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LIQUID COAL CHARACTERISTIC ANALYSIS WITH FOURIER TRANSFORM INFRA RED (FTIR) AND DIFFERENTIAL SCANNING CALORIMETER (DSC)

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Abstract

The aim of this study is to identify the value of compounds contained in liquid coal by using Fourier Transform Infra-Red (FTIR) and Differential Scanning Calorimeter (DSC). FTIR was used to analyse the components contained in liquid coal, while the DSC is done to observe the heat reaction to the environment. Based on the Fourier Transform Infra-Red (FTIR) test results it is shown that the compound contained in the liquid Coal consisting of alkanes, alkenes and alkyne. These compounds are similar compounds. The alkanes, alkenes and alkynes compounds undergo complete combustion reaction with oxygen and would produce CO_2 and water vapour [$H_2O_{(g)}$]. If incomplete combustion occurs, the reaction proceeds in the form of Carbon Monoxide CO gas or solid carbon and H_2O. Combustion reaction that occurs in all these three compounds also produces a number of considerable energy. And if it has higher value of Carbon then the boiling point would be higher. From the Differential Scanning Calorimetric (DSC) test results obtained some of the factors that affect the reaction speed, which are the temperature, the reaction mixture composition, and pressure. Temperature has a profound influence in coal liquefaction, because if liquid coal heated with high pressure, the carbon chain would break down into smaller chains consisting of aromatic chain, hydro-aromatic, or aliphatic. This then triggers a reaction between oil formation and polymerization reactions to form solids (char).

Keywords: Identification, Calorific value, Liquid coal.

1. Introduction

Coal is one of the fossil fuels formed from organic sedimentary rocks, primarily from plants residue, and are formed through a coal formation process. The main elements consist of Carbon, Hydrogen and Oxygen. Coal is also an organic rock that has physical properties and chemical compound that can be found in various forms. Anthracite coal is classified on the highest grade black coal shimmering metallic (86-98% C, 8% moisture content), Bituminous (68-86% C, 8-10% moisture content) and Lignite or brown coal (carbon levels below 60% and moisture content 35-75% by weight). Usually, coal type used is the Anthracite Coal ($C_{240}H_{90}O_4NS$) and Bituminous ($C_{137}H_{97}O_9NS$) which is containing high levels of carbon and a relatively low water moisture level. While Lignite utilization is still less because of a lower carbon value and has a moisture content of 35-75% [1].

The liquefaction process is just simple, which is converting solid coal into a liquid product, at high hydrogen temperature and high pressure with the implementation of a catalyst and solvent media. Coal liquefaction can be done in two ways, namely the indirect liquefaction process and directly liquefaction [2, 3].

In order to ensure the element content as well as the brown coal feasibility as a fuel, it is needed a liquefaction process which must passes through several stages. After the coal melting process a physical testing and chemical testing should be followed, to ensure the liquid coal can be used as oil [4]. In the coal liquefaction quality testing process, an adequate technology is required to detect the elements content contained in liquid coal [5]. On the liquid coal analysis, the contact area parameters and dissolve time is strongly influence the hydrocarbon chain of alkanes and alcohol [6].

The constraint encountered in the tar process, is the compound complexity, so that it is necessary to do a pre separation process in order to facilitate the further utilization. The separation process commonly used for example is the use of fractionation distillation using a reactor based on the component boiling point differences. The tar component separation which has many types of components, such as hydrocarbon fractions ranging from mild to heavy fraction would result an efficiency constraints process and requires considerable large energy for the distillation process [7]. There are several materials that can be used as a stationary phase, namely aluminium and carbon [8, 9]. The use of solvents is crucial in reducing the sulphur content and can cut a covalent bond [10, 11]. There is an evaluation for coal-to-liquids (CTL) plants by using carbon capture and sequestration [12]. The influence and transformation of coal mineral matter during hydrogenation would also be taken account [13, 14].

