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ERL 93-0813

Process Flowsheet Computer Simulation

CPUB

Plastic Wastes Conversion
Involving
Batch Reactor Thermal Cracking
of Polyethylene

ERL 93-0813



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ERL 93-0813

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Plastic Wastes Conversion
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Batch Reactor Thermal Cracking
of Polyethylene

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August 13, 1993

Attention: Professor Toogood

coal processing section at section
The ~~Synthetic Fuels Research Laboratories (SFRL) division~~ of CANMET - EMR is directed by Dr. J. Kelly. The ~~division~~ is principally involved with the research and development of coal processing to transform raw material into products such as heavy oils and petroleum fuels. Among such areas of research includes the recycling of waste plastics such as polyethylene and converting the waste into alternative fuels, oils, lubricants and petrochemicals. This report involves the generation of a computer process flowsheet simulation modelling the thermal cracking of polyethylene. The simulation results is compared with that of the actual experimental data.

The report is entitled "Process Flowsheet Computer Simulation - Plastic Wastes Conversion - Batch Reactor Thermal Cracking of Polyethylene" and has been prepared by me and is my fourth work term report. I would like to thank Dr. H. Seoud, Dr. M. Ikura and Dr. M. Stanciulescu for their assistance in preparing this report.

Sincerely,

R. J. Tuling
90049617

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Summary

The purpose of this report is to determine ^{whether with the help of the pen one could determine the optimum} the maximum A-olefin/N-paraffin ratio from polyethylene thermal cracking ^{operating conditions to maximize} for a given set of ~~temperature~~ conditions. The ratio value is a factor in determining the feasibility of converting plastic wastes into products such as ^{with the} oils, lubricants, petrochemicals and synthetic fuels. ^{lubricants}

This report addresses the ability of a computer process simulation to accurately model the thermal cracking of polyethylene in a batch stirred tank reactor (BSTR). In the report, simulations modelling the thermal cracking of both eicosane and pentadecane-eicosane are considered. The simulation results are compared to the experimental GC results to determine the validity of the model.

The process simulation and the data generated are discussed. A description of the simulation is given. The results from the simulation and comparisons are shown, conclusions drawn and recommendations made.

Optimal conditions were determined by the results from the simulations. The maximum A-olefin/N-paraffin ratios for eicosane involved a reactor temperature of 170°C with 30-70°C reflux temperatures. The maximum ratios for the pentadecane-eicosane mixture occurred at the same reaction temperature since increased product yield was considered. ^{these temperatures are much lower than the "}

It is recommended that a more thorough literature search be done to produce improved simulations that model the process more closely. Further research and development is recommended as well to determine new and different methods to simulate the process.

actual operating temperatures, as they are derived from an equilibrium model and the kinetics of the reaction are not taken into consideration.

Conclusions

~~The process simulation and A-olefin and N-paraffin~~ ^{simulated} distributions of thermally cracked polyethylene was ~~effectively modelled~~ by the Aspen Plus software although the simulation reaction temperatures were lower than desired.

The experiment involved computer simulation of thermally cracked eicosane and a pentadecane-eicosane mixture. The total olefins and paraffins, A-olefins and N-paraffins and the A-olefin/N-paraffin ratios were compared, graphed and discussed.

The A-olefin/N-paraffin ratio ^{simulated} distributions for thermally cracked eicosane showed that the reactor ^{simulated} temperature of 170°C with ^{simulated} reflux temperatures of 30-70°C provided the optimal conditions for the maximum ratio under the given conditions. The ratio distributions for thermally cracked pentadecane-eicosane showed that the optimal ^{simulated} reactor temperature was 210°C for maximum A-olefin/N-paraffin ratios although the ^{simulated} reaction temperature of 170°C produced a higher yield of A-olefins. ^{simulated}

An indepth detailed study of the process simulation is recommended to improve the exactness of the computer model.

Recommendations

The Aspen Plus flowsheeting program must be studied again to determine if different block models, components, temperatures and other optional parameters may be able to duplicate the experimental data more effectively.

Difficulties arose in the Aspen Plus program concerning reflux block simulation warnings and erratic system crashing. Allocating the program memory to a different section on the hard drive may prevent program malfunctions.

A literature search should be done to develop an improved way to represent the thermal cracking process of polyethylene on the Aspen Plus process simulation program. Alternatively, other process flowsheet programs such as Hysim and ChemCad should be used to compare the results.

1. Introduction

1.1 Background

In modern society where environmental awareness is increasing, recycling and reusing of waste material has become a rising obligation to government and industry. The CANMET-ERL branch of Energy, Mines and Resources has developed methods to thermally crack linear low-density polyethylene (~~LLDPE~~) so that products such as oils, lubricants, synthetic fuels and petrochemicals may be produced [1, 2].

1.2 Objectives

The main objective involves varying reactor and reflux temperature parameters of a thermal cracking process simulation involving eicosane and a mixture pentadecane-eicosane as the initial reactant feeds. From the manipulation of temperature maximum A-olefin/N-paraffin ratios may be optimized for product formation. The distribution of the A-olefin/N-paraffin ratios are compared to and correlated with the GC run distributions.

1.3 Method

The principal method involves a computer process flowsheet simulation of thermal cracking of eicosane involving a ~~continuous flow reactor~~ modelling a batch reactor. The reactor and reflux temperatures are each specified at three temperatures and combinations of these are entered for each run.

2. Materials and Method

2.1 Computer Process Flowsheet Simulation with Aspen Plus: Modelling of Batch Reactor Thermal Cracking of Polyethylene

The process flowsheet involved is displayed in Figures 1 and 2. In the process (Figure 1) a predetermined amount of polyethylene material is fed into the batch reactor (BSTR). Nitrogen is allowed to purge the air from the system in order that combustion does not occur which would otherwise interfere with thermal cracking. After purging, the reactor temperature is gradually increased to 450-600°C at atmospheric pressure. Liquid-solid polyethylene component material starts to thermally crack, recycle through the refluxer (hot traced heat separator) and re-enter the reactor for further cracking. Eventually, vapour components begin to separate out in the refluxer and enter the water-cooled condenser. The components are condensed at a specific temperature and separated into vapour and liquid phases. GC analysis of the liquid reflux, liquid condensate and vapour condensate streams is completed to determine the olefin-paraffin weight distributions and the olefin/paraffin ratios for each carbon number.

Reactor. In Figure 2, the Aspen Plus simulation is shown. In the process, the batch reactor is modelled by a continuous-flow stirred tank reactor (CSTR) since the batch stirred tank reactor (BSTR) model requires that the reaction kinetics and stoichiometry parameters be predetermined [3].

The reactor is an RGIBBS block model which considers simultaneous multiple phases without chemical reaction (physical thermal cracking) and accounts for chemical equilibrium [3]. RGIBBS calculates vapour phase equilibria by Gibbs free energy minimization for the determined products while satisfying atom balances. Thus, atomic formula must be defined for each feed and product component through the data bank. Reactor temperature and pressure parameters must be defined as well [3]. In the simulation, the reactor temperature parameters were set for 170°C, 190°C and 210°C at atmospheric pressure.

Unlike the RBATCH block model, RGIBBS does not require reaction stoichiometry or chemical reaction kinetics to be specified. The flexibility of restricted equilibria specifications such as moles of product produced, percentage of a feed component that does not react and temperature approaches to individual extents of reaction allow RGIBBS to be the most suited reactor model [3].

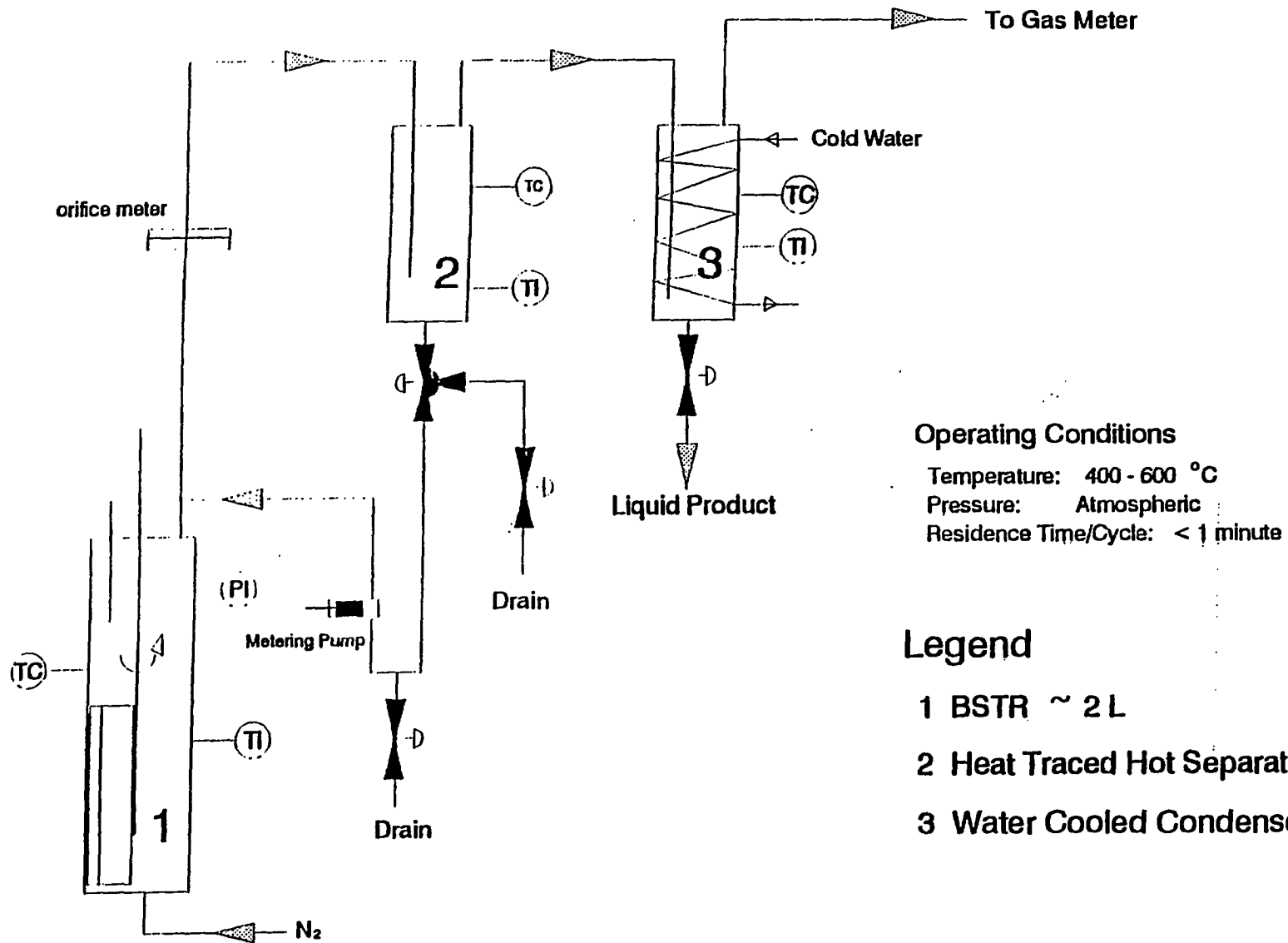
Refluxer and Condenser. In Figure 2, both the refluxer and condenser are modelled by FLASH2 blocks. The separator performs vapour-liquid equilibrium calculations to form both vapour and liquid outlet streams [3]. The calculations are completed at various temperatures and at atmospheric pressure (1 atm). The

refluxer temperature parameters were set at 30°C, 50°C and 70°C.
The condenser temperature was set at 15°C.

