AN APPRAISAL OF THE MACSIM SIMULATION ROUTINE IN ITS APPLICATION TO AN ALKYLATION PLANT

by

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TITLE : An Appraisal of the MACSIM Simulation Routine In Its Application to an Alkylation Plant

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SCOPE AND CONTENTS:

The object of the program was to develop general guidelines for the art of simulation, and then to show how simulation could be used in practice.

A digital computer simulation was assembled to describe the operation of the Shell aklylation plant at Bronte, Ontario. The solution of the steady-state mass and energy balances provided a working simulation on which to demonstrate the modeling and simulation techniques which are presented.

The simulation was used to predict the operating costs and to assess the technical feasibility of five plant case studies.

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1.0 CHEMICAL PLANT SIMULATION

Digital simulation is becoming an accepted tool for studying the interactions among individual pieces of equipment, or groups of equipment, in a chemical plant. A simulation can be used both to evaluate alternate proposals suggested to improve the operation of an existing plant, or to evaluate a proposed plant design. Based on criteria involving cost and technical feasibility, many proposals and alternate operations can be readily evaluated once the simulation has developed.

The steady-state simulation of a chemical or a petroleum plant is complicated by two factors. First, many of the processing units that must be described are mathematically complex and may also be highly non-linear. Secondly, recycle streams exist in many chemical processing plants. The description of the feed (flow and thermodynamic state) to a processing unit such as a reactor or a separation unit, depends not only on the operation of the equipment preceeding the unit, but also on the performance of the unit itself, and on following units because of recycle. Thus, the steady-state solution must be obtained usually by an iterative calculation of the mathematical models used to describe the process. Hand calculations of the tedious, repetitive, non-linear models required to describe a process could lead to exhorbitant expenditure of manual labour with a high probability of error.

1.1 The "PACER" and "MACSIM" Simulation Executives

The executive routine used in this simulation controls the storing and transfer of information, and the execution of the various mathematical models used in a study.

The PACER (Process Assembly Case Evaluator Routine) executive was written by Professor P.T. Shannon and H. Mosler(M2). The MACSIM (McMaster Simulator System) is a modified version of PACER developed by the Department of Chemical Engineering at McMaster University. A detailed description of the MACSIM executive can be found in Chapters 2, 3 and 4 of reference (C2). The executive can only deal with the steady-state behaviour of a process. No process computations are performed by the executive program; it only transfers information from one model to the next in a logical prescribed sequence. Thus mathematical models are written to describe the various units making up the process. Not all process equipment need be modeled. The relative importance of the various units, and its effect on the questions to be answered, determine whether it is simulated, and the level of sophistication of the simulation that is required.

The MACSIM simulation system is based on the concept of modularity. The executive program controls the execution of the modules which are mathematical models representing pieces of equipment in the overall simulation. The basic premise upon which the mathematical models are formulated is as follows: all input information to a module (feed and operating parameters) is known; the module is required to calculate and to specify the output information. Modules can be easily added, improved or removed. Thus, the description of one equipment in the plant can easily be altered or improved by changing only the particular module.

The executive program requires an analog of a plant flow sheet called the "information flow diagram". The information flow diagram informs the executive of the structure of the process to be studied. That is to say, the information flow diagram indicates the modules (mathematical models) used to represent the processing equipment, process controllers, simulation optimizers and controllers, and the connecting streams through which information is passed from module to module. Thus, just as a plant is a set of equipments with connecting pipes carrying material, the simulation is a set of modules described by mathematical models connected by streams transferring information. In most cases, the modules and the lines of information flow in the simulation correspond to processing equipment and process streams in the plant. However, there need not be, and frequently there is not, a one-to-one correspondence between simulation modules and processing equipment, and lines of information flow and process streams.

1.2 Objectives of the Present Study

During the past decade there has been an increasing use of digital computers in the steady state simulation of chemical processes. This is manifested by the ever increasing number of chemical industries which are forming separate simulation groups to work with research teams, designers and plant operators to improve the efficiency of the total technical team and to optimize present and future processes.

Experience and proficiency in simulation has been shown to be expensive to obtain, both in the cost of highly technical personnel and in computer time. It therefore becomes imperative that the effectiveness and the efficiency of these simulation teams must be improved by providing general and specific guidelines in the practice of simulation, just as these guidelines have been developed for design teams over the past fifty years. Hence one of the main objectives of this investigation is to review one of our previous simulation studies and to delineate the shortcomings and mistakes in this work, to generalize some of the developed procedure and to make recommendations concerning future programs.

This "know-how" has been generated by putting the simulation to work. That is, the simulation has been used to investigate changes in operating conditions, process layout, equipment size, feed purity etc. To measure the correct response to these changes, the economics of the process are required. For a complete economic evaluation, a sensitivity analysis should be included to ascertain the relative importance of each element of the total set of input information to the simulation. In this way the maximum knowledge of the process can be obtained.

2.0 DEVELOPMENT OF THE SIMULATION

The simulation of the Alkylation unit within Shell Canada's refinery, located at Bronte, Ontario, will be used to demonstrate some of the general principles of simulation and how a simulation may be used as an aid in directing future operations and/or programmes. The Alkylation plant is an ideal one to use for this purpose since it is fairly large, complex and the units within it are highly interactive.

In this chapter, a general description of the plant will be presented together with the development of the information flow diagram from the general process flowsheet. In later chapters, the evolution of the various models and the total simulation is presented to demonstrate the requirements and pitfalls within any given simulation. Specifically this presentation concentrates on the philosophy associated with the formulation of the models required for any given level of simulation. Many factors, such as the end use of the simulation (i.e. questions to be answered), the relative importance of the model and the state of total knowledge, must be evaluated, if the equipment is to be described effectively and the model is to be used efficiently within the computer. Since several levels of sophistication may exist for any given model, the justification for each must be evaluated.

Some of the experiences with these aspects of simulation and the philosophy related to model formation have been generalized in the discussion of the models that are presented in this chapter of the thesis.

2.1 Description of the Alkylation Unit

Alkylates are used to improve the octane rating of motor gasoline. The alkylates are produced from the reaction of propylene and butylenes with an excess of isobutane in the presence of sulphuric acid which acts as a catalyst. The excess isobutane must be separated from the product alkylate, combined with fresh olefin and isobutane feed, and recycled back to the reactor. The olefin and isobutane feed streams are not pure and the propane and butane, which are the main impurities would add to the recycle volume, and are therefore removed as byproducts. Thus the plant has three product streams: alkylate, propane and butane. The description which follows relates to the present operation of the unit.

The flow sheet of the alkylation unit can be broken into three sections, as shown in Figures 2.1(a), 2.1(b) and 2.1(c). The first section is the reactor and the initial separator circuit, and it is followed by the depropanizer and deisobutanizer circuits, removing propane and butane plus alkylate.

2.1.1 Reactor and Separator Circuit

The organic feed to the reactor, is a combination of two recycle streams, one from each of the columns, and an olefin-rich, plus an isobutane-rich feed stream. This combined reactor feed first passes through a coalescer to remove water. It is then fed to the Stratco reactor, along with an equal volume of sulphuric acid. The Stratco reactor is a large horizontal shell containing cooling coils to remove most of the heat of reaction, and an impeller. The emulsion that is formed is acid continuous.

If the acid strength is above 89%, and the temperature is between 45°F and

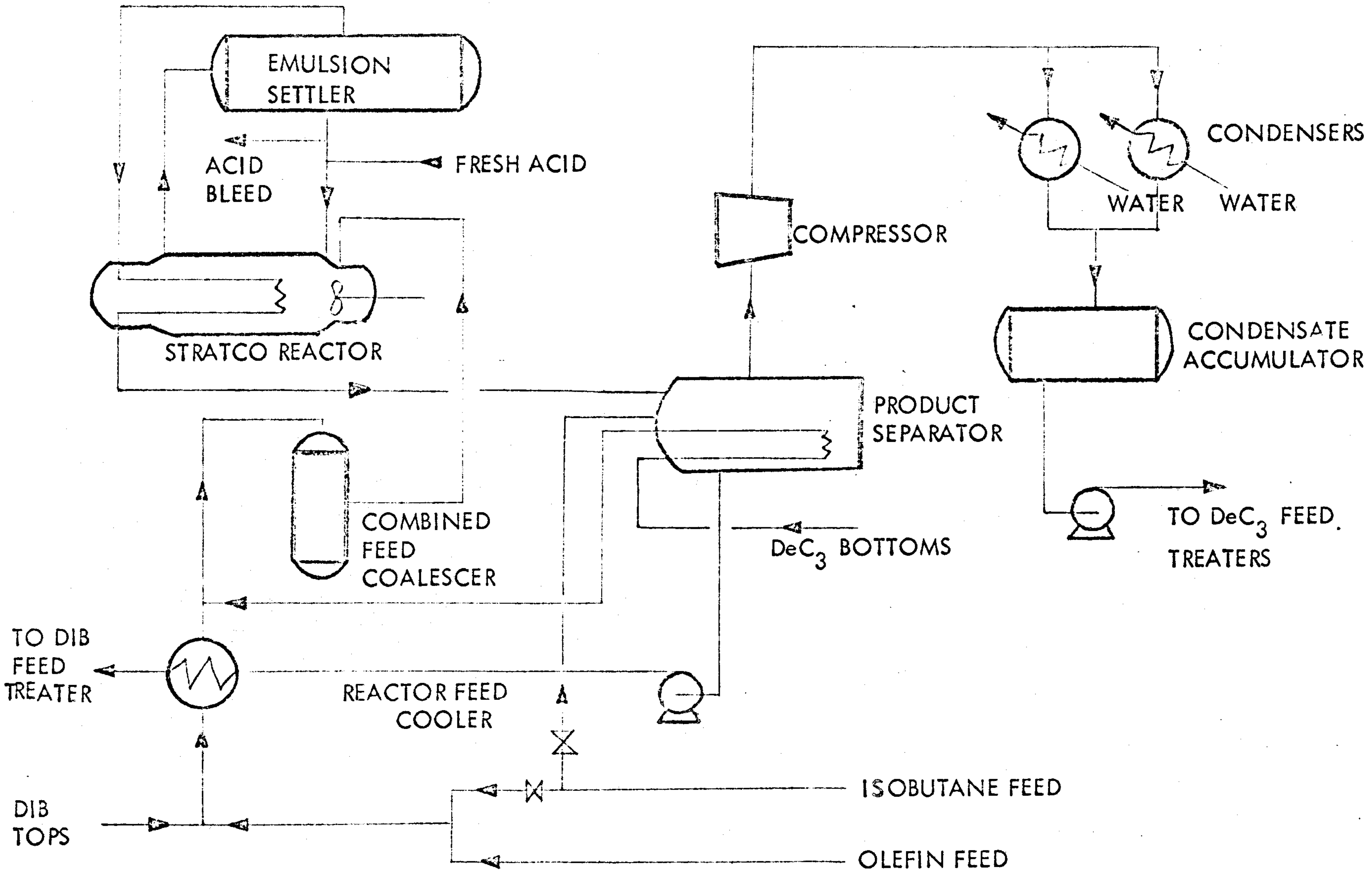


FIGURE 2.1(a) : Plant Flow Sheet of the Reactor-Separator Circuit

55°F, desirable alkylate is produced, and undesirable side reactions are minimized. The reaction rate of the olefins with the isobutane is very high, and as a result, no olefins leave the reactor. The production of alkylate in the reactor is controlled by its ability to remove the heat of reaction and maintain the temperature at the desired level. The propane and butane fed to the reactor are inerts. The emulsion of acid, alkylates, propane, butane, and isobutane leaves the reactor at high pressure (ca. 80 p.s.i.g.) and enters an acid-emulsion settler.

In the acid-emulsion settler, shown above in the reactor in Figure 2.1(a), the acid and organic phases are separated. The acid is recycled to the reactor. Before entering the reactor, some of the acid is bled off and fresh acid added; this compensates for the dilution of the acid catalyst by water from the organic feed, and the "acid oil" produced by side reactions. The organic phase from the settler is passed through a throttling valve and then through the reactor heat exchanger coils, where it removes some of the heat of reaction. From the reactor coils, the flow enters a flash drum called the product separator.

The product separator splits the organic reactor effluent. The overhead vapor is mainly propane,isobutane and butane, and is the depropanizer feed. The remaining liquid contains alkylate, butane, isobutane and some propane, and is the feed for the deisobutanizer column. Additional heat may be added to the product separator to change the relative amounts of vapor and liquid from this separator. The bottoms recycle from the depropanizer, which has already been partially cooled to about 80°F, is further cooled in the product separator heat exchanger coils before entering the reactor. In this way, an additional heat load is supplied to the product separator.

The product separator pressure is used to control the vapor flow. The vapor is compressed in a three-stage centrifugal compressor, and then condensed. If the condensers cannot liquify the total flow, the product separator pressure is raised above the base level to reduce the load on the condensers.

2.1.2 Depropanizer Circuit

The liquified vapor flow from the product separator is pumped under high pressure to the depropanizer (DeC_3) circuit as shown in Figure 2.1(b). Any entrained acid and water is removed by caustic washers and water settlers. The feed passes through a bottom-to-feed heat exchanger, a steam heater, where any desired temperature is obtained, and then into the depropanizer. The overhead is a high-purity propane stream that is sold as LPG. The underflow is partially cooled and then passes through the product separator heat exchanger coils. This stream contains only a few percent propane.

2.1.3 Deisobutanizer Circuit

The liquid flowing from the product separator is fed to the deisobutanizer (DIB) circuit. Entrained water and acid are removed in a caustic wash and coalescer train as shown in Figure 2.1(c). The column feed quality is adjusted in a bottoms-to-feed exchanger. The reboiler is gas fired. The bottoms flow is the product alkylate, and the vapor side draw is a butane-rich product. The distillate flow contains butane, most of the isobutane, and propane. This stream is recycled back to the reactor.

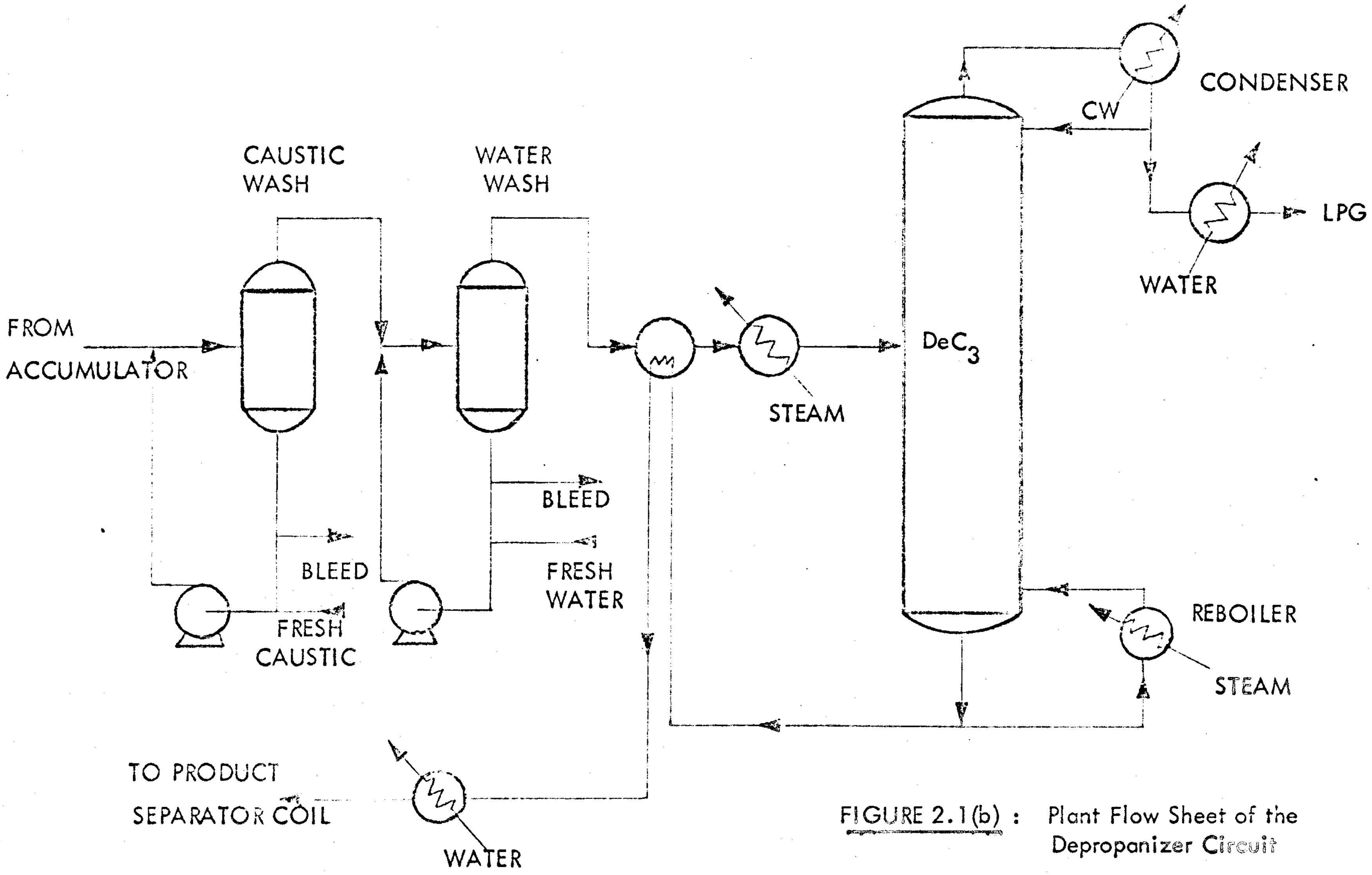


FIGURE 2.1(b) : Plant Flow Sheet of the Depropanizer Circuit

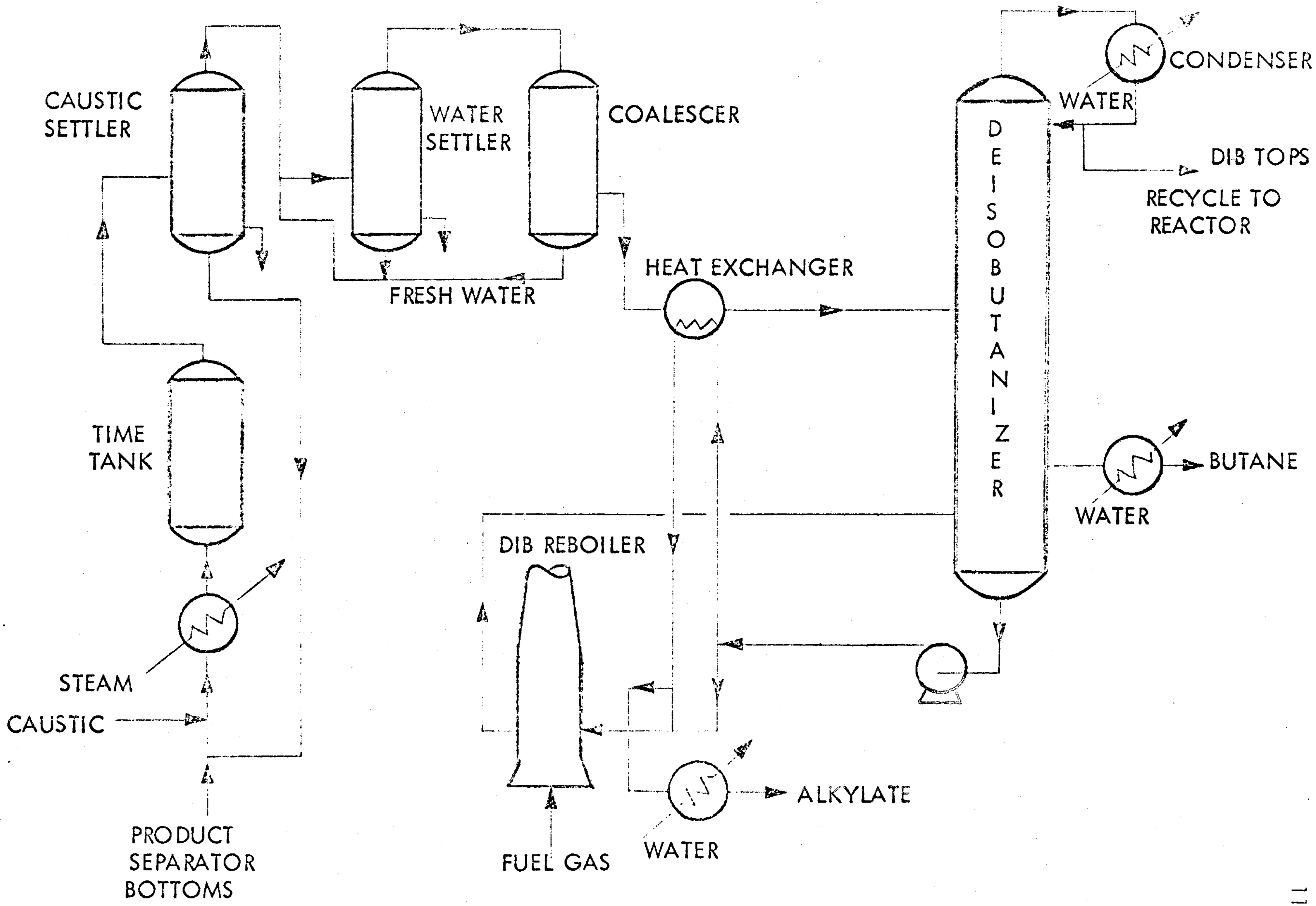


FIGURE 2.1(c) : Plant Flow Sheet of the Deisobutanizer Circuit

2.2 Construction of Information Flow Diagram

An information flow diagram is required for the MACSIM simulation system. The information flow diagram describes the transfer of information (stream composition and thermodynamic variables), from model to model, just as the piping transfers fluid from equipment to equipment in the actual plant. The plant flow sheet, as discussed in Section 2.1, must be thoroughly understood before an information flow diagram is generated.

The models in the information flow diagram describe plant operations or plant equipment. There need not be a one-to-one correspondence between equipment on the flow sheet, and the modules of the information flow diagram. Modules may be required at mixing points, or to describe the acid make-up, where no such equipment actually exists in the plant. Conversely, it may be decided to group several equipments, such as the deisobutanizer column, the condensers, the reboiler, and the reflux coalescer into one module.

The full description of the plant equipment, and its operation will be presented in Section 2.3 along with the detailed presentation of each model, and the philosophy of its development. This section will only demonstrate the conversion of a flow sheet into an information flow diagram, and its description. The fine points, such as why some pieces of equipment were grouped into one module, will be presented with the detailed description of that module.

