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Study on Coal Gasification Kinetics

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Abstract—*Coal-based conventional power generation technology is a foremost cause of carbon dioxide emissions, which have adverse affect on global warming. Coal gasification has emerged as a clean coal technology which utilizes coal more effectively for power generation and meeting stringent environmental regulations. Integrated gasification combined cycle (IGCC) is being developed as a clean and effective power production plant worldwide. Study on gasification kinetics plays a key role for rate determining process in coal gasifier. Coal gasification reactions in gasifier are divided into three phases like pyrolysis of coal, gasification of char and gas reactions. Characteristics of coal gasification depend on type of coal and gasification medium. Study of gasification reaction mechanism and its reactivity is important for designing and operation of gasifier. This paper reports coal gasification kinetics by reviewing literature on gasification. In this paper reaction rate and activation energy are also reported for different kinetic models.*

Keywords: *coal, gasification, kinetics, reaction rate, activation energy.*

1. INTRODUCTION

Coal is a major energy source for electric power generation in several regions of world. Increase in public awareness toward probable environmental impacts of coal combustion, reducing convention use of coal for power generation. Scientists have made enormous effort to develop a new technology for power production with less environmental impacts. Coal gasification is considered as a clean coal technology for power generation [1]. Coal gasification is completed in two steps; coal pyrolysis and char gasification. Rate of char gasification is slower than the rate of pyrolysis. Char gasification mainly depend upon the design, construction and operating parameters of gasifier. So the kinetic study of char plays a significant role under different gasification conditions. Several investigations have been done on the coal char gasification. Gasification rate depend on the pressure, temperature, composition of gasifying regent, type of the coal, conditions under which char produced and mineral matters present in char which act as catalyst [2]. In this paper attempt has been made to compile the kinetic data obtained from literature.

2. CHAR GASIFICATION KINETICS

Kinetic study of lignite char in CO_2, H_2 and steam atmosphere in packed bed balance reactor (PBBR) system has been reported by [2]. They reported that the experimental results are best perceived by volume reaction model for char gasification in H_2 medium and unreacted core shrinking model for char gasification in CO_2 and steam medium.

Unreacted core shrinking model:

$$1-(1-X)^{1/3}=\bar{K}t \tag{1}$$

Volume reaction model:

$$-\ln(1-X)=K_v P_A^n t=K't \tag{2}$$

Where X is defined as the ratio of the gasification carbon to the initial carbon in the coal, t: time, K_V is the volume reaction rate constant.

Activation energy of char in CO_2, H_2 and steam gasification medium are reported as 149.1, 196.6 kJ and 138.3 kJ mol^{-1} respectively.

[3] Studied the gasification kinetics of Indonesian coal char in CO_2 medium under elevated pressure in pressurized drop tube furnace. They reported that the gasification of char is gas-solid reaction for which conversion rate is divided into two reaction rates such as intrinsic and apparent reaction rate because oxidant diffuses into a surface of particles. Rate equation for non reactive core model is expressed as;

$$\frac{dX}{dt}=kP_{CO_2}^n(1-X)^{2/3} \tag{3}$$

Where k: Apparent reaction coefficient, n: Apparent reaction order, X: Carbon conversion, t: Reaction time, P_{CO2}: CO_2 Gas concentration.

In non reactive coal model, it is assumed that the reaction occurs on the spherical surface of unreacted shrinking sphere carbon. [3] modified the nth order rate equation to (when total pressure of the system changes):

$$\frac{dx}{dt} = A\, e^{-(E/RT)} P_{CO_2}^{n} P_{total}^{m} (1 - X)^{2/3} \quad (4)$$

A: Pre-exponential factor, E: Apparent activation energy, R: Gas constant, T: Gasification temperature

They also reported that the apparent activation energy at high temperature (1100°C to 1400°C) was 71.5 kJmol^{-1} and intrinsic activation energy at low temperature (900°C to 1000°C) was 144 kJ mol^{-1}.

[4] Reported the gasification kinetics of South Australian low-rank coal, Bowmans coal, under CO_2 and H_2O medium in single-particle reactor. They reported that the gasification rate of coal is independent of particle size at a given temperature and same gasification medium. On the basis of this statement they distinguish two kinetic models: homogenous and shrinking core model. They recommended homogenous model for the modeling of Bowmans coal gasification.

For CO_2 gasification:

$$k = 1327 \exp(-10\,945/T) \quad (5)$$

For H_2O gasification:

$$k = 261\,276 \exp(-15\,733/T) \quad (6)$$

K: gasification rate constant, T: temperature.

Activation energy for CO_2 and H_2O are reported as 91 kJ mol^{-1} and 131 kJ mol^{-1} respectively.

[5] Reported the gasification behavior of two types of coal char under CO_2 or steam medium in pressurized drop tube furnace. They reported that the surface area of char increases rapidly i.e. up to approximately six times the initial char surface area size as gasification progresses. The change in surface area and reaction rate is described with the help of random pore model.

Random pore model:

$$\frac{dx}{dt} = k_p (1 - x)\sqrt{1 - \Psi \ln(1 - x)} \quad (7)$$

Grain model:

$$\frac{dx}{dt} = k_g (1 - x)^{2/3} \quad (8)$$

Where T: time, K_p and K_g reaction rate constants, x conversion ratio of char, Ψ dimensionless parameter $\Psi = 4\pi L_0 (1 - \epsilon_0)/S_0^2$, S_o: initial specific area, L_o pore length, ε_o porosity per unit volume of solid.

Fig. 1 shows the comparison of gasification rate obtained from experiment and models.

