



Evaluation of Chemical Constituents of Crude Oil

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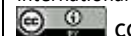
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Abstract

The chemical constituents of crude oil were evaluated in this study. Crude oil is used for many purposes. It is commonly used for production of fuel and in traditional medicine for various purposes. Some people also use crude oil as antidote for poisons. Analysis of the chemical constituents of crude oil was carried out with the use of GC (model No. 7890B) and MS detector (model 5977A). Several chemical constituents with various functions were detected in the crude oil. Some of the chemical constituents detected have been reported to be used for the production of some fuels, pesticides, volatile compounds, fragrance, food additives and antimicrobial agents. This study therefore showed that various important chemicals/compounds useful in traditional medicine and for industrial uses are present in crude oil, thereby making it a good raw material for industrial and medicinal purposes. However, some constituents of crude oil are known to be able to cause toxicity, making crude oil a toxic substance.

Keywords: Crude oil; Chemical constituents; Fuel; Industrial; Traditional medicine.

1. Introduction

Crude oil, a naturally occurring unrefined petroleum product composed of hydrocarbon deposits and other organic materials. Crude oil can exist in several forms such as aliphatic, alicyclic and aromatic compounds. Most of these compounds when exposed to at a given lethal dose are known to be toxic to different biomass in the ecosystem [1, 2]. It is believed to have harmful effects when consumed, but also believed to cure some skin diseases [3].

Crude oil spillage on soil generally retards plant growth [4], decreases aeration by occluding air spaces between soil particles thereby creating a condition of anaerobiosis [5] and causes root stress in plant which also reduces leaf growth [6]. Within our rural population, crude oil is orally ingested for medicinal purposes. It is claimed to be an antidote for poisons and a cure for various gastrointestinal disturbances [7]. The ingestion of crude oil either orally or through polluted marine species represents a pathway for delivery of potential toxicants to the human system. Over the years, local population has used crude oil or its fraction for the treatment of various ailments such as gastrointestinal disorders, burns, foot rot, leg ulcer, poisoning and even witchcraft and is mostly administered orally [8, 9].

Crude oil in various oil producing areas of Nigeria has caused devastating socio-economic problems and health hazards to communities and explorers, and for this reason, the search for daily bread by oil workers may become a harvest of ill health, diseases and even in extreme cases death [10]. Petroleum hydrocarbons or carbon-containing compounds are converted into free radicals or activated metabolites during their oxidation in the cells. These activated metabolites react with some cellular components such as membrane lipids and produce lipid peroxidation products which may lead to membrane damage [11]. The acute toxicity of crude oil is usually attributed to low molecular weight hydrophobic petroleum hydrocarbons that penetrate into lipid membranes and cause death by narcosis [12]. Larger compounds, such as alkyl PAHs with three or more rings that are less soluble in water, contribute less to acute toxicity because they are taken up more slowly than low molecular weight compounds, however, they are reported to be associated with chronic and sub-chronic toxicity owe to the fact that, their metabolism usually yields metabolites that are more toxic than their parent compound [13].

There is need to evaluate the chemical constituents of crude oil due to its wide use in traditional medicine and for other industrial purposes. The knowledge of its chemical constituents will show various areas its application will be required. This therefore warranted research into the present study.

2. Materials and Methods

2.1. Crude Oil used

The crude oil used in this study was obtained from Port Harcourt, Nigeria.

