SIMULATION OF FLUID CATALYTIC GRACKING OPERATION

Ihab H. Farag and Kun-Yung Tsai

Department of Chemical Engineering, University of New Hampshire, Durham, N.H. 03824-3591, U.S.A.

<u>Abstract</u>. Since its introduction in 1942 the fluid catalytic cracking (FCC) has been the most important and widely used process for the production of gasoline from heavy distillates. In most refineries the capacity of the FCC unit is second only to that of the crude distillation unit. Often an FCC unit is referred to as the heart of a modern refinery oriented toward maximum production of gasoline.

The basic step in the FCC process is the recirculation of the catalyst through the reactor, stripping and regenerator. In the reactor system the hydrocarbon feed is heated and cracked. Coke (or carbon) may be produced and may deposit on the catalyst reducing its activity and selectivity. When the catalyst is circulated to the regenerator carbon is burned off causing the heating of the catalyst before its return to the reactor part. The products from the reactor are separated in a main fractionator into gas and liquid streams normally including a recycle feed to the reactor.

The operation of an FCC unit requires the manipulation of a large number of controlled variables affecting its performance. Major process variables such as reactor temperature, catalyst circulation rate, catalyst inventory and recycle feed rate can be varied to influence the product yields and to accommodate widely different feedstocks. Unpredictable variation can occur in feed stock, catalyst quality and equipment performance. Most normal variation can be accommodated by a small change in operating conditions.

For a new plant, comparison of actual versus predicted performance provides a valuable check on the validity of the design correlations and a guide for future laboratory and engineering research.

The objectives of the present work are to simplify the complicated FCC process variables and to develop a computer model to simulate the operation of an FCC at different conditions. This includes the prediction of the effects of the operating variables on the reactor product yields. These products include fuel gas, C_3 , C_4 gasoline, light gas oil and coke. The model provides a good base for troubleshooting and debottlenecking and may be useful in optimal control of the FCC.

<u>Keywords</u>. Modelling, Oil Refining, catalytic cracking, Prediction, Iterative methods, fuel gas, light gas oil.

INTRODUCTION

Since the first fluid catalytic cracking (FCC) went on stream in 1942, catalytic cracking has been the most important and widely used process for the production of gasoline from heavy distillates, and hence the major means for increasing the ratio of light to heavy product from crude oil. In most refinery, the capacity of catalytic cracking is second only to that of crude distillation unit. Often an FCC unit is referred to as the heart of a modern refinery oriented towards maximum gasoline production.

The basic steps in the process have remained essentially the same. The catalyst is circulated through the reactor where the hydrocarbon feed is heated and cracked, through a stripping section into the regenerator where carbon is burned off, reacting and heating the catalyst, and back to the reactor. Entrained catalyst losses from the reactor and regenerator are limited to low level by cyclone separation. Reactor products are separated in a main fractionator into a gas stream and a liquid stream, normally including a recycle feed to the reactor.

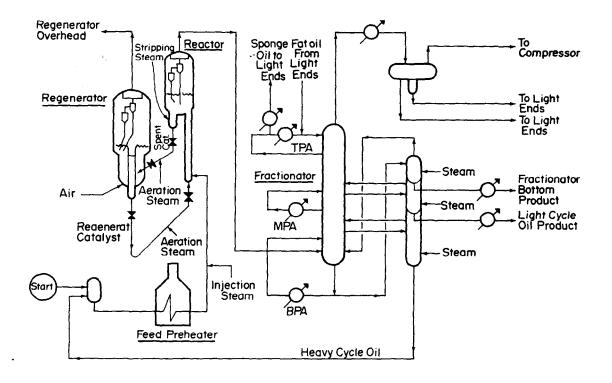


Figure 1 FCC Process Flow Diagram

Catalytic cracking is a very flexible process. Major process variables such as reactor temperature, catalyst circulation rate, catalyst inventory and rate of recycle feed can be varied to meet the demand of product yields and to accommodate widely different feedstocks.

The FCC unit combines a reactor and a regenerator with fractionation and gas plant auxiliaries. Its operation requires the manipulation of a large number of controlled variables having direct effects on the unit performance. Unpredictable variation can occur in feedstock, catalyst quality and equipment performance. Most normal variation can be compensated by a small change in the operating conditions provided that the critical equipment such as the gas and air compressors have adequate flexibility.