Figure 1

PLASTIC WASTE CONVERSION

Batch Stirred Tank Reactor



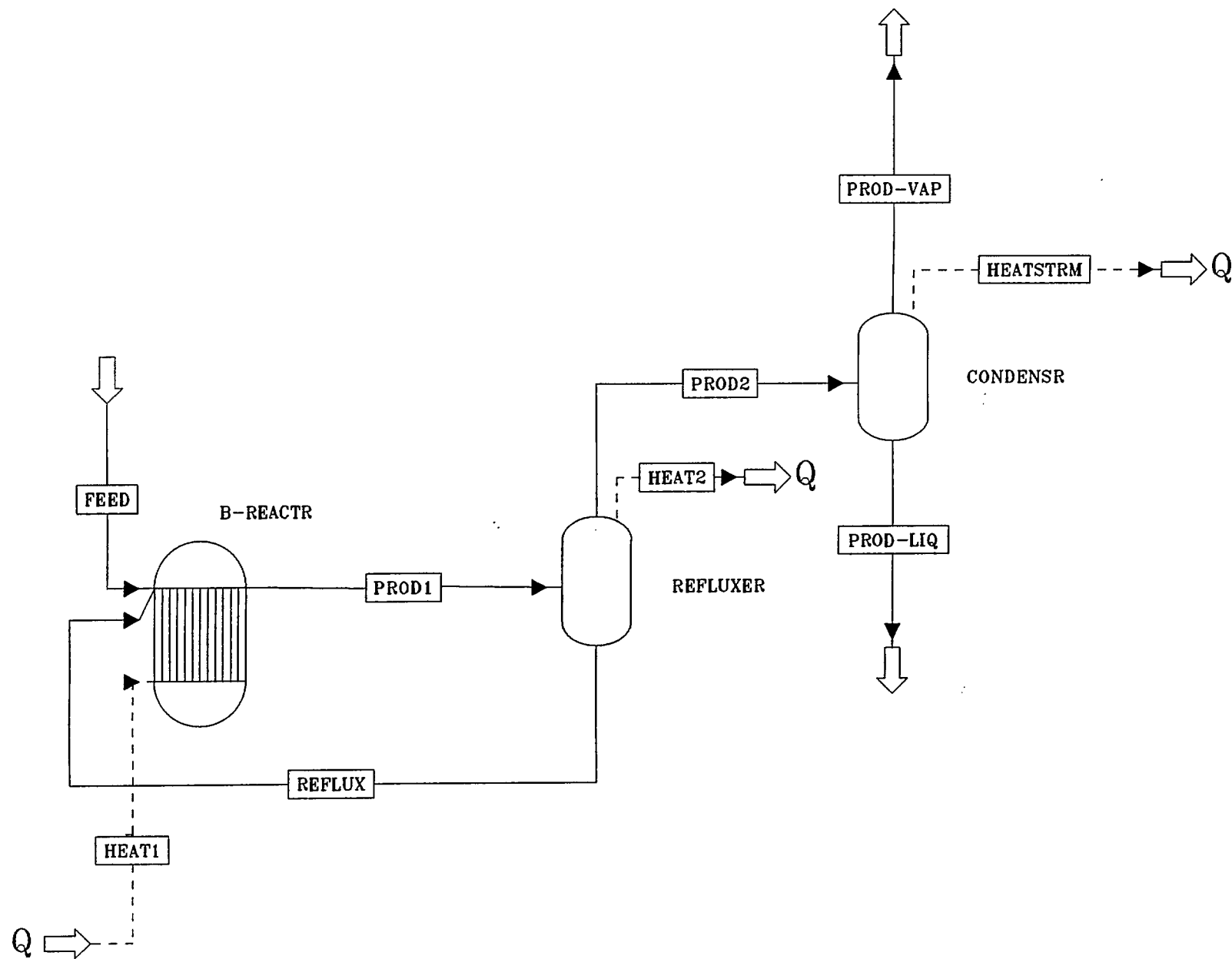


Figure 2: ASPEN PLUS Eicosane Thermal Cracking Simulation Process

3. Results and Discussion

3.1 Process Flowsheet Simulation: Component Distribution of Thermally Cracked Eicosane

Figure 3a compares the olefin and paraffin distribution of eicosane (100 kg/hr feed rate) according to weight percentage versus carbon number after thermal cracking at 170°C. Temperatures for the reflux were determined negligible and essentially had no effect on the component distributions. The distribution of olefins appears to be acute at C4-C5. At C5 the olefins comprise roughly 80 % of the total weight percentage. From C6 to C20 the weight percentage appears negligible. The overwhelming distribution of C4 and C5 liquid olefin components is a result of entering isomeric C4 and C5 olefins such as isobutane, cis and trans-2-butene, 1,3-butadiene, 3-methyl-1-butene, 2-methyl-1-butene, cis and trans-2-pentene and 2-methyl-2-butene into the data bank. These components were accounted for since the GC data from the condensate liquid and gaseous streams showed evidence of the compounds. A-olefin and N-paraffin components from C1 to C20 were added to the data bank as well (Appendix).

Figure 3b shows an enlarged section of Figure 3a from C6 to C24. The region contains solely A-olefins and N-paraffins which comprise 6.30% of the total product from PROD1 (Figure 2). The distribution of both is logarithmic although a slight decrease in C9 paraffins is evident. The amount of olefins is greater than the amount of paraffins which is favourable since a maximum olefin/paraffin ratio is desired for product formation. Figure 3c depicts the A-olefin/N-paraffin ratio distribution of cracked eicosane from C1 to C24. All the ratio values are greater than 1.0 with C9 having the highest value of 2.20 as a result of a lower paraffin value. Ratio values were negligible for C1, C2 and C17-C24. The rest of the values remained in the range of 1.50-1.95.

In Figure 4a the distribution of olefins and paraffins is essentially identical to that of Figure 3a with the exception of an increase in C4 and a decrease in C5 components at 190°C. The increase in temperature resulted in components being cracked further. In Figure 4b the distribution of A-olefins and N-paraffins resulted in a logarithmic spread. Olefins dominated paraffins throughout the distribution as a result of a higher reaction temperature causing an possible optimal maximum for A-olefin products. When Figure 4b is compared to Figure 3b the increase in reaction temperature appears to result in an acute increase in components of lower carbon numbers. The weight percentage increased from 0.39 to 1.13 for C9. The total weight percentage of A-olefins and N-paraffins was lowered to 4.45 % as compared to 6.30% as shown in Figure 3b since the temperature was increased to 190°C. The decrease in the A-olefins and N-paraffins may have resulted from an increase in temperature causing more isomers and branched

components to be formed during polymerization (Figure 4a). Figure 4c shows the A-olefin/N-paraffin ratio gradually decreasing with increasing carbon number. When compared to Figure 3c a sharp contrast is evident. The ratios in Figure 3c are relatively consistent whereas the ratios in Figure 4c are decreasing. The ratios appear greater in Figure 4c (0.95-6.10) thus suggesting that optimum reactor conditions is nearly reached.

Figure 5a portrays the overall olefin and paraffin distribution from C1 to C24 at 210°C. The amounts of C4 and C5 isomers have increased when compared to Figures 3a and 4a. The trend suggests that as the reaction temperature is increased the A-olefins reform to produce isomeric and polymeric compounds. As a result, only 1.94% of A-olefins and N-paraffins were produced. In Figure 5b the components from C6 to C24 are again logarithmically distributed. The A-olefins are dominant but not to the same extent as that shown in Figure 4b. Again, the total weight percentage appears to be slowly decreasing with increasing reaction temperature. Figure 5c depicts the ratio for the selected olefins to be relatively consistent (1.3-2.5) with the exception of C3 and C9 which appear to duplicate the data from the GC readings (Figure 9a and 9c). It is evident that the A-olefin/N-paraffin ratios displayed in Figure 4c with a reactor temperature of 190°C produces the maximum A-olefin/N-paraffin ratio (0.98-6.1).

Thermally Cracked Eicosane

Olefin and Paraffin Distribution

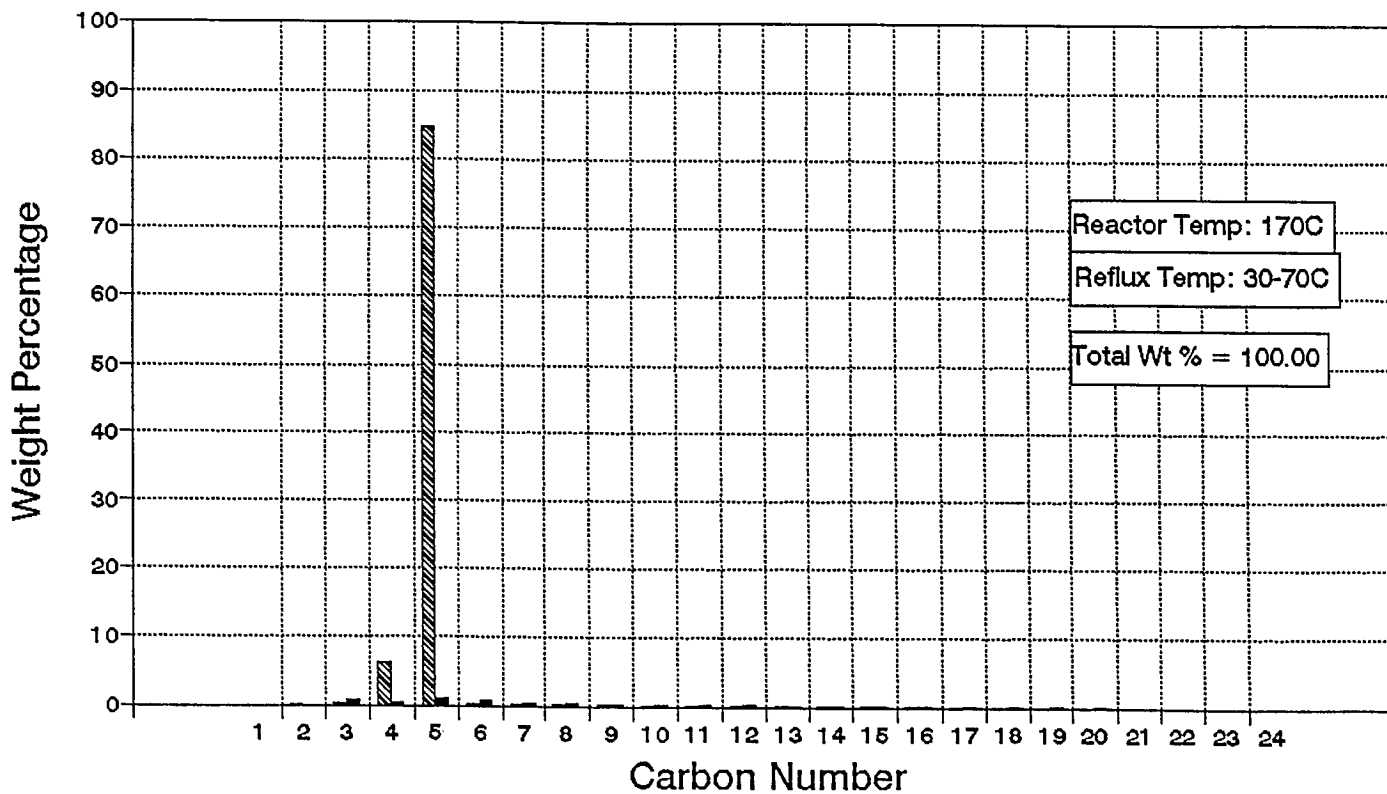
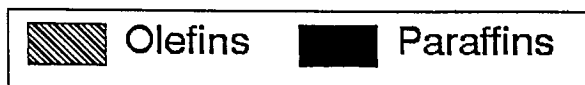


Figure 3a



Thermally Cracked Eicosane

A-Olefin and N-Paraffin Distribution

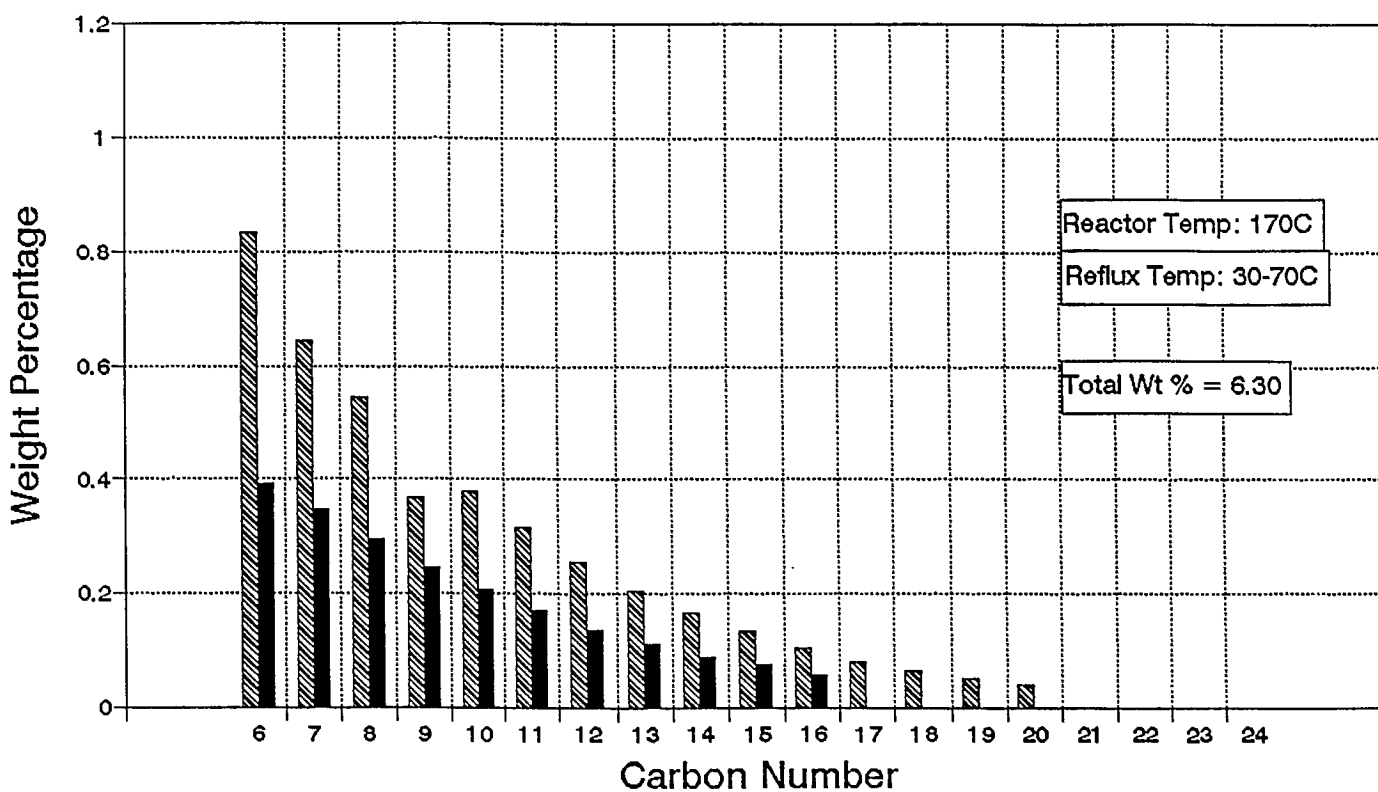
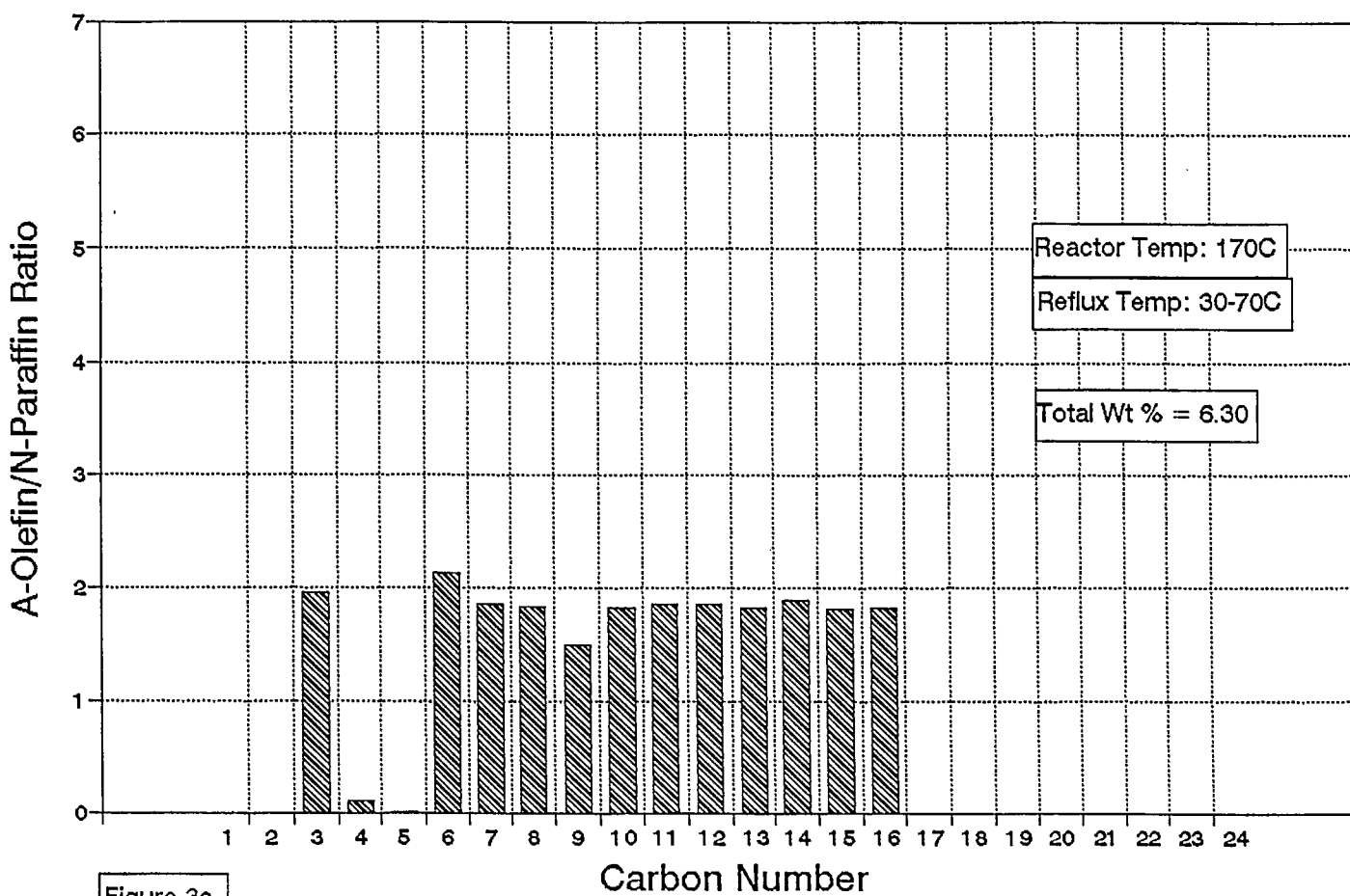