2.2. Determination of Chemical Constituents of Crude Oil

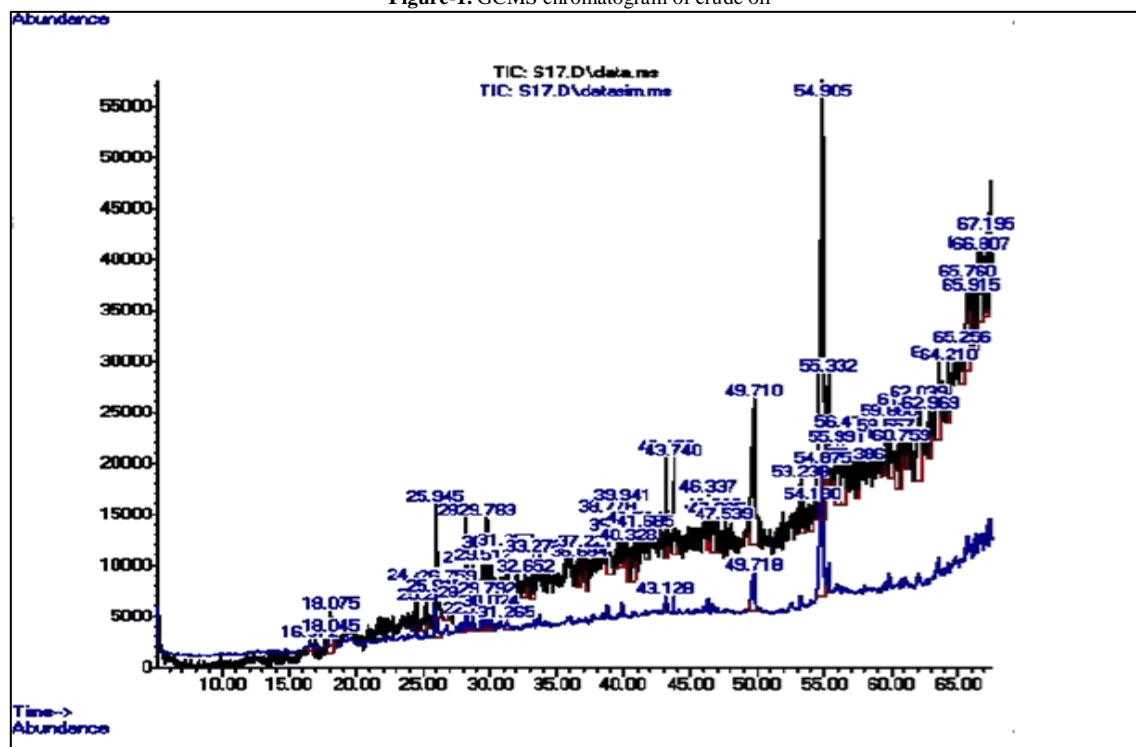
The evaluation of the chemical constituents of crude oil was carried out with the use of GC (model No. 7890B) and MS detector (model 5977A) using the method of Imai, *et al.* [14]. According to the method, the GC-MS used was equipped with column: Agilent HP 5MS ultra Inert (350°C) 30 m × 250 μm × 0.25 μm. Helium was used as the gas with flow: 0.7 ml/min, pressure: 4.4867 psi and average velocity: 30.641 cm/seconds. The injection volume used was 1 ml with an inlet temperature of 250°C, split flow 14 ml/min and split ratio 20:1. The oven temperature of 60°C was used with 1 min equilibrating time, maximum oven temperature of 350°C, and a total run time of 35.857 min. Chemical constituents of the crude oil were identified by matching the spectra of the chemical constituents in the crude oil which are to be identified with the mass spectra of reference compounds which are contained in the database of National Institute of Standards and Technology (NIST 14). The amount of the chemical constituents detected/suggested to be present in the crude oil were then expressed as area percent which is comparable to the total peak area.