The compound identification and the reaction rate in the liquid coal are necessary. Compounds contained in a liquid coal should be known to be used as reference materials for the new fuel production. While the coal calorific value identification contained in the liquid coal is very important to know the heating rate and the relation with the liquid coal thermal fragmentation.

2. Material and Methods

The research method is to produce the coal liquefaction process. While, the material used in the liquefaction process consists of Lignite (browncoal) as seen in Fig. 1, solvents and catalysts. The reason to choose lignite utilization is because lignite as a type of coal has low carbon content and a high water content that cannot be used as a solid fuel. A low quality coal in general is built from a small hydrocarbon aromatic group which has many cross links and functions which is very reactive on a rapid and broad cutting bonds activity along with the liquefying process. A low coal quality could produce more liquid product than high quality coal. The solvent used is 1-methyl naphthalene and the catalyst used is the Fe ore.

Fig. 1. Lignite (Brown coal).

The coal liquefaction steps in the process including the selection of the coal that will be liquefied, the process of coal crushing to produce coal powder up to 200 mesh size. The coal powder, catalyst and solvent were added to the 500 ml capacity autoclave. This process takes place at a temperature of 400 °C and a pressure of 20 bar, until the tar appear. Pyrolysis is the method to separate between the liquid and dreg. Pyrolysis was done by using a flow reactor by controlling the fluid flow rate. Tar was filled in the container in the reactor which was already filled with catalyst with a certain weight. The reactor column was then located inside the furnace. The furnace was then heated to a certain temperature, while the tar and gas was then flown together with a constant flow speed. Tar was then vaporized and separated along the reactor. The product result is in a form of liquid and solid.

3. Experimental Design

In the testing process, some test equipments are used, such as the Fourier Transform Infra-Red (FTIR) as seen in Fig. 2, Differential Scanning Calorimeter (DSC) as seen in Fig. 3 and XRD is for the validation and the potential use of liquid coal as a new fuel.

The Fourier Transform Infra-Red (FTIR) test procedure is as follows: Liquid coal as a sample is located in the FTIR container and put in the FTIR apparatus. Switch the FTIR apparatus on. The test result is in a print-out in a form of graph which is showing the peak points (FTIR spectrums), and the wave positions. This file also shows the liquid coal compounds. This file could also be read in a form of Microsoft Excel (table) file.

The steps in the Differential Scanning Calorimeter (DSC), is by filling in a 30.0 mg liquid coal in the DSC container. The container with the sample inside was then located in the DSC apparatus. The apparatus was then switched on a constant temperature of 30°C for one minute. After that, heat the oven with a rate of 20 °C/minute until 445 °C.

To get the liquid brown coal to be tested from the raw brown coal material, a research installation was set up as seen in Fig. 4.

Fig. 2. FTIR-8400S Shimadzu.

Fig. 3. Perkin Elmer DSC 4000.

