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Letter of Appreciation

Dear Dr. Firman A. Noor

On behalf of the Editor-in-Chief of JESTEC, Prof. Dr. Mushtak Al-Atabi, and the Editorial Board, I would like to thank you for your contribution in reviewing the following paper submitted to our journal.

LIQUID LIGNITE COAL COMPOUND AND DREGS ANALYSIS USING GAS CHROMATOGRAPHY-MASS SPECTROMETRY (GC-MS) AND X-RAY POWDER DIFFRACTION (XRD)

I am confident that with your continuous support and commitment, we will be able to maintain the quality and value of JESTEC.

With best regards

Yours sincerely

Dr. Abdulkareem Sh. Mahdi Al-Obaidi, CEng MIMechE
Executive Editor, Journal of Engineering Science & Technology
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Journal of Engineering Science and Technology (JESTEC)

REVIEW FORM

Title of paper:

LIQUID LIGNITE COAL COMPOUND AND DREGS ANALYSIS USING GAS CHROMATOGRAPHY-MASS SPECTROMETRY (GC-MS) AND X-RAY POWDER DIFFRACTION (XRD)

For sections A & B, please tick a number from 0 to 5, where 0 = strongly disagree and 5 = strongly agree.

A. Technical aspects

	0	1	2	3	4	5
1. The paper is within the scope of the Journal.	□	□	□	□	√	□
2. The paper is original.	□	□	□	□	√	□
3. The paper is free of technical errors.	□	□	□	□	√	□

B. Communications aspects

	0	1	2	3	4	5
1. The paper is clearly readable.	□	□	□	□	√	□
2. The figures are clear & do clearly convey the intended message.	□	□	□	√	□	□
3. The length of the paper is appropriate.	□	□	□	√	□	□

C. Comments to the authors (You may use another sheet of paper.)

1. The Coal is then crushed until a form of powder. The coal powder size is 200 mesh. (page 3). A reason is needed why 200 mesh. (Reference)
2. The coal liquification process is under a temperature of 400 °C and a 20 bar pressure, until tar appears. The liquefied coal process is done to separate the liquid coal from coal tar and waste. (Page 3). Please clarify why 400 °C and a 20 bar pressure is chosen. (Reference).

D. Recommendation (Tick one)

1. Accepted without modifications.	√
2. Accepted with minor corrections.	□
3. Accepted with major modification.	□
4. Rejected.	□

E. Comments to the editors (These comments will not be sent to the authors)

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LIQUID LIGNITE COAL COMPOUND AND DREGS ANALYSIS USING GAS CHROMATOGRAPHY-MASS SPECTROMETRY (GC-MS)AND X-RAY POWDER DIFFRACTION (XRD)

Abstract

The aim of this study is to identify compounds contained in liquid coal by using Gas Chromatography-Mass Spectrometry (GC-MS) and X-Ray. GC-MS is used to analyse the compounds contained in coal liquefaction, while the X-ray is used to analyse the compounds homogeneity contained in the liquid coal dregs.Compounds contained in liquid coal. The dominant compounds are methyl and naphthalene. Naphthalene is an aromatic hydrocarbon crystalline white solid form and a form of two united benzene rings. These compounds are volatile, easy to evaporate even in solid form, the vapour produce is flammable. Hydrocarbon compounds are the main substance making up the fuel. When compared with the hydrocarbon group that most of the molecule is most stable found in many organic compounds, the methyl groups are usually part of a larger molecule. The methyl reactivity depends on the substituents adjacent. Methyl groups can be very active. The hydrocarbon homogeneity influence in the liquid coal dregs is very strong because it has a high ionic strength and has a polar property and a high melting point. This is supported by the composition of the hydrocarbon compound remaining in the liquid coal dreg is more than the other compounds composition. This shows that coal residue still can be processed into a new fuel.

