Iranian Journal of Chemical Engineering
Vol. 4, No. 1 (Winter), 2007, IAChE

Research note

Study of Carbon Black Production with Optimized Feed to Predict Product Particle Size

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Abstract

Carbon black or soot is a carbon rich material which is widely used as a modifier and filler. Usually carbon black is produced via thermal decomposition of heavy hydrocarbons. This process is too complex to be modelled fundamentally. In this study, the effect of reaction feed composition on the soot production yield was studied experimentally in a lab-scale reactor. The soot production was optimized based on feed Composition and economical aspects. The effects of reaction time and temperature on the product particle size produced using the optimized feed were also investigated experimentally. Then a semi-empirical model was developed to predict soot particle size as a function of reaction time and temperature. The model has been validated upon the experimental data successfully.

Keywords: *Carbon Black, Mathematical Modelling, Soot Particle Size, BMCI, Feed Composition*

Introduction

Carbon black is produced by mean incomplete combustion and/or thermal decomposition of heavy hydrocarbons. In most carbon black production processes, thermal decomposition of hydrocarbons (C_xH_y) is used to produce carbon black efficiently as:

$$C_xH_y \rightarrow x\,C + y/2\,H_2 \qquad (1)$$

There are four main methods of lamp, channel, furnace and acetylene to produce carbon black. These methods differ in the type of energy supply and the type of hydrocarbons in feed and operating conditions. These parameters affect product properties directly. Today, about 90% of the world production of carbon black is produced by means of incomplete combustion of heavy aromatic hydrocarbons using the furnace method [1]. The quality of hydrocarbons as feedstock has an important effect on product properties. The quality of the hydrocarbons is measured by the *BMCI* factor (Bureau of Mines Correlation Index) which is defined as:

$$BMCI = 48640/(B.P.) + 473.7\,(sp.gr.) - 456.8 \qquad (2)$$

Where *B.P.* is average boiling point (^oC) and *sp.gr.* is the specific gravity of feed at 25 ^oC
The common feed of soot production plants

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are coal tar, aromatic substances extracted from heavy oils (furfural extracted) and cracked fuel oil (CFO).The BMCI factor and domestic price of these hydrocarbons are presented in Table 1. The composition of these hydrocarbons in the feed affects both the yield and properties of the product. In this study, we have tried to determine the optimum feed composition based on the operational and economic aspects. Choosing the proper feed, the effect of operating conditions such as the reaction time and the temperature on soot particle size has been studied experimentally and theoretically.

Experimental study

All experiments were conducted in the lab-scale reactor. This reactor works based on the furnace method and is composed of four sections: primary fire (pre-heating), feedstock vaporization, main reaction zone (particle formation and growth) and quenching (finishing). A schematic diagram of this reactor is shown in Fig. 1.

This reactor has an internal heat exchanger to adjust the desirable temperature. In addition, controllable quenching is made possible by spraying water to adjust the reaction time. The soot particle size reported in this study is determined with the standard test method ASTM D1765.

By carrying out several experiments in this reactor under the same operating conditions, the BMCI parameter of the feed was changed (with feed composition) and the weight of the used feed to produce the unit weight of carbon black (gr/gr) in each experiment was measured. The experimental results are shown in Figure 2.

There is a linear relation between BMCI and the cost of feed with the feed composition. By using this linearity and the curve fitting of the experimental data in Fig. 2, Fig. 3 is presented to show the relation of the production cost of the unit weight of carbon black with the furfural extracted composition in the feed. Here we assume a maximum allowable composition of CFO in the feed, which is 30%. Thus, the optimized feed composition to produce carbon black was determined economically. This composition is presented in Table 1.

In the next step, several experiments with the optimal feed composition were conducted in the same reactor in different reaction times and temperatures and the effects of these operating conditions on the soot particle size were investigated. The results are presented in Table 2. These data were then used to verify the model.

