GLOBAL JOURNAL OF PURE AND APPLIED SCIENCES VOL. 10, NO. 3, JUNE 2004: 429 - 434
COPYRIGHT(C) BACHUDO SCIENCE CO. LTD. PRINTED IN NIGERIA. ISSN 1118-0579

APPLICATION OF MICROSOFT EXCEL PROGRAM FOR PREDICTION OF FLUID CATALYTIC CRACKER PERFORMANCE

P. N. JOSIAH and S. S. IKIENSIKIMAMA

(Received 28 September 2001; Revision accepted 18 June 2002)

ABSRACT

In the analysis of engineering systems in general , emphasis has been placed on the use of Fortran programs .In this paper, a simple method for predicting the performance of systems using Microsoft Excel has been presented. The method has been applied to the prediction of fluid catalytic cracking (FCC) kinetics at a constant temperature of 548°C and a catalyst-to oil ratio of 4 , using the four-lump model. Results show that the maximum yield of gasoline occurs at a space velocity of 10 hr^{-1} and this corresponds to a coke yield of 4.6% and a gas-oil conversion of 82% by weight. These agree well with published data, suggesting that the method is reliable for predicting system performance. A very important merit of the method is that it is both simple and fast.

KEYWORDS: Catalytic Cracking, Riser Reactor, Kinetic Modeling

INTRODUCTION

Catalytic processes have over the years been exploited beneficially to meet the needs of an increasingly developing society. By any standard, be it capacity, catalyst cost, or product value, fluid catalytic cracking remains the largest catalytic process in the world. Fluid catalytic cracking (FCC) in its simplest sense, is a process in which a catalyst is used to break down heavy oil into lighter hydrocarbons of higher economic value at temperatures between 510°C to 540°C. The process plant consists of three units namely the transfer line (riser) reactor, where almost all the endothermic cracking reactions and coke deposition on the catalyst occur, the particle separator which acts as a disengaging chamber for separating catalyst from gaseous products by stripping steam, and the regenerator in which spent catalyst is reactivated by using air to burn off the deposited coke. Apart from catalyst reactivation the regeneration process provides the heat required by the endothermic cracking reactions.

The literature is relatively rich in the modeling and analysis of fluid catalytic cracking (FCC) reactions. Weekman (1968) proposed a three-hump kinetic description of the fluid catalytic cracking process and other theoretical as well as experimental and semi-empirical studies were conducted by several independent workers.Notable among them are Wojciechowski (1968), Kuo and Wei(1969),Wang(1974),Corella,Fernandez and Vidal (1986), Oliveria and Biscaia (1989), Lee-Chen-Huang (1989). Such descriptions have been supported by further work, Kraemer et al (1990), Groten and Wojciechowski (1993).

Application of kinetic models for simulation purposes has been limited to the use of Fortran computer programs. A basic requirement for such programs is that the different equations describing the kinetics of the reactions must be solved analytically. Although the availability of standard analytical solutions and numerical methods makes it relatively easy to develop such programs, they suffer two major drawbacks. Each time the value of a process variable is changed, the program must be compiled and the result file be edited before one can access the influence of the variable so changed on product yields. Apart from this weakness, such results cannot be viewed graphically except another program or a subroutine is developed for this purpose. At best, such results can be printed out for onward plotting using windows utilities. In this work, a simple numerical method has been automated on an electronic spreadsheet and used to predict the performance of fluid catalytic cracking process, and the method has successfully eliminated the drawbacks of the conventional method in use.

Kinetic Modeling and Parameter Estimation

Kinetic schemes of varying complexities have been proposed as descriptors of fluid catalytic cracking reactions. In this work, the four-lump model proposed by Lee, Chen and Huang (1989) was adopted. Details of the model can be found in their paper but the pertinent equations are as follows:

P. N. JOSIAH, Department of Chemical Engineering, University of Port Harcourt, Port Harcourt, Nigeria
S. S. IKIENSIKIMAMA, Department of Chemical Engineering, University of Port Harcourt, Port Harcout, Nigeria

$$dy_1/dtv = -(K_{12}\,Y_1^2 + K_{13}\,Y_1^2 + K_{14}\,Y_1^2)\varphi \tag{E1}$$

$$dy_2/dtv = (K_{12}\,Y_1^2 - K_{23}Y_2 - K_{24}Y_2)\,\varphi \tag{E2}$$

$$dy_3/dtv = (K_{13}\,Y_1^2 + K_{23}\,Y_2)\,\varphi \tag{E3}$$

$$dy_4/dtv = (K_{14}Y_1^2 + K_{24}Y_2)\,\varphi \tag{E4}$$

$$\varphi = \mathrm{Exp}(-\alpha tc) \tag{E5}$$

Equation E1 – E5 is a system of differential-algebraic equations (DAE) solvable by Gear's (1971) method. For the purpose of this study, equation E5 was substituted in E1 through E4 and the fourth order Runge-Kutta (Rk4) was then implemented in the visual basic for application (VBA) environment of Microsoft excel. The rate constant Kij for each reaction is related to the pre-exponential factor, Ko and the activation energy, Ea as

$$Kij\,(T) = K_o \exp(-Ea/RT) \tag{E6}$$

Similarly, the catalyst deactivation constant, α is given by

$$\alpha\,(T) = K_o \exp(-Ea/RT) \tag{E7}$$

In order to estimate the constants, k_{12}, k_{13}, k_{14}, k_{23}, and k_{24}, equation E6 and E7 were linearized and the data of Lee, Chen and Huang (1989), was used to estimate the adjustable parameters, K_o and Ea/R using the least square technique, giving rise to the following expressions:

$$\alpha(T) = \mathrm{Exp}(21.8678 - (16000/T)) \tag{E8}$$

$$\varphi(T) = \mathrm{Exp}(-\alpha\, t_c) \tag{E9}$$

$$K_{12}(T) = \mathrm{Exp}(13.3859 - (8000/T)) \tag{E10}$$

$$K_{13}(T) = \mathrm{Exp}(15.729 - (11000/T)) \tag{E11}$$

$$K_{14}(T) = \mathrm{Exp}(11.848 - (8800/T)) \tag{E12}$$

$$K_{23}(T) = \mathrm{Exp}(10.0014 - (7870/T)) \tag{E13}$$

$$K_{24}(T) = \mathrm{Exp}(8.0346 - (6980/T)) \tag{E14}$$

Equations E8 – E14 were combined with E1 – E5 for the implementation of the fourth order Runge-Kutta (Rk4) algorithm.

The velocity of gas and solid in the riser may differ, the ratio between these two velocities is defined as the slip factor

$$S = V_v/V_c \tag{E15}$$

The catalyst hold-up can be expressed as

$$H = CCR \times S \times V_R \times \rho_F/G_F \tag{E16}$$

Assuming no slip conditions, $S = 1$

Let $CCR/G_F = C/O$ be defined as the circulation rate of catalyst per unit mass of feed. Then

$$H = C/O \times V_R \times \rho_F \tag{E17}$$

The catalyst residence time is given by

$$t_c = H/CCR = V_R \times \rho_F/G_F \qquad \text{E 18}$$

The gas oil space-time is given by

$$t_v = H/G_F = t_c \times C/O \qquad \text{E 19}$$

Technical Development

The automation of the electronic spreadsheet consists of three sub-activities namely:

1. Design of user interface
2. Code programming
3. Graphics Design.

In the first activity, efforts were directed at designing a screen with which the user interacts with the simulator. Fig 1a is a sample interface, which has been designed in such a manner that allows the user to vary either the catalyst recycle - to- feed rate ratio (C/O), or the reaction temperature, either one at a time or simultaneously. The effect of such change on the performance of the process is instantly reflected on the interface, in a tabular display.

The next step in the automation of the spreadsheet is the code-programming step. Basically there are three methods for code programming. The most elementary and commonly used method is that of writing the terms of an equation in columns and writing formula in each cell of a spreadsheet. Another method ,which is more superior to the former is to write macros on module sheets which are embedded .An advanced form is to write codes in the visual basic for applications environment of excel. such codes represent the fourth-order Runge-Kutta algorithm for solving the differential equations that describe the fluid cracking kinetics. The codes are then enhanced by making them to interact with the user-interface. Once this is done, a single click on the user-interface generates the required results for each change in the operating variables.