The information flow diagram for the alkylation study is shown in Figure 2.2. First consider the reactor area. Module 3 describes the reactor and the flash coils, while module 4 represents the acid settler. Also, modules 14 and 11 are required to

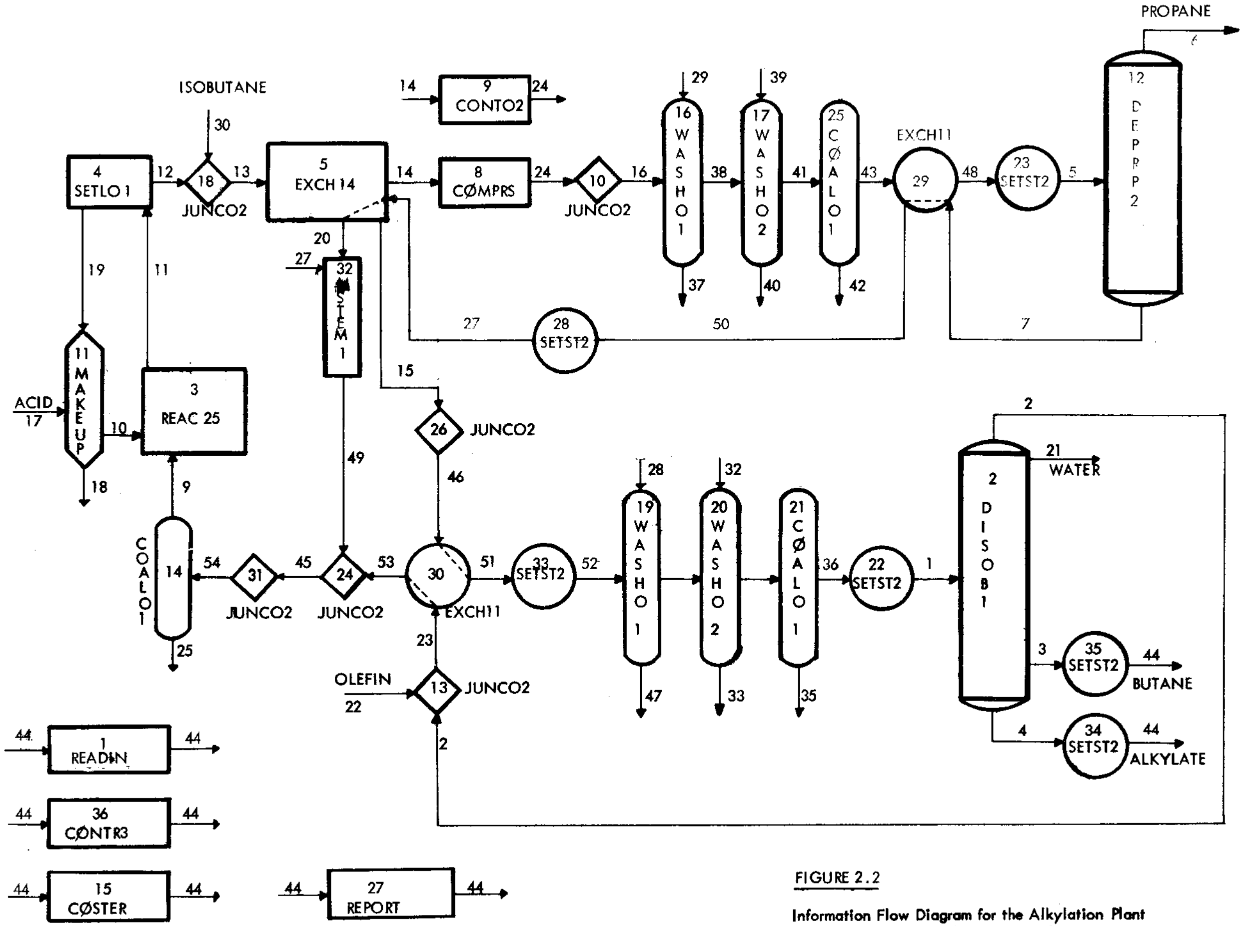


FIGURE 2.2

Information Flow Diagram for the Alkylation Plant with Comprehensive Models describe the feed coalescer, and the acid make-up operation. Module 18 is a mixer that allows the entry of a feed stream into the system.

The product separator and the vapor control loop is important. Module 5 describes the product separator and the internal heat exchanger coils. Module 8 represents a line pressure drop, the centrifugal compressor, and the vapor condensers. Module 9 describes the pressure control loop, and 10 is the high pressure pump. Module 32 is a dummy model of the product separator that is used in the recycle loop to reduce calculation time, and will be explained in Section 2.3.4.

Next the depropanizer circuit must be converted. Modules 16, 17 and 25 are needed to describe the acid wash, the water wash, and the coalescer. Module 29 is the bottoms to feed exchanger, and 23 is the steam heater for the feed. The depropanizer, as well as the reboiler and the condenser are combined to form module 12. The depropanizer bottoms recycle is cooled in module 28 before entering the product separator coils.

The deisobutanizer feed leaves the product separator as a liquid. It is pumped by module 26 to a process heat exchanger 30, where it cools part of the reactor feed, and is then steam heated in module 33. Before this stream is fed to the deisobutanizer it is caustic washed, water washed and coalesced in modules 19, 20 and 21, and then heated in module 22. Module 2, the deisobutanizer, represents the column, the reboiler, the bottoms-to-feed exchanger, the reflux coalescer, as well as the overhead condenser and the side-draw condenser. Modules 34 and 35 represent coolers for the product alkylate and butane.

Modules 13, 24 and 31 are mixers for the combination of the recycle and feed streams to the reactor. Module 1 is used to read in a physical property package. Module 15 does the final cost summing and reports the cost, as well as the values of some important parameters from the solution of case being studied. Module 36 is a special control module for the isobutane feed, and its function will be explained in Section 3.3.

Now each of the modules of the information flow sheet must be developed. The reader will be presented with the basic philosophy of model building, and its application, as each of the widely different modules are formulated.

2.3 Development and Description of Models

Large plant simulation is used to study the interaction of equipment rather than the isolated performance of a single piece of equipment for a fixed feed. The aims of a simulation study are stated in the questions to be asked. The development of a model will depend on the questions to be answered by the simulation, and how the equipment it describes, contributes to the answering of the questions. "How important is the model to the simulation, and to the questions to be answered?", is the dominant criteria used for developing an individual model.

In the final analysis, the state of knowledge of the phenomena occurring in any equipment may determine the final formulation of the model, although the desired level of sophistication may be defined by criteria relating to the end use of the simulation. The state of knowledge is defined by plant operating experience, and by the information available in the literature, including physical properties and equilibrium data.

The application of simple models in a total simulation is an important first-step in any development of an overall plant model. Simulation studies answer questions about the interaction of equipment. Initial studies with simple models are essential in determining the extent to which various models influence the answers to the questions asked. It is often found that the relative importance of a given model only becomes apparent after the interaction of all units has been studied. Those models which have been suggested to be important in the initial study should then be described in as much detail as possible; otherwise the accuracy of the simulation is dictated by the accuracy of these models.

2.3.1 Stratco Reactor

Even without a preliminary simulation, it is obvious that the reactor model is the most important. The octane rating of the alkylate, and thus its dollar value, depends on the amount of each of the alkylate isomers produced in the reactor.

The Stratco reactor is a horizontal shell operated at about 80 p.s.i.a., and contains cooling coils and an impeller. The organic feed is a combination of C_3 and C_4 olefins and normal paraffins, isobutane, and some pentanes. The second feed is an equal volume of acid. The impeller circulates the acid-continuous emulsion around the cooling coils to remove the heat of reaction. The reactor effluent is settled; the organic phase is passed through a throttling valve, and vaporized further in the cooling coils of the reactor. Most of the acid phase is recycled to the reactor.

The reaction mechanism is very complex, and the quality of the alkylate produced is affected by many variables. Past reactor operation, and observations reported in the literature (J1, A1, P1, C1, P2), point to the following variables affecting reactor operation and alkylate quality:

1. High isobutane-to-olefin ratios promote the production of desirable alkylate.
2. Higher acid strengths, result in higher alkylate quality.
3. Reactor temperatures below 45°F produce too high a viscosity with the ensuing excessive mixing power requirements. On the other hand, increasing temperatures above about 55°F results in poor alkylate quality, and increased acid dilution from side reactions.
4. Increased mixing improves alkylate quality.
5. Lower olefin space velocity results in higher alkylate quality.

To describe the kinetics of the reaction, many sets of equations have been proposed. A partial set of some of the possible reactions were proposed by Crowe, Sutton and Gleave during an initial reactor study(M1), but it is noted that the reactions for the polymerization of propene, and the reactions of normal butene are not included.

(i) $iC_4 + iC_4^{=} \longrightarrow C_8$

(ii) $C_8 + iC_4^{=} \longrightarrow C_{12}$

(iii) $C_{12} + iC_4 \longrightarrow C_5 + C_{11}$

(iv) $C_{11} \longrightarrow C_8 + C_3^{=}$

(v) $iC_4 + C_3^{=} \longrightarrow C_7$

(vi) $iC_4 + 3C_3^{=} \longrightarrow C_8 + C_5^{=}$

(vii) $iC_4 + C_5^{=} \longrightarrow C_9$

(viii) $C_7 + C_5^= \longrightarrow C_9$

(ix) $iC_4 + C_8 \longrightarrow 2C_6$

This list must also be extended when the various isomers of C_7, and greater, products are considered.

Our ability to describe the performance of an alkylation reactor is still quite limited. The reactor operation in the plant is guided by the aforementioned five variables that affect, in some way, the quality of alkylate produced. Four levels of sophistication of reactor modeling will be discussed.

The first level is a simple setter model, based on the normal operating conditions. The amounts of each isomer produced is calculated from the flowrate of olefin feed times a constant factor. No account is taken of the effect of the reactor temperature. The second level of sophistication is based on a set of possible reactions and one set of input-output plant reactor data. The extent of conversion for each of the proposed reactions was obtained using linear programming. The third level of sophistication is the one used in the present study. The reactor temperature was not calculated from a heat balance, but was set, based on plant operating experience, at a constant value above the feed temperature. Average data for the reactor operation under twenty-one distinctly different operating conditions were used in a linear regression analysis to relate output flows of each component to input flows. Higher level models would include a description of the heat transfer rate in the coils, and/or kinetic expressions to describe the reaction rate within the required flow and temperature ranges.

Level-1, STIR01(M1)

The level-1 model is based on general reactor operating conditions. Variables such as acid strength, stirring rate, reactor temperature, and isobutane-to-olefin ratio are not considered. All olefins are assumed to react completely, and the amount of each C_7 and C_8 isomer produced, is a constant times the propene and butene feed rates respectively. The amount of pentane, C_9 and C_9+ produced is a constant. One mole of isobutane is assumed to react with one mole of olefin. The reactor temperature is set at a reasonable value, and a heat balance calculates the amount of heat that the heating coils would have to remove.

This model is very satisfactory for initial interaction studies, particularly when applied over a small range of feed compositions. This model will err in the prediction of the amount of each alkylate isomer produced as the feed deviates from that used to establish it.

Level-2, REAC11(M1)

The level-2 model is similar to the level-1 model, except that the amount of each isomer produced is calculated from a set of rate equations. A likely set of reactions was chosen from the literature(A1). Linear programming techniques were used with these equations to choose the best set of rate constants to fit a set of input -output analysis for the reactor.

This was found to be only slightly better than "STIR01" since there was loss of accuracy when the feed rates deviated from the conditions under which the constants were derived. Again, the effect of temperature is not considered. A far more powerful model could have been developed using this formulation if a number of sets of reactor operating conditions and flows had been available at the time.

Level-3, REAC25

This is the model that is presently used in the simulation study. During the summer of 1967, a set of 21 data points describing the reactor feed, effluent and operation was collected$^{(F1)}$. A reactor model could now be developed that was applicable over a wider range of feed flows and compositions. The model would still suffer from the lack of knowledge concerning the fundamental mechanism involved.

The outlet flow of the C_5 and greater components could be predicted knowing the reactor temperature, and the inlet flow rate of the C_3, C_4, and C_5 components. The 21 sets of data points were regressed to give an equation of the form:

$$\begin{aligned}\text{Iso-Octane} = \quad & C1 + C2{+}\text{Propane} + C3{*}\text{Propene}\\ & {+}C4{*}\text{Isobutane} + C5{*}\text{N-Butane}\\ & {+}C6{*}\text{I-Butene} + C7{*}\text{N-Butene}\\ & {+}C8{*}\text{I-Pentane} + C9{*}\text{Temperature}\end{aligned} \tag{2A}$$

where the chemical names represent the flow of that component in pound moles per hour. A set of constants is calculated for each of the products.

The reactor temperature was found to be $8^{\circ}F$ above the feed temperature for a very wide range of operating conditions and feed temperatures. This was used to set the reactor temperature, and then a heat balance was performed to calculate the heat to be removed in the reactor coils.

The isobutane usage is calculated from plant factors times the feed of each olefin. The production of alkyl sulphate, assumed to be the acid diluent other than water, is calculated as a function of acid strength, temperature, and isobutane-to-olefin ratio. The olefins are assumed to be completely reacted. The propane and butane are assumed to be inert.

The model performs well over a range of feed concentrations. It does include the effect of temperature, and indirectly, the effect of isobutane-to-olefin ratio. The effects of acid strength and mixing, two very important variables, are not included since the 21 sets of data points did not include measurements of these variables.

There are several changes that should be made to the present model. First, since propane and butane are both inerts, the effect of their feed flows should be combined,and not included separately. Second, there should be some estimate of the effect of the acid strength, even if it is a simple linear relationship. Also, some higher power terms, perhaps of the isobutane, should be included. More significance should be given to forms of the correlation equations that reflect the state of knowledge (theoretical or operational), rather than arbitrary linear forms that include all the measured variables.

Higher Level Models

Before a higher level model is developed, the effort to develop the model must be justified, based on the additional questions the new model will answer in the overall simulation study. Future reactor models, allowing extrapolation with confidence to feed conditions and operating parameters well outside the present limits, involve two areas of description: the reaction kinetics and/or the heat transfer

(i) The kinetics, which at present are not completely understood, and mass transfer with chemical reaction could be described by fundamental equations. Activation energies would have to be incorporated in the kinetic rate constants so that extrapolation to other temperature conditions would be possible. Moreover, the degree of stirring, which effects the mass transfer, the heat transfer, and the heat generated by viscous dissipation would have to be included. Also, acid activity would have to be included in the rate expressions.

(ii) By describing the heat transfer phenomena in the exchanger coils, a better prediction of the reactor temperature would be available for a kinetic model. Moreover, changes in operating conditions, or the addition of equipment could be evaluated. For example, the effect of placing a freon chiller to cool the hydrocarbon before it entered the exchanger coils could be evaluated. Similarly, some of the hydrocarbon could bypass the exchanger. This would allow a lower pressure in the coils, thus producing a greater temperature difference over the reactor coils, and hence, greater heat transfer. The description of the heat transfer would require an extremely complicated description of two-phase flow and boiling heat transfer. Such a description would involve a large commitment of time.

2.3.3 Depropanizer

The depropanizer feed is the overhead from the product separator. The vapor is condensed, caustic and water washed, and the water is removed in a colescer before entering the distillation column. The feed is mainly isobutane, butane and propane, with small amounts of propene and pentanes. The column operating at about 280 p.s.i.a., has 37 Koch Flexitrays, with the feed tray being 19 from the top.

The reboiler is steam heated.

The depropanizer has two purposes:

1) To remove propane from the system, so as to reduce the recycle volume to the reactor.

2) To produce a high purity propane product.

In actual plant operation, the depropanizer is controlled so as to maintain the propane concentration in the bottoms flow below a maximum allowable level to minimize the recycle back to the reactor. To achieve this control, the column is run at maximum condenser capacity. In plant operation, when the bottoms purity specification is obtained, the additional condenser capacity is used to produce an LPG distillate product of highest purity (normally greater than 95% propane).

Several distinctly different models were developed to describe the depropanizer. Initially, a linear splitter model was used in which the fraction of each component in the feed leaving in the overhead was specified. This model was used to study the interaction of the column with other units in the initial simulation studies. The final model, which is discussed below, was based on the Fenske equations(F2), and the Gilliland plot(G1). The Petryschuk model(P3), based on the relaxation technique as originally suggested by Ball(B1), was adapted to the MACSIM system(M1) to study the depropanizer. Later, Brown and Williams(M3) developed a correlation model based on the response of the Petryshuk model to changes in feed composition, reflux ratio and draw-off rate. It had been hoped that this model would retain the accuracy of the sophisticated Petryschuk model, while requiring less storage space and execution time.

Modeling the depropanizer, which is a relatively simple column to describe, points out one of the basic rules of equipment modeling: "The model must be constructed to act, and to react, in the same way that the actual plant equipment would act and react." This implies that a detailed knowledge of the control or operating procedures must be built into any model. It will be shown that a column model based on the bottoms purity control, and using a simple distillation technique, reacts far more realistically in this instance than a comprehensive model based on classical distillation parameters such as product-to-feed ratio, and reflux ratio.

Earlier Models

The Petryschuk plate-to-plate model(P3) was used to replace the simple splitter model in earlier studies of the depropanizer. Several of the problems encountered were:

(i) Excessive execution time required per loop (five minutes on IBM 7040).

(ii) Excessive storage required.

(iii) The model would not respond to changes in the propane content of the feed in the same way the plant column did, since the reflux ratio and the product flow rates had to be specified.

The model did, however, very accurately describe the column operation for a specified feed and operating conditions.

In an attempt to reduce the execution time and the program storage required, a correlation model, DCOR01 was developed(M3). The Petryschuk program was used to generate a set of outlet flows for a given set of feed compositions, reflux ratios, and product-to-feed ratios. This set of predicted output compositions was regressed against the feed composition, and the operating parameters. The constants obtained from the regression analysis were used to develop a correlation depropanizer model. The model was much faster and required less computer storage space than the Petryschuk model. It still, however, required that the reflux ratio be known; more seriously, it would not respond to feed composition changes in the same way that the controlled plant column would. Also, the range of feed and operating parameters used to develop the model were not wide enough, and the feed to the model in later studies on the whole plant was often outside the range of the model.

Final Model, DEPRP2

The Frenske equations$^{(F2)}$, as indicated below, were used to calculate the minimum reflux ratio, and the component distribution in the product.

$$\log \frac{X_D \quad (1 - X_B)}{X_B \quad (1 - X_D)} = N \log \alpha \tag{2B}$$

where X_D and X_B are the mole fractions of a component in the distillate and bottoms respectively, and α is the relative volitility. N is the minimum number of stages for a specified separation. The minimum reflux ratio is obtained from the equation

$$\text{RMIN} = \left[\frac{X_D^{LK}}{X_F^{LK}} - \left(\frac{\alpha^{LK}}{\alpha^{HK}} \; \frac{X_D^{HK}}{X_F^{HK}} \right) \right] \left[\frac{\alpha^{HK}}{\alpha^{LK} + \alpha^{HK}} \right] \tag{2c}$$

where the superscripts LK and HK refer to the light key and heavy key respectively (propane and isobutane), and the subscripts D and F refer to the distillate and the feed respectively. The relative volitility is α and X is a mole fraction. A linear equation representing the low reflux ratio portion of the Gilliland plot, which is an empirical plot of a function of the actual stages and the minimum stages versus a function of the reflux ratio and the minimum reflux ratio, is used to determine the reflux ratio required for the specified separation. Then, knowing the reflux ratio, the condenser duty can be calculated.

The model has not been extended to search for the operating conditions that correspond to the maximum condenser duty. Instead, knowing the number of ideal stages, a required recovery of propane, and the fraction of propane in the distillate, the output flows from this column are specified. In fact, the total flow and composition of the two outlet streams can be calculated directly. Moreover, it is not difficult to choose the proper value of propane recovery to yield a required propane content in the bottoms.

The model, when the recovery of propane, rather than a product-to-feed ratio, is specified will react properly to a change in propane composition in the feed. The distillate and the bottoms flow rates are very non-linear functions of the total feed flow, but are more directly affected by the fraction of propane in the feed. It was found that earlier models would not react to a change in propane content of the feed at a constant feed flowrate, unless the propane recovery was the parameter used.

The next stage of development would be to search for a propane recovery that will satisfy a specified maximum propane content in the bottoms, subject to a condenser duty limitation. This search would be done initially at a reasonable propane concentration in the distillate (98%) and then the exact value, that would correspond to the maximum condenser duty, would be found by a second search. A model with these specifications would respond to changes in feed flow and composition in the same way that the actual unit would respond.

The use of the Fenske equations must be evaluated since they rely on the assumptions:

(i) constant relative volitility.

(ii) constant model overflow.

(iii) ideal feed-plate location.

The first two assumptions are reasonable for the accuracy required, when considering a system of propane, butane, and isobutane. The assumption of an ideal feed plate location is the weakest. If a wide range of feed compositions are to be evaluated, a more exact method of calculating the column performance might have to be considered. If the present model is to be applied over a wide range of feed compositions, its accuracy should be evaluated by comparing these predictions with those of the Petryschuk model(P3). This can be done external to the simulation, as it should be.

2.3.3 Deisobutanizer

The liquid flow from the product separator is caustic and water washed, and the water is removed in a coalescer before it is fed to the deisobutanizer. The column feed contains approximately 75% normal butane and isobutane; the remainder is made up of the alkylate, propane and pentanes. The column contains 80 Koch Flexitrays with the feed on tray 31, and a vapor side-draw near the bottom on tray 74. The reboiler is gas-fired. A reflux coalescer is used to separate water from the reflux.

The three main purposes of the column are:

(i) To remove the product alkylate.

(ii) To remove butane from the system so as to reduce the recycle volume to the reactor.

(iii) To return as much as possible of the isobutane back to the reactor.

The plant operation of the column is based on controlling the bottom of the column to a Reid vapor pressure. Almost all of the isobutane fed to the column leaves in the distillate, and is recycled to the reactor. This is accomplished by controlling the condenser and reboiler heat fluxes, and the vapor side-draw rate. In practice, the flow rate of the butane side-cut is increased until its isobutane content exceeds the allowable limit.

Models for multicomponent distillation columns as indicated in the discussion of the depropanizer, require a large amount of storage and execution time. When a vapor side-draw is included, the problem is even more complex. A simple splitter model is only sufficient for initial plant studies. There are a number of plate-to-plate models available in the literature, and several of them have been evaluated by Petryschuk(P3). The Petryschuk model was adapted to include a side-draw by Powell and Kitcher(M1). When this program was inserted into the MACSIM system, it required excessive execution time and storage. A correlation model, DCOR02, was developed using the modified Petryschuk program to describe the deisobutanizer(M3). The correlation model was similar in theory to DCOR01, in Section 2.3.2, developed to describe the depropanizer. The model proved to be unreliable. The correlation equations were developed over too narrow a range of feed compositions. Also, the form of the equations chosen, and the variables used to predict outlet flows and compositions, were dictated only by the regression analysis, and fundamental and theoretical equations and variables were not used.

Present Model DISOB1

The present model illustrates the same rule of model development, as did the depropanizer model: "Make the model respond to feed changes in the same way that the plant equipment would respond." Thus, classical models that require a reflux ratio or a product-to-feed ratio, may be of limited use in a simulation when the feed composition is not known initially. The actual plant column is controlled, and the effect of the control should be included in the model.

A typical column feed and the corresponding product stream compositions are shown in Table 2.1. It can be seen, that under desired plant operation, all the propane goes overhead, and all C_6 and heavier components leave the column in the bottoms flow. Thus, only the distribution of the C_4 and the C_5 components in the three output streams need to be described. Furthermore, there is never any isobutane in the alkylate or any pentanes in the distillate. In addition, the plant is run to a maximum isobutane specification in the side-draw. On the basis of these observations and recalling the three main purposes of the column, the model DISOB1 was developed. It was found, as in the case of the propane in the depropanizer, that the recovery of butane in the side cut was the "best" variable to use to describe the flow in the side-cut.