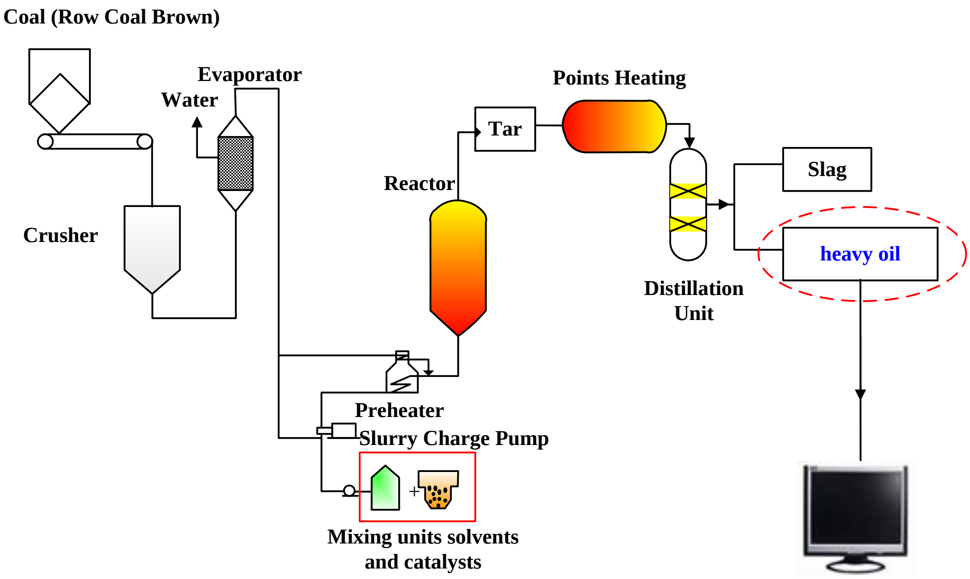

Fig. 4. Research installation.

4. Results and Discussion

Based on the Fourier Transform Infra-Red (FTIR) test results, as seen in Fig. 5, it can be explained that at 2924.09 cm^{-1} wave number is obtained by the alkyne compound. In a condition of 28652.72 cm^{-1} wave number, compounds formed is the alkanes of Methylene. If the compounds of alkanes undergo with a complete combustion reaction with oxygen, then it will produce CO_2 and water vapour [$H_2O_{(g)}$]. If incomplete combustion occurs, the reaction result is in the form of carbon monoxide CO gas or solid carbon and H_2O.

As seen in Table 1 the combustion reactions that occur in the alkane compound also produced a number of considerable energy. If the alkane compounds have a high carbon value then the boiling point will be much higher. On the wave number of 2358.94 to 1913.39 cm^{-1} Hydrocarbon compounds are double (C = C) and at a number of 1602.85 cm^{-1} Hydrocarbons number triplicate (C≡C). Hydrocarbon having duplicate or triplicate is mentioned as Alkene. Alkene is a sensitive compound, it is flammable. While the physical compound of Alkene is ease of an addition reaction, polymerized, substitution and combustible. The addition reaction occurs on a compound which has a double or triple bonds. The Alkene and Alkanes has double and triple bonds with other atoms, on the addition reaction, the molecular compound has a double bonds and absorbing atom clusters so that the double bonds change to single bonds. The polymerization is two molecules with more than one cluster function, which would result a big molecule with a more than one cluster function followed by shifting small molecules.

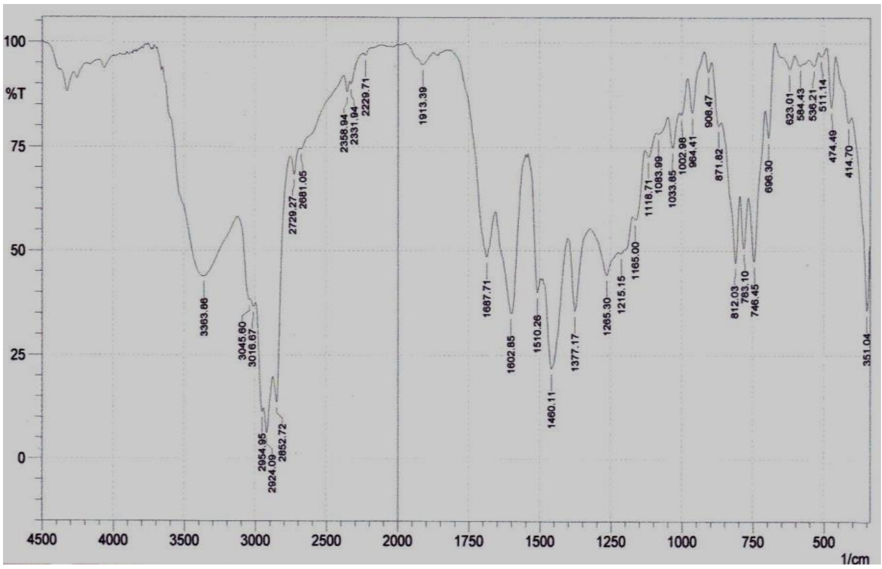

Fig. 5. Results of FTIR testing.