As a final step, the chart wizard on the standard menu bar is used to draw graphs of key variables against some performance indicators. In this work, five of such graphs: Product Yields versus conversion,

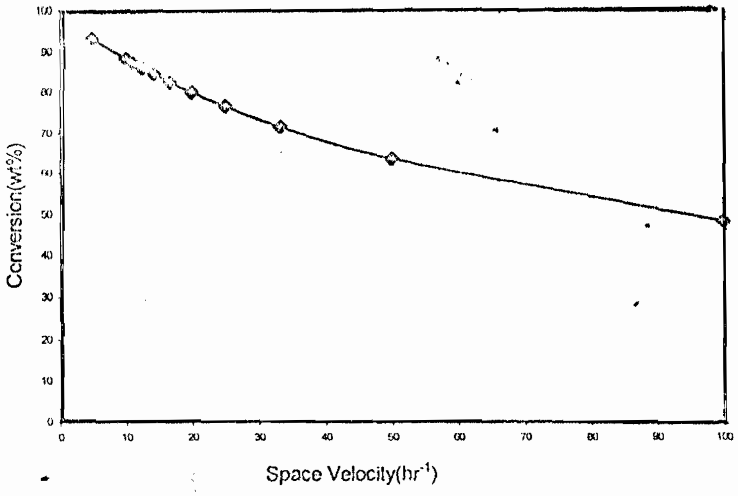

Figure 1:Effect Of Space Velocity On GasOil conversion

Conversion versus space velocity, Gasoline yield versus space velocity Yield, Coke Yield coke yield versus gas-oil conversion, and Gasoline Yield versus conversion, have been designed. A single mouse click on the appropriate sheet tab causes a display of a profile. Note that each change on the input section of the user-interface is reflected on both the tabular display and the graphs. The only legitimate means of changing data on the tabular display is through the code-interface interaction since the tabular display and the graphs are highly protected. More so, unauthorized persons cannot have access to the code by any means.

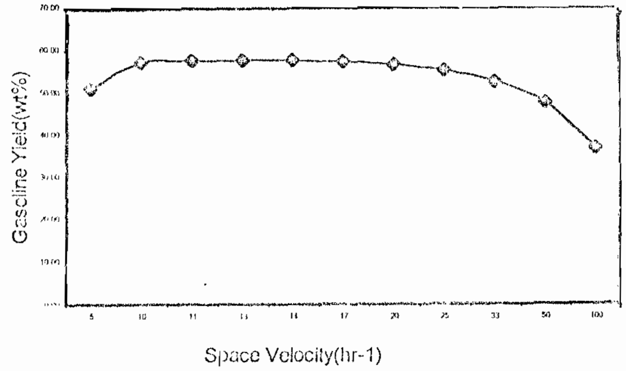

Figure 2:Effect Of Space Velocity On Gasoline Yield

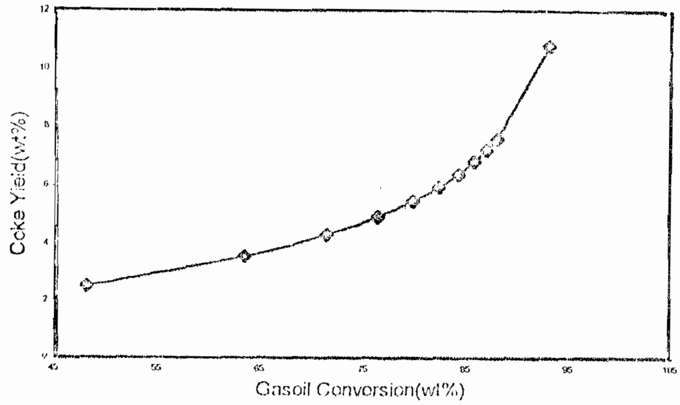

Figure 3:Effect Of Conversion On coke Yield

RESULTS AND DISCUSSION

For the purpose of demonstrating the use of Excel as a tool for simulating the behaviour of systems, this study was conducted at a fixed temperature of 548 °C and a catalyst-to-oil ratio of 4 and the results are as discussed below.

