

# In-situ Characterization of an Iron based Fischer Tropsch Catalyst using DRIFTS

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## Introduction

The Fischer-Tropsch (FT) synthesis catalysed by iron is a well-established, industrial process for the production of synthetic fuels, waxes and many other chemicals. The activity and selectivity of these Fischer-Tropsch synthesis catalysts can be influenced by the nature of the catalytic active species that exist on the catalyst surface. The properties of these surface species are determined by their composition and structure on the atomic scale. To this effect there have been numerous reports in literature which attempt to link surface properties (such as adsorption characteristics) to bulk properties and selectivity of Fischer Tropsch catalysts.

Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) is a technique that permits a study of catalyst-reactant interactions by noting the interaction of a surface with gaseous species. It is thus an ideal technique for studying heterogeneous catalysts such as Fischer-Tropsch (FT) catalysts under reaction conditions. Consequently numerous reports have appeared on the use of this technique in FT studies, both for studying of adsorption behaviour and for assessing the rates of reactions [1-3].



## Materials and Methods

The importance of being able to study catalysts under in-situ conditions has long been recognised. Changes during the course of reaction may not be readily detected by performing before and after type analysis. During chemical reaction for example, the presence of reactant and products at elevated temperatures and possibly at elevated pressures are known to influence the surface composition and arrangement of adsorbent atoms. Sintering, poisoning, coking and surface segregation of one or more components may occur, all of which may have profound effects on the course of the reaction as a function of time.

In this project the adsorption behaviour of an iron based FT catalyst has been investigated by means of DRIFTS. The study was done in order to correlate the active sites on the catalyst to the adsorption behaviour of the probe molecules. Thus, preliminary studies have been performed *in-situ* in a Thermo Spectra-Tech high temperature/pressure cell using (i) H<sub>2</sub> as a reductant gas and (ii) CO as a probe molecule. Variables investigated include gas pressure and temperature.

## Results and Discussion

Table 1: Peak assignments for adsorbed CO species in figure 1

Species	Wavenumber (cm <sup>-1</sup> )
Bridged carbonyl 	1940, 1965
Linear carbonyl 	2016

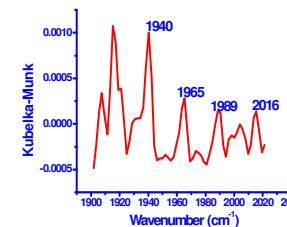


Figure 1: Typical DRIFTS spectrum for adsorbed CO (T = 250°C, P = 10 bar)

The electronic state of Fe after H<sub>2</sub> reduction is predominantly Fe<sup>0</sup> as evidenced by the presence of the linear carbonyl when CO is adsorbed (figure 1). Apart from adsorbing linearly, CO does adsorb in a bridging manner (CO bridged carbonyl = 1940 and 1965 cm<sup>-1</sup>). The bridge-type CO species are considered more active for the FT reaction than linear-type CO [3], which hardly influences the catalytic activity.

## Significance

The production of liquid fuel from natural gas (GTL) via the Fischer-Tropsch (FT) synthesis process is currently an attractive option for monetizing natural gas that has potential to revolutionize the fuel industry [4]. The major factors supporting this drive towards GTL are the high price of crude oil and global growth in demand for clean diesel fuel [4]. Iron based catalysts are the system of choice for FT due to them being relatively cheap than their cobalt counterparts, also their high metal dispersion and long life make them more preferable.

Therefore, by being able to fully understand how active sites on the iron based FT catalyst influence its activity and selectivity. One can be able to manipulate the chemical composition of these catalysts to influence the FT activity and selectivity.

## References

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