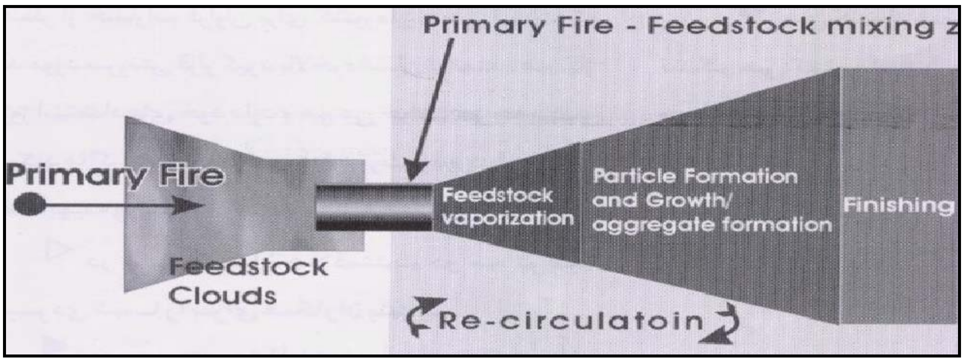

Figure 1. The reactor of carbon black production in the furnace method

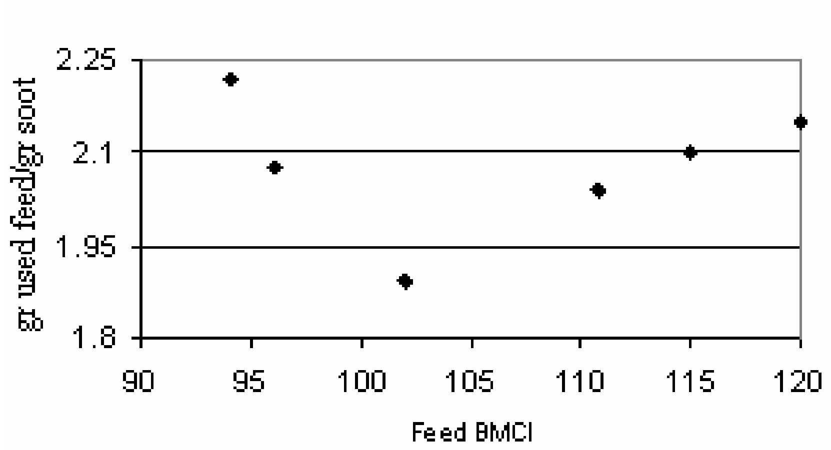

Figure 2. Effect of feed BMCI on the amount of feed used to produce unit weight of carbon black

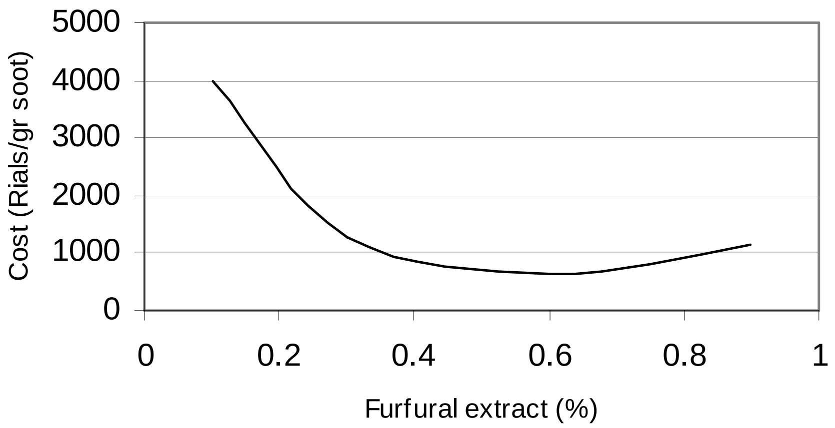

Figure 3. Production cost of unit weight of soot versus furfulal extract composition of the feed

Table 1. Specification and optimized composition of feed components

Feed Component	Ave. BMCI	Price (Rial/kg)	Optimized Feed Composition (%)
Furfural extracted	82.5	252	55
Coal tar	147	807	15
CFO	117	307	30