Figure 3b



Thermally Cracked Eicosane

A-Olefin/N-Paraffin Ratio Distribution



Thermally Cracked Eicosane

Olefin and Paraffin Distribution

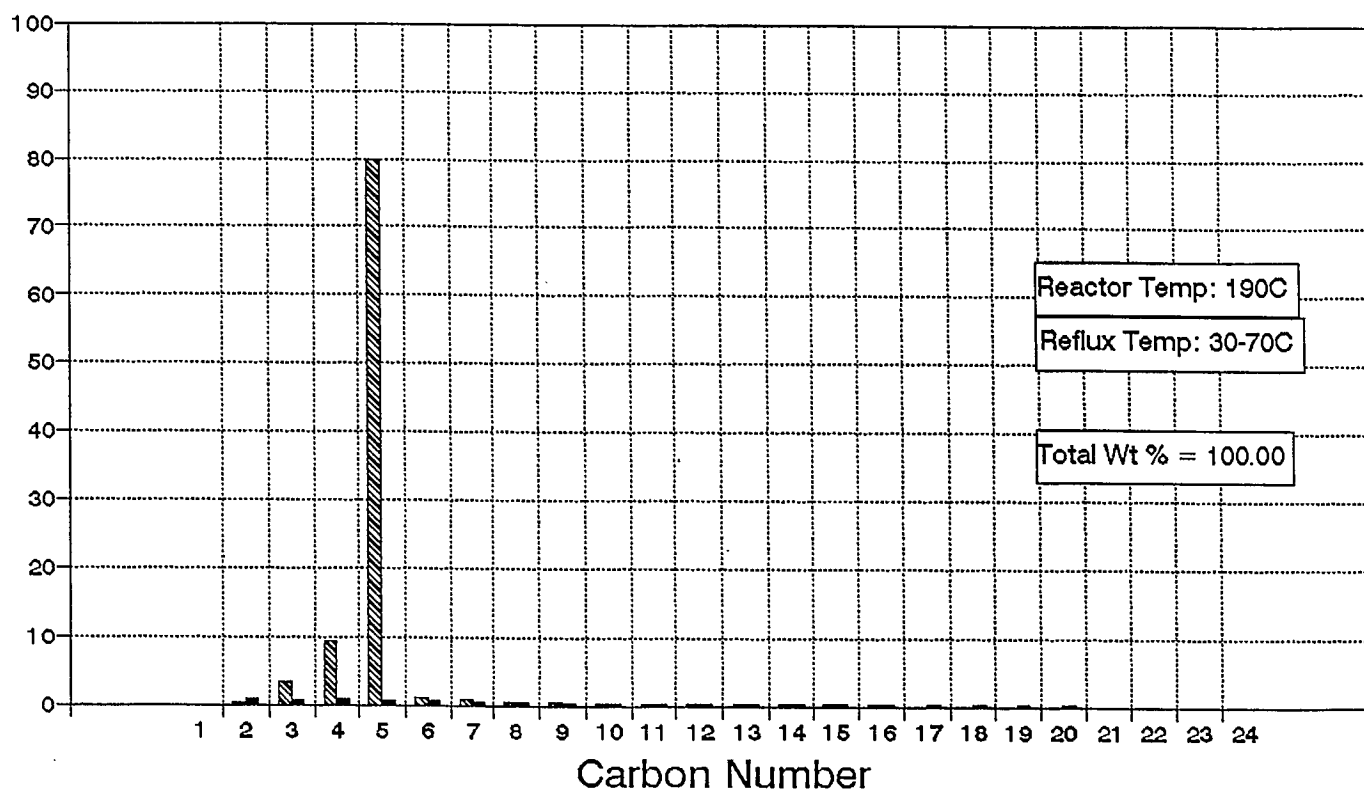


Figure 4a



Thermally Cracked Eicosane

A-Olefin and N-Paraffin Distribution

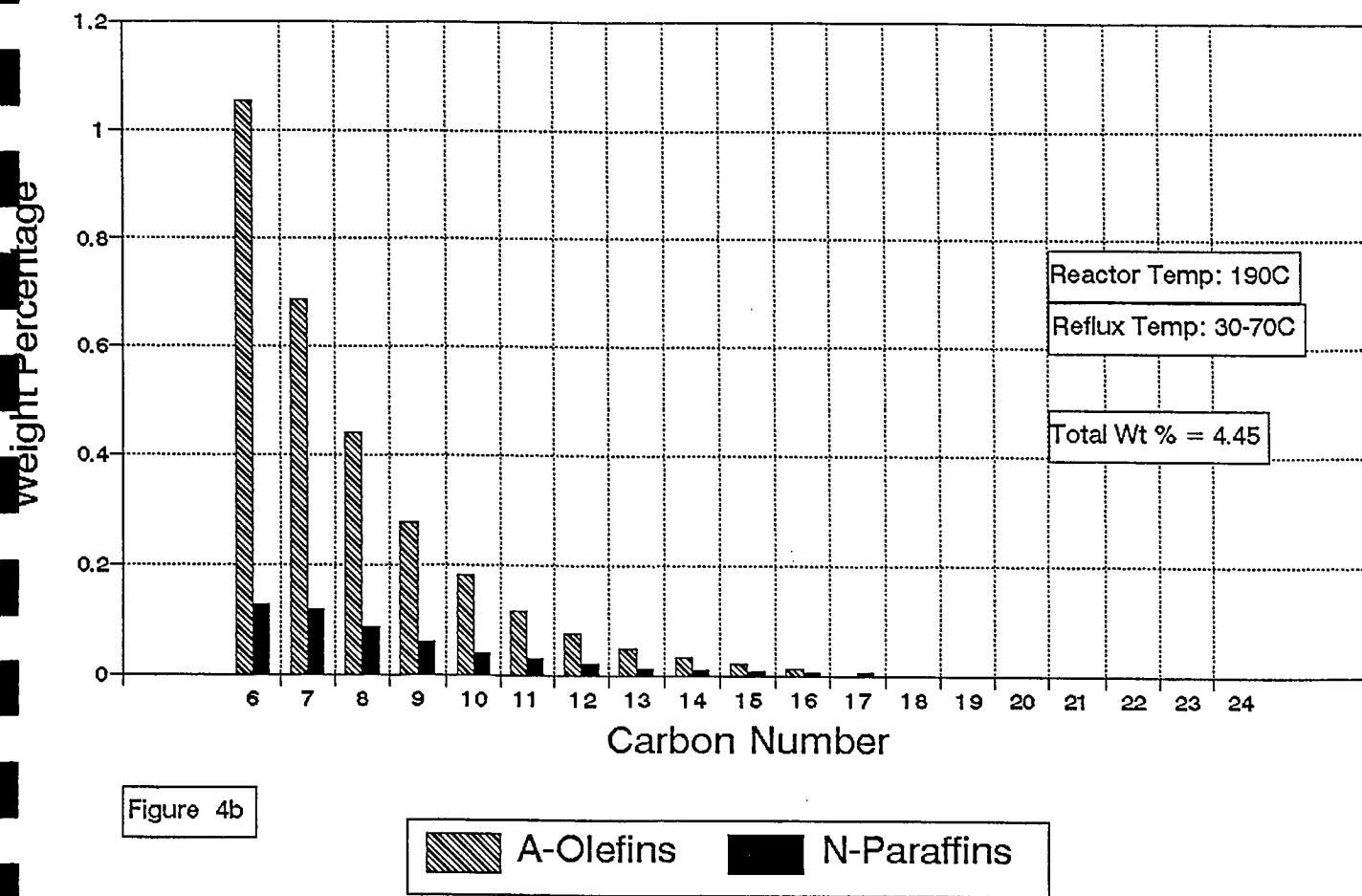


Figure 4b

Thermally Cracked Eicosane

A-Olefin/N-Paraffin Ratio Distribution

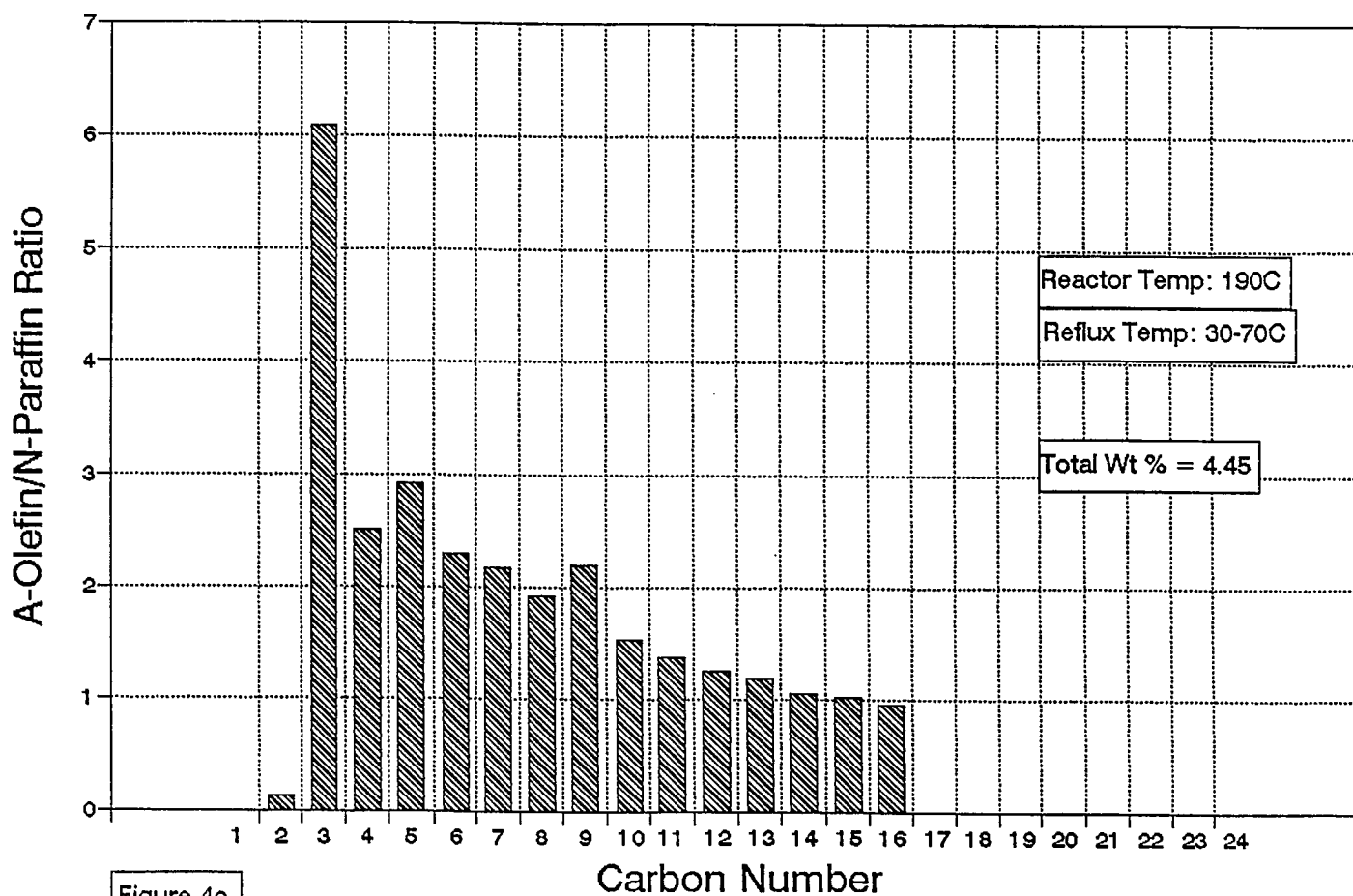


Figure 4c

Thermally Cracked Eicosane

Olefin and Paraffin Distribution

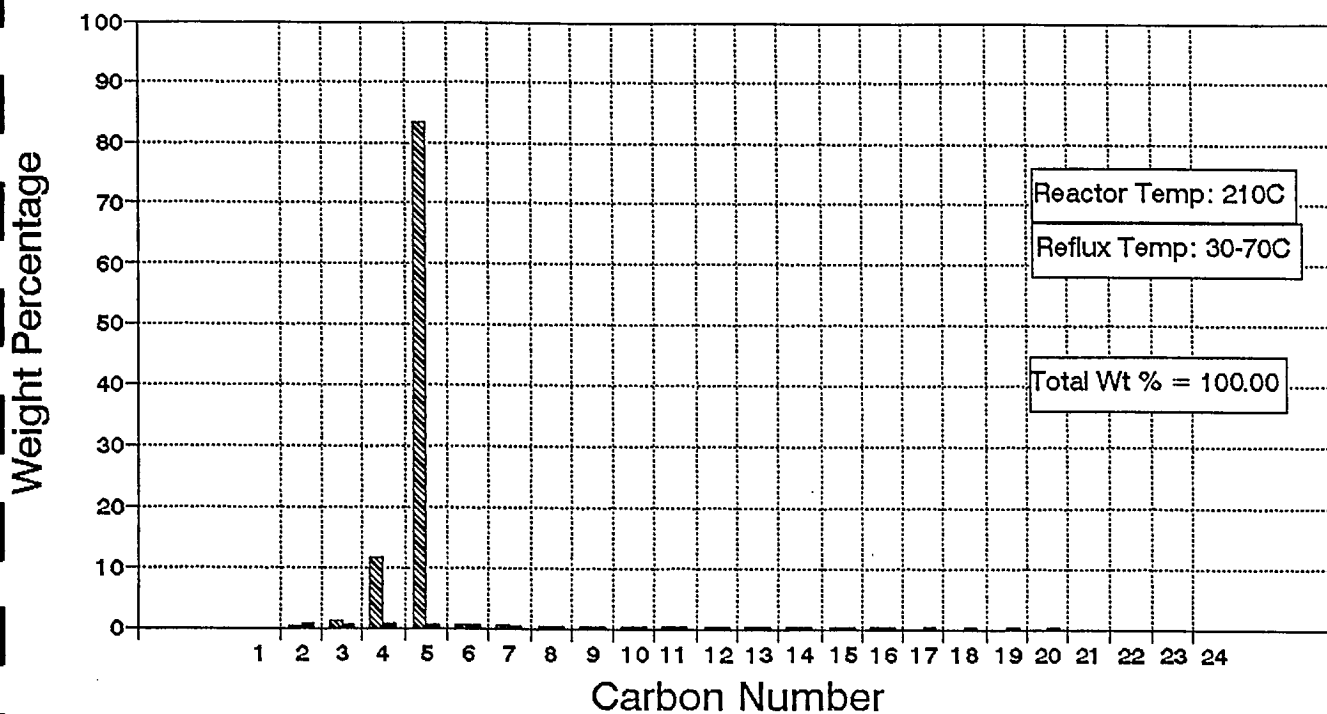


Figure 5a



Thermally Cracked Eicosane

A-Olefin and N-Paraffin Distribution

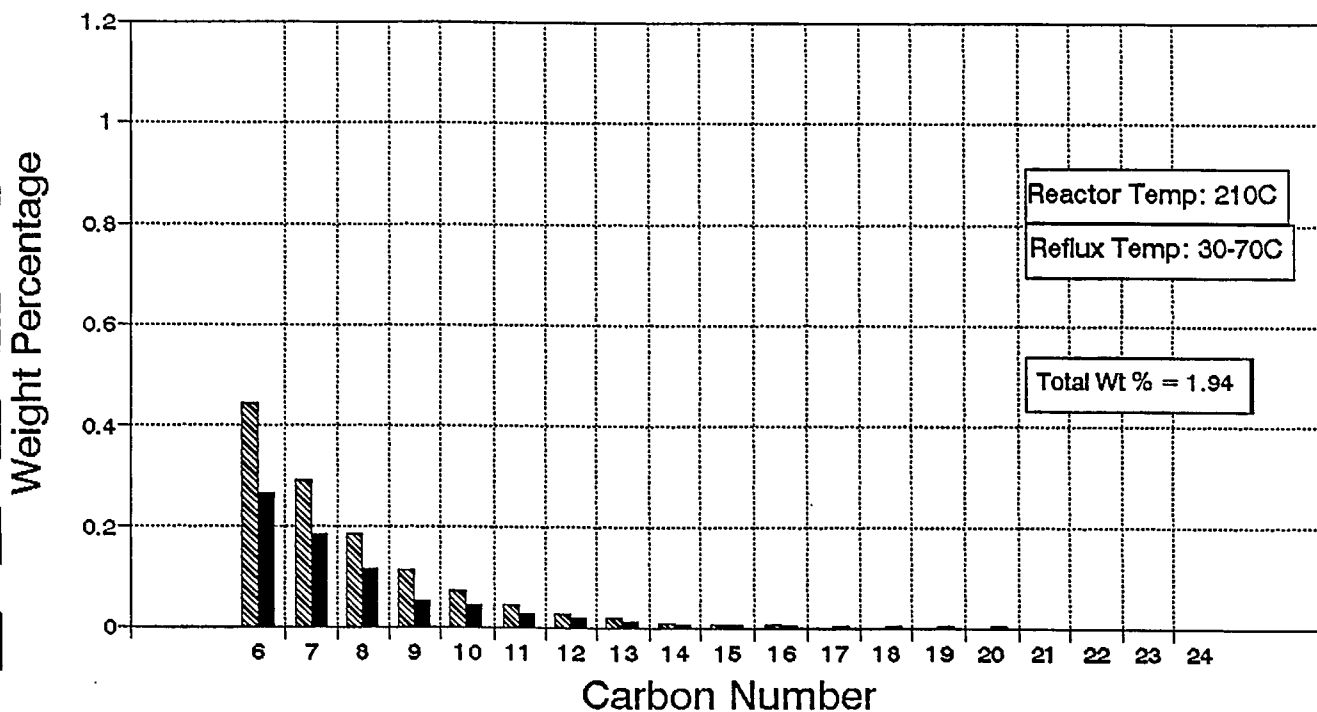
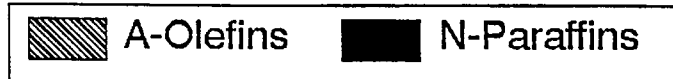
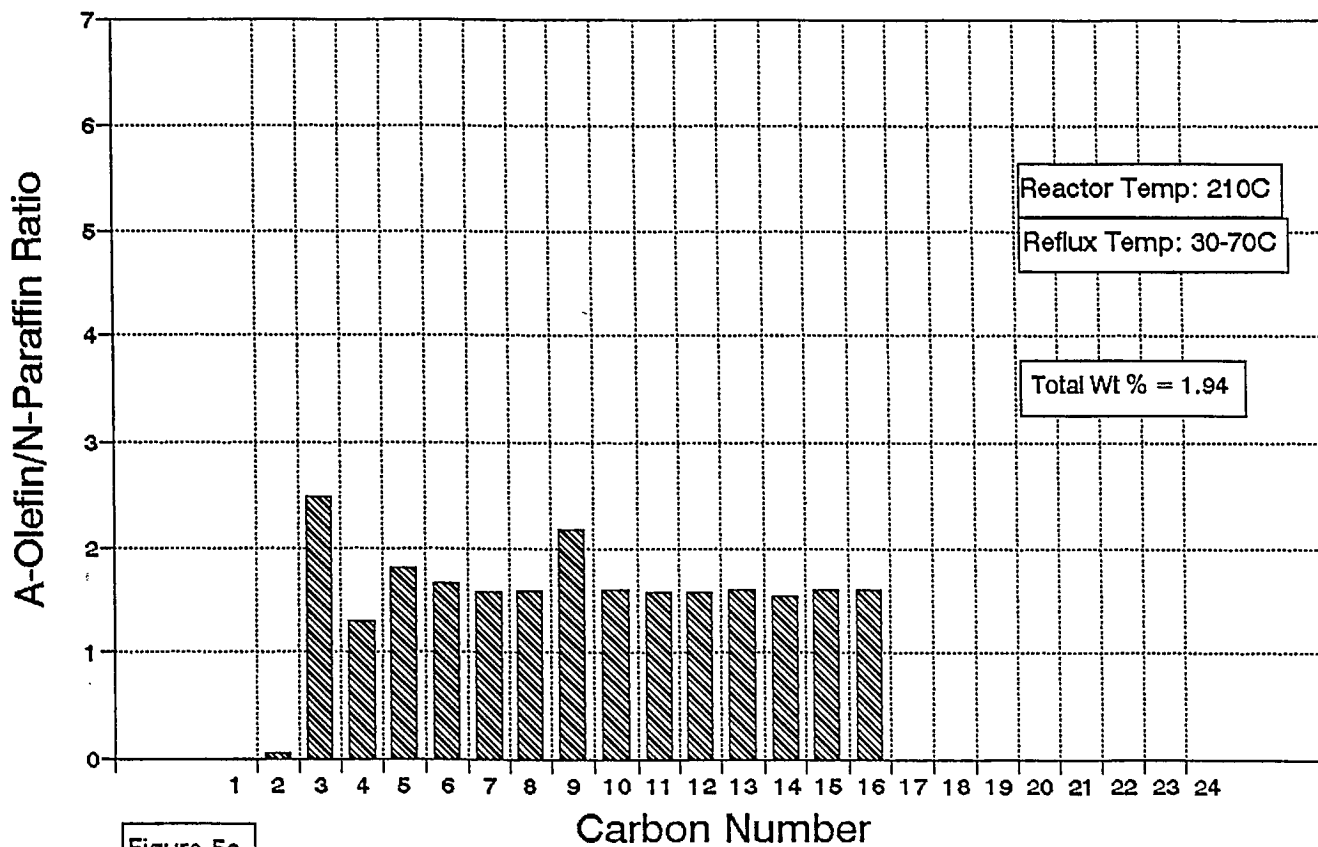


Figure 5b



Thermally Cracked Eicosane

A-Olefin/N-Paraffin Ratio Distribution



3.2 Process Flowsheet Simulation: Component Distribution of Thermally Cracked Pentadecane-Eicosane

Figures 6a to 8b are similar to the previous experiments except that the feed stream contains a mixture of pentadecane and eicosane in a 1:1 ratio (100 kg/hr feed rate). Figure 6a shows an increase of weight percentage to 87% of isomeric C5 compounds as compared to 80-84% from Figures 3a, 4a and 5a. Figure 6b shows an enlargement from C6 to C24. The distribution is uniform with the exception of C9. The A-olefins appear to dominate the N-paraffins at C9 even more. At C9 on the GC chromatograms, C9 often has the highest A-olefin/N-paraffin ratio (Figures 9a and 9b). With the mixture of pentadecane and eicosane in the feed stream the total weight percentage for these olefins and paraffins is 5.01% which is a decrease from the results containing an exclusive eicosane feed stream. The decrease is explained by the mixture of eicosane with pentadecane in the feedstock. More isomeric and polymeric olefins and less A-olefins and N-paraffins were produced. Figure 6c shows the ratio distribution to be similar to the previous. The range was from 0.80 to 1.4.