Hydrocarbons, which has two or three bonds is a saturated compound. On a saturated compound it is possible to increase hydrogen. If a saturated compound be reacted with hydrogen, it could produce a single product. The triple bonds compound is stronger than the double or single bonds compound. The bonds distance or the combine length is shorter compared with the double and single bond compound. The shorter the compound bonds the stronger the bonds. The adhesion and cohesion activity and the sediment structure column dissolved between two particles is an important parameter in the liquefied coal processing [8].

Table 1. Alkane wave numbers, cluster function and compound.

Compound	Cluster Function	Wave numbers (cm-^{1})
Alkene (stretching vibration)	≡C-H	2924,09
Alkanes Aromatic rings	=C-H	3045,60 and 3016,67
Alkanes of Methylene	C-H	28652,72
Alkyne	C≡C	2358,94; 2331,94; 2229,4 ;1913,39
Alkenes (buckling vibration)	C=C	1602,85
Alkanes from substituted aromatic deformation	C-H	812,03 and 746,45
Sulphur (elongation vibration)	S=O	1265,3

Based on the Differential Scanning Calorimeter (DSC) test results, Fig. 6, the results obtained a reaction rate of heat transfer from the system to the environment (heat released by the system to its environment). It is characterized by an increase in the ambient temperature around the system. This reaction is known as the exothermic reaction which is a reaction that releases heat, heat flows from the system to the environment. The reaction then lowering the enthalpy results a smaller product enthalpy than the reagent enthalpy. Therefore, the enthalpy change is characterized as negative.

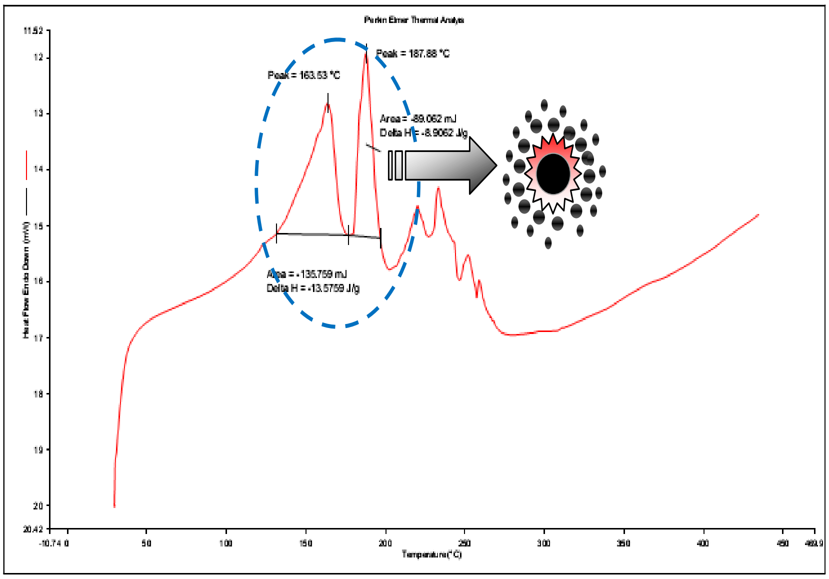

Fig. 6. Differential Scanning Calorimeter (DSC).

The reaction changing is characterized by the blast that spontaneously took place. The burst occurs at a temperature from 163.53 to 187.88 °C at a rate of heat transfer which is released into the environment between 89.062-135.759 mJ and the enthalpy values from 8.9062 to 13.5759 J/kg. In this case the energy released is greater than the energy received.