TABLE 2.1 : AVERAGE FEED AND EXIT FLOW OF EACH COMPONENT FOR THE DEISOBUTANIZER

		Percent of each entering component leaving in the exit streams		
Percentage of FEED	COMPONENT	TOP	S/C	BOTTOMS
4.6	nC_3	100.0	0.0	0.0
0.0	$C_3^=$	100.0	0.0	0.0
37.2	LC_4	97.5	2.5	0.0
39.3	nC_4	38.0	57.6	4.4
0.4	$iC_4^=$			0.0
0.4	$nC_4^=$	0.0		
0.9	nC_5	0.0		
3.4	iC_5	0.0		
0.0	$iC_5^=$	0.0		100.0
13.8	C_6^+	0.0	0.0	100.0

Future Model

Any future model developed to describe the operation of the deisobutanizer must include the effect of the control system. A possible method would be one that would start with the heavier components, and then add the lighter components to the bottom flow, until the desired Reid vapor pressure was obtained. Then the component flows in the side-draw and the distillate might be calculated using a Fenske approach, since the remaining $C_3 - C_4 - C_5$ mixture would be close to 90% normal butane plus isobutane. A model of this type would predict exit flows similar to the flows that would be produced by the controlled plant column. In developing a model of this type, it is essential to have an accurate plate-to-plate model available to check the flows that the model predicted for the converged plant solution.

2.3.4 Product Separator

The product separator is very important in the simulation of the alkylation plant. The organic reactor effluent, after leaving the reactor heat exchanger coils, is split into two streams. The lighter components leave as vapor, and enter the depropanizer circuit, while the heavier components leave as liquid, and are fed to the deisobutanizer circuit. An error in this model causes errors in the feed flow and composition to both of the columns.

The product separator is a low pressure flash drum, and contains a heat exchanger coil. The vapor-liquid reactor effluent from the reactor heat exchanger coils is fed to the product separator where it flashes further. Additional heat is added to the product separator as the bottoms from the depropanizer, at a controlled temperature, is further cooled in the heat exchanger coils. The product-separator pressure is controlled and the temperature adjusts according to this pressure and the heat input in the following way. If the vapor flow is too great for the downstream condenser capacity, the product separator pressure rises, thus reducing the vapor flow. The pressure continues to rise until the vapor flow does not exceed that which can be condensed.

Initial Model

Initial plant studies can be carried out using a simple component splitting model to represent the product separator, along with another simple temperature setter to fix the temperature of the bottoms stream from the depropanizer which passes through the coils of the product separator on its way back to the reactor. Under these conditions, however, the two exit flows from the product separator to the depropanizer and the deisobutanizer would not reflect the heat transferred in the reactor or the heat transferred in the product separator coils.

Comprehensive Model, EXCH14

The product separator model must search for an operating temperature, at a specified operating pressure, so that a heat balance around the unit is satisfied. This obviously implies that the total input enthalpy must equal the total output enthalpy. On the other hand, the amount of the feed that is flashed depends on the operating temperature.

The reactor temperature is set by the reactor model. With this temperature, the amount of heat that must be removed in the reactor coils is calculated through a heat balance on the reactor. Since the quality of the product separator feed is not defined, the feed to the product separator model is taken to be the liquid leaving the acid settler, and the heat load calculated for the reactor coils is considered as input heat to the product separator model.

At any temperature, the vapor and liquid flows from the product separator must be calculated. The derivation of the flash calculation is given in Appendix (7.2). Then the exact operating temperature, at a specified operating pressure, must be found so that the model satisfies a heat balance. A reguli-falsi search routine is used to find the exact operating temperature that satisfies the heat balance.

It is necessary for the product separator model to be calculated twice during one MACSIM loop, once after the reactor so as to define the column feeds, and once at the end of each MACSIM loop to cool the newly calculated depropanizer bottoms. To avoid recalculating of EXCH14 at the end of the loop, a simple model MSTEM1 was written. It modifies only the depropanizer-bottoms recycle stream leaving the cooling coils of the product separator. The outlet composition is set equal to the new depropanizer bottoms composition, but the temperature is set equal to the previously calculated value for the exit stream from the heat exchange coils. As the simulation nears convergence, the error introduced by this model rapidly approaches zero.

2.3.5 Compressor Control

The vapor from the product separator is compressed and condensed. If the condenser is not overloaded, the product separator pressure remains at the base value of 17.7 p.s.i.g. If the condenser duty is exceeded, the product separator operating pressure is increased and this,in turn,acts to reduce the amount of vapor produced.

Two modules are used to describe this control loop. The module COMPRS represents three pieces of equipment in the alkylation unit:

(i) The pipeline, and the corresponding pressure drop between the product separator and the compressor.

(ii) The centrifugal compressor.

(iii) The condensers.

The pipeline pressure drop, the compressor exit pressure, and the condenser operating pressure are all calculated as a linear function of the flow rate. The equations used are linear fits of plant pressures over a range of vapor flow rate. The second model, CONT02, considers the condenser to be overloaded if the calculated compressor discharge pressure is less than the condenser operating pressure. If the condenser is not overloaded, the control module takes no action.

If the condenser is overloaded, the control module assumes command of the product separator and the pressure drop-compressor-condenser modules. A reguli-falsi search is used to determine the lowest product separator pressure, above the base value of 17.7 p.s.i.a., that will reduce the amount of vapor produced, and relieve the overloading at the condenser. Once the minimum allowable product separator pressure is determined, CONT02 allows the MACSIM calculation to continue in the specified order.

2.3.6 Heat Exchangers

Chemical plants often employ a large number of heat exchangers for the recovery of heat, and the control of processing streams. Often the questions to be answered by simulation studies involve heat recovery studies and heat-and-mass interactions. In addition, the utility usages required for temperature control may represent a sizeable portion of the operating costs. Moreover, operating restrictions on feed temperatures may require that the temperatures be accurately known. To describe unit operations that involve interactions between heat and mass (for example, a reactor or a flash drum),an accurate knowledge of both heat and mass inputs is required if the equipment performance is to be properly described. Utility costs, such as water and steam, will be useful in an economic evaluation.

The level of sophistication used in describing heat transfer operations is dictated by the importance of the performance of the model on the questions to be answered by the simulation study. Models range from simple temperature setting models, to models that depend on the flow rates and fluid characteristics in order to predict the amount of heat being transferred. Heat exchanger models, therefore, can be subdivided into two groups:

(i) Temperature settlers where only one outlet temperature is important.

(ii) Temperature of both exits streams must be predicted given input flows, temperatures and exchanger size.

Setting Model, SETST2

In initial simulation studies, process heat exchangers can be replaced by temperature-setting models. In the final study, setting modules can be used to describe a perfectly-controlled heat exchanger using steam, or some other utility, to maintain a stream temperature at a specified set point. The model can also calculate the required utility usage to produce the desired temperature.

Both Exit Temperatures Required, EXCH11

A setting model may not be sufficient if both exchanger feeds are process streams, and the outlet temperatures of each are important. The effectiveness factor method(K2) can be employed to describe the performance of an exchanger when the product of the overall heat transfer coefficient and the area is known. The calculation is direct, and no iterating is required to obtain the outlet temperatures if the overall coefficient and the heat capacities can be assumed to be independent of temperature.

The model EXCH11 contains the effectiveness factors for eight types of shell-and-tube exchangers: counter current, parallel, crossflow with four mixing patterns, parallel-counter flow with multiple pass, and condensing or evaporating systems. The type of exchanger is indicated in the equipment vector, and the correct effectiveness factor relation is used to calculate the outlet temperatures. Heat capacities are calculated using the physical property package as described in Section 2.3.10.

2.3.7. Acid-Emulsion Settler

The acid-emulsion settler separates the acid and the organic phase leaving the reactor. The organic phase from the settling drum flows to the product separator and the acid phase returns to the Stratco Reactor. General plant operation has indicated that there is very little acid carry-over into the organic effluents.

It was originally thought that the settler operation might contribute more to "acid loss" than was believed by the plant operating personnel. This conclusion was reached from experimental work done on a scale model of the settler by Gilmour and Chappell(M1). These experiments indicated an acid carry-over of 61 barrels per day as compared to a value of 3.6 as suggested by the operating personnel. This low value was obtained from plant operation by determining the caustic usage in the distillation column treaters and measuring the acid removed in an acid leg in the product separator. Further study revealed that the main cause of "acid loss" was not carry-over from the settler, but was caused by dilution of the acid catalyst caused by water in the feed streams, and reactions occurring in the Stratco reactor to produce "acid oils". The "acid oils" are a large range of acid-soluble materials that are referred to in the component list as propyl sulphates.

Final Model, SETL01

The model employed to describe the settler is a simple setting model. An average value of the acid carry-over, 3.6 barrels per day, is supplied as an equipment parameter. The model assumes that the acid phase contains all the water, alkyl sulphate and sodium sulphate. Thus, some of these components also leave in the hydrocarbon effluent because of the acid carry-over.

2.3.8 Coalescers, Caustic and Water Washers

The feed to each column is washed with caustic to neutralize the acid carried over from the acid emulsion settler. Then,any caustic carry-over is removed in a water wash tank. Finally, water is removed in a coalescer.

These three models are only important to the simulation study in that they affect the water and acid added or removed from the system. The caustic wash is a simple acid-caustic reactor, and the water wash is a dilution tank. Temperature affects the performance of all three models since the solubility of water in hydrocarbons is a function of temperature. Each model uses the subroutine FSOL to calculate the amount of dissolved water in the hydrocarbon according to the equation:

$$\text{Dissolved Water} = \quad (\text{moles of component } i)(\exp(C1(i) - \frac{C2(i)}{T}) \qquad (2D)$$

where C1 and C2 are constants for each component, and T is the absolute temperature(T1).

The amount of entrained water leaving with the hydrocarbon is calculated from a specified efficiency of removal of entrained water. The value of this parameter must be determined from a water balance on each unit. Thus, each of the models, WASH01, WASH02, and COAL01, calculates the amount of water leaving with the hydrocarbon to be the sum of the dissolved water and a specified fraction of the total entrained water in the unit.

2.3.9 Acid Makeup, MAKEUP

Plant operation of the Stratco reactor requires that 45 to 50% of the total acid and hydrocarbon feed be acid of a specified strength. Water in the organic feed to the reactor and "acid-oil" produced in the reactor dilute the acid. Present operation of the acid bleed system does not allow weak acid to be bled and fresh acid to be added continuously. Instead, fresh acid is added batchwise whenever the acid strength drops below the desired concentration for the alkylation reaction. It is important to note that the cost of acid required to maintain the activity of the acid catalyst at the desired level, as calculated from the present study, exceeds the total cost of steam, electricity and cooling water. Hence, any reactor model should pay particular attention to the loss of acid.

An unsteady-state process, like the batch addition of acid, cannot be described by MACSIM. Instead, the flow of makeup acid must be assumed to be constant to maintain the acid feed at a constant flow and concentration. The module that calculates the required acid makeup and waste-acid flows is unique in that an outlet stream, the reactor acid feed, is specified in the EN list, and an input stream, the makeup acid, is calculated.

The makeup model has two input streams: the acid from the emulsion settler, and the fresh makeup acid. The two outlet streams are the acid feed to the reactor, and the acid waste stream. The acid strength of the reactor feed must be specified in the EN vector, and the total flow of this stream is calculated knowing that it is a specified fraction of the total reactor feed volume. Then, if the strength of the makeup acid is known, the module will calculate the flow of the waste stream, the required flow of makeup acid, and the composition of the acid feed to the reactor. Five linear equations consisting of an overall mass balance, and four component balances (on water, acid, alkyl sulphate, and sodium sulphate) are sufficient to describe the performance of the acid makeup model. It is assumed that the composition of the waste stream is equal to the composition of the acid recycle to the makeup model.

2.3.10 Physical Property Calculations

Many of the models require physical property data. A physical property package was developed to avoid one function statement, and one set of physical property data in every model where a physical property was required. One subroutine reads all the required data into a physical property block, and the other two subroutines can be called from any model to calculate physical properties using the data stored in this block. A complete description of the physical property calculations, and all the regression coefficients are given in reference (M3).

The first groups to study the alkylation plant proposed a list of 17 required physical properties. Li (M1) regressed all the required data, for each of the twenty-six components, against temperature in degrees Fahrenheit, and obtained a set of constants for each component for each property. Later, when the models to describe the unit operations were developed, only five of the physical properties were actually required for each component: molecular weight, heat of vaporization as compared to water, and liquid heat capacity, liquid density, and K-equilibrium ratio at 18.0 p.s.i.a., all as a function of temperature.

READIN

This subroutine is executed only once, at the start of the simulation study. It reads in each set of correlation coefficients for temperature, for each component for each physical property that is required, and stores them in the physical property data block. In addition, it reads in the code that specifies which of the several parametric equations, in the property calculating subroutines, is to be used for the calculation of each physical property.

PROCAL and PROMIX

These two subroutines calculate the required physical properties, and can be called from any model used in the information flow diagram. PROCAL is called if the physical property, at a specified temperature, is required for each component. If, instead, a property is required for a known mixture of components, such as a feed stream, PROMIX is called. PROMIX calls PROCAL to evaluate the property of each component at a given temperature. Then, with a given composition of the mixture, this subroutine calculates the property for the mixture, weighting each property according to the amount of the component that is in the defined mixture.

2.3.11 Costing and Reporting Module

To summarize a case study, and in order to have an economic evaluation, as well as an estimate of the technical feasibility, a reporting module is required. The function of such a model, is the presentation of only the pertinent parameters that characterize the case being studied. The report must be complete in itself, and any parameter presented should be in sentence or tabular form.

The main function of the COSTER module is the evaluation of the cost of feeds, products and utilities. There are many possible costs that can be included in an analysis, and there are many different methods of including such costs. In the alkylation study, the difference in costs between case studies of an existing plant are to be compared. Thus, costs that may be assumed to be constant from case-to-case, such as capital, inventory, and maintenance costs, as well as other fixed costs, are not included. The value of the materials flowing in the plant, or the utilities associated with each operation can be carried with each stream list (SN), with each equipment parameter list (EN), or can be evaluated as required in an overall costing module. It was decided to perform all the costing in one module, COSTER, that requires a cost matrix which includes utility costs, as well as the cost per component in the input feeds, and the values of the product streams.

The COSTER module also evaluates two functions used by Shell to reflect the economics of operation of the case being studied. The cost function is defined as the sum of the utility costs, the caustic, isobutane, and olefin feed costs, plus the net cost of the makeup acid. The profit function is defined as the value of three product streams, alkylate, butane and propane, minus the cost function.

As long as the purity of the propane and butane product streams is above a minimum purity specification their value can be expressed in dollars per barrel. No penalty was included for failure to meet this specification because the present simulation ensured the purity of these streams.

The value of the alkylate depends on its composition and this is reflected by the magnitude of the octane number. Thus the octane number must be evaluated, and with the value of an octane-barrel, the value of the alkylate product stream is determined. The value of the isobutane and olefin feed streams is assumed to be the sum of the equivalent thermal value of each component in each of the feed streams.

The flow and the value per day of each of the feeds, products and utilities are calculated for the case being studied. In addition, the corresponding values for a base case are also presented for the purpose of comparison. The profit function and the cost function are presented per day and per barrel of alkylate for the case study being evaluated and for the base case. Also the difference between the cost and profit functions for the base case and the particular trial is presented to provide a direct comparison of the economic merits of the two cases.

The second function of the costing module is to monitor specific flows and operating variables in the converged solution. Any flow, composition or operating parameter can be compared to an average or a limiting value, and printed out.

This final check on the converged solution, along with the cost summary, can supply the user of the simulation with most of the information that is required. The user does not have to search through the final equipment matrix for all equipments, and the stream matrix for all streams in order to locate the few values that will characterize a particular case study.

In the present alkylation study, the following parameters are reported:

(i) The product separator pressure.

(ii) Any correlation limits that are exceeded in the reactor model.

(iii) Strength and volume fraction of the acid in the reactor.

(iv) The depropanizer condenser duty and vapor velocity in the column.

A sample printout of the operating cost summary and the summary of the process and correlation limits are given in Figures 2.3(a) and 2.3(b)

In summary, the complete stream matrix and the complete equipment matrix will be important during the time that the simulation is being developed. When this initial phase is complete, any parameter that is important to the solution should be presented in a report of form presented here, rather than in a matrix of many numbers, most of which are not critical to the case being studied.

FIGURE 2.3(a) : OPERATING COST SUMMARY

Run Number 2

Conditions Shell Alkylation Simulation - Enriched I-C4 Feed

Summary of Material Flows		Quantity per day		Value per day	
		Run No.2	Base Case	Run No.2	Base Case
Feeds	Isobutane (bbls)	990.	1576.	3080.	4857.
	Olefin (bbls)	3180.	3180.	9132.	9132.
	Sulphuric Acid (bbls)	75.	74.	648.	645.
	Caustic (100 lbs.)	11.	11.	39.	39.
Products	Alkylate (bbls)	1881.	1923.	7950.	8114.
	Propane (bbls)	723.	839.	2604.	3020.
	Butane (bbls)	1131.	1552.	3981.	5464.
Utilities	Steam (50 psig) (1000 lbs)	68.	84.	26.	32.
	Steam (200 psig) (1000 lbs)	327.	301.	124.	114.
	Fueld (MM Btu)	495.	510.	140.	144.
	Electricity (Kw)	32376.	32928.	204.	207.
	Cooling Water (1000 gals.)	3052.	3077	34.	34.

The debutanized R-3 octane rating of the alkylate is 104.52

	Run No.2	Base Case	Difference
Cost function per day	13426.3	15205.4	-1779.16
Profit function per day	1109.1	1392.0	- 282.93
Cost function per bbl. of alkylate	7.137	7.907	- 0.7706
Profit function per bbl of alkylate	0.590	0.724	- 0.1347

FIGURE 2.3(b) : SUMMARY OF PROCESS AND CORRELATION LIMITS

The following limits have been exceeded in the reactor module

The correlation limit of 52.5 is exceeded for STRMI (1,16) which is 56.0

The DC3 vapor velocity is 5.05 and the present limit is 13.00 cubic feet per second
The DC3 overhead condenser duty is 10.09 and the present limit is 10,00 million Btu per hour

The product separator pressure control was not required and the pressure remained at the base value of 17.7 psia

The fresh make-up acid is 99.20% acid. The acid feed to the reactor is 48.0% of the total flow and is 91.00 weight % acid and 1.63 weight % water.

3.0 ESTABLISHING A BASE CASE

The base case provides a set of conditions and economic worths against which alternate proposals can be compared. Furthermore, there will be parameters within various modules that cannot be obtained theoretically, and must be set on the basis of the performance of the model for the base case.

To establish the actual flows, compositions and temperatures in Shell's alkylation unit, the plant was operated under constant feed and operating conditions for four hours. In this case, many more engineers, operators and students were assembled and, with this close supervision, the process was run under conditions which approximated steady-state as closely as possible. The flow concentration and operating data, shown in Table 3.1 , are from that plant run; these data represent the base case. It is important to have these data available, not only to test the overall simulation, but also to test the individual models as they are developed. Moreover, the experience with the simulation discussed in this thesis has indicated that it is advantageous to have one set of plant data to test all models. This leads to easier incorporation of the models into the overall simulation later. This problem is more acute when a number of models of difficult levels of sophistication are developed at the same time. It must be emphasized, however, that models should be tested on more than one set of operating conditions.

3.1 Initial Study with Simple Models

Initial plant studies should be performed with simple setting and splitting models in order to establish the importance of various models in the overall simulation and to

TABLE 3.1 : MASS BALANCE FROM PLANT TRIAL AND FROM BASE CASE SIMULATION STUDY

(Simulation Study Flows in Brackets)

TREAM		TOTAL FLOW	PROPANE	PROPENE	BUTANE	ISOBUTANE	N-BUTENE	I-BUTENE	N-PENTANE	I-PENTANE	C6+
eactor	- Feed	1732.0	190.9	65.0	498.0	854.0	56.7	60.0	4.9	1.5	0.0
		(1730.8)	(191.3)	(65.0)	(490.8)	(854.3)	(58.0)	(61.6)	(2.3)	(6.5)	(1.0
	- Effluent	1561.6	189.4	0.0	507.1	689.5	0.0	0.0	8.4	32.7	132.1
		(1563.6)	(191.3)	(0.0)	(490.8)	(689.2)	(0.0)	(0.0)	(5.0)	(30.9)	(156.4)
eed	- Olefin	498.0	122.0	65.0	116.0	80.0	55.4	58.6	0.0	1.5	0.0
	- Isobutane	234.4	21.5	0.0	108.4	95.5	3.2	3.2	0.5	2.1	0.0
		(232.3)	(21.1)	(0.0)	(107.5)	(94.7)	(3.2)	(3.2)	(0.5)	(2.1)	(0.0)
epropanizer	- Feed	839.6	166.4	0.0	239.0	429.3	0.0	0.0	4.9	0.0	0.0
		(837.8)	(162.9)	(0.0)	(250.3)	(413.5)	(1.3)	(1.5)	(0.8)	(6.5)	(1.0)
	- Propane	144.3	142.0	0.0	0.0	2.3	0.0	0.0	0.0	0.0	0.0
		(145.3)	(143.1)	(0.0)	(0.1)	(2.1)	(0.0)	(0.0)	(0.0)	(0.0)	(0.0)
	- Bottoms	695.3	24.4	0.0	239.0	427.0	0.0	0.0	4.9	0.0	0.0
		(692.5)	(19.8)	(0.0)	(250.2)	(411.4)	(1.3)	(1.5)	(0.8)	(6.5)	(1.0)
eisobutanizer	- Feed	955.0	44.5	0.0	376.5	355.7	3.7	3.9	8.4	32.7	132.1
		(958.1)	(49.5)	(0.0)	(348.0)	(370.4)	(1.9)	(1.6)	(4.7)	(26.6)	(155.4)
	- Overhead	537.0	44.5	0.0	143.0	347.0	1.3	1.4	0.0	0.0	0.0
		(539.8)	(49.5)	(0.0)	(124.6)	(362.9)	(1.3)	(1.5)	(0.0)	(0.0)	(0.0)
	- Side Cut	258.0	0.0	0.0	217.0	8.5	2.4	2.5	8.3	15.0	0.0
		(227.2)	(0.0)	(0.0)	(204.3)	(7.5)	(0.6)	(0.1)	(1.4)	(13.3)	(0.0)
	- Alkylate	160.0	0.0	0.0	16.5	0.2	0.0	0.0	0.1	17.7	132.1
		(191.1)	(0.0)	(0.0)	(19.1)	(0.0)	(0.0)	(0.0)	(3.3)	(13.3)	(155.4)

develop experience with the mathematical problems associated with it (e.g. convergence promotion).