3. Results

Table-1. Chemical constituents of crude oil

Name of compound	Retention time (min)	Area %
2-Nonynoic acid	18.075	1.84
1-Hexyne, 5-methyl-	24.472	1.19
4-Octyne	25.247	1.07
3-Octen-1-ol, (Z)-	25.945	2.21
7-Octen-1-ol, 3,7-dimethyl-, (S)-	28.233	1.87
1,8-Nonadiyne	29.512	1.21
10-Undecyn-1-ol	30.055	1.08
1,4-Pentadien-3-ol	31.257	1.58
Cyclobutanone, 2-methyl-2-oxiranyl	32.652	0.94
1-Heptanol, 7-chloro-	36.684	0.81
1-Pentadecene, 2-methyl-	37.227	0.91
Cyclopropanecarboxylic acid, dodec-9-ynyl ester	38.778	1.83
3-Heptene, 4-propyl-	39.941	1.23
Ethyl angelate	40.328	1.00
2,4-Hexadien-1-ol	40.794	1.83
Nipecotic acid	41.685	1.04
Formic acid, 2-ethylhexyl ester	43.158	1.98
Nitrous acid, cyclohexyl ester	43.740	2.18
(E)-6-Methylhept-4-en-1-ol	46.337	1.29
1,5-Hexadiene, 2,5-dimethyl-	46.686	1.06
13-Methyltetradecanal	47.035	0.87
1-Nitro-bicyclo[6.1.0]nonan-2-one	47.539	0.85
7-Bromoheptanoic acid	49.710	6.99
Dodecane, 1-fluoro-	53.238	1.73
Cyclopentaneundecanoic acid	54.905	19.81
Pentafluoropropionic acid, 10-undecenyl ester	55.332	2.40
9-Octadecenal	55.991	2.44
Tridecanal	56.417	2.49
Carvone oxide, trans-	59.557	0.81
Undec-10-ynoic acid, undecyl ester	59.868	1.75
Heptenyl tiglate, 3Z-	60.527	1.86
1-Heptafluorobutyryloxy-10-undecen	60.759	1.10
1,12-Tridecadiene	61.108	1.07
Dodecyl acrylate	62.039	3.41
1-Octyn-3-ol	63.589	2.58
1-Trifluoroacetoxy-10-undecene	64.210	1.06
Z-10-Pentadecen-1-ol	65.256	1.18
(R)-(-)-(Z)-14-Methyl-8-hexadecen-1-ol	65.760	3.01
Citronellol	66.381	2.56
6-Octen-1-ol, 3,7-dimethyl-, formate	66.807	2.37
Oxirane, (7-octenyl)-	67.195	1.99

Figure-1. GCMS chromatogram of crude oil



4. Discussion

The chemical constituents detected in crude oil are presented in [table 1](#) and the chromatogram presented in [figure 1](#). The chemical constituents suggested to be present in crude oil possess various biological, nutritional and industrial properties. 7-Octen-1-ol, 3,7-dimethyl-, (S)- and 2-Nonenoic acid, methyl ester are food additives which are used as flavouring agents. According to [Human Metabolome Database HMDB \[15\]](#), 3-Octen-1-ol, (Z)- and 3-Nonen-1-ol, (E)- are found in fruits. They are flavouring ingredients which is reported to belong to the class of organic compounds known as fatty alcohols. These are aliphatic alcohols consisting of a chain of at least six carbon atoms. (Z)-3-octen-1-ol is considered to be a fatty alcohol lipid molecule. Its biological roles include as nutrient, energy source and membrane stabilizer. The industrial applications include as surfactant and as emulsifier. This suggests crude oil may possess emulsifying properties. 1,8-Nonadiyne was used as starting reagent in the synthesis of 2,6-hexadecadiynoic acid, 2,6-nonadecadiynoic acid and 2,9-hexadecadiynoic acid which are novel synthesized acetylenic fatty acids as potent antifungal agents [16]. 1,8-Nonadiyne is reported to undergo one-step hydrosilylation reaction for attaching acetylene-terminated alkyl monolayers to nonoxidized crystalline silicon surfaces [17]. 10-Undecyn-1-ol has been reported to possess antifungal activity [18]. Some of these properties of the constituents detected in crude oil showed that it may be useful as or in production of certain antifungal.

1,4-Pentadien-3-ol is used as a starting material for asymmetric epoxidation [14, 19] and as a useful building block in the synthesis of natural product [20, 21]. Angelates are the salts and esters of angelic acid. Angelic acid esters have been reported as active components of herbal medicine which is used against a wide range of many health disturbances such as pains, fever, gout, heartburn, loss of appetite, among others [22]. These and more supports the use of crude oil in traditional medicine. This may also be one of the reasons why traditional medicine practitioners use crude oil for treating fever and other diseased conditions.