The objectives of the present work are the development of a computer model to simulate the operation of an FCC unit at different conditions. Specific objectives include:

- 1 Prediction of the effect of the operating variables on the reactor product yields. The operating variables include the reactor temperature, combined feed ratio, catalyst to oil ratio, space velocity and feed preheat temperature. The products of interest are fuel gas, propane (C₃), butane (C₄), gasoline, light gas oil and coke.
- 2 Prediction of the operating conditions

of the reactor and the regenerator for a given conversion. The operation of some equipment, such as the gas compressor, may become a critical part of the operation if the gas products reach the capacity limit of the gas compressor. The model, therefore, would provide a good base for troubleshooting.

3 - Supplying additional information to plant operators to adjust the operation to be as close to the limits of any critical equipment as possible. The model could therefore, provide a base for future optimal control.

FCC PROCESS DESCRIPTION

Generally the FCC complex, shown in figure 1, is divided into four major sections, which are 1 - Riser and Reactor, 2 - Regenerator-Flue gas handling, 3 - catalyst circulation 4 - Fractionation. Fresh feed and heavy cycle oil (HCO) are preheated then injected into the bottom of the riser, atomized with steam and then contacted with hot regenerated catalyst. Most of the conversion occurs in the riser. The reactor serves as a separator of the catalyst and the vapor which is sent to fractionation. The stripped spent catalyst is transferred into the regenerator. The reactor operating conditions - temperature and catalyst hold-up vary over a considerable range depending on the catalyst, feedstock and desired conversion level. In the regenerator the carbon deposited on the spent catalyst is burned off with air at high temperature to restore the catalyst activity.

The hot regenerated catalyst is returned to the base of the riser and admixed with oil and the cycle is repeated. The catalyst circulation rate is controlled by the presure difference between the reactor and regenerator. The regenerator flue gases pass through cyclones to remove and return the entrained catalyst then pass through a separator to remove particles greater than 5 μ m.

Catalyst circulation is accomplished by maintaining a density difference between the regenerator and the riser. The circulation rate is not measured, it must be calculated from the heat balance.

In the fractionator section the reactor effluent is fractionated into selected products streams, e.g. C_2 gas, C_3/C_4 gas, debutanized gasoline, light cycle oil (LCO) and heavy cycle oil (HCO).

OPERATING VARIABLES

In addition to the feedstock and catalyst, FCC product yields and qualities are determined by a large number of operating variables, which may be divided into independent and dependent variables. The major independent variables are those that can be controlled directly and include: 1 - Reactor Temperature, 2 - Recycle Rate, 3 - Feed Preheat Temperature, and 4 - Space Velocity. The dependent variables include: 1 - catalyst circulation rate, 2 - regenerator temperature, 3 - Regenerator air rate and 4 - conversion. Several operating variables are interrelated, e.g. when reactor temperature is increased at constant feed and preheat temperature conditions the following changes are observed: increased catalyst/oil ratio, increased conversion, increased regenerator temperature, increased C_3 , C_4 , gas and debutanized gasoline and decreased LCO yield.

Conversion is often thought of as the major independent variable of operation. It is a useful parameter for correlating the yield and the operating conditions, and is a measure of the severity of the FCC commercial operation. Many yields and product quality measures and economic factors have been related to conversion and the effects of feed quality, reactor temperature and catalyst activity may to a large extent be lumped in the conversion parameter.

The detailed effects of changing conversion depend upon the manner in which conversion is changed, i.e. by changing temperature, space velocity, catalyst activity etc. However, the general trends are similar; the increase in conversion increases the yield of gasoline and all light products up to 80% conversion level in most cases. Higher conversion cause an increase in the rate of undesirable secondary reactions decreasing olefin and gasoline yields.

To operate an FCC unit in a stable condition the reactor and regenerator must be simul-

taneously heat balanced and carbon balanced. The preferred control variable for carbon balance is the catalyst circulation rate, which can be adjusted by the pressure difference between the reactor and the regenerator. The preferred control variable for heat balance is the preheater temperature, which is controlled by the fuel rate to the preheater. Therefore the reactor temperature and the catalyst circulation rate are considered as the two most important variables.