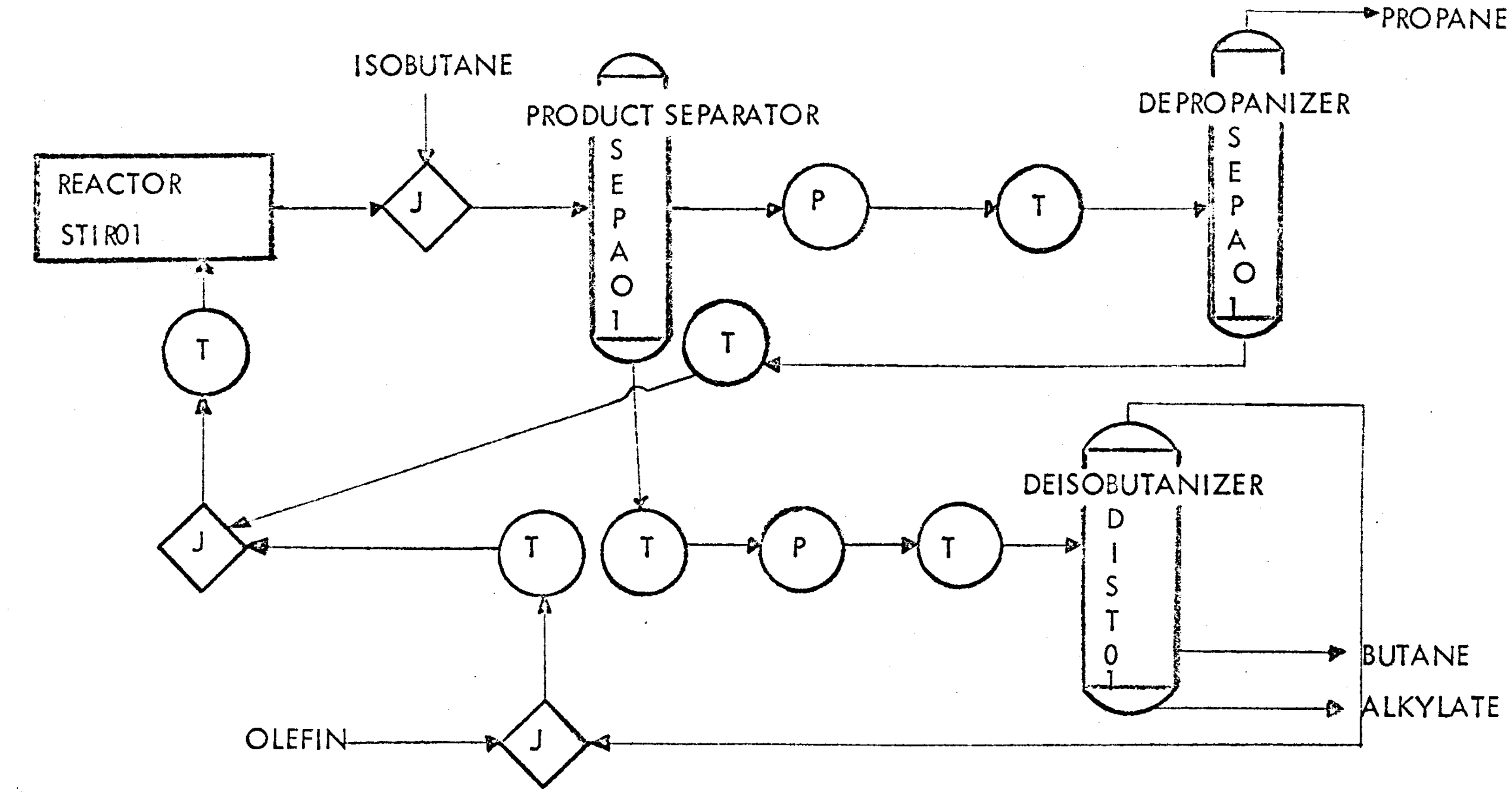
The flow sheet for the initial alkylation plant studies is shown in Figure 3.1. The simple reactor model,"STIR01", plus temperature and pressure setting models were used. The product separator model and the models for the two distillation columns specify the exit flows of each component in the outlets as a set fraction of the feed of that component. The required settings for these models were determined using the base data set.

Once the initial simulation is developed, convergence promotion techniques (0-1) (K-1) can be applied. The component flows in the main recycle streams are adjusted according to equation 3a:

$$\overset{\text{Adjusted}}{F_{i,\theta}} = C_i \times (\overset{\text{Calculated}}{F_{i,\theta}} - F_{i,\theta-1}) \tag{3a}$$

where $F_{i,\theta}$ is the flow rate calculated for component i at the θ'th iteration, and C_i is a constant for component i, and depends on the process (0-1). Thus,the convergence promotion subroutine adjusts the newly calculated flow of component i, based on the previous value and the present one, to accelerate the convergence to the steady-state solution. Convergence promotion becomes essential when the simple models are replaced by sophisticated models (usually non-linear) that require a large amount of computer time. Some difficulties have been encountered when applying these linear techniques on plant studies containing non-linear models.

From studies using the initial information flow diagram, models requiring



T	Temperature Setter
P	Pressure Setter
J	Mass Balance Junction

FIGURE 3:1 Information Flow Diagram for the Alkylation Plant Using Simple Setting and Splitting Models

more sophistication can be defined. The models are listed in order of importance to the present study:

(i) The product separator to define the flows to both distillation columns.

(ii) The reactor which controls the production of alkylate, the loss of acid, and the heat generation in the system.

(iii) The debutanizer and depropanizer models, since they define the production of propane, butane and alkylate, and recycle to the reactor.

(iv) The process heat exchangers to describe the heat recovery, and the interaction between the heat and the mass balance.

(v) The compressor-condenser system with its control loop that interacts with the product separator when the condenser is overloaded.

Once the required models and the required level of sophistication are defined by the questions to be answered, the models can be developed. Each model should then be tested under a wide range of conditions, including the base set of data, before it is inserted into the initial plant simulation or used to replace an existing model. Once incorporated in the overall simulation, models may still require some parameter adjustment.

3.2 Parameter Adjustment

As each new model replaces the simple one describing the base case, no drastic changes should occur. The sophisticated models must be added one at a time, and then the simulation should be allowed to iterate for 4 or 5 loops. The component flows, and the temperature for the major plant streams should be printed after each iteration. If there is a drift away from the converged, base-case values, adjustment of the empirical parameters within the model may be required. The parameters and sets of parameters that required adjustment in the alkylation study are discussed below:

(i) The heat transfer-area product, UA, had to be adjusted for the heat exchanger in the product separator and for process heat exchangers (modules 29 and 30 in the information flow diagram). The design value, supplied by Shell, could only be used as an approximation since fouling had occurred, and the flow rates were different than the design flow rates.

(ii) Both distillation models required that the recovery of the paraffin product be specified as a fraction of its flow in the feed. This parameter had to be adjusted in order to obtain the base set of exit flows from the columns.

(iii) Shell engineers indicated that the heats of reaction, as reported by Putney(P1), were slightly high. The reported values, as used in the reactor model, were adjusted in order to fit the plant trial mass and heat balance around the reactor and the product separator.

(iv) The efficiency of removal of the entrained water in the washers and coalescers was adjusted so that an overall water balance for the plant could be achieved.

3.3 Isobutane Buildup

After all the models had been incorporated into the information flow diagram, a steady buildup of the isobutane in the feed to the reactor was detected. When a convergence promotion routine was used, this buildup only increased more rapidly and the solution became unstable, even though the initial estimates used for the recycle streams were very close to the correct base case values. Discussions with the Shell personnel indicated that this phenomena is also observed in actual plant operation. It is difficult to define the required isobutane feed. Thus, isobutane is fed to the plant at approximately the correct rate. Then, if a buildup or depletion is detected in the recycle level of isobutane, the feed flow is adjusted, just as it would be in actual practice.

This phenomena can be explained by examining the ways in which the isobutane inventory in the unit can change. The main loss of isobutane is due to its reaction with olefins, and this usage is determined by the amount of olefin being fed to the alkylation unit. Isobutane can leave the unit in the propane or in the butane product streams from the distillation columns. However, the amount of isobutane in these streams is a plant operating parameter that is carefully controlled. Thus, the amount of isobutane leaving in the propane and in the butane is a very insensitive function of the amount of isobutane in the column feeds. The depropanizer overhead must be a specified propane purity (minimum of 95%). The deisobutanizer is controlled to a maximum allowable isobutane content of the side draw (normally less than 3%). Thus, if too much isobutane is fed to the alkylation plant, the isobutane inventory in the plant increases.

The steady-state solution of a case study will be over-specified if the total flow and the composition of both the olefin and the isobutane feeds are specified. A control module, CONTO3, was developed to monitor the isobutane flow in the recycle to the reactor. If a constant increase or decrease, within a specified tolerance, is detected between consecutive iterations, CONTO3 changes the total isobutane feed so that its isobutane content is decreased or increased by an amount equal to the change between iterations.

3.4 Base Case Mass Balance

The base case mass balance is shown in Table 3.1, along with the mass balance from the plant trial (which the base case is intended to describe). A hydrocarbon balance over all the input and outlet streams (including the organic content of the propyl sulphate) was in error by only two pounds per hour for a feed rate of over 39,000 pounds per hour.

Three errors have been noted in the plant trial mass balance, as supplied by Shell:

(i) There should be no change in normal butane flow across the reactor.

(ii) The ratio of isopentane-to-normal pentane is high due to analytical problems at the time of the plant trial run.

(iii) Too much of the butane fed to the product separator remains as liquid, and is fed to the deisobutanizer.

It must be stated for a fixed set of feeds and for a fixed set of equipment parameters (EN vectors), there exist an infinite set of solutions. Each one of the solutions can be characterized by the level of isobutane in the main plant recycle. This is due to the way in which the plant is operated in order to return as much as possible of the isobutane that is fed to the depropanizer and to the deisobutanizer back to the reactor. The amount of isobutane leaving the alkylation unit in the propane or in the butane product streams is a very insensitive function of the isobutane content of the feed to the columns. This problem will be discussed further in Section 4.1.1 as a case study.

4.0 SIMULATION STUDIES

Once a base case has been established, the simulation is ready to answer the questions for which it was written. A report of the economic result, as well as the flows, and the technical feasibility, is generated for each case. From these reports, the answers to questions concerning operating parameters, material costs, and plant sensitivity can be readily evaluated, and will be directly comparable to the answers from alternate questions.

In this study, a number of questions have been selected to demonstrate the use of the simulation, and the relative importance of certain aspects of the modeling. Each of these case studies is discussed in detail. A general discussion of plant sensitivity analysis follows the presentation of the case studies.

4.1 Case Studies

All case studies were run using the same feed and operating conditions as in the base case except one. In this way, the effect of a particular change could be followed throughout the entire plant. Obviously, this leads to a sensitivity analysis in which the change in concentration, temperature or flowrate, and finally, operating costs, can be compared with the unit change in an operating parameter or a feed condition, etc. Five selected examples to illustrate the use of the simulation follow.

4.1.1 Internal Change - Increase level of Isobutane Recycle

It has been observed that there are an infinite number of solutions for one set of equipment parameters and feeds, based on the amount of isobutane in the recycle to the reactor, a situation which also occurs in the actual plant. The initial estimate of the isobutane in the reactor feed was raised 200 pound moles per hour above the base case flow of 854. With this increased isobutane recycle, the octane rating of the alkylate was increased from 104.38,for the base case, to 105.24. The increased isobutane flow in the recycle raised the total organic feed volume to the reactor by approximately 10%. This increase in flow should have caused an increase in acid usage for three reasons:

(i) More water in the organic feed to the reactor.

(ii) More acid required to maintain the acid-to-organic feed ratio to the reactor.

(iii) Increased temperature of reactor feed.

but the acid usage decreased by five barrels per day. Actually,the important point in this case is that a higher isobutane-to-olefin ratio in the reactor reduces the amount of acid-oil produced. This factor more than offsets the other factors which tended to increase the acid usage. This result was surprising, and was contrary to the expected acid usage at higher recycle volumes.

The cost function was reduced by $40 per day since the reduction in acid costs far exceeded the slight increase in utility usage. The profit function, due to reduced acid use, and increased octane rating of the alkylate, increased by $121 per day. This case study is technically feasible for all models, with the possible exception of the deisobutanizer. The present model for this column is insufficient to determine the technical feasibility of operation, the basic restriction being the overhead condenser capacity.

4.1.2 Control Set Point Change - Increase Temperature of Flow to Product Separator Heat Exchanger Coil

Operating experience has suggested that the plant is sensitive to heat input to the product separator through the product separator heat exchanger coil. Temperature of this stream (i.e. bottoms from the debutanizer column) is controlled via a chilled-water cooler. Normal operation (base case) uses a set-point temperature of 80°F out of the exchanger, that is, for the feed to the coils of the product separator. Two case studies were evaluated: the first with the control point seeting of 85°F and the other with a setting at 90°F.

The resultant increase in the heat flux will produce more vapor in the product separator. This effect may cause an increase in the product separator pressure if the condensers become overloaded. Table 4.1 shows the results for the product separator feed, vapor and liquid flow rates, as well as the operating temperature and pressure for the three control temperatures. The rise in the product separator pressure almost compensates for the increased heat flux. There is only a small increase in the main recycle back to the reactor. The increase in flow to the depropanizer, and the decrease in the flow to the deisobutanizer is mainly butane and isobutane.

Thus,there is a slight decrease in the amount of butane removed from the system in the deisobutanizer side-cut. The propane flow to the depropanizer was unchanged. This study implies that the limitation on the capacity of the depropanizer feed condensers function efficiently in preventing any major upset from occurring. The cost function and the profit function for the two cases are practically the same as for the base case. Both case studies appear to be technically feasible.

TABLE 4.1 : EFFECT OF TEMPERATURE TO PRODUCT SEPARATOR HEAT EXCHANGER COIL ON PRODUCT SEPARATOR OPERATION IN THE ALKYLATION PLANT

EXCHANGER COIL FEED TEMPERATURE °F	PRODUCT SEPARATOR OPERATION				
	FLOWS (lb.mole/hr.)			PRESSURE	TEMPERATURE
	FEED	VAPOR	LIQUID	p.s.i.a.	°F
80	1798.6	840.8	957.8	18.03	31.32
85	1803.4	849.9	953.5	18.26	32.16
90	1849.5	865.9	983.6	18.63	32.61

Further studies in other areas of the plant involving changes in set points could evaluate the effect of changing the operation of the two distillation columns. These case studies could be used to weigh the economics of trying to remove more inerts from the system (propane and butane).

4.1.3 Change in Piping - Isobutane Fed Directly To the Reactor

The isobutane may be fed to the product separator (as in the Shell plant trial from which the base case was developed) or it may be fed directly to the reactor. By feeding the isobutane to the product separator, some of the propane and butane, which are inerts, will be removed by the distillation columns, thus reducing the recycle volume, and thus the reactor space velocity. But, this mode of operation will remove some of the olefins in the isobutane feed, and they will not be reacted.

Because this case study was run with the same amount of isobutane in the reactor feed, as in the base case, there was almost no change in the economics. However, the deisobutanizer feed was reduced by 8%, and most of this difference was isobutane. The column could have been run to recover more butane product, and thus to reduce the recycle volume. Both of these factors would increase profit. It must also be noted that the water in the isobutane feed increased the reactor acid usage by three barrels per day.

Changes in piping, along with adjustments in operating conditions, offer many opportunities for increasing profit. The effects of introducing the feed stocks (isobutane and olefin) into the reactor, the product separator, or the two distillation columns can be easily evaluated using the present simulation.

4.1.4 Change in Feed Composition - Enriched Isobutane Feed

The present isobutane feed contains 41 mole percent isobutane, but a potential feed contains 62 mole percent isobutane. Moreover, the proposed feed would contain substantially less butane and slightly less propane. A feed of this composition would be introduced into the reactor, rather than the product separator, and so this case study would be directly comparable to the base case.

The solution of this case study indicated that only 990 barrels per day of the enriched isobutane feed would be needed to provide the required isobutane to react with the olefin feed, as compared to 1576 barrels per day of the present feed. The cost function, using the same cost figures for the components of the isobutane feed as used for the base case, was reduced by $1779 per day. However, the profit function was reduced by 283 dollars since the isobutane feed contained less olefins, less butane, less propane, and as a result, there was less alkylate, butane, and propane produced.

It must be noted that this case study was performed by changing only the isobutane feed so that the effect of this one change could be studied. In actual operation of the plant, a number of changes, including the flow of olefin feed, and the operation of both distillation columns, would be made to take full advantage of the reduced volumentric flows resulting from the new feed.

4.1.5 Error in a Physical Property - Decrease K-Equilibrium for Butane in the Product Separator

Many of the comprehensive models require physical properties. Errors in the calculated value of a physical property may arise from two sources. First, the initial physical property date may not be accurate. Secondly, further errors may be introduced when the initial data is regressed for use in the computer. One incorrect data point in a set will introduce an error into the regression coefficients. Further error may arise when using the regression equation to calculate a physical property if the form of the equation chosen for the regression does not reflect the theoretical dependence of the property on the independent variable.

The base case was re-run using a value for the equilibrium constant of butane in the product separator that was 20% low. The converged solution indicated a 2.7% increase in the deisobutanizer feed, and a 3.0% decrease in the combined recycle from the two distillation columns. These changes appear to be small. However, the reduced recycle to the reactor resulted in an increase of 0.23 in the octane number. Also, since the deisobutanizer was already overloaded at the base case conditions, a further increase in the feed is undesirable.

Thus, such an error in the equilibrium constant for butane would have predicted too high an octane number, and would have predicted a need for a larger deisobutanizer column than was required. The predicted profict was only $32 per day too high.

An error in the equilibrium constant produced an error in the cost function. The sensitivity of the system and the resultant cost of an error in knowledge can be described by a sensitivity analysis. This topic will be presented in the following section.

4.2 Sensitivity Analysis

The end uses of a simulation are many. Not only can the steady-state operation of the plant be predicted for any set of operating and feed conditions, but a sensitivity analysis can also be performed. The sensitivity of the plant cost to an incremental change in one operating variable, or an error in knowledge of a physical property or a model parameter can be studied. For example, the sensitivity of the profit function with respect to an error in the equilibrium constant, as indicated in Section 4.1.5 would be given by:

$$\frac{(\Delta\ \text{Profit Function})\ /\ (\text{Profit Function})}{(\Delta\ \text{K-Equilibrium})\ /\ (\text{K-Equilibrium})}$$

Although the change in the cost, or in the profit is of great importance, the change in equipment size may be the required result if the simulation is to be used for design purposes.

The concept of a sensitivity analysis can be employed in many aspects of simulation. It can be used to better understand the operating characteristics of a plant, and in the training of operating personnel and engineers. Sensitivity analysis can be used, along with a simulation, to study the economic repercussions of an error in knowledge of a design parameter. Also, the sensitivity analysis has vast pedagogical potential when coupled with a simulation. The effect of an error in knowledge in one specific equipment can be traced throughout an entire plant, and the relative importance of many factors can be compared.

5.0 EXPERIENCES WITH LARGE SYSTEM SIMULATION

The development of a working simulation and cost analysis of a complex plant has provided valuable experience in large system simulation. The various modeling techniques and the case studies have already been presented. Now, a larger view of general simulation topics are presented. The questions to be answered are first discussed. Then, the choosing of a stream list, the identification of recycle problems, the formulation of models, and the development of a physical property package are discussed. All these topics depend on the questions to be answered.

5.1 The Questions to be Answered

A steady-state simulation employing MACSIM concepts is an excellent tool with which questions relating to interactions between units in large chemical, metallurgical or petroleum processing plants can be answered. It is very important that these questions be very precisely and accurately stated if the simulation is to yield accurate answers with a minimum expenditure of man hours and computation time. Based on these questions, the engineer must decide which chemical species must be included in the stream list and which species should be excluded. Also, he must decide what equipment to model, and what equipment not to model, based only on the questions to be answered.

In an industrial environment, only these specific questions must govern the development of the simulation. It must be remembered, however, that this present work with the alkylation plant was carried out in a university environment and therefore considerable detail was included in the original simulation(M3) because of its pedogogical value. Moreover, it represented an experience in solving general simulation problems for complex processes and allowed experimentation with various modeling techniques. For this reason, an overall general simulation was developed in this case. At the same time, the simulation was to provide information relating to the following tasks or questions:

The simulation should be able to

(i) Evaluate the effects of different olefin and isobutane feed compositions and feed entry points to the plant.

(ii) Describe the heat and mass flow interactions between the reactor and product separator.

(iii) Describe the reactor performance for different feed and operating conditions.

(iv) Describe the water flow in the plant.

(v) Describe the compressor-condenser loop as it functions in the overall plant.

(vi) Evaluate the importance of the present control systems in the steady-state performance of the plant.

(vii) Perform a cost study involving feed, product and operating utility costs.

The task of preparing a simulation, while answering the above questions, provided a realistic definition of the purpose of the simulation. In addition, a large amount of experience was gained in convergence-promotion techniques, large system sensitivity analysis, and the problems encountered with interactions between heat and mass balances. The alkylation simulation was an excellent tool to test the MACSIM technique, and some of the results of work include recommendations that are presented in Section 7.1.

5.2 Formulation of the Stream List

The stream vector contains the flow per unit time of every component that is considered in the simulation study. Choosing the proper chemical species to be included in the stream list is of great importance. If the component list is too small or incomplete, the flow will not be properly described and the entire simulation will be ineffective. If too many unnecessary components are included, storage requirements and execution time far exceed that required for adequate description of the process.

Choosing the correct stream list, if done systematically, is not difficult, and will result in a concise description of the material flow within the simulation. It must be emphasized that this step should be done correctly since the problems encountered when changing the stream list in the middle of a simulation study are extremely time consuming. Unexpected problems will occur even weeks after a stream list has been altered.

The choice of components for the stream list depends on the questions to be answered by the simulation. Initially, the stream list should be made as complete and as large as possible. Any component that exists in a plant stream should be included. To ensure that no components are omitted, the plant flow sheet should be checked equipment-by-equipment for known components. Then, this stream list is contracted, remembering that it is better to include an unnecessary component than to discard a required component. Each component of the stream list is examined for each piece of equipment in the plant flow sheet, and for each module of the information flow diagram. The following questions are asked:

(i) Is the component a major flow component for the module or equipment?

(ii) Is the component a "critical" or a "key" component to the operation or performance of the module or equipment?

(iii) Is the "behaviour" of the component the same as the "behaviour" of some other component in the module or equipment?

(iv) Is a chemical analysis available, or can it be calculated for the component in the module or equipment?

After asking these questions for each module in the information flow diagram, and each equipment in the plant flow sheet, the stream list can be sorted in two ways. First, components having the same behaviour and properties, or components that are not analyzed separately, can be grouped together. Secondly, components whose flows are very minor, and which do not affect the questions to be answered by the simulation, should be deleted from the stream list.

The stream list for the Alkylation simulation is shown in Table 5.1. Examples of grouping of components can be seen in position 10 for the "acid oils", in position 16 for the cis and trans isomers, as well as in positions 28, 29, 30 and 31.

Whenever possible, the components should be arranged in some logical order. In this study, the five non-organic components were placed first from positions 6 to 10. Then the hydrocarbons were listed, roughly in order of decreasing volitility. It is also important that the component in the stream list be in the form of the species in the plant, and not in the form in which the plant analyzes for it.