Keywords: Identification, compound, homogeneity, dregs, liquid coal

Nomenclatures

C	Carbon
H	Hydrogen
N	Nitrogen
O	Oxygen
S	Sulphur
CO_2	Carbon Dioxide
H_2O	Water
CO	Carbon Monoxide

1. Introduction

Coal is formed from organic sediments derived from plant remains. Coal is a fossil fuel with Carbon, Hydrogen and Oxygen elements inside.Coal could be found in many Chemical and physical forms. Coal is a kind of organic rock) Coal is classified as anthracite as the highest coal grade, it has a black colour, shimmering metallic with 86-98% carbon content and 8% water content, bituminous with 68-86%carbon content and 8-10% water content and lignite with 60% carbon level content and a large content of 35-75%). In general, the use of coal is anthracite coal ($C_{240}H_{90}O_4NS$) and bituminous ($C_{137}H_{97}O_9NS$) containing a high carbon content and still a relatively low water level. While the lignite coal moisture content is still very high (35-75%) and a low carbon content (60%), which resulting a lack of using lignite coal for fuel [1]. The lignite coal utilization for combustion are in cement kilns [2]; gasification [3-5]; supported materials [6] and liquid coal [7-18].

Simply, the coal liquefaction process is a solid coal converting process into a liquid product, at a high hydrogen temperatures and pressures with the aid of a catalyst and a solvent media. The direct and indirect liquefaction are the methods used in the coal liquefaction process [19]. To make sure that the liquefied coal is suitable for fuel, some phase sequence could be follow in the coal liquefaction process. To make sure that the liquefied coal is suitable for fuel, it is necessary to follow the chemical and physics test [20]). In the testing process toward the coal liquefaction quality it is required an adequate technology to detect the elements content contained in the liquid coal [21]. The alkane length and alcohol hydrocarbon chain is highly influenced by the contact area parameter [11].

In the liquefied coal production process, the problem faced is the tar processing as an effect of the problem complexity, so that a separation process is needed. The separation process commonly used, for example is the fractional distillation using a reactor based on the difference the components boiling point. The tar component separation relatively composed of many types of components ranging from light fraction hydrocarbon to heavy fractions hydrocarbon. It would generate the process efficiency constraints and requires a large energy for the distillation process [22]. There are several materials that can be used as the stationary phase being aluminium and carbon [23-24]. The use of solvents is crucial in reducing the sulphur content and can cut the covalent bonds [19,17, 25-26].

The liquid coal calorific value identification contained is very important to know the heating rate and the thermal fragmentation relation to liquid coal. While coal dregs should be analysed to determine the carbon left in the dregs, it would determines the liquid coal dregs feasibility to be reprocessed into a new fuel.

2. Material and Methods

The research method is by doing a coal liquefaction process. The materials used in the liquefaction process consist of lignite (brown coal), solvents and catalysts. The reason to utilise lignite is because this type of coal has low carbon content and a high water content that cannot be used as a solid fuel. The low rank coals are generally composed of small aromatic groups containing many cross-functional relationships and highly reactive in a rapidly and extensively breaking the bond during the liquefaction process.

Fig.1. Lignite (Brown Coal).

The steps in coal liquefaction process are the sort of coal to be liquefied. The coal used is lignite. The Coal is then crushed until a form of powder. The coal powder size is 200 mesh. The coal powder is then feed in the autoclave with other materials such as the catalyst and the solvent material. The autoclave capacity is 500 ml. The coal liquification process is under a temperature of 400 °C and a 20 bar pressure, until tar appears. The liquefied coal process is done to separate the liquid coal from coal tar and waste. The testing process is using Gas Chromatography-Mass Spectrometry (GC-MS) and X-Ray.

3. Experimental Design

In the testing process, some test equipments are used, such as the Gas Chromatography-Mass Spectrometry (GC-MS) as seen in Fig. 2 and X-Ray Powder Diffraction (XRD)as seen in Fig. 3.

