



Energy, Mines and
Resources Canada

Énergie, Mines et
Ressources Canada

AA

CANMET

Canada Centre
for Mineral
and Energy
Technology

Centre canadien
de la technologie
des minéraux
et de l'énergie

FOR REFERENCE
NOT TO BE TAKEN FROM THIS ROOM

SHORT REPORT ON ACTIVITIES AS A CONSULTANT FOR CATALYST APPLICATION IN
TAR- AND COAL-HYDROCRACKING

Contract No. 93984

G.C.A. Schuit

SYNTHETIC FUELS RESEARCH LABORATORY

Periods: October, November 1977 and March 1978

ERP/ERL 78-26 OFF 60

4P
01-209

ENERGY RESEARCH PROGRAM

ENERGY RESEARCH LABORATORIES

REPORT ERP/ERL 78-26

CANMET LIBRARY

SHORT REPORT ON ACTIVITIES AS A CONSULTANT FOR
CATALYST APPLICATION IN TAR- AND COAL-HYDROCRACKING

Contract No. 93984

Periods: October, November 1977, March 1978

by

G.C.A. Schuit

INTRODUCTION

In the following a short survey is given of my activities at the CANMET laboratories in Ottawa during the period October 1977 to March 1978. The scope of these activities were as given in contract no. 93984 and are essentially defined by giving advice on catalytic aspects of coal- and tar-hydrocracking.

To arrive at the objects stated, reports were studied on hydrocracking of Athabasca bitumen to become sufficiently acquainted with the problems. In special discussions with Dr. A. Hardin and Dr. M. Ternan, coal hydrocracking and coal gasification were analyzed in some detail as concerned the influence and the choice of appropriate catalysts. A series of discussions were arranged on these subjects where experts in the various fields such as structure of coal, chemical engineering of hydrocracking processes, analytical studies on the products and catalysis studies took part in the analysis of certain sub-problems. The discussions were introduced by me starting from a more academic point of view after which the participants analyzed the models critically on basis of their experience. At the end of the session it was attempted to set up a working model that allowed further research to be planned.

Two reports were written to summarize some of the results of the discussions. They represent my personal view on the problem but it can be said that this was strongly influenced by the contribution of the various participants. One report discusses the first step in the hydrocracking. It relies very much on the experience at CANMET on the hydrocracking of Athabasca bitumen in particular as concerns the pilot-plant reports and the analysis of the products. The second report starts from the question whether one should apply catalysts for the gasification of Athabasca hydrocracking residue by steam and O_2 . It may be helpful to elucidate the method of approach somewhat more extensively. It starts from two assumptions.

(a) To understand heterogeneous catalysis, it is necessary to have a sufficient knowledge of the properties of the solid state of the catalyst since this allows to a certain extent to define what might occur at the surface. This assumption is based on early work in the Shell laboratories at Amsterdam where it led to theories such as from Cossee regarding the

mechanism of the Ziegler-Natta polymerization, of Voorhoeve and Farragher on the hydrodesulfurization reaction and of Sachtler on metal alloy catalysts. It is now generally accepted in industrial research and has been shown to be of great value for zeolite catalysts (Union Carbide, Mobil Oil), selective oxidation (SOHIO) and catalytic reforming (Chevron, UOP, Exxon).

- (b) Any industrial catalytic process that aims at optimal selectivity is bound to end up in using multi-functional catalysts that are often very complicated combinations of different solids. The multifunctionality - we believe - arises automatically because the majority of the reactions envisaged occur or can be made to occur as a sequence of elementary steps, each of which needs its own special catalyst. The consequence of this model is the need for a basic mechanistic model for the reaction mechanism. That for the coal-hydrocracking was derived from the CANMET-data while the model for the pitch gasification was borrowed from the literature on hydrocarbonoxidation.

GENERAL CONCLUSIONS

The extensive work at the CANMET laboratories on the hydrocracking of Athabasca bitumen is unique in that it produced considerable information on the reactions occurring during thermal hydrocracking of heavy feedstocks. It showed thermal hydrocracking to be a feasible operation for the processing of Athabasca bitumen. Moreover, it added valuable information to the modes of operation of catalysts and re-introduced the application of carbon supported catalysts, earlier applied in the pre-war German coal hydrocracking. For instance, it was found that catalysts of the Fe-based type do not increase the rate of cracking but eliminate coke formation, i.e. the catalyst made the reaction more selective. The essence of the report written on the subject was that this could be rationalized according to a model in which the catalyst operates by interfering with the thermal chain reaction in facilitating chain transfer by H_2 by dissociative adsorption on its surface followed by donation of the hydrogen atoms to the radicals.

Another aspect considered in the report, again based on CANMET work, is the colloid chemistry of the coal particle-catalyst particle system. It is argued that both types of particles should remain in contact for some time in order to allow hydrogen transfer from the second to the first. "Sticking" times should not be too short (because of the necessity for sufficient hydrogen transfer) nor too long (because of blocking of the catalyst by the coal particle). Since "sticking time" is mainly determined by the major catalyst component, the support, it is to be expected that it is different for a carbon support and an inorganic support. It is argued from early German experience that carbon supports are superior in this connection. This model seems to reflect the tendency in Athabasca hydrocracking research to apply coal based catalysts. The second report produces an attempt to theoretically predict catalysts for the interaction of carbonaceous materials (Residue from Athabasca hydrocracking) with oxygen and steam. The predictions were compared with experimental data from the literature. It was predicted that MoO_3 or Fe_2O_3 would be the most appropriate choices. This is now being checked in the laboratory.

SOME ADDITIONAL REMARKS

I found the collaboration with the scientists of the CANMET laboratories highly rewarding. They form a group of very capable, intelligent workers who are dedicated to their research. It was a great pleasure to discuss the various catalytic problems with them and I retained a great respect for their scientific achievements. The organization of the research, enabling cooperation of experts in various, widely remote fields, such as structure of coal, organic reaction mechanisms, analytical research, catalytic processes and chemical engineering, appears well suited to perform research on complex problems such as coal- and tar-hydrocracking. Indeed, for the central research problem, the hydrocracking of Athabasca bitumen, it is obvious that the CANMET laboratories are well in advance of the rest of the world both as concerns large-scale application as in their understanding of the reaction mechanism. Moreover, the catalysis group has performed interesting results on catalysts for the hydrocracking and for hydrorefining of the products of the hydrocracking.

Due to the success in these fields it may be expected that activities will tend to grow in the near future. Although the present manpower is adequate for the moment and of high quality, there is reason to assume that the growth will necessitate an increase in the number of participating scientists and professionals.

Finally, I would like to especially thank Dr. Hardin and Dr. Ternan for their extensive help and cooperation which made my stay most enjoyable. Dr. Basil Parsons and Dr. Jean Denis are also thanked for their friendly reception and moral support.