TABLE 5.1 : STREAM VARIABLES LIST FOR ALKYLATION SIMULATION

Location	Information	Units
1	Stream Number	
2	Stream Flag	
3.	Total Flow	lb.moles/hour
4	Temperature	°F
5	Pressure	p.s.i.a.
6	Flow of Water	lb.moles/hour
7	Flow of Sulphuric Acid	"
8	Flow of Sodium Hydroxide	"
9	Flow of Sodium Sulphate	"
10	Flow of Propyl Sulphate	"
11	Flow of C2 and Lighter	"
12	Flow of Propane	"
13	Flow of Propene	"
14	Flow of Normal Butane	"
15	Flow of Isobutane	"
16	Flow of Normal Butene	"
17	Flow of Isobutene	"
18	Flow of Normal Pentane	"
19	Flow of Isopentane	"
20	Flow of Isopentene	"
21	Flow of C6	"
22	Flow of 2,3-Dimethylbutane	"
23	Flow of C7	"
24	Flow of 2,4-Dimethylpentane	"
25	Flow of 2,3-Dimethylpentane	"
26	Flow of C8	"
27	Flow of Iso-Octane	"
28	Flow of 2,4-Dimethylhexane	"
	2,5-Dimethylhexane	"
	2,2,3-Trimethylpentane	"
29	Flow of 2,3,4-Trimethylpentane	"
	2,3,3-Trimethylpentane	"
	2,3-Dimethylhexane	"
30	Flow of C9	"
31	Flow of C10 and Greater	lb.moles/hour

5.3 Indentification of Key Recycle Components

Recycle creates problems in the steady-state simulation of chemical processes. The solution to a case study must be obtained by iterative rather than direct calculations. Early in the simulation, the recycle must be examined for two reasons. First, the important recycle components must be identified. Also, the possibility of a steady build up of one or more components, as in the case of isobutane, must be examined.

The first case is well known and easily identified. It is important to identify the major recycle components, since special attention must be given to them in all models in the recycle loop. The description of the flow of these components constitutes the major task of modeling the many separation processes that occur in a recycle loop. Looking now at the alkylation plant, several observations can be made:

(i) C6 and heavier components do not recycle.

(ii) Olefins do not recycle since they are completely reacted.

(iii) Acid, propyl sulphate, sodium hydroxide and sodium sulphate are not recycle components in the main plant recycle.

From these three observations, the only important components of the main plant recycle are:

(i) water
(ii) propane
(iii) butane
(iv) isobutane
(v) pentane
(vi) isopentane

The two pentanes may be considered of secondary importance because of their low flow rates, and because a large percentage of the pentanes are removed from the system at the deisobutanizer. Thus the description of the main recycle loop, which is made up of the reactor and the three main separation equipments (product separator, depropanizer and deisobutanizer), is mainly a description of the flow of water, propane, isobutane and butane; obviously the reactor must consider many more components. This description of the recycle, and the separation processes, puts the development of models in the proper perspective. These are the important recycle components and, therefore, they are the ones to be given prime consideration in modeling and in the gathering of physical property data.

The recycle of heat is also very important. There is a strong interaction between the heat and the mass balances in the plant, both in the reactor, and in the product separator. Thus the temperature of the main recycle, as well as its total flow, must be accurately described.

The second reason for the close examination of the recycle is the possibility of a steady buildup of one component. Often this problem is not discovered when simple, linear models are used to describe the process. Inerts or impurities, often removed by purging, are not the compounds that build up in a chemical plant. The removal of isobutane from the alkylation plant is a very insensitive function of the internal flows within the plant. Primarily, the reaction with olefins in the Stratco reactor accounts for the isobutane usage. The amount reacted is almost entirely dependent on the amount of olefin present, and on no other conditions. The only other route by which isobutane leaves the alkylation plant is in the propane or the butane product streams. However, both columns are controlled to allow as little as possible isobutane to leave in these streams; consequently, the exit concentrations of isobutane in these two products is a very insensitive function of the isobutane content of the feed to the columns.

Plant operation is designed to keep isobutane within the system. Thus, if too much isobutane is fed to the plant, a build up will occur. Examination of the plant operation indicates that this does occur, and the amount of isobutane being fed, for a constant olefin feed rate, is continually being adjusted by the operators to achieve the desired control.

This phenomena creates two problems. First a converged solution cannot be obtained if there is a change in component flows from iteration to iteration. Secondly, the isobutane feed flows will be incorrect, and this will affect any economic evaluation that is performed.

There are some general characteristics of this material build up problem that was encountered here. It can be seen that this increase in inventory will arise for those components which enter into the process as feed and/or reaction products, and then recycle. In addition, if the removal of these components, either by reaction or in an exit stream, is a non-linear function of its flowrate within the plant, then, unless adequate control schemes are included in the process or operating procedures, the flow of these components will either increase or decrease continually. Any control scheme must then monitor and fix the component flow or concentration. Just as control must be exercised in the real plant, so it must be included in the simulation.

5.4 Model Development

Although each module of each simulation study is unique, there are five cardinal rules of model development that can be applied to any large steady-state simulation of a chemical plant.

(i) Formulation of every model must only be influenced by the questions to be answered by the simulation.

(ii) A MACSIM - like simulation is a tool to study the interaction among many models, rather than the performance of one or two very complex models.

(iii) Start with simple models and replace them as their importance becomes known.

(iv) Models should be specific to a given simulation rather than general.

(v) Construct models so that they operate with the same specifications and constraints as the actual plant.

It is to be noted that there is a certain similarity with all of these rules but the specific points are underlined since all of these rules must be applied to any simulation study. Further amplification is indicated below.

Models must be developed to assist in the answering of questions asked of the simulation. The questions to be answered, and the important flow components must be kept in view at all times. A sophisticated model, or a sophisticated section of a model, is a costly waste of time and resources if it contributes nothing of value to the questions to be answered. Conversly, one weak model that has not sufficiently described a particular operation which is critical in answering the simulation questions, may negate the work done on many other sophisticated models. For example, all possible reactions between the organic and the acid phases might be described in order to accurately predict the required acid makeup. However, if the solubility of these components in acid was not well known, the question to be answered - acid usage - could not be accurately described. On the other hand, if the performance of the settler had been described in terms of drop-size distribution, but this distribution could not have been predicted for the discharge stream from the reactor, then this particular settler model would have been of no use in the simulation.

It cannot be emphasized enough that the power of a MACSIM-like system is in the study of interactions among process equipment, rather than in the performance of one very complex model. There always seems to be a tendency to develop very sophisticated models when they are not required. A sophisticated model may be required to answer some of the questions that have been posed, but the main objective of the simulation is still the study of interactions.

Simulation studies must start simply. Efficiency of time alone dictates this rule. It is often impossible to tell what areas of the plant require sophisticated models until a model of the plant has been assembled. Simple reactor models, along with temperature and pressure setters, and linear splitting models must comprise the initial simulation of the plant. Perhaps some of the questions may be able to be answered using a simulation comprised of simple modules. As one uses this simple simulation of the plant to answer the questions, it rapidly becomes very obvious which models require sophistication, and which modules are sufficiently sophisticated, even in their very simple form.

Experience has shown that the development of general models, as opposed to specific models, in most cases, is not justified. The only exception to this rule is the simple temperature and pressure setting models, the linear splitting models, and the junction or mixing models that can be used to assemble the initial simple plant simulation. The general principle that an engineer should be able to "select modules off the shelf" when he assembles a plant simulation is an excellent concept, but seems to be as difficult to achieve in practice as the concept of choosing general hardware "off the shelf" for any specific plant. When a model is developed,it is very difficult to guess all of the uses to which that model will be put; some modification always seems to be necessary. On the other hand, after experience has been gained in any specific modeling area, in most cases, revisions required for a given system are very easily incorporated into existing models. In situations where some generalization is possible, it should probably be incorporated as it was in EXCH11.

Finally, the rule that is most often overlooked is, "Construct a model based on the same specifications and constraints under which the plant equipment operates". This rule contains two sections: operating specifications, and operating constraints. In order to develop a model that responds in the same way as the plant equipment and its control system does, operating specifications must be an integral part of the model. The depropanizer operates to a maximum propane content in the bottoms, and the deisobutanizer is operated to a maximum isobutane concentration in the butane side-cut. To properly model these units, these operating specifications must be incorporated; the conventional specifications of reflux ratio and product-to-feed ratios, which are useful in design calculations, may not be useful in simulation models for distillation columns. This point was most important in the alkylation plant simulation since the general design model did not describe the actual plant operation and its response to a variety of feed compositions.

Plant operating restrictions must also be included in a model. If the solution of the simulation suggests operation beyond the capacities of any of the equipment, then it is not a meaningful simulation of actual plant operation. Flowrates, condenser capacities, compositions, temperatures, and pressures that would result in non-allowable plant or equipment operation must be detected by a model, and an error message printed out. Otherwise, a technically unfeasible solution to a case study may be accepted.

5.5 Development of a Physical Property Package

A modular approach to physical property calculation provides a concise package and allows additional properties to be easily added. The package described in Section 2.3.10 contains one subroutine to read in the physical property constraints, one subroutine to calculate physical properties, and one subroutine to calculate the physical property for a specified composition. This section discusses the compiling of physical property data, and the regression of this data.

The physical properties that must be obtained, and their accuracy, depend on the questions to be answered by the simulation. For example, if a heat balance is of little importance, average heat capacities may be sufficient. It must also be stressed, as in the case of model development, the cardinal rule is "start simple". More precision can be included if it is necessary. It must also be stressed that great care must be taken in preparing a set of physical properties for future use. When the simulation of the alkylation plant was initiated, seventeen physical properties were collected and regressed before the actual requirements were ascertained. In actual fact only five of these properties were found to be needed to answer all questions that had been proposed.

The regression of physical property data, usually against temperature, can lead to several problems if not carefully done. First, the basic premise of all regression techniques is that the form of the equation used relates to the fundamental background of the phenomena to be described. Although this is more important for regressing experimental data containing significant but random errors, it is also an important consideration in the fitting of physical properties. As an example, it was found that a simple polynomial form was not sufficient to relate the liquid-vapor equilibrium constants at 18 psia with temperature. Although the polynomial was used for all other physical properties it was found that a logarithmic dependence on temperature, as indicated by theory, was necessary to obtain the required accuracy.

5.6 Summary and Contributions to Knowledge

An accurate working simulation of the steady-state behaviour of the Shell alkylation unit at Bronte, Ontario has been assembled and tested. This simulation incorporates a costing analysis that includes feed, product, and operating utility costs. A number of case studies were performed to test the simulation and to provide data for a sensitivity analysis. In addition to a complete description of the process and the simulation, the experience gained from the development of a simulation for a large complex plant has been presented, and can be summarized as follows:

(i) New modeling techniques have been tried and evaluated.

(ii) The necessity of including control modules, as well as convergence promotion techniques, in order to obtain a solution to a case study, has been demonstrated.

(iii) The MACSIM Simulation system has been tested with a large complex plant in which there are interactions between the mass and energy balances.

(iv) Guidelines for the development of a simulation of any process are presented for questions concerning the preparation of the stream list, model development, and the identification of recycle problems.

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7.1 Flash Equation for Product Separator

The flash calculation is used to predict the equilibrium distribution of vapor and liquid produced when a multicomponent mixture is flashed. The equilibrium constant K is assumed to be only a function of temperature and pressure.

Consider a flash drum with inlet liquid flow F, and exit vapor and liquid flow V and L respectively. Overall and component mass balances give the equations:

$$F = V + L \tag{7A}$$

$$F X_i = V y_i^f + L x_i^f \tag{7B}$$

where X_i is the mole fraction of component i in the feed, and y_i^f and x_i^f are the mole fractions of component i in the exit vapor and liquid streams respectively.

But x_i^f and y_i^f are related by the equilibrium constant K_i

$$y_i^f = K_i \; x_i^f \tag{7C}$$

Substitute Equations 7A and 7B in 7C, and define ψ to be $(\frac{L}{F})$. But the sum of the mole fractions in the vapor must equal one.

$$\sum_{i=1}^{n} \left[\frac{x_i}{1 - \psi (1 - \frac{1}{K_i})} \right] = 1 \tag{7D}$$

An iterative technique can be used to find the value of ψ which is $\frac{L}{F}$, for which the following function of ψ tends to zero.

$$f(\psi) = \sum_{i-1}^{n} \frac{x_i}{1 - \psi \; (1 - \frac{1}{K_i})} - 1 \tag{7E}$$

The Newton-Raphson method is used in the iterative search of a ψ for which $f(\psi)$ approaches zero.

$$\psi_{new} = \psi_{old} - \frac{f(\psi)}{f'(\psi)} \qquad (7F)$$

where

$$f'(\psi) = \sum_{i=1}^{n} \left[\frac{-X_i \left(1 - \frac{1}{K_i}\right)}{\left(1 - \psi\left(1 - \frac{1}{K_i}\right)\right)^2} \right] \qquad (7G)$$

7.2 Suggestions for the Improvement of the MACSIM System

The MACSIM executive is a MAP version of PACER that was written for the McMaster IBM 7040 by Dr. W. Fleming. It was not possible to alter the executive during the Alkylation study, but several recommendations for future revisions are presented, based on the experience obtained while using the system.

(i) The order of calculation for the modules should always be specified by the user, and the section of the executive that calculates this could be deleted.

(ii) The debugging printout from the executive should be controlled by a large number of specific switches, perhaps in the EN vector of each equipment, rather than by the variable KSETS which often produces far more than the desired information.

(iii) All printout of stream and equipment vectors should be limited to only those with non-zero numbers.

(iv) The variable KSETS should not be used for printout control in any module that is written. All modules used in a simulation should contain their own print switches in the EN or ENC vectors.

(v) It is not necessary that all streams used in the simulation be stored. Those to be saved can be indicated by the "stream flag" (second position in the stream vector). This position in the stream vector will not be required once the order of calculation is specified.

(vi) Not all streams need to be tested during the check for convergence.

APPENDIX 7.3

Base Case Input Data

```
$ENDCH
C      ********MACSIM COMMON DECK, FOR ALKALATION.  APR.30,1968. T.T.****
       COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
       COMMON AEN(4,102),ENC(50,20),NOPP,X,XMOLE(26),PPSC(17,26),PPMX(17)
       COMMON  SN(75,31),DELS(31), KPM(50,10),KUS(75),KPS(3)
       COMMON  SNC(75,1),DELSC(1),STRMCI(5,1),STRMCO(5,1), KVOID
       COMMON  KSEM( 75,3),  NELIST(70,2),  NAME(50),  NAME2(50)
       COMMON  KEFLAG(50),  KSFLAG( 75),  NECALL(50)
       COMMON  TITLE(24), KE1(50), KE2(50), KE3(50), KSPRNT(10)
       COMMON               NSLMAX,  NSCLMX
       COMMON  NELMAX,  NECLMX,  NEMAX,  NSMAX,  NEQUIP
       COMMON  N2MAX,  N3MAX,           KRET,  KRET2,  KRET3
       COMMON  NOAEN,  NOEN,  LIMIT,  LIMIT2,  LIMIT3
       COMMON  CS(150),BI(150)
       COMMON  LOOP,  KBACK,  KBACK2,  KARDS,  KPRINT,  KONV
       COMMON  KRUN,           KCLEAN,  LOOPS,  NOGO,  MCHAIN
       COMMON  NCHAIN,  KOUNT2,        NLIST,  LIST
       COMMON  NUS,  NUSMAX,  NPS,  NPSMAX,  NUS1,  NUS2
       COMMON  NUS3,  KCV1,  KCV2,  KCV3,  NE2,  NE1MAX
       COMMON  NE2MAX,  NE3MAX,  KES,  KES2,  KPLOOP
       COMMON  NEUSED,  NSUSED
C      ******************************************************************
ENDCO
  SHELL ALKYLATION SIMULATION

   1     0     0    10     0     0    50     0 111111111 1 11
  36     7    36    60    10    20    31     0     0    26
  34                                                        PROCESS MATRIX
   1 READIN            44   -44
   2 DISOB1  DIB        1    -2    -3    -4   -21
   3 REAC25 REACTR      9    10   -11
   4 SETL01            11   -12   -19
   5 EXCH14 PR SEP     13    27   -14   -15   -20
   8 COMPRS            14   -24
   9 CONT02            14   -24
  10 JUNC02  PUMP      24   -16
  11 MAKEUP  ACID      19    17   -10   -18
  12 DEPRP2 DEPROP      5    -6    -7
  13 JUNC02             2    22   -23
  14 COAL01            54    -9   -25
  15 COSTER            44   -44
  16 WASH01            16    29   -38   -37
  17 WASH02            38    39   -41   -40
  18 JUNC02            12    30   -13
  19 WASH01            52    28   -31   -47
  20 WASH02            31    32   -34   -33
  21 COAL01            34   -36   -35
  22 SETST2            36    -1
  23 SETST2            48    -5
  24 JUNC02            53    49   -45
  25 COAL01            41   -43   -42
  26 JUNC02            15   -46
  27 REPORT            44   -44
```

```
   28 SETST2                  50   -27
   29 EXCH11 E-6010            7   -45    -50    -48
   30 EXCH11 E-6002           46    23    -51    -53
   31 JUNC02                  45   -54
   32 NSTEM1                  20    27    -49
   33 SETST2                  51   -52
   34 SETST2                   4   -44
   35 SETST2                   3   -44
   36 CONT03 I-C4             44   -44
   31                                                            EQUIPMENT VECTORS
2.                 .587             .033             .70              .90
.30                .50              .45              .10
3.                 .0               .0               1.               5.
1.                 7.               340.             .926
4.0                3.6
0.0
5.                 36300.           17.7             18.
29.                                 0.0
9.0                                                  0.01             2.
5.                 20.7511          0.0              2.               1.
10.                80.              325.             0.               0.
1.0
11.                0.992            0.91             0.48             9.
13.                1.               7.               50.
12.                30.              .891             120.             7.
15.                .985             847.
13.0                                95.0
1.0
14.                .80
0.0
15.                13.                               75.
0.38               0.38             0.282            0.0063           0.011
16.0               0.20             7.0
0.0
17.0               0.20             7.0
0.0
18.0
1.0
19.0               0.20             7.0
0.0
20.0               0.20             7.0
0.0
21.0               0.80
0.0
22.0               170.0            0.0
0.0
23.                196.             2.               847.
7.
24.0
1.0
25.0               0.80
0.0
26.                38.              225.
1.0
27.                9.
.0                                                                    100.
28.                80.              7.               104.             15.
7.
29.                44000.           1.
```

```
7.              7.
30.             12000.          1.
7.              7.
31.
1.0
33.             142.            1.              938.7           0.
7.
34.             80.             7.              115.            15.
7.
35.             90.             7.              101.            15.
7.
36.             9.              3.              .003            30.
.0
    6                                                EQUIP CONTROL VECTORS
2.                                              104.            15.
                6.              .9
.0
.0
5.                              10.             7.              6.
17.             7.              0.              0.              0.
0.0
0.0
13.                             10.             7.
0.0
0.0
0.0
18.0                            5.0             7.0
0.0
0.0
0.0
24.                                             7.
0.0
0.0
0.0
31.                             5.              7.
.0
.0
.0
     0                                                    STREAM VECTORS
9.              .0              1731.           43.8644         95.
1.1549
.0              191.31          65.             490.78          854.27
58.00           61.61           2.32            6.46            .0
.0              .09             .0              .25             .26
.0              .16             .07             .16             .01
.01
10.             .0              1256.           51.8320         70.
108.61          1120.                                           44.21
0.0
0.0
0.0
0.0
0.0
27.                             690.7           80.
.0
.0              19.8                            247.4           412.4
1.3             1.5             .8              6.4
.0              .10             .0              .25             .26
.0              .15             .07             .15             .015
```

```
.015
22.             1.              500.5           42.             14.7
2.
0.0             122.0           65.0            116.0           80.0
55.4            58.6            1.5
0.
0.0
0.0
28.0            1.0             40.016          50.0            180.0
39.09                           0.926
0.0
0.0
0.0
0.0
0.0
29.0            1.0             10.2375         50.0            318.0
10.0            0.0             0.2375
0.0
0.0
0.0
0.0
0.0
30.             1.              236.            38.             80.
2.
.0              21.13182        .0              107.4836        94.6926
3.1729          3.1729          .4957           2.0822
.0
0.0
0.0
32.0            1.0             208.0           50.0            225.0
208.0
0.0
0.0
0.0
0.0
0.0
39.0            1.0             30.5            50.0            325.0
30.5
0.0
0.0
0.0
0.0
0.0
   0                                            STREAM CONTROL VECTORS
  31                                              COMPONENT TOLERANCES
                                .1              .01             .01
.1              .1              .1              .1              .1
0.001           0.001           0.001           0.001           0.001
0.001           0.001           0.001           0.001           0.001
0.001           0.001           0.001           0.001           0.001
0.001           0.001           0.001           0.001           0.001
0.001
   0                                                 PREFERRED STREAMS
   2                                          ADDITIONAL EQUIP VECTORS
15.0            45.             1.26                            3.48
2.94            3.55            3.55            3.8             3.8
0.0                             1.16            1.16            3.97
4.13            3.24            3.24            3.8             3.8
0.0                             4.15            3.6             3.52
```

```
8.68                3.5
30.0                22.0            4.0             6.0             3.0
17.0                28.0            29.0            11.             12.
15.                 9.
36.                 5.
   1    36                                                     CALCULATION ORDER
   1     1     3     2     4     2    11     2    18     2
   5     2     8     2     9     2    10     2    16     2
  17     2    25     2    29     2    23     2    12     2
  29     2    28     2    32     2    26     2    30     2
  33     2    19     2    20     2    21     2    22     2
   2     2    13     2    30     2    24     2    31     2
  14     2    27     2    36     3    34     1    35     1
  15     1
   2     9    27                                            STREAMS PRINTED
               5                                          PHYSICAL PROPERTIES
               1               11               1              2
 0.1801600E 02 -0.             -0.              -0.
 0.9810000E 02 -0.             -0.              -0.
 0.4000000E 02 -0.             -0.              -0.
 0.1421000E 03 -0.             -0.              -0.
 0.1980000E 03 -0.             -0.              -0.
 0.3006800E 02 -0.             -0.              -0.
 0.4409400E 02 -0.             -0.              -0.
 0.4207800E 02 -0.             -0.              -0.
 0.5812000E 02 -0.             -0.              -0.
 0.5812000E 02 -0.             -0.              -0.
 0.5610400E 02 -0.             -0.              -0.
 0.5610400E 02 -0.             -0.              -0.
 0.7214600E 02 -0.             -0.              -0.
 0.7214600E 02 -0.             -0.              -0.
 0.7013000E 02 -0.             -0.              -0.
 0.8617200E 02 -0.             -0.              -0.
 0.8617200E 02
 0.1002000E 03 -0.             -0.              -0.
 0.1002000E 03
 0.1002000E 03
 0.1142000E 03 -0.             -0.              -0.
 0.1142000E 03
 0.1142000E 03
 0.1142000E 03
 0.1282500E 03 -0.             -0.              -0.
 0.1422800E 03 -0.             -0.              -0.
               6               11               1              2
 0.1000000E 01 -0.             -0.              -0.
-0.            -0.             -0.              -0.
-0.            -0.             -0.              -0.
-0.            -0.             -0.              -0.
-0.            -0.             -0.              -0.
 0.3620000E 00 -0.             -0.              -0.
 0.4570000E 00 -0.             -0.              -0.
 0.4420000E 00 -0.             -0.              -0.
 0.5450000E 00 -0.             -0.              -0.
 0.5160000E 00 -0.             -0.              -0.
 0.5800000E 00 -0.             -0.              -0.
 0.5600000E 00 -0.             -0.              -0.
 0.6230000E 00 -0.             -0.              -0.
 0.5940000E 00 -0.             -0.              -0.
 0.6300000E 00 -0.             -0.              -0.
```

```
 0.7040000E 00 -0.            -0.              -0.
 0.7040000E 00 -0.            -0.              -0.
 0.7960000E 00 -0.            -0.              -0.
 0.7960000E 00 -0.            -0.              -0.
 0.7960000E 00 -0.            -0.              -0.
 0.8160000E 00 -0.            -0.              -0.
 0.8160000E 00 -0.            -0.              -0.
 0.8160000E 00 -0.            -0.              -0.
 0.8160000E 00 -0.            -0.              -0.
 0.9920000E 00 -0.            -0.              -0.
 0.1052000E 01 -0.            -0.              -0.
            7              12               2              2
 0.1800000E 02 -0.            -0.              -0.
 0.3370000E 02 -0.            -0.              -0.
-0.            -0.            -0.              -0.
-0.            -0.            -0.              -0.
-0.            -0.            -0.              -0.
 0.3500000E 02 -0.            -0.              -0.
 0.3500000E 02 -0.            -0.              -0.
 0.3500000E 02 -0.            -0.              -0.
 0.3183333E 02  0.4833333E-01 -0.              -0.
 0.3045889E 02  0.4838889E-01 -0.              -0.
 0.2951889E 02  0.4738889E-01 -0.              -0.
 0.2569444E 02  0.7294444E-01 -0.              -0.
 0.3925222E 02  0.4772222E-01 -0.              -0.
 0.3582333E 02  0.6083333E-01 -0.              -0.
 0.3582333E 02  0.6083333E-01 -0.              -0.
 0.4400667E 02  0.5566667E-01 -0.              -0.
 0.4400667E 02  0.5566667E-01 -0.              -0.
 0.5027778E 02  0.6277778E-01 -0.              -0.
 0.5027778E 02  0.6277778E-01 -0.              -0.
 0.5027778E 02  0.6277778E-01 -0.              -0.
 0.5808111E 02  0.6561111E-01 -0.              -0.
 0.5808111E 02  0.6561111E-01 -0.              -0.
 0.5808111E 02  0.6561111E-01 -0.              -0.
 0.5808111E 02  0.6561111E-01 -0.              -0.
 0.5808111E 02  0.6561111E-01 -0.              -0.
 0.5808111E 02  0.6561111E-01 -0.              -0.
           17              21               3              2
  -0.               -0.           -0.
  -0.               -0.           -0.
  -0.               -0.           -0.
  -0.               -0.           -0.
  -0.               -0.           -0.
  -4.88040E 03      1.44368E 01   -7.28131E-06
  -6.85093E 03      1.81815E 01   -1.20715E-05
  -6.69163E 03      1.80048E 01   -1.17771E-05
  -5.18631E 03      1.06313E 01   -1.12911E-06
  -5.61591E 03      1.29087E 01   -5.11979E-06
  -5.26768E 03      1.07812E 01   -1.44842E-06
  -5.62085E 03      1.27715E 01   -5.27266E-06
  -7.00107E 03      1.34919E 01   -3.58334E-06
  -6.38888E 03      1.24424E 01   -2.98350E-06
  -7.09311E 03      1.44224E 01   -5.31812E-06
  -3.26512E 03      1.01366E 00   +1.12630E-06
  -3.26512E 03      1.01366E 00   +1.12630E-06
  -8.41156E 03      1.34505E 01   -2.27858E-06
  -8.41156E 03      1.34505E 01   -2.27858E-06
  -8.41156E 03      1.34505E 01   -2.27858E-06
```

```
   -8.59512E 03      1.35143E 01     -4.87632E-06
   -8.59512E 03      1.35143E 01     -4.87632E-06
   -8.59512E 03      1.35143E 01     -4.87632E-06
   -8.59512E 03      1.35143E 01     -4.87632E-06
   -1.06507E 04      1.71613E 01     -7.57032E-06
   -1.06507E 04      1.71613E 01     -7.57032E-06
              13                14              4                  2
  0.3486420E 01 -0.4492820E-03 -0.1473570E-05 0.
 -0.            -0.            -0.            -0.
 -0.            -0.            -0.            -0.
 -0.            -0.            -0.            -0.
 -0.            -0.            -0.            -0.
  0.9229252E 00 -0.1904835E-02 -0.4140946E-05 -0.3000686E-08
  0.7918123E 00 -0.1031659E-02 -0.2242737E-05 -0.1625171E-08
  0.8572489E 00 -0.1172290E-02 -0.2548457E-05 -0.1846708E-08
  0.6728226E 00 -0.5946352E-03 -0.1292685E-05 -0.9367284E-09
  0.6532023E 00 -0.6117243E-03 -0.1329835E-05 -0.9636488E-09
  0.6988615E 00 -0.6465556E-03 -0.1405556E-05 -0.1018519E-08
  0.6988782E 00 -0.6464467E-03 -0.1405319E-05 -0.1018347E-08
  0.5739921E 00 -0.4304691E-03 -0.4679012E-06 -0.
  0.5681185E 00 -0.4429630E-03 -0.4814815E-06 -0.
  0.5950788E 00 -0.4103560E-03 -0.8920782E-06 -0.6464335E-09
  0.5045949E 00 -0.2569895E-03 -0.5586728E-06 -0.4048354E-09
  0.5045949E 00 -0.2569895E-03 -0.5586728E-06 -0.4048354E-09
  0.4405297E 00 -0.1726325E-03 -0.3752881E-06 -0.2719479E-09
  0.4405297E 00 -0.1726325E-03 -0.3752881E-06 -0.2719479E-09
  0.4405297E 00 -0.1726325E-03 -0.3752881E-06 -0.2719479E-09
  0.3955055E 00 -0.1595051E-03 -0.2259774E-06 -0.1637517E-09
  0.3955055E 00 -0.1595051E-03 -0.2259774E-06 -0.1637517E-09
  0.3955055E 00 -0.1595051E-03 -0.2259774E-06 -0.1637517E-09
  0.3955055E 00 -0.1595051E-03 -0.2259774E-06 -0.1637517E-09
  0.3614475E 00 -0.1632716E-03 -0.1774691E-06 -0.
  0.3294951E 00 -0.1369778E-03 -0.1488889E-06 -0.
$IBSYS
```