5. Conclusions

Based on the Fourier Transform Infra-Red (FTIR) test results, it showed that the compounds contained in liquid coal consisting of alkanes, alkenes and alkynes. These compounds are similar compounds. Compounds alkanes, alkenes and alkynes undergo a complete combustion reaction with oxygen gas would produce CO_2 and water vapour [$H_2O_{(g)}$]. If incomplete combustion occurs, then the reaction results are in a form of carbon monoxide, CO gas or solid carbon and H_2O. The combustion reaction that occurs in all three of these compounds also produced a number of considerable energy and if it has a much carbon value then the boiling point will be higher. From the Differential Scanning Calorimeter (DSC) test results, it obtains some of the factors that affect the speed of the reaction, which are the temperature (T), the reaction mixture composition (C) and pressure (P). Temperature has a profound influence in the coal liquefaction, because if liquid coal is given heat under a high pressure, carbon chain will break down into smaller chains consisting of aromatic chain, hydro-aromatic, or aliphatic. This then triggers a reaction there is competition between oil formation and polymerization reactions to form a solid (char).

References

1. Speight, J.G. (2005). *Handbook of coal analysis, chemical analysis a series of monographs on analytical chemistry and its application*. New York: John Wiley & Sons, Inc.
2. Hook, M.; and Aleklett, K. (2009). A review on coal-to-liquid fuels and its coal consumption. *International Journal of Energy Research*, 34(10), 848-864.
3. Dong Shi, S.; Wen, L. B.; Wang, Y.; Zhi, G.; and Jian, L.K. (2008). Study on the mechanism of coal liquefaction reaction and a new process concept. *Journal of Coal Science and Engineering*, 14(1), 119-124.
4. Zhang, G.; Qiao, X.; Miao, X.; Hong, J.; Zheng, J.; and Huang, Z. (2012). Experimental study on the effect of coal to liquid on combustion and emission of heavy-duty diesel engine with exhaust gas recirculation. *Applied Thermal Engineering*, 42(2012), 64-70.
5. Hendratna, K. K.; Nishida, O.; Fujita, H.; and Harano, W. (2010). Laboratory scale of liquid coal fuel combustion process and exhaust gas formation. *American Journal of Environmental Sciences*, 6(3), 204-211.
6. Ogonowski, R.; Wójcik, W.; and Jańczuk, B. (2001). The effect of liquids on the interaction between coal particles. *Physicochemical Problems of Mineral Processing*, 35(2001), 43-53.
7. Hessley, R.K.; Reasoner, J.W.; and Riley, J.T. (1986). *Coal science, an introduction to chemistry, technology and utilization*. London: McGraw Hill Publishing Company Limited.
8. Kirk; and Othmer (1994). *Kirk-Othmer Encyclopedia of chemical technology*. New York: John Wiley & Sons.

9. Smith, F.J.; and Braithwaite A. (2001). *Chromatographic methods (*5th ed.*)*, London: Kluwer Academic Publishers.
10. Li, Y.W.; Feng, J.; Xie, C.K.; and Kandiyoti, R. (2004). Analysis of solvent extracts from coal liquefaction in a flowing solvent reactor. *Fuel Processing Technology*, 85(15), 1671-1687.
11. Rong, F.; and Victor, D.G. (2011) Coal liquefaction policy in china: explaining the policy reversal since 2006. *Energy Policy*, 39(2011), 8175-8184.
12. Mantripragada, C.H.; and Rubin, S.W. (2011). Techno-economic evaluation of coal-to-liquids (CTL) plants with carbon capture and sequestration. *Energy Policy*, 9(2011), 2808-2816.
13. Maldonado, J.F.; Hodar; and Utrilla, R.J. (1995). Influence and transformation of coal mineral matter during hydrogenation. *Fuel*, 74(6), 818-822.
14. Hodar, F.J.M.; Utrilla, R.J.; Lamarca, M.M.A.; and Garcia, F.A.M. (1995). Influence and transformation of coal mineral matter during hydrogenation. *Fuel*, 74(6), 818-822.