SIMULATION PROCEDURE

Yield Correlations

Several methods have been developed to correlate the product yields and the operations variable for an FCC process, e.g. Gary's approach [1975] and Ewell and Gadmer [1978] method. The practical approach is to express the weight fraction of C_4 and lighter in the form: $\ln(C_4) = a \times b$, where $\times a$ is the weight conversion, and a and b are constants. Similar equations are used for coke. Gasoline yield is calculated as: conversion - (gas + coke + C_3 + C_4). Figure 2 is a plot of the gasoline yield versus conversion, vol %, at a reactor temperature of 510^{0} C (950 F). At constant conversion the gasoline yield increases with increasing the combined feed ratio CFR.

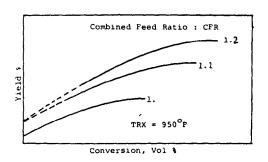


Figure 2 Effect of conversion and combined feed ratio on gasoline yield

<u>Heat Balance</u>

The major heat inputs in a steady state total energy balance are: 1 - Carbon Burning Rate CBR, 2 - Feed preheat and 3 - Torch Oil. The heat outputs are: 1 - feed vaporization and cracking heat and 2 - flue gas. These are shown in Figure 3. Heat balance is performed on the regenerator and reactor.

In the regenerator the circulating catalyst must remove the heat generated from coke burning. Heat inputs include: 1 - heat of combustion of coke and torch oil and 2 - sensible heat of steam, air and torch oil. Heat outputs include: 1 - coke desorption heat, 2 - sensible heat to increase coke, air, steam and torch oil temperatures to

314 5th ICMM

regenerator flue gas temperature and 3 - Radiation and Convection losses. The catalyst circulation rate, CCR is calculated as the Net heat/ $[C_{p,cat}(T_{reg}-T_{react})]$. The amount of coke burned, CBR is calculated from the air rate and flue gas analysis.

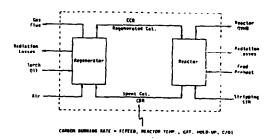


Figure 3 Reactor and Regenerator Heat Balance

In the reactor the heat equation is used to balance the following heat inputs and outputs of reactor. Heat inputs include: 1 - sensible heat from regenerated catalyst, stripping steam and feed preheat and 2 - heat liberated by coke absorption on catalyst. Heat outputs include: 1 - heat of cracking 2 - sensible heat to raise the stripping steam and preheated feed to reactor temperature, and 3 - radiation and convection losses.

Process Model

The maximum reactor temperature is set by the material of construction or by the possible increasing impact of undesirable side reactions. Catalyst circulation rate, which is maintained by density differences, has a maximum physical limit set by the FCC unit. The catalyst inventory is an important controllable variable for a broad operating flexibility. Therefore, the selected model should contain the reactor temperature (TRX), catalyst circulation rate (CCR) and catalyst hold-up. A number of models have been developed, e.g. Shankland and Schmitkons [1947], Van der Baan [1980] three-lump riser model and Wallaston et. al. [1975] model validated with 180 tests from a refinery FCC unit. The model used in the present work may be written in the form

$$x/(1-x) = F(C/0)^n(WHSV)^{n-1}exp(-E/RT_{RX})$$

with the decay exponent, n = 0.65, as recommended by the AMOCO model of Wallaston. The activation energy E was taken to be 25,000 BTU/lbmol constant, independent of temperature and catalyst hold-up. F is a function coefficient and may be computed from known design conditions. In the present model F was assumed to vary linearly with CFR.

Simulation Program Assumptions

The steady-state simulation program developed in the present work was based on the following assumptions: 1 - constant fresh feed

rate, 2 - constant feed and product properties, 3 - Products yields are linear functions of the conversion at a given reactor temperature and combined feed ratio (CFR), 3 - constant regenerator bed temperature 715°C (1320 F) for maximum gasoline production, 4 - constant temperature difference of 30°F between dilute phase and regenerator bed temperature, 5 - coke has an H/C of 0.086 by weight, 6 - complete oxidation of coke to CO_2 , 7 - constant zeolite catalyst activity, 0.05% (wt) of carbon on regenerated catalyst and no poisoning effect, 8 constant heat of desorption of coke from catalyst 1453 BTU/lb, 9 - rate of heat loss is 2% of heat load, 10 - pseudo second order reaction at constant pressure with an activation energy of 25,000 BTU/1bmo1 and a decay exponent of 0.65, and 11 \sim no torch oil is being used.