APPENDIX 7.4

Program Listings in Alphabetical Order

```
$IBFTC COAL01
      SUBROUTINE COAL01
C     WRITTEN FEB.  A. ORLICKAS
C     REVISED MAY  I. SHAW
C
C    -COALESCER MODULE WRITTEN FOR SHELL OAKVILLE SIMULATION
C    -ENTRAINED WATER IS REMOVED ACCORDING TO A SPECIFIED EFFICIENCY
C    -THE EXIT ORGANIC STREAM CONTAINS ENTRAINED AND DISSOLVED WATER
C
C     STRMO(1,J) IS THE EXIT ORGANIC STREAM
C     STRMO(2,J) IS THE EXIT AQUEOUS STREAM
C
C     EN VECTOR
C     1. EQUIPMENT NO.
C     2. FRACTION OF ENTRAINED WATER REMOVED BY COALESCER
C
C     *******MACSIM COMMON DECK, FOR ALKYLATION.  APR.30,1968. T.T.****
      COMMON NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
      COMMON AEN(4,102),ENC(50,20),NOPP,X,XMOLE(26),PPSC(17,26),PPMX(17)
C
      JJ = NOCOMP + 5
C     FENTW --- ENTRAINED WATER IN HYDROCARBON STREAM
C     FWATT --- TOTAL INPUT WATER FLOWRATE
      FWATT = STRMI(1,6)
C     CALCULATE WATER SOLUBILITY AND CHECK WATER BALANCE
      X = STRMI(1,4)
      DO 12 J=1,NOCOMP
   12 XMOLE(J) = STRMI(1,J+5)
      CALL FSOL ( FSOLW )
      IF ( FSOLW .GE. FWATT ) GO TO 20
      FENTW = (FWATT - FSOLW ) * ( 1.0 - EN(NE,2))
      STRMO(1,6) = FENTW + FSOLW
      IF ( STRMO(1,6) .GE. FWATT ) GO TO 20
      STRMO(2,6) = FWATT - STRMO(1,6)
      GO TO 21
20    STRMO(1,6) = FWATT
      STRMO(2,6) = 0.0
C
   21 STRMO(1,3) = STRMO(1,6)
      STRMO(2,3) = STRMO(2,6)
      RATIO = (STRMO(1,6)-FSOLW)/(FWATT-FSOLW)
      DO 30 J=7,10
      STRMO(1,J) = STRMI(1,J)*RATIO
      STRMO(2,J) = STRMI(1,J) - STRMO(1,J)
      STRMO(1,3) = STRMO(1,3) + STRMO(1,J)
   30 STRMO(2,3) = STRMO(2,3) + STRMO(2,J)
C     NO ORGANIC LEAVES IN THE WATER STREAM
      DO 40 J=11,JJ
      STRMO(1,J) = STRMI(1,J)
      STRMO(2,J) = 0.0
   40 STRMO(1,3) = STRMO(1,3) + STRMO(1,J)
C     TRANSFER TEMPERATURE AND PRESSURE
      DO 50 J=4,5
      STRMO(1,J) = STRMI(1,J)
   50 STRMO(2,J) = STRMI(1,J)
C
      RETURN
      END
```

```
$IBFTC COMPRS
      SUBROUTINE COMPRS
C     WRITTEN BY A. ORLICKAS    P. MELNYK
C     REVISED BY I. SHAW SEPT 1968
C
C     MODULE WRITTEN FOR THE SHELL ALKYLATION SIMULATION TO DESCRIBE
C        - THE PRESSURE DROP FROM THE PRODUCT SEPARATOR TO THE COMPESSOR
C        - THE COMPRESSOR
C        - THE CONDENSER FOR THE FEED TO THE DEPROPANIZER COLUMN
C
C     NO EN VECTOR
C
C     ******* MACSIM COMMON DECK, FOR ALKYLATION.  T.T. APR.29,1968.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
      COMMON AEN(4,102),ENC(50,20),NOPP,X,XMOLE(26),PPSC(17,26),PPMX(17)
      COMMON  SN(75,31),DELS(31), KPM(50,10),KUS(75),KPS(3)
C
      JJ = NOCOMP + 5
      DO 20 J=6,JJ
   20 STRMO(1,J) = STRMI(1,J)
      STRMO(1,3) = STRMI(1,3)
C
C     CALCULATE PRESSURE KNOWING FLOW AND ASSUMING IDEAL GAS BEHAVIOR
      PDROP = 2.395E-05*STRMI(1,3)*(STRMI(1,4)+460.0)*0.1788/STRMI(1,5)
C
C     CALCULATE COMLRESSOR OUTLET PRESSURE FROM COMRESSION RATIO
      VFLOW = STRMI(1,3)*(STRMI(1,4)+460.0)*0.1788/(STRMI(1,5) - PDROP)
      IF(VFLOW.GT.4600.0) WRITE(6,151) VFLOW
      RATIO = 15.10 - 0.00267*VFLOW
      NN = KPM(NE,2)
      SN(NN,5) = RATIO*(STRMI(1,5) - PDROP)
      STRMI(1,5) = SN(NN,5)
C     COSTING DATA
      SHTHP = 0.187*VFLOW + 0.1248
      KWPH = SHTHP / 0.746
      ENC (NE,16) = KWPH
C
C     CALCULATE CONDENSER OUTLET PRESSURE AND OPERATING COSTS
      STRMO(1,5) = 0.104*STRMI(1,3) - 13.90
      ENC(NE,17) = 18.48
      ENC(NE,18) = 11.58
C
      RETURN
  151 FORMAT(/124H *** POWER CUTOFF LIMIT TO THE COMPRESSOR HAS BEEN EXC
     1EEDED BUT THE CALCULATIONS ARE CONTINUED USING THE OVERLOAD CONDIT
     2IONS/5X,  15HTHE GAS FLOW IS, F9.0,  35H  BUT THE UPPER LIMIT IS 4
     3600.  ***)
      END
```

```
$IBFTC CONT02
      SUBROUTINE CONT02
C    -WRITTEN FOR THE SHELL OAKVILLE REFINERY SIMULATION
C     THE STREAMS FOR THIS MODULE ARE THE EXIT COMPRESSOR STREAM IN
C      AND THE EXIT CONDENSER STREAM OUT
C
C     EN VECTOR
C     1. EQUIPMENT NUMBER
C     2. OLD PRESSURE DIFFERENCE IN THE SEARCH (SET BY THE PROGRAM)
C     3. NEW PRESSURE DIFFERENCE IN THE SEARCH (SET BY THE PROGRAM)
C     4. CONVERGENCE TOLERANCE FOR THE PRESSURE DROP (NORMALLY 0.1)
C     5. NUMBER OF MODULES TO GO BACK TO TO THE PRODUCT SEPARATOR
C     6. EQUIPMENT NUMBER OF THE PRODUCT SEPARATOR
C     7. CHANGE IN DELP WITH A CHANGE OF 1 P.S.I.   (INITIALLY 20)
C     8. PRINT CONTROL   (NORMALLY 0.0 - NO PRINTING)
C     9. SWITCH FOR DIRECT OR LOOP CALCULATION
C        - DIRECT CALCULATION                1.0
C        - LOOP CALCULATION                  2.0
C     10. LOOP CONTROL   (INITIALLY EQUAL TO 1.)
C     11. OLD PRODUCT SEPARATOR PRESSURE IN THE SEARCH
C     12. NEW PRODUCT SEPARATOR PRESSURE IN THE SEARCH
C     13. DELP AT 17.7 PSIG.  SAVED FOR THE PRESSURE SEARCH
C
C     ******* MACSIM COMMON DECK, FOR ALKYLATION.  T.T. APR.29,1968.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,21),STRMO(5,21),EN(50,20)
      COMMON  ZZ(5753), NOEN, LIMIT, LIMIT2, YY(314), NLIST
C
      DELP = STRMI(1,5) - STRMO(1,5)
      LOOPC = EN(NE,10)+0.1
      NEE = EN(NE,6)
      EN(NE,10) = LOOPC + 1
      IF(LOOPC.GE.2)  GO TO 30
C     EN(NEE,3)  IS THE PRESSURE OF THE PRODUCT SEPARATOR
C
  10  IF(DELP.GE.0.0)  GO TO 40
      EN(NE,3) = DELP
      EN(NE,12) = EN(NEE,3)
      EN(NEE,3) = EN(NE,12) - DELP/EN(NE,7)
      EN(NE,13) = DELP
      MM = EN(NE,5)
      IF(EN(NE,9).EQ.1.0)  NLIST = NLIST-MM-1
      IF(EN(NE,9).EQ.2.0)  NOEN = NOEN-MM-1
      GO TO 60
C
C     SEARCH FOR PRODUCT SEPARATOR PRESSURE SO THAT DELP IS ZERO
  30  EN(NE,2) = EN(NE,3)
      EN(NE,11) = EN(NE,12)
      EN(NE,3) = DELP
      EN(NE,12) = EN(NEE,3)
      AA = EN(NE,3) - EN(NE,2)
      EN(NEE,3) = EN(NE,12) - (EN(NE,12)-EN(NE,11))*EN(NE,3)/AA
      EN(NE,7) = EN(NE,13)/(17.7-EN(NE,12))
      IF(ABS(DELP).LE.EN(NE,4))  GO TO 40
      MM = EN(NE,5)
      IF(EN(NE,9).EQ.1.0)  NLIST = NLIST-MM-1
      IF(EN(NE,9).EQ.2.0)  NOEN = NOEN-MM-1
      GO TO 60
C
  40  EN(NE,10) = 1.0
```

```
      FN(NEE,3) = 17.7
C
   60 IF(FN(NE,8).GT.0.5)  WRITE(6,9999) DELP
C     RESET THE CONVERGENCE MONITOR BACK TO ZERO
      LIMIT2 = 0
      RETURN
C
 9999 FORMAT(   6X,8H DELP = ,F38.5)
      END
```

```
$IBFTC CONT03
      SUBROUTINE CONT03
C     CONTROL MODULE FOR I-C4 BUILDUP IN THE SHELL ALKYLATION SIMULATION
C
C     EN VECTOR
C     1. EQUIPMENT NUMBER
C     2. STREAM NUMBER OF ORGANIC FEED TO THE REACTOR
C     3. NUMBER OF LOOPS BELOW THE ACCELERATION TOLERENCE (3)
C     4. MAXIMUM ABSOLUTE ACCELERATION OF I-C4 FROM LOOP TO LOOP (0.003)
C     5. STREAM NUMBER OF THE I-C4 FEED
C     9. LAST VALUE OF I-C4 TO THE REACTOR (SET BY PROGRAM)
C     10. PRESENT VALUE OF I-C4 TO THE REACTOR (SET BY PROGRAM)
C
C     NO INPUT OR OUTPUT STREAMS REQUIRED
C
C     *******MACSIM COMMON DECK, FOR ALKYLATION.  APR.30,1968. T.T.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
      COMMON AEN(4,102),ENC(50,20),NOPP,X,XMOLE(26),PPSC(17,26),PPMX(17)
      COMMON  SN(75,31), DELS(31), AA(1806), LOOP
      DIMENSION DIFF(10)
C
      CALL XDATA
      LOOP10 = LOOP + 10
      NFEED = EN(NE,2) + 0.1
      NLOOP = EN(NE,3) + 0.1
      NLOOP1 = NLOOP + 1
      EN(NE,9) = EN(NE,10)
      EN(NE,10) = SN(NFEED,15)
      AEN(1,LOOP10) = EN(NE,10) - EN(NE,9)
      IF(LOOP.LT.NLOOP1)  RETURN
      DELS10 = DELS(10)/2.0
      IF(AEN(1,LOOP10).LT.DELS10)  RETURN
C
      DO 20 M=1,NLOOP
      NN = LOOP10 + 1 - M
      MM = NN - 1
   20 DIFF(M) = AEN(1,NN) - AEN(1,MM)
C
      DO 60 M=1,NLOOP
   60 IF(ABS(DIFF(M)).GT.EN(NE,4))  RETURN
C
C
      NIC4 = EN(NE,5) + 0.1
      ADJUST = 1.0 - (AEN(1,LOOP10)/SN(NIC4,15))
      SN(NIC4,3) = 0.0
      DO 100 J=6,31
      SN(NIC4,J) = SN(NIC4,J)*ADJUST
  100 SN(NIC4,3) = SN(NIC4,3) + SN(NIC4,J)
      BB = -AEN(1,LOOP10)
      WRITE(6,9999) LOOP, BB
C
      RETURN
 9999 FORMAT(//  19H AT THE END OF LOOP, I4, 63H  THE TOTAL I-C4 FEED WA
     1S CHANGED TO ADJUST THE FEED OF I-C4 BY, F10.4 //)
      END
```

```
$IBFTC COSTER
      SUBROUTINE COSTER
C
C     WRITTEN BY I. SHAW   COSTING MODULE FOR SHELL ALKYLATION STUDY
C
C     EN VECTOR
C     1. EQUIPMENT NUMBER
C     2. LOCATION OF DENSITY FOR LIQUIDS (13)
C     3.
C     4. TEMPERATURE OF INLET COOLING WATER
C     6. COST IN DOLLARS PER 1000 POUNDS OF LOW PRESSURE (50 PSIG) STEAM
C     7. COST IN DOLLARS PER 1000 POUNDS OF 200 PSIG STEAM
C     8. COST IN DOLLARS PER MM B.T.U. OF  BIB  REBOILER FUEL GAS
C     9. COST IN DOLLARS PER K.W.H. OF ELECTRICTY
C     10. COST IN DOLLARS PER 1000 IMP. GALLONS OF COOLING WATER
C
C     AEN VECTOR
C     ALL COSTS ARE IN DOLLARS PER BARREL UNLESS OTHERWISE STATED
C     1. EQUIPMENT NUMBER
C     2. LENGTH OF AEN LIST
C     3. COST OF PROPANE IN THE ISO-BUTANE FEED
C     4. COST OF PROPENE IN THE ISO-BUTANE FEED
C     5. COST OF N-BUTANE IN THE ISO-BUTANE FEED
C     6. COST OF ISO-BUTANE IN THE ISO-BUTANE FEED
C     7. COST OF N-BUTENE IN THE ISO-BUTANE FEED
C     8. COST OF ISO-BUTENE IN THE ISO-BUTANE FEED
C     9. COST OF N-PENTANE IN THE ISO-BUTANE FEED
C     10. COST OF ISO-PENTANE IN THE ISO-BUTANE FEED
C     11. COST OF ISO-PENTENE IN THE ISO-BUTANE FEED
C     12.
C     13. COST OF PROPANE IN THE OLEFIN FEED
C     14. COST OF PROPENE IN THE OLEFIN FEED
C     15. COST OF N-BUTANE IN THE OLEFIN FEED
C     16. COST OF ISO-BUTANE IN THE OLEFIN FEED
C     17. COST OF N-BUTENE IN THE OLEFIN FEED
C     18. COST OF ISO-BUTENE IN THE OLEFIN FEED
C     19. COST OF N-PENTANE IN THE OLEFIN FEED
C     20. COST OF ISO-PENTANE IN THE OLEFIN FEED
C     21. COST OF ISO-PENTENE IN THE OLEFIN FEED
C     22.
C     23. VALUE IN DOLLARS PER BARREL OF 103 OCTANE(R-3) ALKYLATE
C     24. VALUE IN DOLLARS PER BARREL OF PRODUCT PROPANE
C     25. VALUE IN DOLLARS PER BARREL OF PRODUCT BUTANE
C     26. NET COST IN DOLLARS PER BARREL OF 99 PERCENT SULPHURIC ACID
C     27. COST IN DOLLARS PER 100 POUNDS OF CAUSTIC
C     28.
C     31. STREAM NUMBER OF ISO-BUTANE FEED
C     32. STREAM NUMBER OF OLEFIN FEED
C     33. STREAM NUMBER OF PRODUCT ALKYLATE
C     34. STREAM NUMBER OF PRODUCT LPG
C     35. STREAM NUMBER OF PRODUCT BUTANE
C     36. STREAM NUMBER OF ACID FEED
C     37. STREAM NUMBER OF DIB CAUSTIC
C     38. STREAM NUMBER OF DEPROP CAUSTIC
C     39. EQUIPMENT NUMBER OF THE ACID MAKE-UP MODULE
C     40. EQUIPMENT NUMBER OF DEPROP COLUMN
C     41. STREAM NUMBER OF THE LIQUID LEAVING THE PRODUCT SEPARATOR
C     42. STREAM NUMBER OF ORGANIC FEED TO REACTOR
C
```

```
C
C     ******* MACSIM COMMON DECK, FOR ALKYLATION.  T.T. APR.29,1968.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
      COMMON AEN(4,102),ENC(50,20),NOPP,X,XMOLE(26),PPSC(17,26),PPMX(17)
      COMMON SN(75,31),Q1(1336),TITLE(24),Q2(164),NEMAX,Q3(318),KRUN
C
      DIMENSION  FLOW(7), FLOWBC(7), COST(7), COSTBC(7)
      DIMENSION  UTILTY(5), UTLYBC(5), CSTUTL(5), CSTUBC(5)
      DIMENSION R3OCTN(14),REACHI(9), REACLO(9)
C
C     THE FLOWBC AND THE COSTBC VECTORS ARE THE BASE CASE FLOW AND COSTS
C      OF MATERIAL FOR A  24 HOUR DAY
C     THE UTLYBC AND THE CSTUBC VECTORS ARE THE BASE CASE FLOW AND COSTS
C      OF UTILITIES FOR A  24 HOUR DAY
C     THE R3OCTN VECTOR CONTAINS THE R-3 OCTANE NUMBER OF EACH COMPONENT
C      CONTAINING FIVE OR MORE CARBONS
      DATA FLOWBC / 1576., 3180., 1923., 839., 1552., 74., 11. /
      DATA COSTBC / 4857., 9132., 8114., 3020., 5464., 645., 39. /
      DATA UTLYBC / 84., 301., 510., 32928., 3077. /
      DATA CSTUBC / 32., 114., 144., 207., 34. /
      DATA R3OCTN / 83.2, 92.0, 97.0, 24.8, 109.9, 0.0, 95.5, 100.9,
     1              0.0, 113.9, 91.0, 115.5, 96.0, 96.0 /
      DATA REACHI / 245.6, 91.4, 609.1, 989.0, 52.5, 62.9, 100.0, 25.1,
     1              100.0 /
      DATA REACLO / 92.6, 59.6, 190.6, 634.2, 28.1, 39.1, 0.0, 6.7, 0.0/
C
      CALL XDATA
C
C     CALCULATE VALUF AND FLOW PER HOUR OF THE OLEFIN AND IC4 FEEDS
      AA = 7.481/42.
      NOPP = EN(NE,2)
      X = 60.0
      CALL PROCAL
      DO 20 III=1,2
      I = 10*III-14
      II = AEN(1,III+30)
      FLOW(III) = 0.0
      COST(III) = 0.0
      DO 15 J=7,15
      IJ = I+J
      JJ = J+5
      IF(SN(II,JJ).GT.0.01.AND.AEN(1,IJ).EQ.0.0)  WRITE(6,9983) J,II
      BB = SN(II,JJ)*AA/PPSC(NOPP,J)
      FLOW(III) = FLOW(III)+BB
   15 COST(III) = COST(III) +BB*AEN(1,IJ)
   20 CONTINUE
C
C     CALCULATE THE VALUE AND THE FLOW PER HOUR OF THE ALKYLATE STREAM
      II = AEN(1,33)
      FLOW(3) = 0.0
      OCTANN = 0.0
      DO 30 J=18,31
      FLOWW = SN(II,J)*AA/PPSC(NOPP,J-5)
      FLOW(3) = FLOW(3) + FLOWW
   30 OCTANN = R3OCTN(J-17)*FLOWW + OCTANN
      OCTANN = OCTANN/FLOW(3)