Fig. 2.Agilent 7890A Gas Chromatograph

Fig. 3. RigakuMiniFlexII XRD

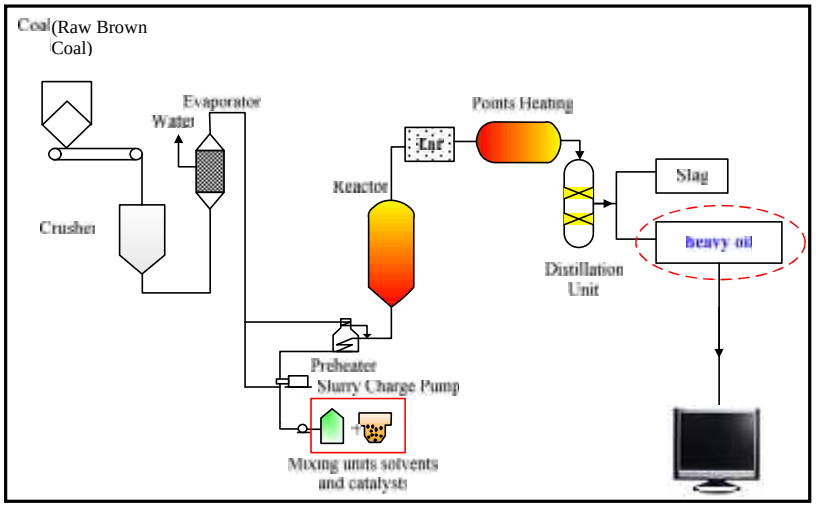


Fig.4.Research Installation.

4. Results and Discussion

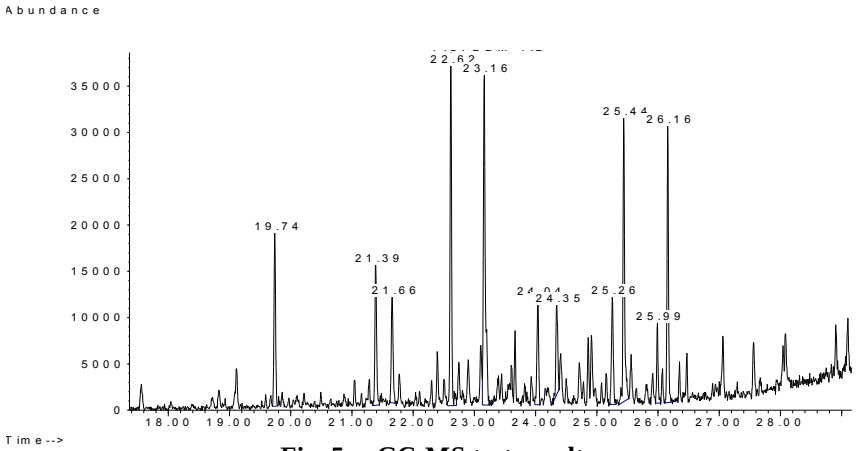
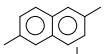
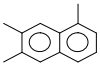
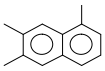
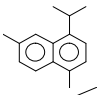
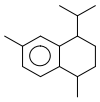
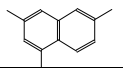


Fig. 5 GC-MS test result.

Table 1 Formula forming compound in liquid coal fuels.

Compound	Formula	Compound shape
Napthale	$C_{10}H_8$	
Napthalene, 2 methil	$C_{11}H_{10}$	
Naphthalene, 1-methyl-	$C_{11}H_{10}$	
Benzene, 1-(2-butenyl)-2,3-dimethyl-	$C_{12}H_{16}$	
Naphthalene, 2,7-dimethyl-	$C_{12}H_{12}$	
Naphthalene, 2,6-dimethyl-	$C_{12}H_{12}$	
Naphthalene, 1,5-dimethyl-	$C_{12}H_{12}$	
Naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-ethylethyl)-, (1S-cis)-	$C_{15}H_{22}$	
Naphthalene, 1,3,6-trimethyl- (CAS)	$C_{13}H_{14}$	
Naphthalene, 1,6,7-trimethyl-	$C_{13}H_{14}$	
Benzene, [1-(2,4-cyclopentadien-1-ylidene)ethyl]-	$C_{13}H_{12}$	
Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-	$C_{15}H_{18}$	

Based on the GC-MS testing result it is found that the chemical content in coal are the naphthalene compound, benzena and methyl groups.

Naphthalene is an aromatic hydrocarbon crystalline, white solid form and the form of two united benzene rings. These compounds are volatile, easy to evaporate even in a solid form, the vapour product is flammable. Hydrocarbons are the main substance making up the fuel. Naphthalene is part of the benzene aromatic hydrocarbon, but not including polycyclic. Naphthalene has a property similar to a gasoline additive to increase the octane number. Naphthalene nature include: the nature of good combustion, does not leave solid gums on machine parts and easy to evaporate. Naphthalene is generally derived from petroleum or coal. The physical property of naphthalene is a substance that is crystal pieces shapes, easy to evaporate, colourless and volatile. Because the naphthalene chemical structures and aromatics nature, then naphthalene like benzene, has a good anti-knock property. Therefore, the addition of naphthalene in gasoline will improve the gasoline quality.