Figure 7a is nearly identical to Figure 6a with the exception of the slight increase in C4 and decrease in C5 olefins. The higher reaction temperature of 190°C produced further cracking of components thus increasing the weight percentage of the C4 compounds. In Figure 7b the distribution is similar to that of Figure 6b. With increased reaction temperature the bulk of the distribution shifted to C6-C8 (0.24-0.49%) in Figure 7b whereas in Figure 6b, the distribution ranged from C17-C20 and appeared to be more spread out (C6-C8; 0.37-0.48%). In Figure 7c, the A-olefin/N-paraffin ratios were similar to those in Figure 6c except Figure 7c had slightly lower values.

Figure 8a, when compared with Figures 6a and 7a shows a trend with increasing reaction temperature. The isomers and polymers in C4 olefins are increasing while the C5 olefins are decreasing thus indicating that reaction temperature is a factor in determining the degree of isomerization and the final distribution of the components. In Figure 8b, the distribution again shows that the thermal cracking process is uniform. Comparing Figures 6b, 7b and 8b displays a trend with increasing reaction temperature. It is shown that the distribution is shifted even further to lower carbon numbers. At a reactor temperature of 210°C, the A-olefins clearly dominate the N-paraffins. Thus the optimal ratio from the experimental simulation temperatures appears to be at 210°C. Figure 8c depicts the A-olefin and N-paraffin ratio to be relatively high when compared to Figures 6c and 7c.