      DO 35 J=11,17
   35 FLOW(3) = FLOW(3) + SN(II,J)*AA/PPSC(NOPP,J-5)
```

```
      COST(3) = (AEN(1,23) + (OCTANN-103.)*0.05)*FLOW(3)
C
C     CALCULATE VALUE AND FLOW PER HOUR OF PROPANE AND BUTANE STREAMS
      AA = 7.481/42.
      NOPP = EN(NE,2)
      DO 50 III=4,5
      II = AEN(1,III+30)
      X = 60.0
      DO 45 I=1,NOCOMP
   45 XMOLE(I) = SN(II,I+5)
      CALL PROMIX(2)
      FLOW(III) = SN(II,3)*AA/PPMX(NOPP)
   50 COST(III) = FLOW(III)*AEN(1,III+20)
C
C     CALCULATE VALUE AND FLOW PER HOUR OF SULPHURIC ACID STREAM
C     ASSUME THAT THE ACID FEED IS 99 PERCENT ACID, IS AT 68 DEGREES F.
C      AND HAS A DENSITY OF 1.8342
      II = AEN(1,36)
      BB = SN(II,7)*98.1/0.99
      BB = BB/(62.4189*1.8342)
      FLOW(6) = BB*AA
      COST(6) = AEN(1,26)*FLOW(6)
C
C     CALCALATE VALUE AND FLOW PER HOUR OF TWO CAUSTIC STREAMS
      MM = AEN(1,37)
      NN = AEN(1,38)
      FLOW(7) = (SN(NN,8)+SN(MM,8))*(40.0/100.0)
      COST(7) = AEN(1,27)*FLOW(7)
C
C
C     SUM ALL UTILITY USAGES
      DO 200 I=1,5
  200 UTILTY(I) = 0.0
      DO 210 K=1,NEMAX
      IF(ENC(K,1).LT.0.1)  GO TO 210
      UTILTY(1) = UTILTY(1) + ENC(K,11)
      UTILTY(2) = UTILTY(2) + ENC(K,12)
      UTILTY(3) = UTILTY(3) + ENC(K,14)
      UTILTY(4) = UTILTY(4) + ENC(K,16)
      UTILTY(5) = UTILTY(5) + ENC(K,17)
  210 CONTINUE
      DO 220 I=1,5
  220 CSTUTL(I) = UTILTY(I)*EN(NE,I+5)
C
C     CHANGE COSTS AND FLOWS FROM HOURS TO DAYS
      TIME = 24.0
      DO 305 I=1,7
      FLOW(I) = FLOW(I)*TIME
  305 COST(I) = COST(I)*TIME
      DO 310 I=1,5
      UTILTY(I) = UTILTY(I)*TIME
  310 CSTUTL(I) = CSTUTL(I)*TIME
      WRITE(6,9999) KRUN, TITLE
      WRITE(6,9998) KRUN, KRUN
      WRITE(6,9997) FLOW(1), FLOWBC(1), COST(1), COSTBC(1)
      WRITE(6,9996) FLOW(2), FLOWBC(2), COST(2), COSTBC(2)
      WRITE(6,9995) FLOW(6), FLOWBC(6), COST(6), COSTBC(6)
      WRITE(6,9994) FLOW(7), FLOWBC(7), COST(7), COSTBC(7)
```

```
      WRITE(6,9993) FLOW(3), FLOWRC(3), COST(3), COSTRC(3)
      WRITE(6,9992) FLOW(4), FLOWRC(4), COST(4), COSTRC(4)
      WRITE(6,9991) FLOW(5), FLOWRC(5), COST(5), COSTRC(5)
      WRITE(6,9990) UTILTY(1), UTLYRC(1), CSTUTL(1), CSTURC(1)
      WRITE(6,9985) UTILTY(2), UTLYRC(2), CSTUTL(2), CSTURC(2)
      WRITE(6,9987) UTILTY(3), UTLYRC(3), CSTUTL(3), CSTURC(3)
      WRITE(6,9988) UTILTY(4), UTLYRC(4), CSTUTL(4), CSTURC(4)
      WRITE(6,9989) UTILTY(5), UTLYRC(5), CSTUTL(5), CSTURC(5)
      WRITE(6,9981)  OCTANN
C
      CSTERC = 15205.4
      RETERC = 1392.5
      B = 7.997
      E = 0.724
      CSTE = COST(1) + COST(2) + COST(6) + COST(7) + CSTUTL(1) +
     1       CSTUTL(2) + CSTUTL(3) + CSTUTL(4) + CSTUTL(5)
      RETE = COST(3) + COST(4) + COST(5) - CSTE
      A = CSTE/FLOW(3)
      D = RETE/FLOW(3)
      CSTDIF = CSTE - CSTERC
      RETDIF = RETE - RETERC
      C = A - B
      F = D - E
      WRITE(6,9980) KRUN
      WRITE(6,9979) CSTE, CSTERC, CSTDIF
      WRITE(6,9978) RETE, RETERC, RETDIF
      WRITE(6,9977) A, B, C
      WRITE(6,9976) D, E, F
C
C
C     CHECK CORRELATION AND EQUIPMENT LIMITATIONS
      WRITE(6,9970)
C
C
C
C     CHECK LIMITS OF REACTOR CORRELATION
      N = AFN(1,42)
      M = 0
      DO 1220 J=12,20
      L = J-11
      IF(SN(N,J).GE.REACLO(L))  GO TO 1210
      M = M+1
      IF(M.EQ.1)  WRITE(6,9966)
      WRITE(6,9965) REACLO(L), J, SN(N,J)
      GO TO 1220
 1210 IF(SN(N,J).LE.REACHI(L))  GO TO 1220
      M = M+1
      IF(M.EQ.1)  WRITE(6,9966)
      WRITE(6,9965) REACHI(L), J, SN(N,J)
 1220 CONTINUE
      IF(M.EQ.0)  WRITE(6,9964)
C
C     CONDENSER DUTY AND VAPOR VELOCITY IN DC2 COLUMN
      N = AFN(1,40)
      VEL = ENC(N,4)/3600.0
      CON = ENC(N,5)/1.0E06
      WRITE(6,9961) VEL
      WRITE(6,9960) CON
```

```
C
C     CHECK PRESSURE CONTROL ON THE PRODUCT SEPARATOR
      N = AEN(1,41)
      IF(SN(N,5).NE.17.7)  GO TO 1300
      WRITE(6,9959)
      GO TO 1310
 1300 WRITE(6,9958) SN(N,5)
 1310 CONTINUE
C
C     PRINT VALUES IN ACID MAKE-UP CIRCUIT
      N = AEN(1,39)
      A = EN(N,2)*100.0
      B = EN(N,4)*100.0
      C = EN(N,3)*100.0
      D = EN(N,11)*100.0
      WRITE(6,9957) A, B, C, D
C
      RETURN
C
 9957 FORMAT(////26H THE FRESH MAKE-UP ACID IS, F7.2,  47H PERCENT ACID.
     1  THE ACID FEED TO THE REACTOR IS, F5.1,  33H PERCENT OF THE TOTAL
     2 FLOW AND IS/ 40X, F7.2,   24H WEIGHT PERCENT ACID AND, F5.2,
     3 21H WEIGHT PERCENT WATER)
 9958 FORMAT(////45H THE PRODUCT SEPARATOR PRESSURE WAS RAISED TO, F6.2,
     1   70H FROM A BASE OF 17.70 PSIA TO CONTROL THE VAPOR LOAD TO THE
     2COMPRESSOR)
 9959 FORMAT(///113H THE PRODUCT SEPARATOR PRESSURE CONTROL WAS NOT REQU
     1IRED AND THE PRESSURE REMAINED AT THE BASE VALUE OF 17.7 PSIA)
 9960 FORMAT( 35H THE DC3 OVERHEAD CONDENSER DUTY IS,F6.2, 52H AND THE P
     1RESENT LIMIT IS 10.00 MILLION BTU PER HOUR)
 9961 FORMAT(//// 26H THE DC3 VAPOR VELOCITY IS, F6.2,  53H AND THE PRES
     1ENT LIMIT IS 13.00 CUBIC FEET PER SECOND)
 9964 FORMAT(///  58H NO CORRELATION LIMITS WERE EXCEEDED IN THE REACTOR
     1 MODULE//)
 9965 FORMAT( 25H THE CORRELATION LIMIT OF,F7.1,   25H IS EXCEEDED FOR S
     1TRMI(1,, I2, 10H) WHICH IS, F7.1)
 9966 FORMAT(/////  62H THE FOLLOWING LIMITS HAVE BEEN EXCEEDED IN THE R
     1EACTOR MODULE/)
 9970 FORMAT(1H1,  /// 20X,  92H S U M M A R Y     O F     P R O C E S S
     1     A N D     C O R R E L A T I O N     L I M I T S//)
 9976 FORMAT(20X, 35HPROFIT FUNCTION PER BBL OF ALKYLATE, F21.3, F19.3,
     1        F20.4)
 9977 FORMAT(20X,33HCOST FUNCTION PER BBL OF ALKYLATE,F23.3,F19.3,F20.4)
 9978 FORMAT(20X, 23HPROFIT FUNCTION PER DAY, F33.1, F19.1, F20.2)
 9979 FORMAT(20X, 21HCOST FUNCTION PER DAY, F35.1, F19.1, F20.2)
 9980 FORMAT(////   67X,  7HRUN NO., I4, 9X,  9HBASE CASE, 11X,  10HDIFF
     1ERENCE/)
 9981 FORMAT(///   9X, 52HTHE DEBUTANIZED R-3 OCTANE RATING OF THE ALKYL
     1ATE IS, F7.2)
 9983 FORMAT(1X, 49H**** NO COST VALUE HAS BEEN READ IN FOR COMPONENT,
     1I3, 11H  IN STREAM, I4, 36H  AND IT HAS BEEN TAKEN AS ZERO ****)
 9985 FORMAT(20X, 15HSTEAM(200 PSIG), 1X, 10H(1000 LBS), F21.0,F14.0,
     1F23.0,F14.0)
 9986 FORMAT(9X, 37HCHANGE IN OPERATING COST  =  (RUN NO ,I3, 5H) - (BA
     1SE CASE), / 35X, 1H=, F8.0)
 9987 FORMAT(20X, 4HFUEL, 14X, 8H(MM BTU), F21.0,F14.0,F23.0,F14.0)
 9988 FORMAT(20X, 11HELECTRICITY,11X,  4H(KW), F21.0,F14.0,F23.0,F14.0)
 9989 FORMAT(20X, 26HCOOLING WATER  (1000 GALS), F21.0,F14.0,F23.0,F14.0
```

```
     1)
9990 FORMAT(/9X, 25HUTILITIES  STEAM(50 PSIG), 2X, 10H(1000 LBS), F21.0
     1,F14.0,F23.0,F14.0)
9991 FORMAT(20X, 6HBUTANE, 14X, 6H(BBLS), F21.0,F14.0,F23.0,F14.0)
9992 FORMAT(20X, 7HPROPANE, 13X, 6H(BBLS), F21.0,F14.0,F23.0,F14.0)
9993 FORMAT(/9X, 19HPRODUCTS   ALKYLATE, 12X, 6H(BBLS), F21.0,F14.0,F23
     1.0,F14.0)
9994 FORMAT(20X, 7HCAUSTIC, 10X, 9H(100 LBS), F21.0,F14.0,F23.0,F14.0)
9995 FORMAT(20X, 14HSULPHURIC ACID, 6X, 6H(BBLS), F21.0,F14.0,F23.0,F14
     1.0)
9996 FORMAT(20X, 6HOLEFIN,14X, 6H(BBLS), F21.0,F14.0,F23.0,F14.0)
9997 FORMAT(9X, 5HFEEDS, 6X, 9HISOBUTANE,11X, 6H(BBLS),F21.0,F14.0,F23.
     10,F14.0)
9998 FORMAT(9X,28HSUMMARY  OF  MATERIAL  FLOWS, 25X, 20HQUANTITY  PER
     1DAY   , 18X, 16HVALUE  PER DAY  /  59X, 7HRUN NO ,I3, 14H    BASE
     2CASE, 13X, 7HRUN NO , I3, 13H    BASE CASE, /)
9999 FORMAT(1H1,//,41X,47H O P E R A T I N G   C O S T   S U M M A R
     1 Y,///,8X,12H RUN NUMBER ,  I3,  //, 8X, 11H CONDITIONS,//
     219X,12A6/19X,12A6//)
      END
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$IBFTC DEPRP2
      SUBROUTINE DEPRP2
C     WRITTEN BY ALAN G. BROWN
C     REVISED BY I. SHAW
C     WRITTEN TO DESCRIBE THE DEPROPANIZER AT SHELL OAKVILLE
C     ******* MACSIM COMMON DECK, FOR ALKYLATION.  T.T. APR.29,1968.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
      COMMON AEN(4,102),FNC(50,20),NOPP,X,XMOLE(26),PPSC(17,26),PPMX(17)
      DIMENSION AK(4),A(4)
C
C     EQUIPMENT VECTOR
C     1. EQUIPMENT NO.
C     2. NO. OF IDEAL STAGES (USUALLY 30)
C     3. FRACTION OF PROPANE IN FEED GOING OVERHEAD (ABOUT 0.86)
C     4. OUTLET TEMPERATURE OF COOLING WATER (ABOUT 120 DEGREES F.)
C     5. LOCATION OF SPECIFIC HEAT IN PHYSICAL PROPERTY PACKAGE
C     6. THE NUMBER OF THE COSTING MODULE
C     7. MOLE FRACTION OF PROPANE IN DISTILLATE (.98 - .99)
C     8.  ENTHALPY CHANGE OF 200 PSIG STEAM IN BTU (847.0)
C     9. REFLUX RATIO (CALCULATED BY PROGRAM)
C     10. MINIMUM REFLUX RATIO (CALCULATED BY PROGRAM)
C
C     ENC VECTOR
C     4. VAPOR VELOCITY IN CUBIC FEET PER HOUR (CALCULATED BY PROGRAM)
C     5. OVERHEAD CONDENSER DUTY (CALCULATED BY THE PROGRAM)
C
      JJ = NOCOMP + 5
      STRMO(1,4) = 75.0
      STRMO(1,5) = 274.7
      STRMO(1,6) = STRMI(1,6)
      STRMO(1,7) = 0.0
      STRMO(1,8) = 0.0
      STRMO(1,9) = 0.0
      STRMO(1,10) = 0.0
      STRMO(1,11)=STRMI(1,11)
      STRMO(1,13)=STRMI(1,13)
      STRMO(1,16)=0.0
      STRMO(1,17)=0.0
      DO 24  I= 19,JJ
24    STRMO(1,I)= 0.0
      STRMO(2,5)= 290.27
      STRMO(2,6) = 0.0
      STRMO(2,7) = STRMI(1,7)
      STRMO(2,8) = STRMI(1,8)
      STRMO(2,9) = STRMI(1,9)
      STRMO(2,10) = STRMI(1,10)
      STRMO(2,11)=0.0
      STRMO(2,13)=0.0
      STRMO(2,16)=STRMI(1,16)
      STRMO(2,17)=STRMI(1,17)
      DO 27 I = 19,JJ
27    STRMO(2,I)= STRMI(1,I)
C
      T = STRMI(1,4)
      SUMI = STRMI(1,12) + STRMI(1,14) + STRMI(1,15) + STRMI(1,18)
      X1 = STRMI(1,12)/SUMI
      X2 = STRMI(1,14)/SUMI
      X3 = STRMI(1,15)/SUMI
C     AK(I) ARE VAPOR-LIQUID EQUILIBRIUM CONSTANTS
```

```
      AK(1) = -0.20045E01 + (0.26305E-01 - 0.428411E-04*T)*T
      AK(2) = -0.90955E00 + (0.91334E-02 - 0.20431E-07*T*T)*T
      AK(3) = -0.11554E01 + (0.11935E-01 - 0.410412E-07*T*T)*T
      AK(4) = -0.493020E00 + 0.43972E-02*T
C     A(J) IS THE RELATIVE VOLITILITY
      DO 18 J = 1,4
18    A(J) = AK(J)/AK(3)
      SUMO1 = ((STRMI(1,12)*EN(NE,3))/(EN(NE,7)*STRMI(1,3)))*SUMI
      XX1 = EN(NE,7)
      STRMO(1,12) = XX1*SUMO1
C     AS A FIRST APPROXIMATION ASSUME ONLY C3 AND IC4 IN DISTILLATE
      XX3 = 1.0 - XX1
      STRMO(1,15) = XX3*SUMO1
      STRMO(2,12) = STRMI(1,12) - STRMO(1,12)
      STRMO(2,15) = STRMI(1,15) - STRMO(1,15)
      SUMO2 = SUMI - SUMO1
      XXX1 = STRMO(2,12)/SUMO2
      XXX3 = STRMO(2,15)/SUMO2
      AAA = A(1)/A(3)
      RR = STRMO(2,12)/STRMO(1,12)
C
C     STAGMN IS THE MIN. NO. OF STAGES OBTAINED FROM THE FENKE EQUATION
C     (I. AND E. C., V24, NO.5 P. 482-5)
      STAGMN = (ALOG(XX1*XXX3/(XX3*XXX1)))/ALOG(AAA)
      STRMO(1,14) = STRMI(1,14)/((((A(1)/A(2))**STAGMN)*RR) + 1.0)
      STRMO(1,15) = STRMI(1,15)/((((A(1)/A(3))**STAGMN)*RR) + 1.0)
      STRMO(1,18) = STRMI(1,18)/((((A(1)/A(4))**STAGMN)*RR) + 1.0)
      DDD = STRMO(1,14) + STRMO(1,15) + STRMO(1,18)
      CCC = (SUMO1 - STRMO(1,12))/DDD
      STRMO(1,14) = STRMO(1,14)*CCC
      STRMO(1,15) = STRMO(1,15)*CCC
      STRMO(1,18) = STRMO(1,18)*CCC
      STRMO(2,14) = STRMI(1,14) - STRMO(1,14)
      STRMO(2,15) = STRMI(1,15) - STRMO(1,15)
      STRMO(2,18) = STRMI(1,18) - STRMO(1,18)
      STRMO(1,3)=0.0
      STRMO(2,3)=0.0
      DO 22 I=6,31
      STRMO(1,3)=STRMO(1,3)+STRMO(1,I)
22    STRMO(2,3)=STRMO(2,3)+STRMO(2,I)
C
C     RMN IS THE MIN. REFLUX RATIO OBTAINED FROM THE FENKE EQUATION
C      (I. AND E.C., V24 ,NO5 P.482)
C     R IS THE REFLUX RATIO OBTAINED BY LINEARIZING A PORTION OF THE
C     GILLILAND PLOT
      RMN = (XX1/X1 - AAA*XX3/X3)/(AAA - 1.0)
      STAG = (EN(NE,2) - STAGMN)/(EN(NE,2) + 1.0)
      R = (1.0 + 1.16*RMN - 1.7*STAG)/(1.7*STAG + .16)
      EN(NE,9) = R
      EN(NE,10) = RMN
C
C     HEAT BALANCE TO CALCULATE THE BOTTOMS TEMPERATURE
      QCOND= 1000.*(0.123966E04+ 0.105203E04*R)
      QREB= 1000.*(0.105620E04*R + 0.152164E04)
      NCOST = EN(NE,6)
      W = QCOND/(EN(NE,4)-EN(NCOST,4))
      ENC(NE,17)= W/10000.
      ENC(NE,12) = QREB/(EN(NE,8)*1000.)
```

```
      NOPP = EN(NE,5)
      X = STRMI(1,4)
      DO 100 J = 1,NOCOMP
 100  XMOLE(J) = STRMI(1,J+5)
      CALL PROMIX(1)
      QFEED =           PPMX(NOPP)*X
      X = STRMO(1,4)
      DO 101 J = 1,NOCOMP
101   XMOLE(J)= STRMO(1,J+5)
      CALL PROMIX(1)
      QDIST =           PPMX(NOPP)*X
      QBOT = QFEED + QREB - QCOND -QDIST
      X = 230.
      DO 102 J = 1,NOCOMP
102   XMOLE (J) = STRMO(2,J+5)
      CALL PROMIX(1)
      STRMO(2,4) = QBOT/PPMX(NOPP)
C     CALCULATE THE VAPOR FLOW AT THE TOP OF THE COLUMN ASSUMING PROPANE
C      AT 128 DEGREES F. , 280.7 PSIA, AND COMPRESSABILITY OF 0.675
      ENC(NE,4) = (R+1.0)*0.675*STRMO(1,3)*10.73*(128.+460.)/280.7
      ENC(NE,5) = QCOND
C
      RETURN
      END
```