Table 2. Soot particle size measured in the different reaction times and temperatures

Run No.	Temperature (K)	Reaction time (Sec)	Particle size (Nm)
1	1800	0.1	45
2	1800	0.15	49
3	1800	0.2	57
4	1800	0.5	66
5	1800	1	72
6	1800	1.5	83
7	1825	1	58
8	1855	1	41
9	1900	1	31
10	1975	1	23
11	2060	1	15

Modelling of soot particle size

Generally, four stages of nucleation, surface growth, coagulation and aggregation of the nucleus and finally, agglomeration, are included in the carbon black production process. These phenomena should be considered in the modelling of carbon black formation to predict its particle size and density under different operating conditions. There are many attempts to study this process in a general model [2-6]. A simple and semi-experimental model is presented to formulate carbon black particle density from hydrocarbon mixtures [4, 5]. In this model, a general equation is presented to predict soot particle density per unit volume of exhaust gas (N) at different temperatures (T) and feed concentrations [m] with the thermal decom-position reaction in the absence of oxygen as:

$$N = C_1[m]\exp(\frac{E}{RT}) \tag{3}$$

E is the activation energy of the reaction and C is a constant parameter related to reactor geometry. This equation was derived assuming a constant reaction time (102 msec) and constant reaction yield (60%). In this study, this model is modified to consider the effect of reaction time with lower limitations. Equation 3 can be rewritten with the definition of soot particle density per unit mass of the carbon parameter (N_0):

$$N_o = \frac{C_2[m].P}{y_{60}.q}\exp(\frac{E}{RT}) \tag{4}$$

where P is the flow rate of the exhaust gas, y_{60} is the soot yield (that is presumed to be 60%) and q is the flow rate of the inlet carbon.

By definition of x as the carbon percentage in the feed and F_{se} as the mass flow rate of the feed entering the reactor, parameter q can be determined by the equation $q= x\ F_{se}$. Assuming carbon density 2 gr/cm^3 and constant x parameter in the feeds (90%-92), equation 4 can be rewritten as:

$$N = \frac{C_3[m]P}{F_{se}}\exp(\frac{E}{RT}) \tag{5}$$

To add the effect of the reaction time, the relation between the reaction time and the soot particle size should be studied. This relation has been investigated experimentally [6]. It is shown that soot particle size number density (*N*) has a linear logarithmic relation when time is sufficient to ensure steady conditions. Figure 4 shows this relation.

This slope of the line in this figure is about 0.33, and therefore the following equation is obtained

$$Ln\,d = 0.33 Ln\,t + A \qquad (6)$$

This means that $d \propto t^{1/3}$. In addition, we know $N \propto d^{-3}$ [7]. Therefore, the simple relation $N \propto t^{-1}$ can be used in the model. This relation had been proved theoretically [8]. Now the effect of the reaction time on the soot particle density is introduced by the following equation:

$$d = C\left(\frac{t\,F_{se}}{[m]P}\right)^{1/3} \exp\left(-\frac{E}{3RT}\right) \qquad (7)$$

This equation is used to predict carbon black particle density and size as a function of the reaction times and temperatures.

Results and Discussion

Soot particle size was measured experimentally using the optimized feed at different reaction times and temperatures. Moreover, the effect of these operating conditions on the particle size is determined theoretically. Activation energy of the reaction and the geometry factor of the reactor is determined. They are written as E=-7510 cal/mol.k and C=1.21x10^7 in equation 7 [7]. A comparison of the experimental data of the soot particle size measured in different reaction times and temperatures with the model prediction (equation 7) has been shown in Figs. 5 and 6.

