CHARACTERIZATION AND UPGRADING OF DIRECT COAL LIQUEFACTION PRODUCTS

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Summary

In order to obtain high quality transportation fuels, raw coal liquid effluents derived from Direct Coal Liquefaction need to be severely upgraded using hydroprocessing. Compare to crude oil, theses effluents are more aromatic, with higher nitrogen and oxygen contents. Based on these characteristics, there are some difficult challenges for the upgrading to meet the transportation fuel specifications. This work presents the characterizations done on feed and effluents of the upgrading of liquids from direct coal liquefaction in order to define the optimal processing and shows that fuels from direct coal liquefaction can be upgraded to meet the most stringent specifications.

Keywords

Direct coal liquefaction, product qualities, GC-2D

Introduction

The worldwide demand of fuels has been intensified in recent years and is expected to continue growing. To satisfy these energy requirements and diversify the source of fuels, the energy industry has to face the challenge of using alternate feedstock in order to produce transportation fuels like gasoline or diesel. One of these feedstock is coal used in direct coal liquefaction product, which give liquid yields higher than indirect road via Syngas and FT (typically 4 to 5 bbl/T coal for the best available processes compared to 3 to 3,5 bbl/T coal on a daf (dry ash free) basis).

Compare to crude oil cuts, these liquids products are highly polyaromatics, with very high contents in nitrogen and oxygen but low content in sulfur. In order to be use as transportation fuel, they have to undergo purification and upgrading in a hydrotreatment/hydrocracking process at very high severities. This work give chemical characterizations of the direct coal liquefaction effluents before and after hydropurification, and show that high qualities products could be obtained using appropriate hydrocracking conditions.

Materials and Methods

Reaction conditions. The upgrading of direct coal liquefaction effluent were carried out in a high-pressure fixed-bed reactor, under 100 to 160 bar of total pressure, at temperatures of 360 to 400 °C and liquid hourly space velocities (LHSV) of 0.25 h^{-1} to 2 h^{-1}, after in situ sulfidation of a base metal hydrotreating/hydrocracking catalyst.

Analysis. Reactor effluents were cooled, condensed and separated into a gas phase and a liquid phase. Liquid phase effluents were analyzed by means of a physical distillation (ASTM D2892) and characterize using standard petroleum analysis and also using a multidimensional gas chromatography device equipped with a flame-ionization detector and cryogenic system[1].

Results and Discussion

A full boiling range liquefied (C5-450°C) effluent was separated into three distillation fractions (naphtha, diesel and VGO cuts). The distillation fractions were then fully characterized using the best available analytical techniques. The chemical composition of the distillation fractions was found to be much more complex compared to conventional petroleum fractions. Global analyses showed that they are particularly enriched in aromatic, naphtheno-aromatic and, to some extend, olefinic compounds. Other key characteristics are the very high contents of nitrogen (N) and oxygen (O) and a very low amount of paraffinic compounds, resulting in poor combustion properties.

Due to the chemical complexity of such cuts, analysis developed for petroleum cuts cannot be applied to the heavier cuts. Among these heavier cuts, particular attention has to be paid to polyaromatics compounds since even in trace amounts, they have particularly inhibiting

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effect for the upgrading catalyst. Theses compounds exhibit inhibitory or refractory behavior to all hydrotreatment reactions depending on their nature, hence, their analytical characterization and reactivity study is essential for the study of the upgrading process.

In order to obtain chemical information related to theses cuts, a chemical analytical characterization was done on several vgo cuts (350-500°C) before and after upgrading. The use of a GC2D-HT device coupled with a time of flight mass spectrometer allows us to identify several typical chemical structure for the direct coal effluents. The 2D elution zones corresponding to chemical families (saturate, polynaphthenes and monoaromatics, diaromatics, triaromatics and so on) have been identified. The high contents of naphtheno aromatics compounds and very low content in paraffins have been confirmed. Using data obtain with an FID detector, GC2D-HT FID have give quantification by chemical family and evolutions of the chemical structure during upgrading (see figure 1 and 2) allow us to better understand the low reactivity of this kind of feed in the hydrocracking upgrading process.

Combined with analysis of the atmospheric distillates obtained during previous studies[2], theses new detailed characterization allows us to optimize the upgrading process. Using appropriate operating conditions and a catalyst system which is able to do the saturation and the opening of aromatics compounds, we were able to obtains diesel fractions of sufficiently high qualities, suitable to be use as transportation fuel with low densities and cetane number higher than 45.

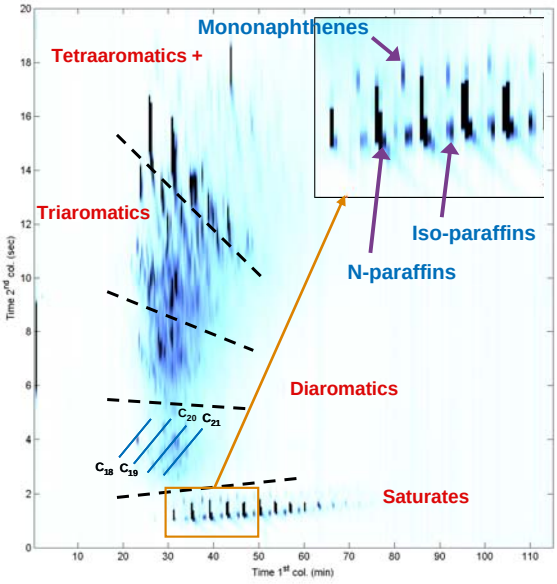

Figure 1: GC-2D analysis of 350+ of direct coal liquefaction effluent

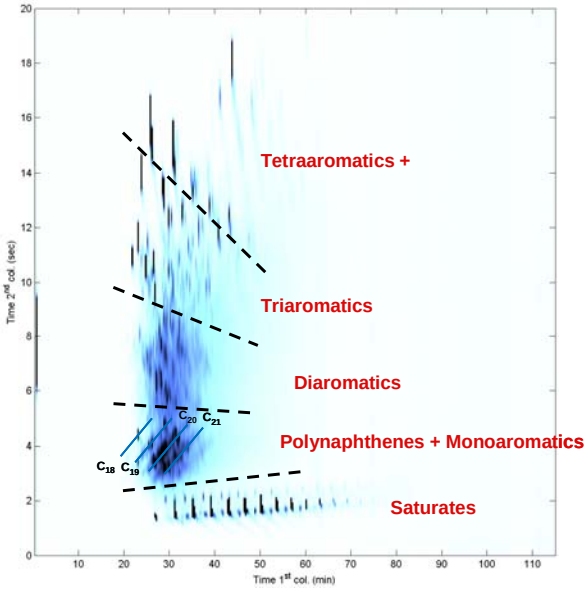

Figure 2: GC-2D analysis of 350+ of direct coal liquefaction effluent after upgrading

References

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