Effect of space velocity on gas oil conversion

Fig 1 shows that the conversion of gas oil is inversely proportional to space velocity. since space velocity is the reciprocal of space time, this can be explained in the context of the gas oil making more contact with the catalyst, leading to more and more of the gas oil being converted to products.

Effect of space velocity on gasoline yield

The yield of gasoline increases progressively from zero to a maximum at a space velocity of 10hr^{-1}.Fig 2 reveals that between a space velocity of 10hr^{-1} and 33hr^{-1},gasoline yield declines steadily and drops sharply as space velocity approaches 100hr^{-1}.This trend is expected since gas oil conversion declines with space velocity.

Effect of gas oil conversion on coke yield

The relationship between conversion and coke yield is as depicted in fig 3.As conversion improves , the yield of coke also increases. It has been established from fig 2 that the best yield of gasoline corresponds to a space velocity of 10hr^{-1} . We also observe from fig 1 that this value of space velocity corresponds to

82% conversion on gas oil with 82% conversion on the x-axis, the coke yield for maximum gasoline yield is 4.6%,from fig 3

CONCLUSION

In this work, a method for automating an electronic spreadsheet has been proposed. It has been used to simulate the kinetics of fluid catalytic cracking of gas oil. The results from the work of Lee-Chen and Huang (1989) agree with those predicted by this method, thus it is reliable and reasonable for conducting simulation studies of engineering systems.

Nomenclature

CCR = Rate of cycling catalyst, kg/hr

C/o = cycling catalyst rate/feedstock mass flow rate

Ea = Activation Energy, KJ/mol

Gf = Feedstock mass flow rate, kg/hr

H = Catalyst hold-up, kg

Kij = Reaction rate constant for reaction of lump i to lump j

Ko = Frequency factor in Arrhenius equation, hr

S = Slip factor

T = Absolute temperature, K

t_c = Catalyst residence time, hr

t_v = Gas oil space time, hr

V_R = Volume of riser, m^3

V_c = Catalyst flow velocity, m/hr

Y_1 = Gas oil weight percent, wt%

Y_2 = Gasoline weight percent, wt%

Y_3 = C_1-C_4 gas weight percent, wt%

Y_4 = Coke weight percent, wt%

Greek letters

α = Catalyst decay constant

ρ = Density of gas oil feed

φ = Activity decay function.

REFERENCES

Corella ,J., Fernandez, A and Vidal, J. M., 1986. Pilot Plant for the fluid catalytic cracking process, .Ind.Eng.Chem.Proc.Des.Dev.25: 554-562

Gear, C. W., 1971. Numerical initial value problems in ordinary differential equations , Prentice Hall, Englewood Cliffs, NY

Groten, W, A and Wojciechowski, B., 1993. The Kinetics of hydrocarbon cracking;. J. catal. 140: 243-261.

Kraemer , D. W; Sedran, U and De Lasa, H, I. 1990. Catalytic cracking kinetics in a novel riser simulator, Chem Eng. Sci 45(8): 2447-2452

Kuo , J. W and Wei, J., 1969. A lumping analysis of mono-molecular reaction systems. Ind.Eng.Chem.Fundam.8: 124

Liang-Sun Lee,Yu-Wen Chen and Tsung-nien Huang, 1989. Four-Lump kinetic model for fluid catalytic cracking process. Can.J.Chem.Eng. 67: 615-619.

Oliveira , L.L and Biscaia, E . C., 1989. Catalytic cracking kinetic models. Ind.Eng.Chem.Res.28: 264-271

Wang, I., 1974. High temperature catalytic cracking, Ph. D dissertation, Fuels Eng. Dept, Univ. of Utah

Weekman, V.W., 1968. A model of catalytic cracking conversion in fixed, moving bed and fluid-bed reactors. Ind. Eng. Chem . Proc. Des. Dev 7: 90-95

Wojciechowski, B. W., 1968. A theoretical treatment of catalyst decay.Can.J.Chem.Eng.46: 48-52