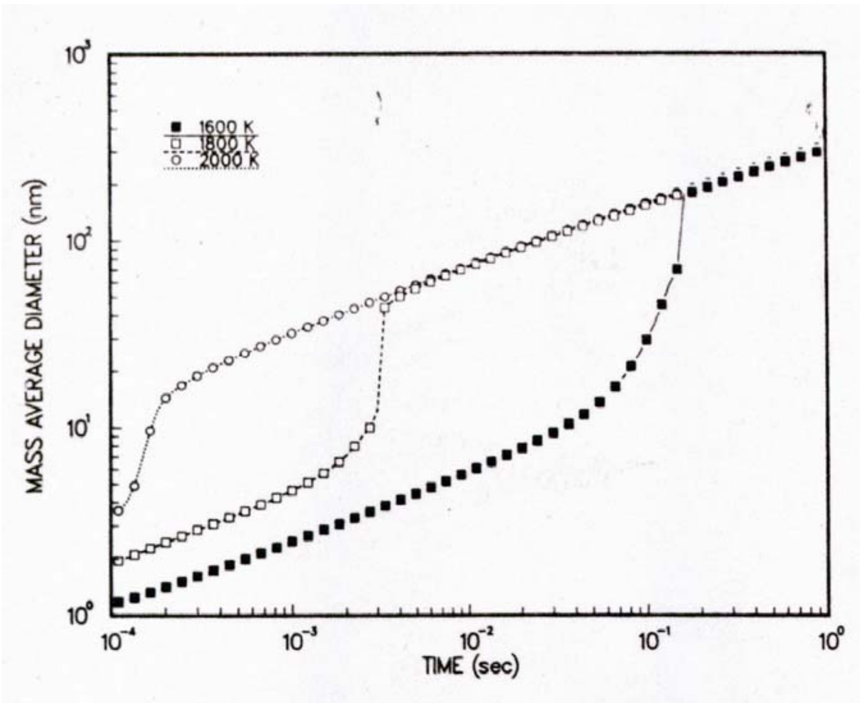

Figure 4. Average diameter of soot particles, according to resident time at different temperatures

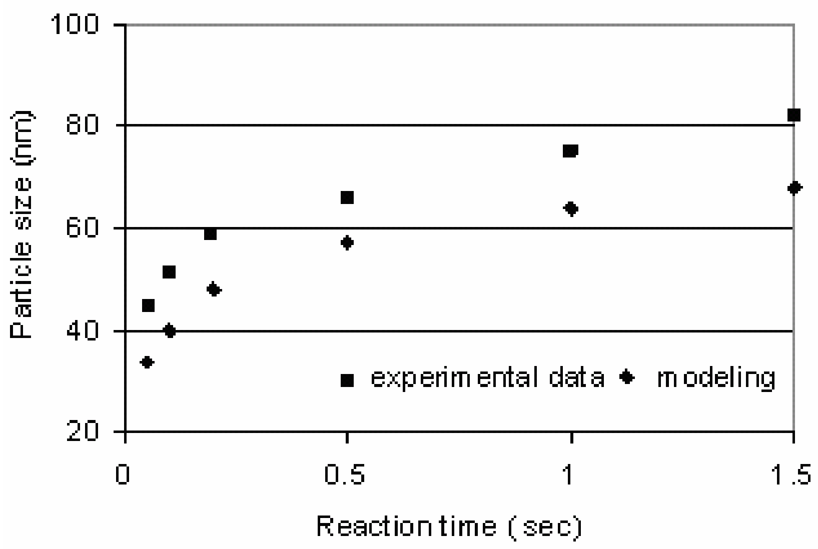

Figure 5. Comparison of model prediction with experimental data of soot particle size in different reaction time