Methyl is an alkyl group containing one carbon atom bonded to three hydrogen atoms (CH_3) derived from methane. When compared with the hydrocarbon group that most of the molecule is a most stable group found in many organic compounds. The methyl groups are usually part of a larger molecule. The methyl group reactivity depends on the substituents adjacent. Methyl groups can be very active. For example, in organic compounds, the methyl groups could hold an attack even strong acids attack.

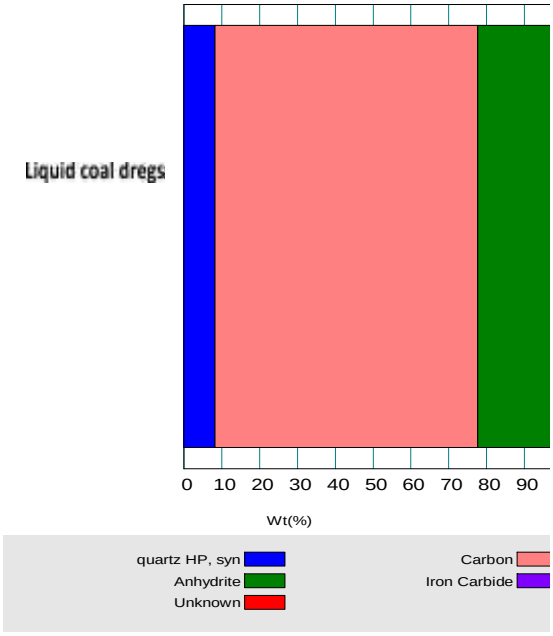


Fig. 6. The Compound content in the liquid coal dregs test result.

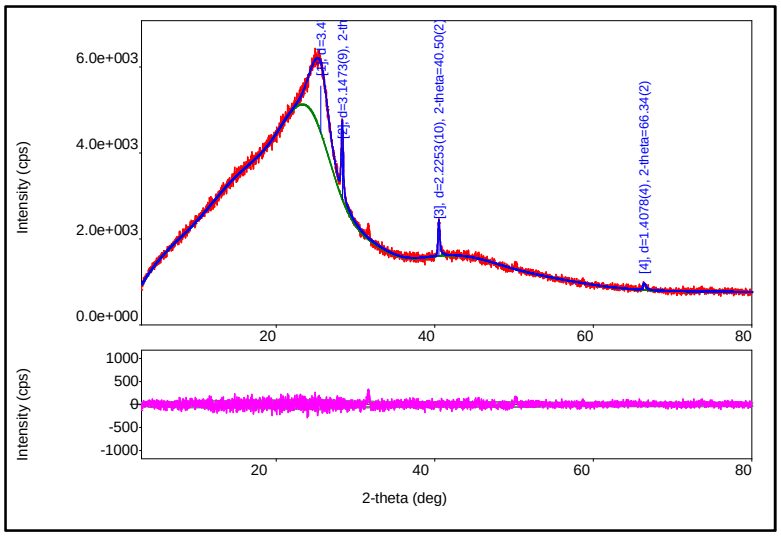


Fig. 7.X-Ray testing result.

Based on figure 6, the X-Ray result test graph to determine the compound content contained in the distillation dregs, where five compounds was found that can be seen in the table below:

5. Conclusions

The dominant compounds contained in liquid coal are Naphthalene and Methyl. Naphthalene is an aromatic hydrocarbon white solid crystalline and form of two united benzene rings. These compounds are volatile, easy to evaporate even in solid form, the vapour product is flammable. The Hydrocarbons compounds are the main ingredients making up the fuel. Methyl is an alkyl group containing one carbon atom bonded to three hydrogen atoms (CH_3) derived from methane. When compared with the hydrocarbon group, that most of the molecule is most stable, which is found in many organic compounds. The methyl groups are usually part of a larger molecule. The methyl group reactivity depends on the substituents adjacent. Methyl groups can be very active.

The hydrocarbon compounds homogeneity influence in the liquid coal dregs is very strong because it has a high ionic strength and has a polar property and a high melting point. This is reinforced by the composition of the hydrocarbon compounds remaining in the pulp liquid coal more than the composition of other compounds. This shows that coal residue still can be processed into a new fuel form.

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