and some died. Animals that ate smaller amounts of PCBs in food over several weeks or months developed various kinds of health effects, including anemia; acne-like skin conditions; and liver, stomach, and thyroid gland injuries. Other effects of PCBs in animals include changes in the immune system, behavioral alterations, and impaired reproduction. PCBs are not known to cause birth defects. [7]

Fig. 11 Amount Change of Products with α

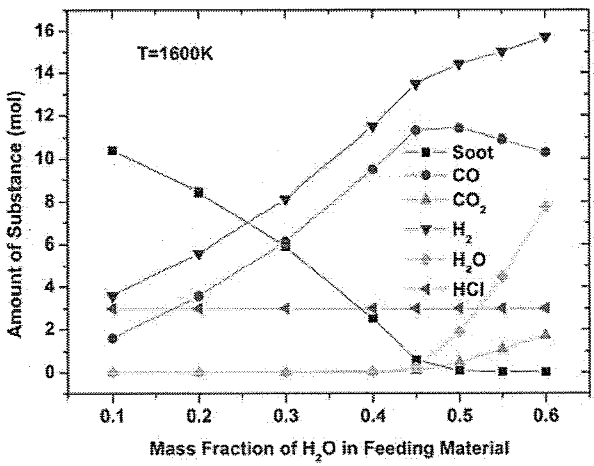
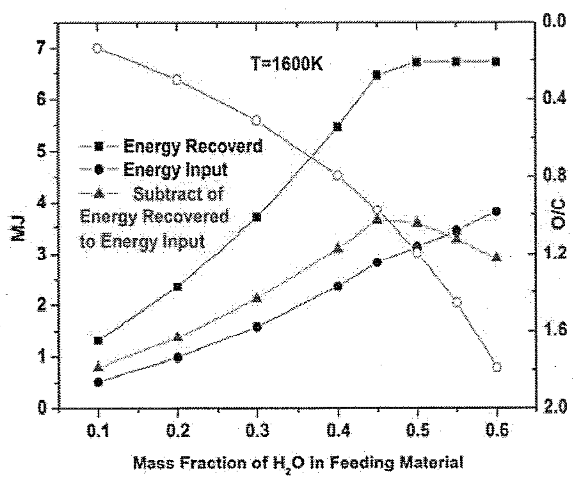


Fig. 12 Amount Change of Q_{in}, Q_{re} and Q_{sub}



According to the same methodology with 2.2, trichlorobiphenyl (one of PCBs) is selected for equilibrium calculations. Figure 11 shows that the amount change of equilibrium products with α when average temperature is 1600 K which is an ideal treatment temperature. Amount of HCl doesn't change with α. With the increase of α from 0.1 to 0.45, amount of CO and H_2 increases while that of soot decreases and steam which reacts completely does not exist in the product. With the increase of α from 0.45 to 0.6, amount of CO decreases while that of CO_2, H_2 and steam, which does not react, increases. When α is near 0.45, steam injected produces relatively large amount of syngas, inhibits the formation of soot in the product and does not cause energy waste with no excessive steam.

As shown in Figure 12, when α increases from 0.1 to 0.6, Q_{in} and Q_{re} both increase but the maximum of Q_{sub} (Q_{in} subtracted from Q_{re}) appears in the range where α is between 0.4 and 0.5 while the molar ratio of O/C is near 1.

CONCLUSIONS

In this paper, according to the real dimension of a 30 kW DC plasma facility, a magnetohydrodynamic model is used to simulate the temperature and velocity fields. The section drawings clearly exhibit the phenomenon of cathode jet and cathode spot. The maximum of velocity gets to 200 m/s near the electrodes, and the maximum of temperature exceeds 20,000 K in arc region. The simulation results supply a valuable reference for the correlative experiment.

Steam injected for syngas recovery from POPs is also calculated. Here, chlorobenzene and trichlorobiphenyl are selected as the POPs agents. The treatment process acts as energy storage - electrical energy is transformed to plasma energy and then stored in the produced syngas. When α increases from 0.1 to 0.6, Q_{in} and Q_{re} both increase, but the maximum of Q_{sub} appears where the molar ratio of O/C is near 1. POPs, which have high calorific value, are difficult to be incinerated. The plasma technology transforms the exothermic potential to truth. A conclusion can be drawn that the plasma-arc technology is an environmentally friendly and economically feasible for the disposal of POPs.

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KEY WORDS

plasma, arc, magnetohydrodynamic, POPs, syngas, recovery