Thermally Cracked Pentadecane-Eicosane

Olefin and Paraffin Distribution

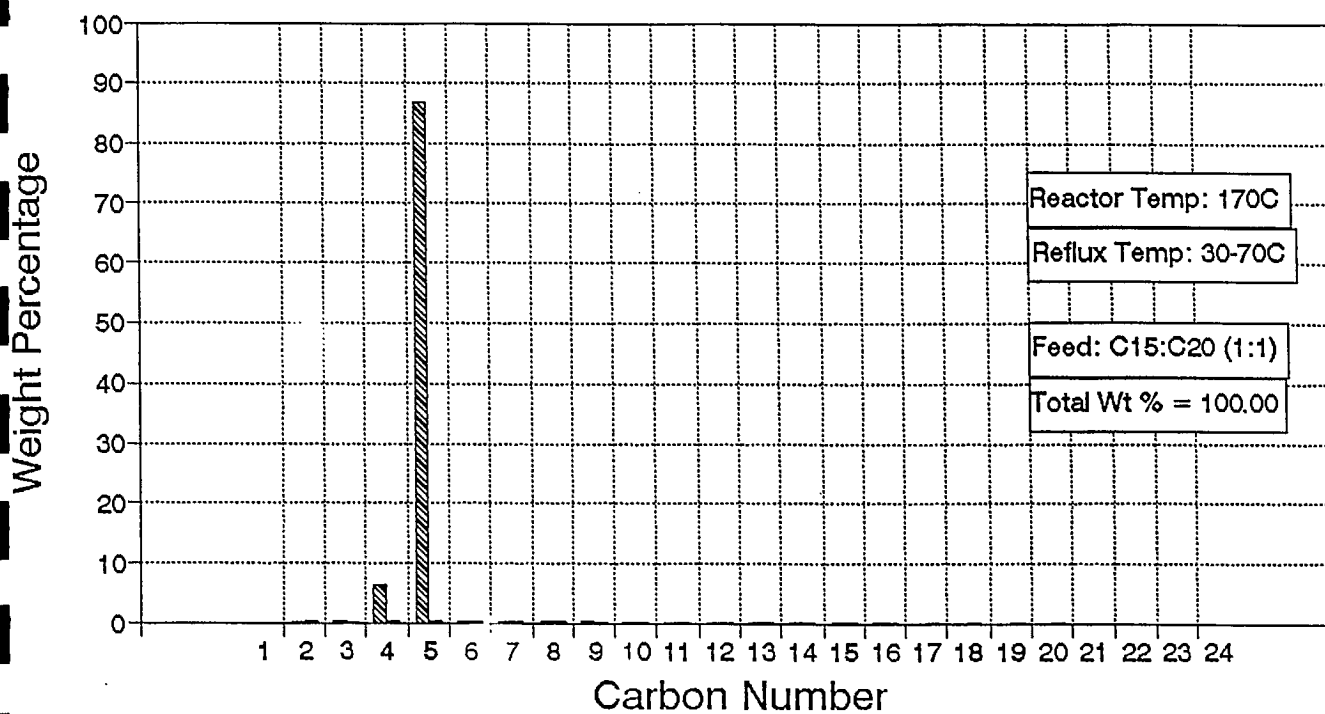


Figure 6a

 Olefins  Paraffins

Thermally Cracked Pentadecane-Eicosane

A-Olefin and N-Paraffin Distribution

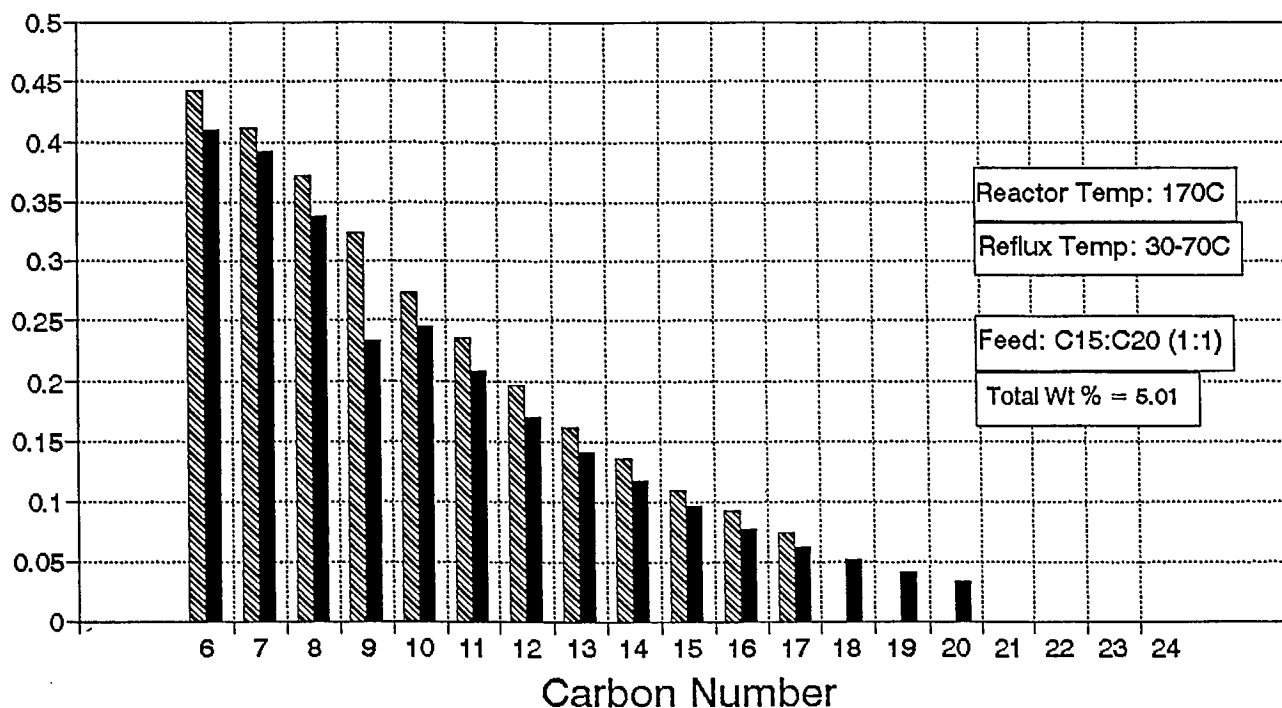
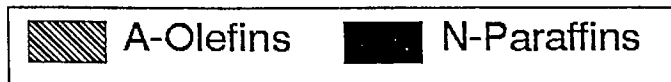
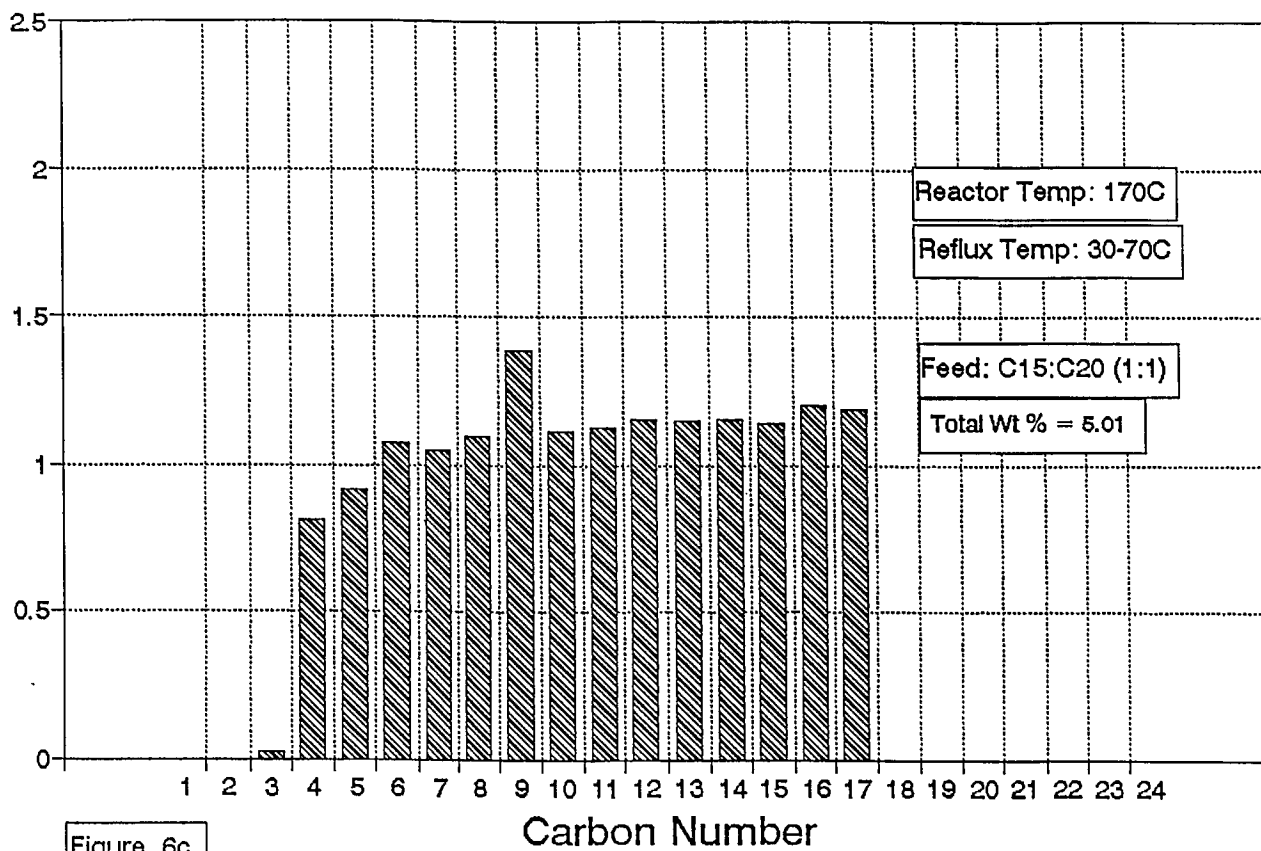


Figure 6b



Thermally Cracked Pentadecane-Eicosane

A-Olefin/N-Paraffin Ratio Distribution



Thermally Cracked Pentadecane-Eicosane

Olefin and Paraffin Distribution

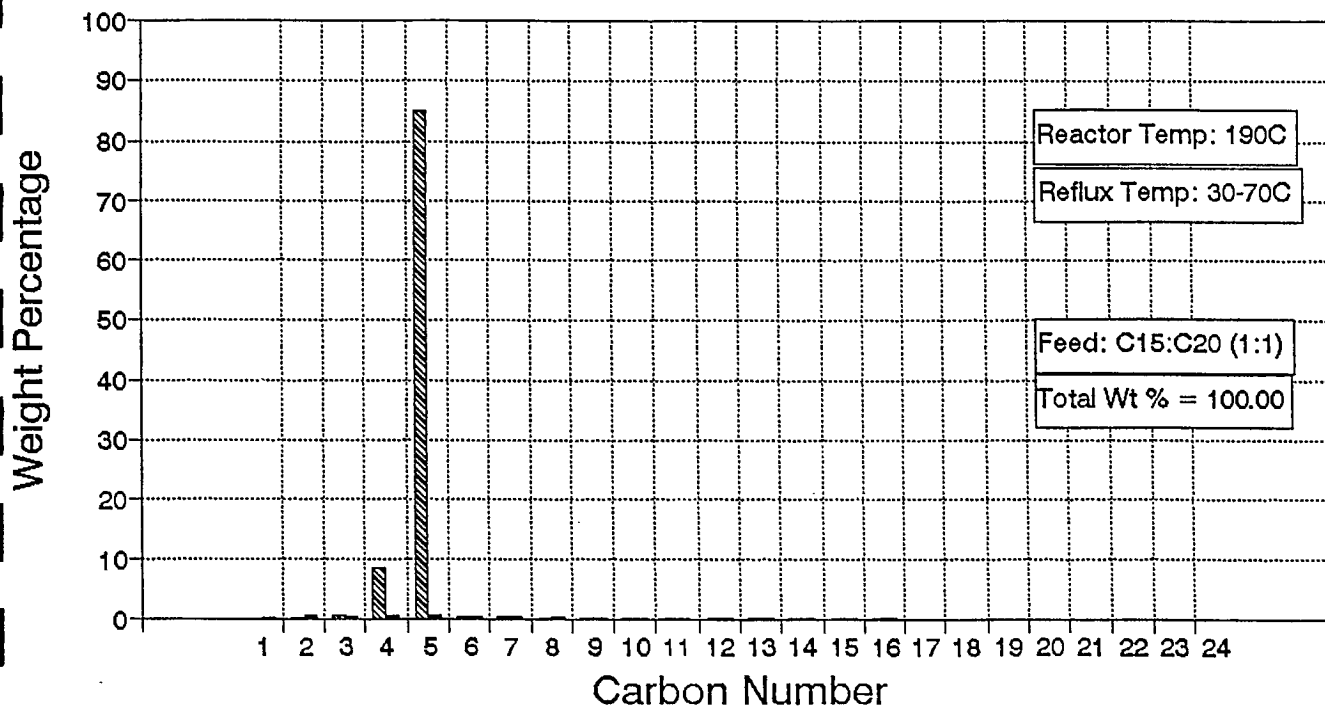
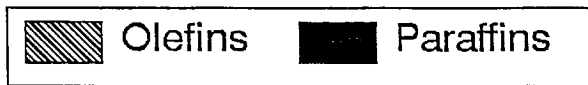