According to [Chemical Entities of Biological Interest \(ChEBI\) \[23\]](#), (2E,4E)-2,4-hexadien-1-ol is described as a medium-chain primary fatty alcohol that is hexan-1-ol with two trans double bonds at positions 2 and 4. It may be used as a fragrance and also as a flavouring agent used to improve the taste of food. It is a primary allylic alcohol, a medium-chain primary fatty alcohol and an alkenyl alcohol. Tridecanal is a flavour and fragrance agents. This means that some chemical constituents of crude oil will be useful in industries where fragrance is required in its production processes.

[Arne and Povl \[24\]](#), reported that nipecotic acid could act as a substrate for GABA uptake in mini-slices of cerebral cortex which is in keeping with the demonstration that it acts as a competitive inhibitor of GABA uptake. [Wahab, et al. \[25\]](#), also reported that Nipecotic acid is a GABA uptake inhibitor which is used in scientific research. Formic acid can inhibit some decay processes and cause feed to retain its nutritive value longer, and so it is reported to be widely used in preserving winter feed for cattle. In the poultry industry, formic acid is sometimes added to feed to inhibit *E. coli* [26, 27]. These compounds detected in crude oil suggests that crude oil will possess antibacterial activity and may also possess the ability to preserve certain food materials.

9-Octadecenal is a food additive (flavouring agent). Carvone oxide is a flavouring and fragrance agent. Carvone is reported to be found naturally in several essential oils and is used in the food and flavour industry [28]. R-(-)-Carvone is reported to be used for air freshening products and, like many essential oils, oils which contain carvones are used in alternative medicine and aromatherapy. S-(+)-Carvone was reported to have a suppressant effect against

high-fat diet induced weight gain in mice [29]. This suggests the use of crude oil in alternative medicine. During storage, *S*-(+)-Carvone is used for prevention of premature sprouting of potatoes [28]. The U.S. Environmental Protection Agency is reviewing a request to register (R)-(-)-Carvone as a pesticide (mosquito repellent) [30]. Citronellol is used in perfumes and for insect repellents [31]. It is reported to be a good mosquito repellent at short distances [32]. Alsters, *et al.* [33], reported that Citronellol is used as a raw material for the production of rose oxide. The presence of these chemical constituents in crude oil showed it may be useful in the synthesis of some pesticides and fragrance products. 1-Octyn-3-ol was reported to be used in the production of synthetic tricolorin A, a novel tetrasaccharide macrolactone that is a natural herbicide [34]. This also suggest crude oil may be used as or in the production of herbicides.

Dodecane is used as a distillation chaser, scintillator component and has been reported to be used as a diluent for tributyl phosphate (TBP) in reprocessing plants [35]. Currently, n-dodecane is said to have garnered attention as a possible surrogate for kerosene-based fuels. This corroborate the fact that crude oil is a source of fuel.

Oxirane, (7-octenyl)- detected in crude oil is also known as 1,2-Epoxy-9-decene. Epoxides are produced on a large scale for various uses. Guenter, *et al.* [36], reported that low molecular weight epoxides are colourless and nonpolar, and often volatile. This may contribute to the reason why some products of crude oil are volatile. Ethylene oxide is widely used to produce detergents and surfactants by ethoxylation. It is also used for other reasons such as sterilization of medical instruments and materials. Epoxides are reported to be alkylating agents, which makes many of them highly toxic [37]. This means that consumption of crude oil will cause toxicity and therefore may be poisonous to human.

5. Conclusion

Several chemical constituents with various functions were detected in crude oil. Some of the chemical constituents detected may be used for various purposes such as production of fuel, pesticides, some volatile compounds, fragrance, food additives and antimicrobial agents. The findings of this study showed crude oil may be useful in traditional medicine and for industrial uses. Some of the constituents detected in crude oil may serve as raw material for industrial and medicinal purposes. However, some constituents of crude oil are able to cause toxicity, making crude oil a toxic substance.

Conflicts of Interest

The authors declare no conflicts of interest.

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