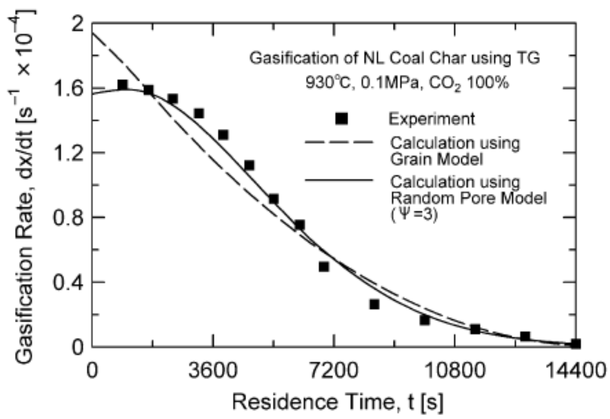

Fig. 1: Gasification rate vs residence time of NL test char measured with TG balance [5].

Activation energy reported for CO_2 was 163kJ/mol and for steam 214 kJ/mol.

[6] Reported that the kinetics of coal char under CO_2 gasifying medium in fixed bed reactor. They reported that the kinetics of char gasification is under chemical control for all studied temperature range. Developed global rate equation:

$$\text{Rate} = \frac{d\alpha}{dt} = (1-\alpha)^{2/3} \cdot 1.1 \times 10^5 \exp\left(-\frac{185 \text{ kJ mol}^{-1}}{R \cdot T}\right) \cdot P_{CO_2}^{0.5} \quad (9)$$

Where α: reaction degree, t: time, R: real gas constant, T: temperature, P_{CO2}: partial pressure of carbon dioxide.

They reported the effect of sample mass on reaction rate by performing gasification reaction with different sample mass. Fig. 2 shows the effect of sample mass on reaction rate, with the decrease in sample mass from 40 to 2.5 mg reaction becomes faster.

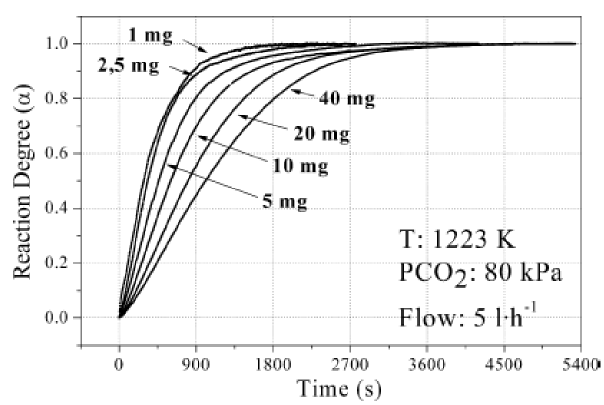

Fig. 2: Effect of mass of sample [6].

To analyze the influence of partial pressure of carbon dioxide on gasification rate, experimental conditions were; Flow: 10l h^{-1}, initial mass: 2.5 mg, temperature: 1223 K, partial pressure of CO_2 varies. It can be seen from the Fig. 3 that as the CO_2 partial pressure increase from 10 to 50 kpa reaction become faster. The time to complete 50% of the reaction were 1130, 750, 510 and 440 s for 10, 20, 40 and 55 kPa. The time to complete 50% of reaction at 60, 70 and 80 kPa was 390s.

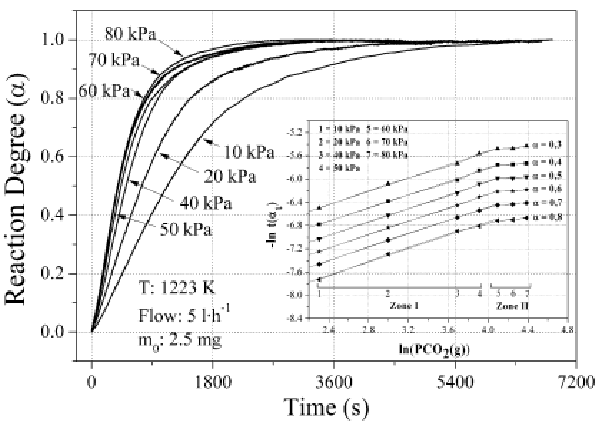

Fig. 3: TG curves for the gasification of char (2.5 mg) at 1223 K and different partial pressure of CO_2 between 10 and 80 kPa [6].

They also reported that the reaction rate is become faster as temperature increases (Fig. 4).

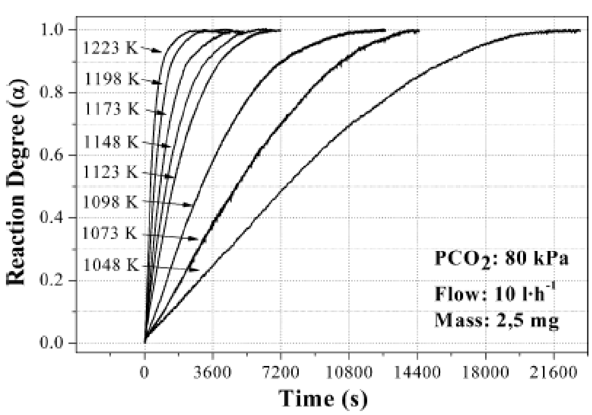

Fig. 4: Effect of reaction temperature on rate of char gasification [6].

3. CONCLUSION

In the above study different kinetic models are reported which describes the rate of gasification reaction. Rate of char gasification reaction is dependent on the type of coal, type of gasifier, gasification medium, reaction temperature and pressure. For different kinetic models activation energies are also reported.

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