Simulation Procedure

The main steps of the simulation procedure, summarized in figure 4, are: 1 - assign TRX, CFR and a starting value of the volume conversion of fresh feed, CONV (also denoted X), 2 - Estimate product yields, 3 - compute material balance around reactor and compute a conversion CONVER. If the difference between CONVER and the assumed value CONV is more than a set value (SETVAL) of 1% the CONV should be adjusted by an amount (CAD) of 0.5 and calculations are repeated starting from step 2, otherwise proceed to 4, 4 - compute product yields and carbon balance, 5 - compute CCR from regenerator

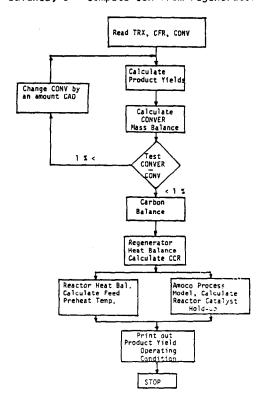


Figure 4 Flow Diagram of Simulation Program

heat balances, 6 - compute feed preheat temperature from reactor heat balance, 7 calculate WHSV from Amoco's model, 8 - calculate the catalyst hold-up on the reactor using the space velocity and the combinedfeed rate in tons/hr, 9 - print outputs.

Extrapolation

Generally feedstock quality is described by a characterization factor K, given by K = $(MABP)^{1/3}/(Sp.gr.60^{O}F/60^{O}F)$, where MABP is the feedstock mean average boiling point in OR. For a highly crackable, generally paraffin feedstock K>12. Intermediately crackable (naphthenic) crudes have K of 11.5-11.6 and a K<11.3 characterizes refractory, generally aromatic, feedstocks. The FCC unit design conditions used were based on a particular feedstock A and very limited data were available. Actual data may be available for a different feedstock B. Therefore the simulation program was run for feedstock B. The analysis of the two feedstocks indicated very close characterization factors K. Therefore the behavior of any property of feedstock A was assumed to follow the same curve shape as the results of the simulation using feedstock B. This assumption permits the extrapolation of the very limited feedstock A data to get the variation of the product yields and of the operating conditions with conversion at any specified temperature and CFR.

RESULTS

The computer model was run to illustrate the FCC unit responses to changes in the operating variables using the same feedstock. Products yields were calculated for various operating conditions.

Three cases were selected for representing typical FCC operations: Case I, maximum gasoline production; Case II, maximum LGO, and Case III constant CFR to study the effect of changing temperature on the conversion. The results were plotted as product yield versus conversion and operating variable versus conversion.

Yield Prediction

Figure 5 is a plot of one of the products C4 yield in % versus the conversion in volume % based on fresh feed. The solid lines are the simulation results using Feedstock B. The circles represent known conditions based on feedstock A. The dashed extrapolated times were drawn through the points of feedstock A such that the lines have the same shape as the computer simulation curves in about 10% conversion range. At the same conversion the yield is different for both feedstocks, although both feedstock have similar distillation range and PONA test. The reasons for this difference are not clearly understood.

Overall, as the conversion increases at con-

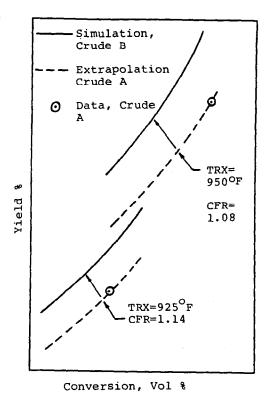


Figure 5 Product Yield versus Conversion

stant reactor temperatures, the yield of fuel gas, C_3 , C_4 and coke increases, the yield of LGO decreases and the gasoline decreases. The drop in gasoline yield is because of over-cracking of gasoline product at higher conversion.