Figure 7a



Thermally Cracked Pentadecane-Eicosane

A-Olefin and N-Paraffin Distribution

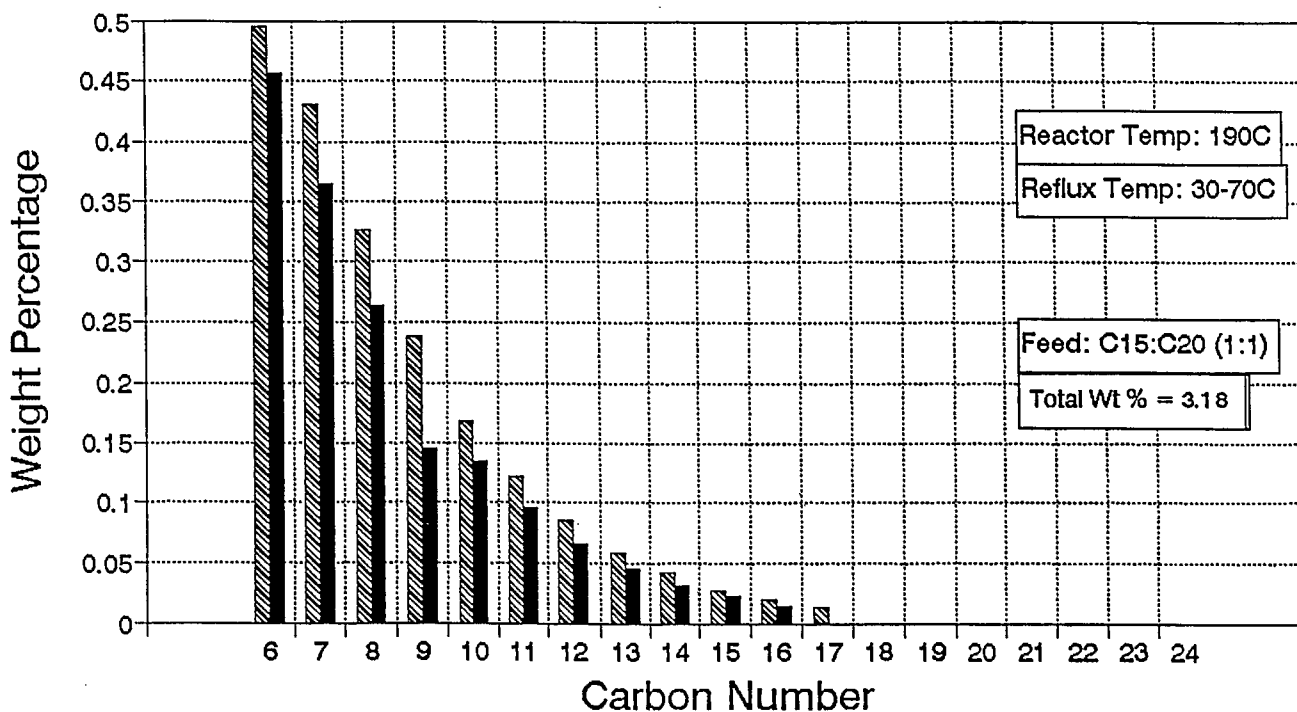
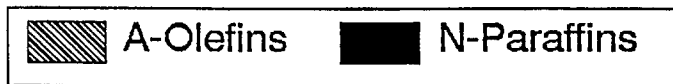
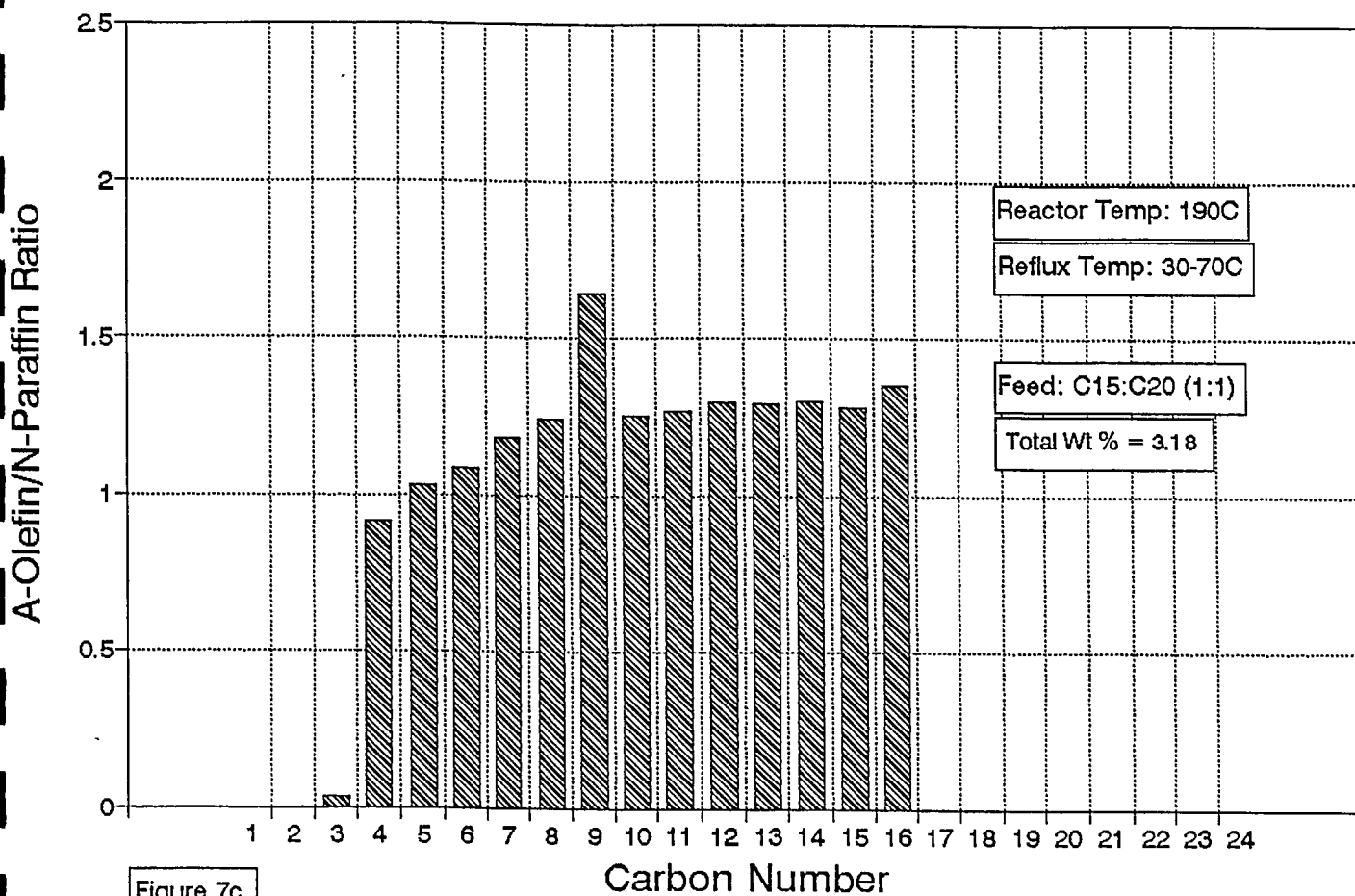