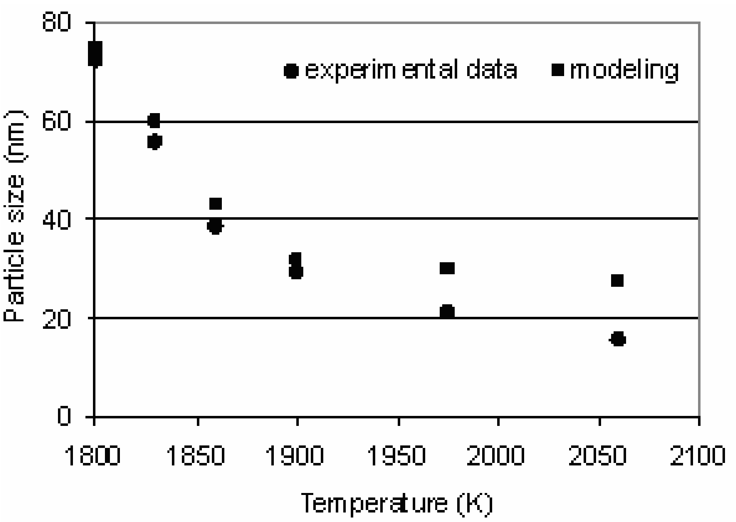

Figure 6. Comparison of model prediction with experimental data of soot particle size in different reaction temperatures

It is shown in these figures that an increase in the reaction time and a decrease in the reaction temperature causes the soot particle size to grow. The prediction of the model is in good agreement with the experimental data. The observed deviation can be attributed to simplifying assumptions in the model and the complexity of the reactions. In addition, there is a soot particle size distribution (soot particle density vs. soot particle size) in the reactor outlet, which varies with the operating conditions. We used the average soot particle size instead of its distribution in this study and this can be a source of error in the model.

The reaction time and temperature affect the rate and progress degree of nucleation, surface growth, coagulation and agglomeration. These phenomena affect the soot particle size independently and cause soot particle size distribution to be generated. Therefore, a detailed study on the effect of the operating parameters on the soot production process needs more complete mathematical modelling, and it is a subject of other studies. [7].

Acknowledgement

We sincerely appreciate the generous help of the head and staff of Iran Carbon Company for cooperating and allowing us to use the lab-scale reactor and the quality control lab of the plant.

Nomenclature

C, C_1, C_2, C_3	Equation constants
d	Soot particle size (nm)
E	Activation Energy (cal/mol k)
F_{se}	Mass flow rate of feed (kg/sec)
N	Soot particle density per unit volume of exhaust gas ($1/m^3$)
N_0	Soot particle density per unit mass of soot (1/kg)
P	Flow rate of exhaust gas (m^3/sec)
q	Flow rate of net carbon entering with feed (kg/sec)
R	Gas constant (J/mol k)
t	Reaction time (m sec)
T	Reaction temperature (k)
y_{60}	Reaction yield (%60)
x	carbon content of feed (%)

References

1. Donnet, J.B., Bansal, R.C. and Wang, M.J., “Carbon black: Science and technology”, New York, Marcel Dekker, (1993).
2. Lockwood, F.C. and Van Niekerk, J.E., “Parametric study of carbon black oil furnace”, Combustion and Flame, **103**, 76, (1995)
3. Zhao, B., Yang, Z., Johnston, M.V., Wang, H., Wexler, A.S., Balthasar, M. and Kraft, M. “Measurement and numerical simulation of soot particle size distribution functions in a laminar premixed ethylene-oxygen-argon flame”, Combus. Flame, **133**, 173, (2003)
4. Tesner, P.A. and Shurupov, S.V., “Soot formation during pyrolysis of Benzene-Xylene mixtures”, Combust. Sci. and Tech., **109**, 401, (1995).
5. Tesner, P.A. and Shurupov, S.V., “Soot formation during pyrolysis of Naphthalene, Anthracene and Pyrene”, Combast. Sci. and Tech., **126**, 139, (1997).
6. Ivie, J.J. and Forney, L.J, “A numerical model of the synthesis of carbon black by benzene pyrolysis”, AIChE Journal, **34**, 1813, (1998).
7. Shakiba, A., “Study of carbon black reactor with optimized feed composition and effect of operating conditions on the particle size distribution” M.Sc. Thesis, Shahid Bahonar University of Kerman, Iran, (2006)
8. Sahebdelfar, S. and Soltanieh, M., “A simple model to predict carbon black particle size in Oil-furnace process”, Proceeding of 10th Iranian Chemical Engineering Conference, Zahedan, Iran, P. 1433 (2005)