Operating Conditions Prediction

The present model results indicate that the coke yield for feedstock B is close to that of feedstock A. Since the operation of FCC is based on satisfying the heat balance, the coke yield will affect the whole operation. The prediction of the variation of operating conditions with conversion was done by drawing a curve through the point of feedstock A with the shape as the simulation results of feedstock B. This approximation is believed to be valid in a 10% conversion range. The effects of changes in catalyst hold-up on conversion are shown in figure 6. At constant reactor temperature an increase in catalyst hold-up will increase conversion. Because of the steep slope of the curve, a large increase in catalyst hold-up will result in only a small increase in conversion due to overcracking of products. Therefore, a large catalyst hold-up will not improve the conversion very much, but will decrease gasoline yield. Similar plots were developed for other operating variables.

The extrapolated dashed curves in figure 6

316 5th ICMM

may be used to predict the variation of operating constraints if the catalyst circulation rate (CCR) was known. The operating range of the main equipment, such as the compressor or heaters, may then be estimated from the high and low limits of CCR at constant reactor temperature.

The major goal of the computer simulation is to run the FCC unit as close to the operating constraints of the equipment as possible and to obtain the best operating conditions that would maximize the yields of the products.

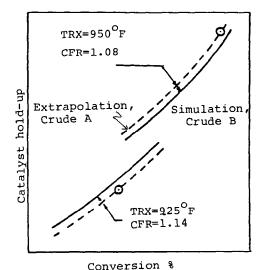


Figure 6 Effects of catalyst hold-up on conversion

CONCLUSIONS

A simplified FCC simulation model was developed assuming, as often done in field operations, that the reactor temperature and catalyst hold-up are the only adjustable variables. The model predicts yields and operating conditions for a given conversion, volume % based on fresh feed.

Even when the feedstock qualities of two feeds are similar it is still possible to get different product yield distribution at the same conversion level. More sophisticated models may be needed to better predict product yields. However the present model is useful in predicting the trend of the operation, if the coke yield remains relatively unchanged.

In the present work the feed quality was assumed to be unaffected by the recycle ratio, and the catalyst activity was assumed to remain constant. The validity of these assumptions should be checked with actual operation data to update the model. Also, the regenerated catalyst was assumed to have a 0.05 wt % carbon deposit irrespective of the operating condition, which may not be the situation in an actual FCC unit.

NOMENCLATURE

- CBR = Carbon burning rate; rate at which
 carbon is burned off the catalyst in
 the regenerator, lbs/hr.
- CCR = Catalyst circulation rate; the weight
 rate of flow of catalyst flowing
 between the reactor and regenerator,
 tons/min.
- C/O = Catalyst-to-oil ratio; ratio of the weight of catalyst circulated to the weight of reactor feed charged.
- CFR = Combined feed ratio; total feed/fresh
 feed.
- E = Activation energy for cracking
- F = Function coefficient, function of feed quality, hydrocarbon partial pressure, instrinsic catalyst activity, and a severity factor reflecting the effective activity at various levels of carbon on the regenerated catalyst.

FF = Fresh feed.

K = Characterization factor.

MABP = Feedstock mean average boiling point in OR.

n = Catalyst decay exponent.

R = Gas constant

TRX = Reactor temperature.

x = 430 conversion, vol % of feed which is converted to material boiling below 430° FVT, and to coke.

WHSV = Weight hourly space velocity; the weight of oil feed per unit time divided by the reactor hold-up.

REFERENCES

Ewell, R.B., and G. Gadmer. (1978). "Design of Catalytic Cracking by Computers", <u>Hydrocarbon Process</u>, (4), p. 125-134.

Gary, J.H., and G.E. Handwerk. (1975).
"Petroleum Refining Technology and
Economics", p. 101, Marcel Dekker, New
York.

Shankland, R.V., and G.E. Schmitkons. (1947).

Proc. Am. Petroleum Inst., 27, (III),
p. 57

Van der Baan, H.S. (1980). "Catcracker Operations", in Chemistry and Chemical Engineering of Catalytic Process, p. 217-233, ed. by R. Prins and G.C.A. Chuit, Sisthoff & Noordhoff, the Netherlands.

Wallaston, E.G., W.J. Haffin, W.D. Ford, and G.J. D'Sousa. (1975). "What Influence Cat. Cracking", Hydrocarbon Process, (9), p. 93-100.