Figure 7b



Thermally Cracked Pentadecane-Eicosane A-Olefin/N-Paraffin Ratio Distribution



Thermally Cracked Pentadecane-Eicosane

Olefin and Paraffin Distribution

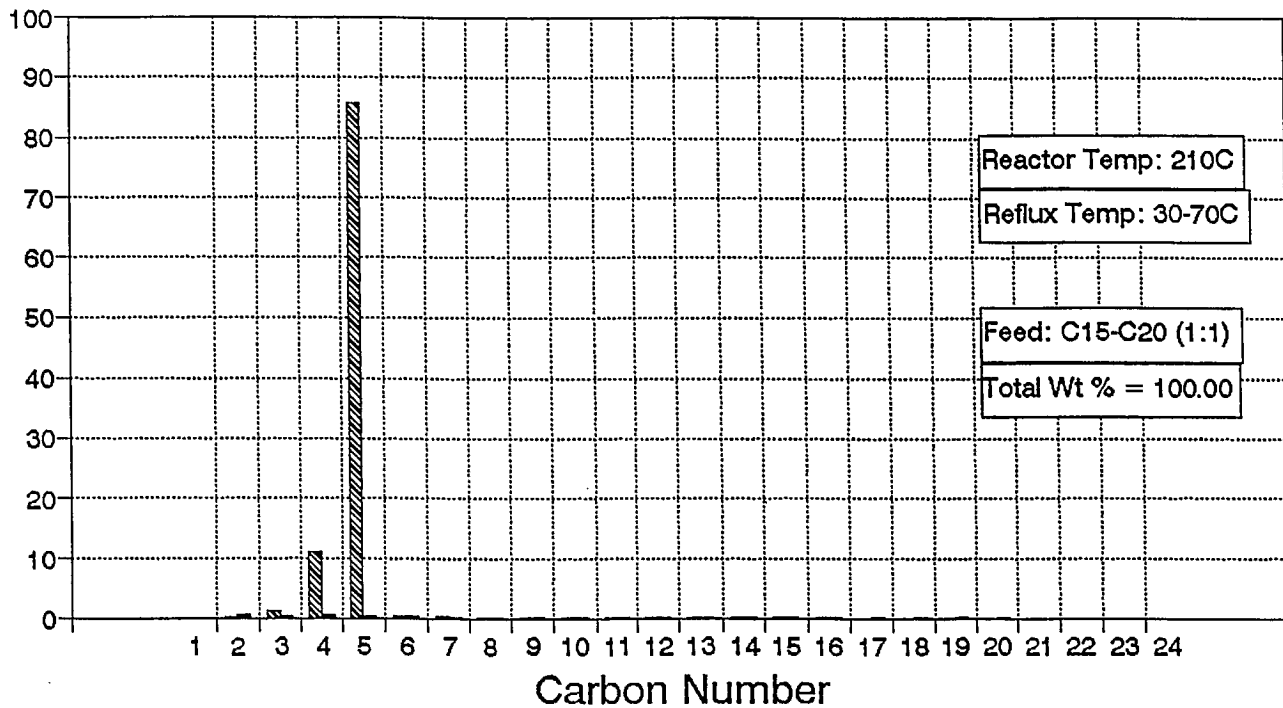


Figure 8a



Thermally Cracked Pentadecane-Eicosane

A-Olefin and N-Paraffin Distribution

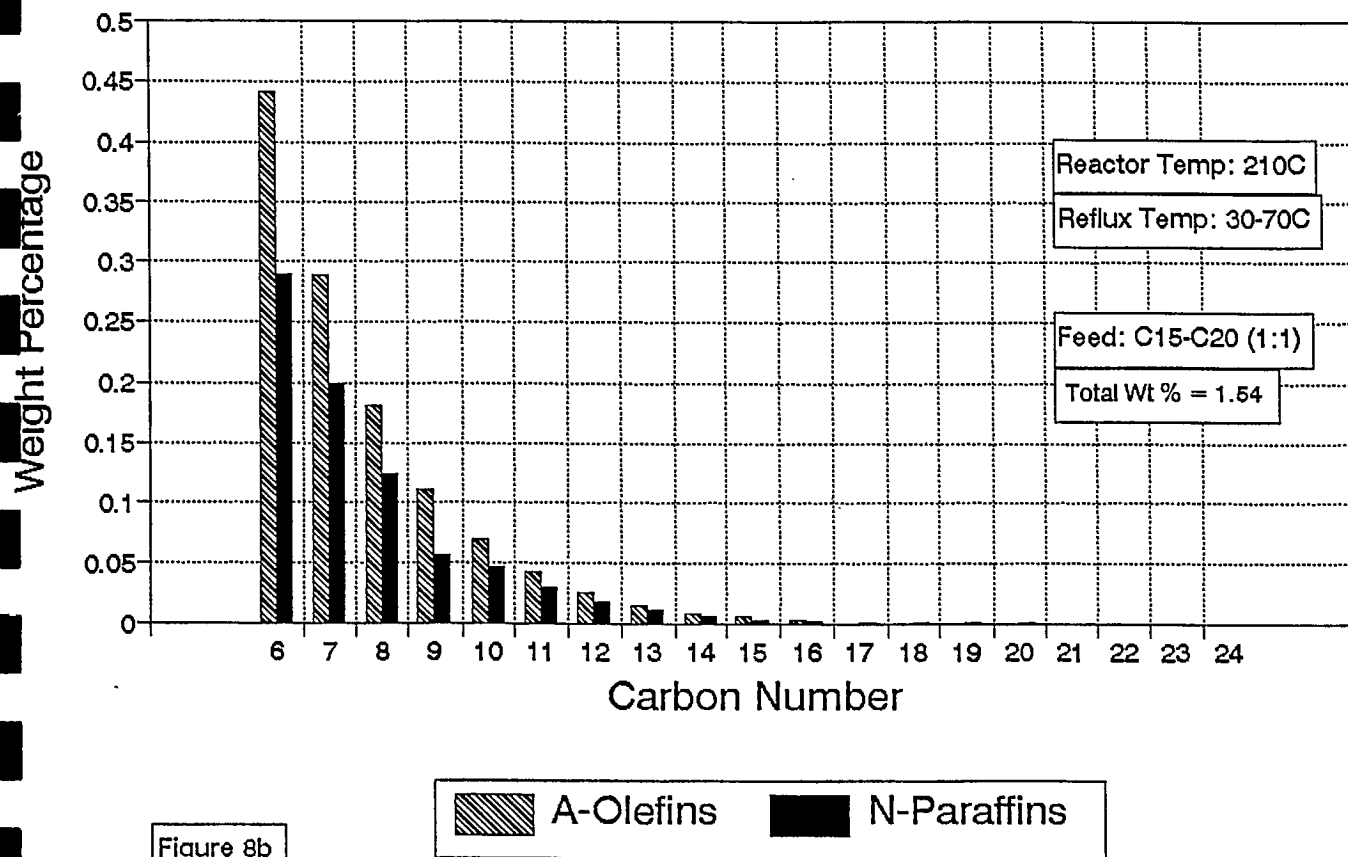


Figure 8b

Thermally Cracked Pentadecane-Eicosane

A-Olefin/N-Paraffin Ratio Distribution

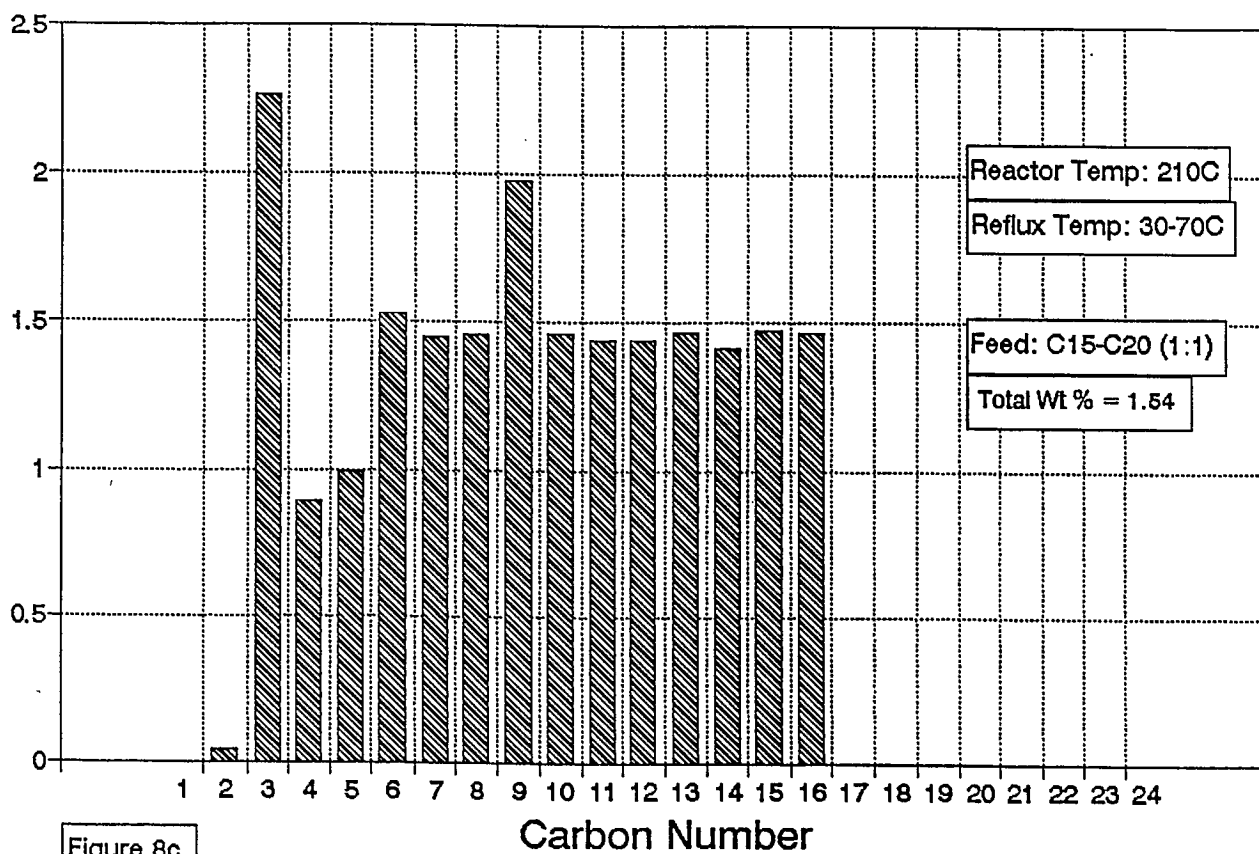


Figure 8c

Thermally Cracked Polyethylene

A-Olefin and N-Paraffin Distribution

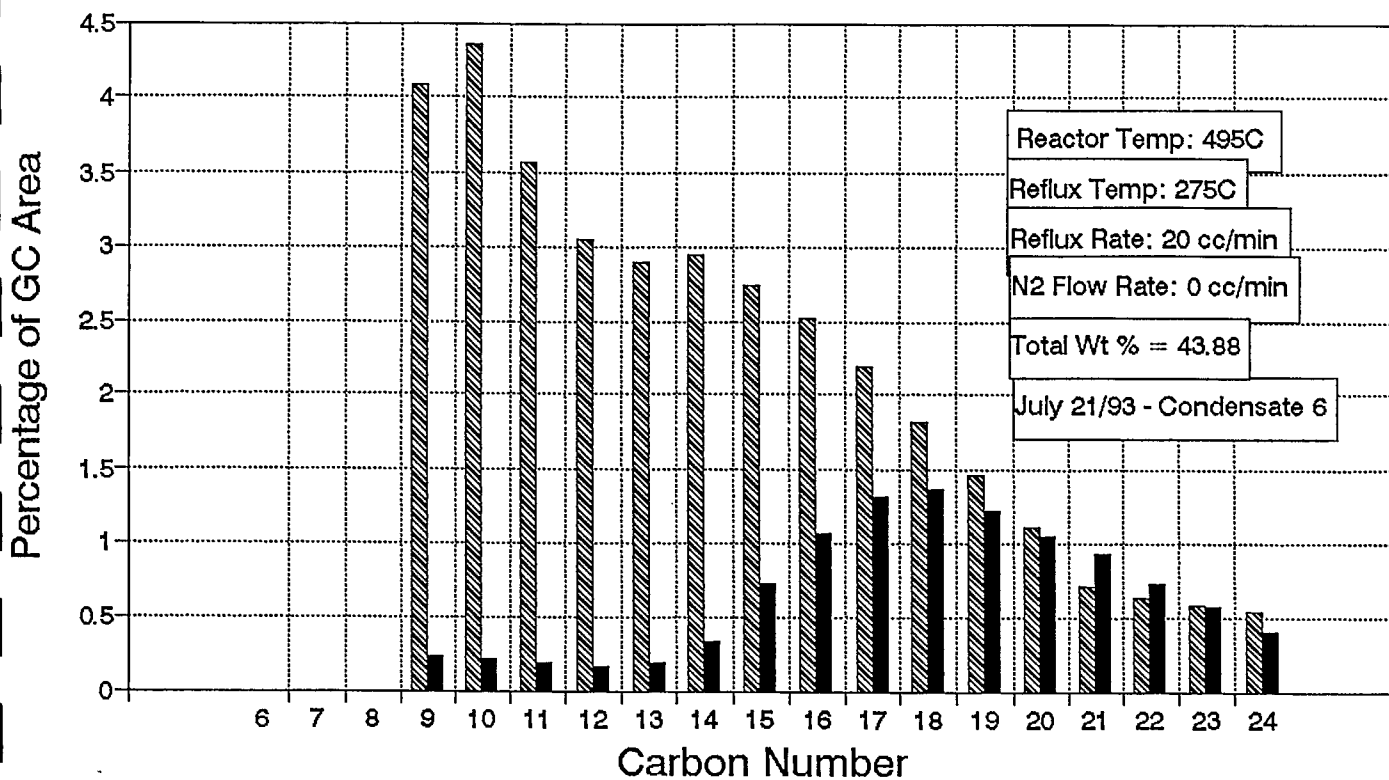
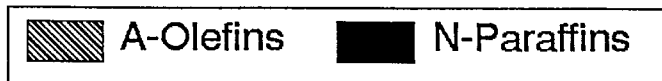
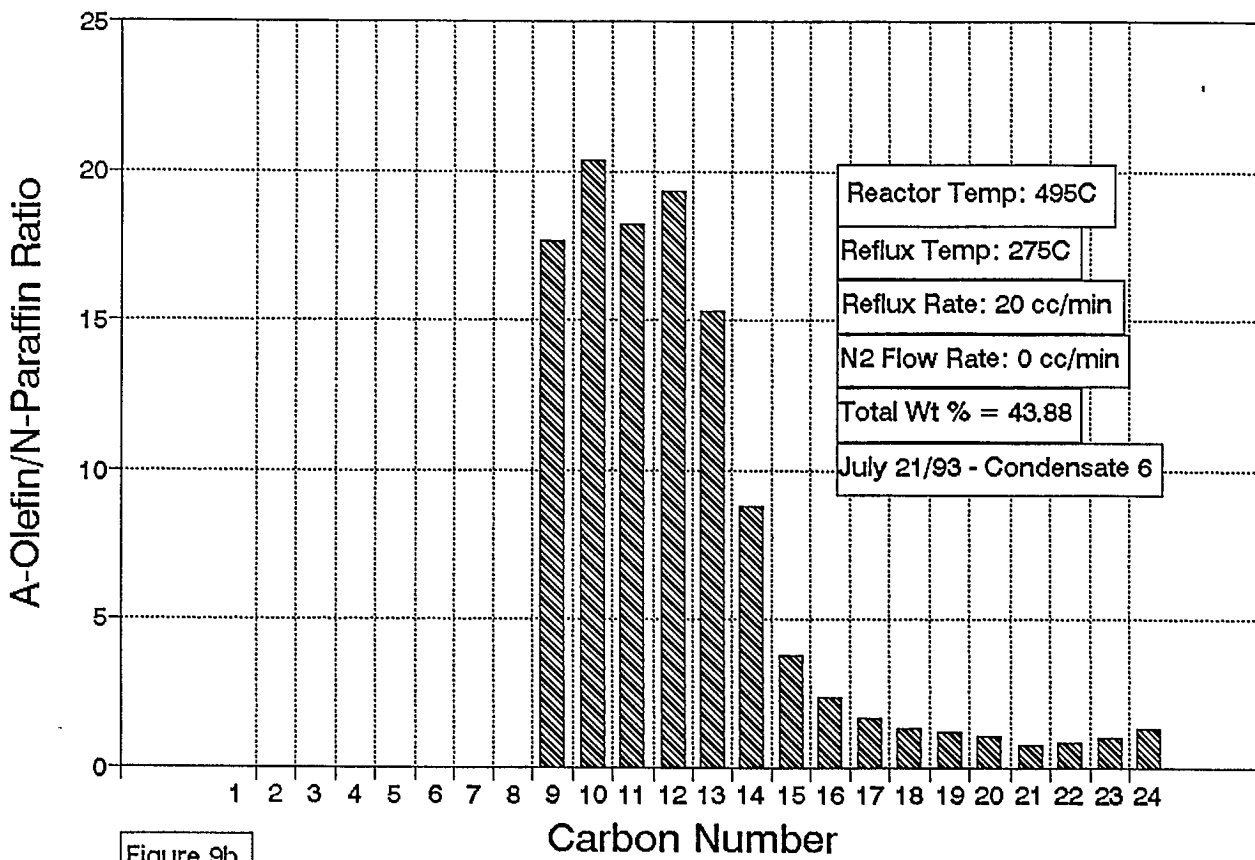


Figure 9a



Thermally Cracked Polyethylene

A-Olefin/N-Paraffin Ratio Distribution



3.3 Gas Chromatography (GC): Component Distribution of Thermally Cracked Polyethylene

Figure 9a portrays actual experimental data obtained from GC analysis. The polyethylene is thermally cracked at a reactor temperature of 495°C and a reflux temperature of 275°C. The distribution was uniform with the olefins decreasing from C9 down to C24 and the paraffins increasing from C9 to C18 and then decreasing down to C24. Olefin and paraffin dominance switched at C20-C21 indicating that the maximum olefin/paraffin ratio was passed. In contrast, switching of dominance is not apparent in the thermally cracked eicosane distributions (Figures 3b, 4b and 5b). In the thermally cracked pentadecane-eicosane mixture, switching of the olefins and paraffins occurred at C9-C10 which is the region where the GC analysis starts to detect the sample. The percentage of GC area value was roughly 4.3% which was considerably greater than the simulation weight percentage value of 1.07% for eicosane and 0.46% for the pentadecane-eicosane mixture.

The computer simulation model was limited since the intended temperatures for the reactor and refluxer could not be attained. In the simulation, the increase in temperature diminished the eicosane to mostly methane product and thus lower temperatures were used. In addition, an infinite residence time for the reactor was assumed.

4. Conclusions

4.1 Analysis of A-Olefin/N-Paraffin Ratio Distributions with Thermally Cracked Eicosane

The A-olefin/N-paraffin ratios obtained in Figure 4c resulted in the maximum A-olefin/N-paraffin ratio for cracked eicosane. The ratios ranged from 0.98 for C16 to 6.1 for C3. The optimal reactor temperature was 190°C with reflux temperatures of 30-70°C. In addition, Figure 3c produced consistent ratios ranging from 1.5 to 2.15. At lower carbon numbers (C3-C7) reactor temperatures of 170°C are preferred whereas at higher carbon numbers (C7-C16) temperatures of 190°C are preferred (Figures 3c and 4c). Depending on the carbon numbers desired either 170°C or 190°C reactor temperatures may produce optimal A-olefin/N-paraffin ratios. Considering the yield of product, the reactor temperature of 170°C may be more advantageous since the total weight percentage is 6.30% as compared to 4.45% at the 190°C temperature.

4.2 Analysis of A-Olefin/N-Paraffin Ratio Distributions with Thermally Cracked Pentadecane-Eicosane

In Figure 8c, the A-olefin/N-paraffin ratios for the reactor temperature of 210°C appear to be the maximum ratios obtained. The values range from 0.8 to 2.3 as compared to 0.76-1.6 and 0.75-1.4

for Figures 6c and 7c respectively. The lower total weight percentage value of 1.54% for Figure 8c (210°C) as compared to values of 5.01 % and 3.18% for Figures 6c and 7c is a disadvantage to the overall yield produced.

The Aspen Plus process flowsheet simulation program was found to be very useful in the understanding and modelling of thermal cracking process of polyethylene. Parameters such as reactor temperature could not be duplicated from experiment since various complications arose in the program software. The distributions of A-olefins and N-paraffins and the ratios were effectively modelled. The need for constant revision is required to perfect the process simulation.

5. References

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6. Appendix

Aspen Plus Quick Reference: Computer Process Flowsheet Simulation Program for Modelling Chemical Systems

1. Using the Pulldown and Popup Menus with the Mouse/Keyboard

When entering ASPEN from the system boot type ASP to enter the program. From DOSSHELL to ASPEN change directories from C:\ to D:\ and type in the subdirectories /MM33/XEQ. Type ASP to enter the program. Do not load ASPEN while in DOSSHELL since RAM memory may not be sufficient for ASPEN to run.

There are various pulldown menus in the main menu bar at the top of the screen [4]:

1) The FILE menu contains New for creating a clear and empty screen, Open for opening work files, Save for saving existing files on screen to the D: drive, Newname for renaming an existing file on screen, Import for bringing backup ASCII files with the extension ".bkp" to the ModelManager program, Export for creating a backup ASCII files of the current program (also Services-Backup menu in FORMS pulldown menu), Print for printing the current flowsheet diagram or selected region and Exit for leaving ModelManager.

2) The FLOWSHEET menu contains Options for controlling the naming, placement and displays of blocks and streams in the flowsheet; Sections for creating a new flowsheet section or dividing the overall flowsheet into smaller sections; Model Menu for showing/hiding the Model Menu on the screen; Find Menu for showing/hiding the Find Menu which is used to locate a block or stream in the diagram; Reorder Ports for eliminating crossing of streams entering/leaving each block; Reroute Streams reroutes the stream(s) selected; Align Blocks for aligning selected or all blocks and streams in the flowsheet; Exchanging Icon(s) for replacing a block icon with a symbolic icon; Unplace Block(s) for temporarily removing blocks from the flowsheet and storing them in the Place menu; Global Data for giving options for global simulation results such as for block heat duty and power, stream temperature, pressure and flow rate.

3) The MODIFY menu contains Edit Text for editing text of a selected block or stream being activated in the Symbol or Draw tool menus in the PFD mode; Font Attribute for changing the size of characters of the selected blocks or streams; Rename for changing the ID name of the selected blocks or streams; Delete for permanently deleting a selected block or stream from the flowsheet.

4) The VIEW menu contains Redraw for cleaning the flowsheet; Zoom In for magnifying a selected region or the centre region on the screen; Zoom Out for shrinking the selected region size; Zoom Full and Zoom Back for displaying the whole flowsheet as large as possible in the workspace and for restoring the flowsheet to the previous zoom level; Centre View for allowing the selected block or stream to be displayed in the centre of the workspace; Preview Mode for allowing the actual flowsheet block and stream IDs and global data to be shown before the diagram is printed; Hide Streams for temporarily deleting streams from the flowsheet.

5) The FORMS menu contains data forms needed to be completed in order for the simulation to be accomplished. The menu contains Next Input for determining the next step required to complete the input specifications for a run; Setup for specifying the default units of measure, stream class and title; Components for specifying the Components.Main form to identify all components; Flowsheet for displaying the Flowsheet.Main form which is equivalent to the flowsheet diagram; Properties for displaying the Properties.Main form to select the option sets to be used in the simulation and to enter optional property specifications (Note: Property Constant Estimation System - PCES - may be used to estimate missing data such as olefins ranging from C22-C50 since the databank only contains C1-C21); Edit Menu/Input for accessing any input or output form and for displaying the menu for the current block or stream; Run Status for checking the error status of the run (Note: The history and output extension files may be checked as well); Stream Summary for displaying a spreadsheet containing all streams; Display Results for displaying the streams or blocks and the results.

6) The RUN menu contains Run which is equivalent to Generate and Submit for executing the calculation of the results; Jobstat for checking the status of the any previous ASPEN PLUS task; Readback for retrieving the results of a completed run that was submitted to run in "background" and storing the results in ModelManager (Note: If runs are executed in "foreground" Readback occurs automatically); Shell for creating a DOS shell to enter DOS commands without leaving ModelManager; Loadsum for loading an ASPEN PLUS summary file from DOS into ModelManager (Note: If the system crashes the results may be obtained in the summary, out or history file extensions); Purge for deleting all results in the present file; Sethost for setting up or continuing a session on a host computer and Endhost for terminating a session on a host computer when ASPEN PLUS/ModelManager reside on more than one computer terminal; Talk for switching to the host computer; Receive for retrieving a file from the host computer and Send for saving a file to the host computer.

7) The PFD menu allows the display of global streams and block data, heat and material balance tables, text and graphics to the diagram. The diagram is uncoupled to the simulation when the PFD mode is active. The PFD menu contains the PFD mode indicator for activating/deactivating the PFD mode; Symbol Menu for displaying extra blocks; Draw Menu for allowing the drawing/adding of objects onto the flowsheet diagram; Segment Editor for showing/hiding the Segment Editor window; Segment Select for selecting graphics segments with the mouse; Layout for creating a simple page layout module to place a frame around a diagram, expand/shrink or rotate a diagram and to print the diagram(s) on one or many pages; Restart PDF resets the PDF settings;

8) The SETTINGS menu contains Grid/Scale for setting the desired appearance for the flowsheet diagram; Printer for setting the HP LaserJet (bitmap) printer and the LPT1 (Parallel) Port designations; Save Settings for saving the printer settings.

Select FORMS from the pulldown menu using left mouse button. For a new setup select Setup or Next Input for updating a file. Note that Next Input creates a new Forms window. In most cases, Next Input should be used when no Forms window has been created.

A Forms window is active when a double line is visible in the window title bar. By clicking the mouse anywhere within the form window the form becomes activated. Located on the top left of each Forms window are 2 boxes - a marked and an unmarked box. The unmarked box closes and cancels a window and the marked box closes and stores the window for later use. Located on the top right of each Forms window is 1 box. Clicked with the left mouse button, the window is deactivated. With the right mouse button a menu appears. Restore reactivates the window, Minimize temporarily stores and Close closes the file and erases it from the screen.

The Forms functions contain commands to be used within each form. Browse Input allows movement to the next form. The Cmnd function followed by other Services functions and the menu items that are to be selected may be used to change data entries. Edit Menu allows movement to any input or results form. Checking the completion status of the simulation is possible as well. The Help function displays useful aids in a specific field, menu item or form. List displays a menu of possible choices and is equivalent to the right mouse button. MaxRestore allows the switching between a Forms window and a full screen forms display. MMhelp displays general help for using ModelManager. Next displays the status of an incomplete form, allows movement to the next menu or form requiring input. PrevMenu displays the menu of the previous form in the menu hierarchy. Results allows only the results from the most previous simulation run to be shown. Services lists a menu that contains various functions that can be performed on forms.

The service menu commands are used for file editing. The Backup command saves the input and graphics information to the disk in the backup ASCII format. The Delete command erases the input from the run. For example, Delete will erase menus such as Design-Spec but will not erase streams, blocks and components. Streams and blocks are deleted from the graphics flowsheet or from the Flowsheet.Main form. The Edit command is similar to that of the ASPENPLUS menu. The Gen-SS command allows the generation of a Lotus-format spreadsheet file. The file may be used in spreadsheet programs such as Lotus 1-2-3, Quattro Pro and Excel. The Gen-Tabl command generates a table of stream results to be displayed on PFD mode drawings. The import command merges the data in a backup file into a current run and is equivalent to MMRestore with /Merge. The Newname command assigns a new Run ID to the current run. The Plot command displays a plot of the data from Report forms. The Purge command deletes all the results from the current run and may be used before saving or submitting new data into a run. The Save command saves the data to the disk without leaving the current form and the file is automatically saved after each submittal run.

To select a menu from a blank field in a form provided that a numerical field is not required, click with the left mouse button to select the desired field and then click with the right mouse button to activate the popup menu. Choose the desired item from the list and click the right mouse button. With the keyboard, use cursor keys to select the field and press F5 to activate the popup menu. Press F1 for Help if necessary.

2. Creating a Process Flowsheet Simulation

(Refer to ModelManager and ASPEN PLUS Installation and Reference for the PC. The Help feature in the Main pulldown menu is useful.) Individual blocks may be chosen from the Menu list on the right column by clicking the right mouse button. The pointer will change to a crosshair and the desired location of the block is selected by a single click (small boxes appear around the block) and is confirmed by a double click.

To erase the location, single click the mouse on the block and click the right mouse button to access the popup menu and select Delete Block. To move the block or stream location, double click the right mouse button

To erase a block selection (crosshair cursor), point to the top right box of the drawing screen where Insert appears and click the right mouse button to deactivate the cursor.

To move an object, point, press and hold the right mouse button on the object and drag the mouse to the desired location.

To select a region, press and hold the left mouse button at the corner of the desired area and drag the mouse to form a box around the region. In order to deselect a region, click the right mouse button away from the selected region.

3. Filling Data into Forms

Setup.Main

-Global units are set to MET and the basis is set to MASS. Units may be modified to suit each simulation using the setup option in the forms. For example, metric units may involve °C instead of K for defining temperature.

Components.Main

-Type ASPENPCD as the databank to be accessed for organic and inorganic compounds. (Aspen Pure Component Databank) [4].

-Click the left mouse button on Alias or Component Name to access the databank then click the right mouse button to list the items in the databank menu. Use the left mouse button to select and enter the desired compound. Continue to select all the compounds that are involved in the simulation in the same manner.

-Enter Comp ID name to identify the compound. Note that the Output ID is automatically named. Type C represents conventional as opposed to Type N - nonconventional.

Flowsheet.Main

-All blocks are automatically identified when the flowsheet diagram is completed in ModelManager Graphics Mode. The flowsheet connectivity including inlet and outlet streams as well as any heat or work streams must be specified and completed [4].

Properties.Main

-For Opsetname enter SYSOP0 for vapour-liquid equilibria at ideal conditions from the popup menu.

-For Free-Water enter SYSOP0, for Solu-Water enter 3 (default) and for True-Comps enter YES. Note that the Henry-Comps and Chemistry fields are left blank as well as the rest of the form [4].

-For producing components with carbon numbers greater than 21 (beyond the range of the data banks) data must be entered. Select PCES and then STRUCTURES to specify the molecular structure of the component [4].

Material Streams

Enter the TEMP, PRES and the basis-FLOW. Specify the Composition Basis and the Total Flow Basis using the popup menu. Usually units of mass/mole and mass/mole fraction are easiest to manipulate. Enter the Total Flow in specified units from the popup menu.

-The values for NPHASE (number of phases, default=2), PHASE (default=V), FREE-WATER (NO), MAXIT (maximum number of flash iterations (default=30), TOL (flash convergence tolerance, default=0.0001) and FLASH-OPTION (NOFLASH). Note that only the initial material stream is specified since the other streams are

dependent on the initial stream [4].

Stream.Main

-For each stream in the simulation Temp and Pres must be specified. Units are to be in MET. It is necessary to specify all initial conditions entering the first stream. Initial conditions involve specifying the COMP BASIS and TOTAL FLOW BASIS. The most convenient bases to use would be that of mole or mass fraction.

-All subsequent streams are automatically calculated provided that two specific parameters are defined such as temperature and pressure [4].

RGibbs.Main

The RGibbs reactor is recommended in most single-phase chemical reaction-separations.

-Enter the reactor parameters such as TEMP, PRES, CHEMEQ (chemical equilibrium=YES), NPHASE (default=2) and VAPOUR (YES). Optional values such as MAXIT (default=30) and TOL (default=0.0001) [4].

Tear.Main

The purpose of the tear stream is to solve design specifications of the flowsheet iteratively with recycle loops [Sec 20-1].

-All streams present are entered under COMPS and a default value of 0.0001 appears under TOL which represents the convergence tolerance. Labels such as PH (pressure-enthalpy default), P (pressure), E (enthalpy) and NONE are selected under STATE [4].

Flash2.Main

-The reflux and condenser vessels are modelled with the FLASH2 block since only single stage separators are needed [Sec 11-6]. Other blocks such as SEP2 are more suited for other simulations involving separation of components.

-The parameters needed to be entered are the TEMP, PRES, NPHASE (number of phases, default=2), ENTRN (liquid fraction entrained, default=0), MAXIT (maximum iterations, default=30) and TOL (flash convergence tolerance, default=0.0001) [4].

4. Running the Process Simulation

-After saving the file using the File pulldown menu commands, the Run pulldown menu is accessed. Generate is selected in order to generate the file and then Submit is chosen to execute the file. Enter the MODE (background), GETRIDOF=Yes (the history and output files are saved and may be used to update/correct errors via any DOS editor) and SAVEMOD=No. The Next command (F4) submits the file for execution [4].

-After the run is executed the file is save immediately as a backup file on the hard drive using the Services command (F2) in the Forms pulldown menu.

-Note that when corrections are made to the file the Run procedure must be repeated and the file must be saved.

5. Troubleshooting Warnings/Errors

In order to correct errors in the simulation the exact cause must be determined. Accessing any DOS editor will reveal the simulation in printed code. Entering a DOS editor may be achieved directly through the ModelManager using the Services command in the Forms pulldown menu or through DOS after exiting ASPEN PLUS [4].

-After entering the editing program the cause or the errors and warnings is revealed. The problem may then be dealt with in ASPEN PLUS. Many causes of the error are due to incorrect data which inhibits the calculations of mass and energy balances surrounding each individual block in the flowsheet. Incorrect stoichiometric balancing of reaction equations will result in error as well [4].