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$IBFTC DISOB1
      SUBROUTINE DISOB1
C     WRITTEN BY I. SHAW AUGUST 1968
C     APPROXIMATE MODEL OF THE DIB COLUMN IN THE SHELL ALKYLATION STUDY
C
C     EN VECTOR
C     1. EQUIPMENT NUMBER
C     2. FRACTION OF INPUT N-C4 REMOVED IN SIDE CUT (0.55 - 0.65)
C     3. MOLE FRACTION I-C4 IN SIDE CUT (0.02 - 0.04)
C     4. FRACTION OF INPUT N-C4 OLEFIN LEAVING IN OVERHEAD (ABOUT 0.70)
C     5. FRACTION OF INPUT I-C4 OLEFIN LEAVING IN OVERHEAD (ABOUT 0.90)
C     6. FRACTION OF INPUT N-C5 LEAVING IN SIDE CUT (ABOUT 0.30)
C     7. FRACTION OF INPUT I-C5 LEAVING IN SIDE CUT (ABOUT 0.50)
C     8. FRACTION OF INPUT I-C5 OLEFIN LEAVING IN SIDE CUT (ABOUT 0.45)
C     9. MOLE FRACTION N-C4 IN THE ALKYLATE (ABOUT 0.10)
C
C     ENC VECTOR
C     1. EQUIPMENT NUMBER
C     4. OUTLET TEMPERATURE OF COOLING WATER (104.)
C     5. EQUIPMENT NUMBER OF COSTING MODULE
C     6. MAXIMUM ALLOWABLE REFLUX RATIO (CALCULATED BY THE PROGRAM)
C     7. LOCATION OF COX CHART RATIOS IN PHYSICAL PROPERTIES (6)
C     8. FRACTIONAL EFFICIENCY OF REFLUX COALESER (ABOUT 0.9)
C
C     ********MACSIM COMMON DECK, FOR ALKYLATION.  APR.30,1968. T.T.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
      COMMON AEN(4,102),ENC(50,20),NOPP,X,XMOLE(26),PPSC(17,26),PPMX(17)
C
C
      STRMO(1,4) = 80.
      STRMO(2,4) = 168.
      STRMO(3,4) = 381.
C
      STRMO(1,5) = 111.7
      STRMO(2,5) = 126.7
      STRMO(3,5) = 133.7
C
      STRMO(1,6) = 0.0
      STRMO(2,6) = 0.0
      STRMO(3,6) = 0.0
C
      DO 20 K=7,10
      STRMO(1,K) = 0.0
      STRMO(2,K) = 0.0
   20 STRMO(3,K) = STRMI(1,K)
C
      DO 40 K=11,13
      STRMO(1,K) = STRMI(1,K)
      STRMO(2,K) = 0.0
   40 STRMO(3,K) = 0.0
C
C     SET SOME OF THE N-C4 AND I-C4 FLOWS
      STRMO(1,14) = 0.0
      STRMO(2,14) = STRMI(1,14)*EN(NE,2)
      STRMO(3,14) = 0.0
      STRMO(1,15) = 0.0
      STRMO(2,15) = 0.0
      STRMO(3,15) = 0.0
C
```

```
      STRMO(1,16) = STRMI(1,16)*EN(NE,4)
      STRMO(2,16) = STRMI(1,16) - STRMO(1,16)
      STRMO(3,16) = 0.0
C
      STRMO(1,17) = STRMI(1,17)*EN(NE,5)
      STRMO(2,17) = STRMI(1,17) - STRMO(1,17)
      STRMO(3,17) = 0.0
C
      STRMO(1,18) = 0.0
      STRMO(2,18) = STRMI(1,18)*EN(NE,6)
      STRMO(3,18) = STRMI(1,18) - STRMO(2,18)
C
      STRMO(1,19) = 0.0
      STRMO(2,19) = STRMI(1,19)*EN(NE,7)
      STRMO(3,19) = STRMI(1,19) - STRMO(2,19)
C
      STRMO(1,20) = 0.0
      STRMO(2,20) = STRMI(1,20)*EN(NE,8)
      STRMO(3,20) = STRMI(1,20) - STRMO(2,20)
C
      DO 80 K=21,31
      STRMO(1,K) = 0.0
      STRMO(2,K) = 0.0
   80 STRMO(3,K) = STRMI(1,K)
C
      STRMO(1,3) = 0.0
      STRMO(2,3) = 0.0
      STRMO(3,3) = 0.0
      DO 200 J=6,31
      STRMO(1,3) = STRMO(1,3) + STRMO(1,J)
      STRMO(2,3) = STRMO(2,3) + STRMO(2,J)
  200 STRMO(3,3) = STRMO(3,3) + STRMO(3,J)
C
C     SET OUTLET FLOWS OF N-C4 AND I-C4
      STRMO(3,14) = (STRMO(3,3)/(1.0-EN(NE,9))) - STRMO(3,3)
      STRMO(3,3) = STRMO(3,3) + STRMO(3,14)
      STRMO(2,15) = (STRMO(2,3)/(1.0-EN(NE,3))) - STRMO(2,3)
      STRMO(2,3) = STRMO(2,3) + STRMO(2,15)
      STRMO(1,14) = STRMI(1,14) - (STRMO(2,14)+STRMO(3,14))
      STRMO(1,15) = STRMI(1,15) - (STRMO(2,15)+STRMO(3,15))
      STRMO(1,3) = STRMO(1,3) + STRMO(1,14) + STRMO(1,15)
C
C     CALCULATE CONDENSER AND REBOILER DUTY ON THE BASIS THAT THE COLUMN
C      IS RUN AT THE MAXIMUM OVERHEAD CONDENSER RATE OF 19 MM BTU/HOUR
      DO 500 J=1,NOCOMP
  500 XMOLE(J) = STRMO(1,J+5)
      TTT = ((STRMO(1,4)-32.0)/1.8) + 273.0
      H2OLAM = (1187.219-0.0015735*TTT*TTT)*18.016
      NOPP = ENC(NE,7)
      CALL PROMIX(1)
      RMAX = (19.0E+06/(H2OLAM*PPMX(NOPP))) - 1.0
      ENC(NE,6) = RMAX
      DO 510 J=1,NOCOMP
  510 XMOLE(J) = STRMO(2,J+5)
      TTT = ((STRMO(2,4)-32.0)/1.8) + 273.0
      H2OLAM = (1187.219-0.0015735*TTT*TTT)*18.016
      NOPP = ENC(NE,7)
      CALL PROMIX(1)
```

```
      SIDCUT = H2OLAM*PPMX(NOPP)
      ENC(NE,14) = (19.0E+06+SIDCUT)/1.0E+06
      NN = ENC(NE,5) + 0.1
      ENC(NE,17) = (19.0E+06+SIDCUT)/(1000.0*10.0*(ENC(NE,4)-EN(NN,4)))
C
C
C     CALCLATE FLOWS OF WATER AS CHANGED BY REFLUX CONDENSER
      DO 300 J=1,NOCOMP
  300 XMOLE(J) = STRMO(1,J+5)
      X = STRMO(1,4)
      CALL FSOL(FSOLW)
      STRMO(1,6) = FSOLW + (STRMI(1,6)-FSOLW)/(ENC(NE,8)*RMAX+1.0)
      STRMO(4,3) = STRMI(1,6) - STRMO(1,6)
      STRMO(4,4) = STRMO(1,4)
      STRMO(4,5) = STRMO(1,5)
      STRMO(4,6) = STRMO(4,3)
      DO 320 J=7,31
  320 STRMO(4,J) = 0.0
C
      RETURN
      END
```

```
$IBFTC DIST01
C
C
C     SUBROUTINE DIST01  (DISTILLATION - SIMPLE MODULE)
C     REVISED BY T. TOONG      FEB.20.1968
C     *THIS MODEL PERMITS SETTING OF FRACTIONS OF FEED COMPONENTS TO BE
C     *TAKEN OFF AS OVERHEAD STREAM (1ST OUTPUT STREAM), SIDE STREAM
C     *(2ND) AND BOTTOM STREAM (3RD)
C
C
C     *ONE INPUT STREAM AND THREE OUTPUT STREAMS
C     *MAXIMUM NUMBER OF FLOW COMPONENTS IS 26
C
C
C     EQUIPMENT VECTOR -
C     1. EQUIPMENT NUMBER
C     2. SPECIFIED OVERHEAD STREAM TEMPERATURE, DEG F
C     3. SPECIFIED SIDE STREAM TEMPERATURE, DEG F
C     4. SPECIFIED BOTTOM STREAM TEMPERATURE, DEG F
C     5. SPECIFIED COLUMN PRESSURE, PSIA
C
C
C     EQUIPMENT CONTROL VECTOR (OPTIONAL) -
C     1. EQUIPMENT NUMBER
C     2. FLAG
C     3. LENGTH OF EN LIST (FOR PRINTING)
C
C
C     STREAM VECTOR -
C     1. STREAM NUMBER
C     2. STREAM FLAG
C     3. TOTAL FLOW,LB MOLES/HR
C     4. TEMPERATURE, DEG F
C     5. PRESSURE,PSIA
C     6. FLOW OF COMPONENT 1, LB MOLE/HR
C     7. ETC.
C
C
C     STREAM CONTROL VECTOR - NOT REQUIRED
C
C
C     ADDITIONAL EQUIPMENT VECTOR -
C     1. EQUIPMENT NUMBER
C     2. LENGTH OF AEN VECTOR
C     3. TO 5. (BLANK)
C     6.,7.,8.,.....  FRACTIONS OF ALL THE FEED COMPONENTS IN OVERHEAD
C                     STREAM, FOLLOWED BY FRACTIONS OF ALL THE FEED
C                     COMPONENTS IN SIDESTREAM
C
C
C
C
      SUBROUTINE DIST01
C     *********MACSIM COMMON DECK, FOR ALKYLATION.  APR.30.1968. T.T.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,21),STRMO(5,21),FN(50,20)
      COMMON AEN(4,102),ENC(50,20),NODP,X,XMOLE(26),PRSC(17,26),PRMX(17)
C     ******************************************************************
      CALL XDATA
C     CALCULATING FLOWS IN THE OUTPUT STREAMS
```

```
      DO 1 I=1,NOUT
    1 STRMO(I,3)= 0.
      JJ= 5+NOCOMP
      DO 2 J= 6,JJ
      J1= J+NOCOMP
      STRMO(1,J)= STRMI(1,J)*AEN(1,J)
      STRMO(2,J)= STRMI(1,J)*AEN(1,J1)
      STRMO(3,J)= STRMI(1,J)-STRMO(1,J)-STRMO(2,J)
      DO 2 I=1,NOUT
    2 STRMO(I,3)= STRMO(I,3)+STRMO(I,J)
C     SETTING TEMPERATURES AND PRESSURES OF OUTPUT STREAMS
      DO 10 I=1,NOUT
   10 STRMO(I,4)= EN(NE,I+1)
      DO 11 I=1,NOUT
   11 STRMO(I,5)= EN(NE,5)
      RETURN
      END
```

```
$IBFTC EXCH11
      SUBROUTINE EXCH11
C     REVISED BY   I. SHAW   JANUARY 1968
C
C     THE PROBRAM CALCULATES THE OUTLET TEMPERATURE DIRECTLY FOR
C      8 TYPES OF HEAT EXCHANGERS USING EFFECTIVENESS FACTORS
C     THE PRODUCT OF THE AREA AND THE HEAT TRANSFER COEFF. IS READ IN
C
C     STRMI(1,1) IS THE INLET TO THE TUBE SIDE
C     STRMI(2,1) IS THE INLET TO THE SHELL SIDE
C     UA IS THE THERMAL CONDUCTANCE OF THE EXCHANGER
C     Z IS THE EFFECTIVENESS FACTOR FOR THE EXCHANGER
C     CMAX IS THE LARGER OF THE TWO THERMAL CAPACITANCES
C     CMIN IS THE SMALLER OF THE TWO THERMAL CAPACITANCES
C
C     EN VECTOR
C     1.0 EQUIPMENT NUMBER
C     2.0 UA
C     3.0 EXCHANGER TYPE
C       -COUNTERCURRENT                                          1.0
C       -PARALLEL                                                2.0
C       -CROSSFLOW, BOTH STREAMS UNMIXED                         3.0
C       -CROSSFLOW, BOTH STREAMS MIXED                           4.0
C       -CROSSFLOW, STREAM CMIN UNMIXED                          5.0
C       -CROSSFLOW, STREAM CMAX UNMIXED                          6.0
C       -PARALLELCOUNTER FLOW WITH N SHELL PASSES                7.0
C       -CONDENSING OR EVAPORATING SYSTEM                        8.0
C     4.0 NUMBER OF SHELL PASSES IF PARALLELCOUNTER FLOW
C     5.0 FOR CONDENSING OR EVAPORATING SYSTEM
C       -FLUID CONDENSING OR EVAPORATING ON TUBE SIDE            1.0
C       -FLUID CONDENSING OR EVAPORATING ON SHELL SIDE           2.0
C     6. LOCATION OF HEAT CAPACITY COEFFICIENTS FOR FLUID IN TUBE SIDE
C     7. LOCATION OF HEAT CAPACITY COEFFICIENTS FOR FLUID IN SHELL SIDE
C
C     ******* MACSIM COMMON DECK, FOR ALKYLATION.  T.T. APR.29,1968.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
      COMMON AEN(4,102),ENC(50,20),NOPP,X,XMOLE(26),PPSC(17,26),PPMX(17)
      DIMENSION TAVE(2),CP(2)
C
C
      IF(STRMI(1,3).LT.0.1.OR.STRMI(2,3).LT.0.1)  GO TO 103
      NTYPE = EN(NE,3)+0.001
      UA= EN(NE,2)
      IF(NTYPE.EQ.8) GO TO 80
  600 DO 2 KK=1,2
      TAVE(KK) = (STRMI(KK,4)+STRMO(KK,4))/2.
      X = TAVE(KK)
      NOPP = EN(NE,KK+5)
      DO 1 J=1,NOCOMP
    1 XMOLE(J) = STRMI(KK,J+5)
      CALL PROMIX(1)
    2 CP(KK) = PPMX(NOPP)
      IF(STRMI(1,4).LT.STRMI(2,4))  GO TO 3
      CH = CP(1)
      CC = CP(2)
      THIN= STRMI(1,4)
      TCIN= STRMI(2,4)
      GO TO 4
    3 CH = CP(2)
```

```
      CC = CP(1)
      THIN= STRMI(2,4)
      TCIN= STRMI(1,4)
    4 IF((CC-CH).LE.0.0) GO TO 5
      GO TO 6
    5 CMIN= CC
      CMAX= CH
      GO TO 7
    6 CMIN= CH
      CMAX= CC
C
    7 GO TO(10,20,30,40,50,60,70,80), NTYPE
C
   10 X=(1.0-CMIN/CMAX)
      Y= EXP(-(UA*X)/CMIN)
      Z = (1.-Y)/(1.-(CMIN*Y/CMAX))
      GO TO 90
   20 Z = (1.-EXP((-UA/CMIN)*(1.+(CMIN/CMAX))))/(1.+(CMIN/CMAX))
      GO TO 90
   30 X=(CMIN/UA)**0.22
      Y=(UA*CMIN*X)/(CMIN*CMAX)
      Z = 1.-EXP((EXP(-Y)-1.)*(CMAX/(CMIN*X)))
      GO TO 90
   40 X=UA/CMIN
      Y=UA/CMAX
      Z = X/((X/(1.-EXP(-X)))+(Y/(1.-EXP(-Y)))-1.)
      GO TO 90
   50 X=CMIN/CMAX
      Y=UA/CMIN
      Z = (1.-EXP(-X*(1.-EXP(-Y))))/X
      GO TO 90
   60 Z = 1.-EXP(-(CMAX/CMIN)*(1.-EXP(-UA/CMAX)))
      GO TO 90
   70 X= CMIN/CMAX
      Y= SQRT(1.0+X**2.0)
      S= UA/CMIN
      E = 2./(1.+X+Y*((1.+EXP(-S*Y))/(1.-EXP(-S*Y))))
      IF(X.EQ.1.0) GO TO 78
      R = ((1.-E*X)/(1.-E))**EN(NE,4)
      Z= (R-1.0)/(R-X)
      GO TO 90
   78 Z = (E*EN(NE,4))/(1.+(EN(NE,4)-1.)*E)
      GO TO 90
   80 MM = EN(NE,5)+0.001
      NN = 1
      IF(MM.EQ.1) NN=2
   83 TAVG = (STRMI(NN,4) + STRMO(NN,4))/2.
      X = TAVG
      NOPP = EN(NE,NN+5)
      DO 84 J=1,NOCOMP
   84 XMOLE(J) = STRMI(NN,J+5)
      CALL PROMIX(1)
      Z = 1. - EXP(-UA/PPMX(NOPP))
      STRMO(MM,4) = STRMI(MM,4)
      STRMO(NN,4) = STRMI(NN,4)-Z*(STRMI(NN,4)-STRMI(MM,4))
      IF(ABS(TAVG - (STRMO(NN,4)+STRMI(NN,4))/2.).LT.5.)   GO TO 108
      GO TO 83
C
```

```
 90 THOT= THIN-(Z*CMIN*(THIN-TCIN)/CH)
    TCOLD= TCIN+(Z*CMIN*(THIN-TCIN)/CC)
    IF(STRMI(1,4).GT.STRMI(2,4))  GO TO 91
    STRMO(1,4)= TCOLD
    STRMO(2,4)= THOT
    GO TO 92
 91 STRMO(1,4)= THOT
    STRMO(2,4)= TCOLD
 92 AVE1= (STRMO(1,4)+ STRMI(1,4))/2.0
    AVE2 = (STRMO(2,4) + STRMI(2,4))/ 2.0
    YY = ABS(AVE2-TAVE(2))
    ZZ = ABS(AVE1-TAVE(1))
    IF(YY.LT.5..AND.ZZ.LT.5.)  GO TO 108
    GO TO 600
C
103 STRMO(1,4)= STRMI(1,4)
    STRMO(2,4)= STRMI(2,4)
    WRITE(6,105) NE
105 FORMAT(//22H ***** BYPASS MODULE   , I4,39H    BECAUSE OF NO FLOW C
   1ONDITIONS *****)
108 JJ = NOCOMP+5
    DO 109 K=1,2
    STRMO(K,3) = STRMI(K,3)
    DO 109 J=5,JJ
109 STRMO(K,J) = STRMI(K,J)
    RETURN
    END
```

```
$IBFTC EXCH14
      SUBROUTINE EXCH14
C                             IAN SHAW  JANUARY 1968
C
C     THIS MODEL PREDICTS THE VAPOUR AND LIQUID COMPOSITION AND THE
C       OUTLET TEMPERATURE OF A LIQUID STREAM TO BE PARTIALLY OR
C       FULLY FLASHED IF THE PRESSURE AFTER FLASHING IS SPECIFIED
C     FLASHING OCCURES IN THE SHELL BUT THE HOT FLUID IN THE TUBES
C       UNDERGOES NO PHASE CHANGE
C     THE UA FOR THE EXCHANGER IS READ IN AND IS NOT CALCULATED
C     AN ADDITIONAL POSITIVE OR NEGATIVE HEAT LOAD TO THE STREAM BEING
C       FLASHED CAN BE ADDED FROM THE EN VECTOR. THE STRATCO REACTOR
C       HEAT LOAD IS ADDED TO THE PRODUCT SEPARATOR FEED IN THIS MANNER
C
C     STRMI(1,J) IS THE LIQUID INPUT TO BE FLASHED
C     STRMI(2,J) IS THE STREAM TO THE HEAT EXCHANGER TUBES
C     STRMO(1,J) IS THE VAPOUR STREAM AFTER FLASHING
C     STRMO(2,J) IS THE LIQUID STREAM AFTER FLASHING
C     STRMO(3,J) IS THE STREAM FROM THE HEAT EXCHANGER TUBES
C
C     EN VECTORS
C     1. EQUIPMENT NUMBER
C     2. UA FOR THE HEAT EXCHANGER
C     3. INITIAL PRESSURE AT WHICH FLASHING CALCULATION IS DONE
C     4. PRESSURE AT WHICH EQUILIBRIUM CONSTANTS WERE EVALUATED
C     5. ADDITIONAL HEAT INPUT IN B.T.U./HOUR IF REQUIRED
C     6. INITIAL TEMPERATURE USED IN SEARCH FOR THE FLASH TEMPERATURE
C     7. FINAL FLASHING PRESSURE (CHANGED IN CONTROL MODULE)
C     8. PRINT SWITCH SET AT 0.0 TO SUPRESS PRINT IN TEMPERATURE SEARCH
C
C     ENC VECTORS
C     1. EQUIPMENT NUMBER
C     2. EQUIPMENT IDENTIFIER
C     3. LENGTH OF EN LIST TO BE PRINTED
C     4. LOCATION OF HEAT CAPACITIES FOR LIQUIDS
C     5. LOCATION OF COX CHART RATIOS
C     6. LOCATION OF EQUILIBRIUM CONSTANTS AT 18 PSIA
C     7. LOCATION OF HEAT CAPACITIES FOR FLUID IN EXCHANGER TUBES
C
C     ******* MACSIM COMMON DECK, FOR ALKYLATION.  T.T. APR.29,1968.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
      COMMON AEN(4,102),ENC(50,20),NOPP,X,XMOLE(26),PPSC(17,26),PPMX(17)
      DIMENSION XX(26)
      DIMENSION DIF(20), TDIF(20)
      NITMAX = 20
C     XX(J)  MUST BE DIMENSIONED AT LEAST AS LARGE AS  NOCOMP
C     DIF(J)  AND  TDIF(J)  MUST BE DIMENSIONED TO NITMAX
C
C
      TOL1 = 0.0001
      TOL2 = TOL1*100.0
C
C     CALCULATE THE INPUT ENTHALPY ABOVE 32 DEGREES F.
C     ENTHI1 IS THE INPUT ENTHALPY OF STRMI(1) ABOVE 32 DEGREES F.
C     ENTHI2 IS THE INPUT ENTHALPY OF STRMI(2) ABOVE 32 DEGREES F.
      X = STRMI(1,4)
      NOPP = ENC(NE,4)
      DO 3 J=1,NOCOMP
    3 XMOLE(J) = STRMI(1,J+5)
```

```
      CALL PROMIX(1)
      ENTHI1 = PPMX(NOPP)*(STRMI(1,4)-32.)
      IF(STRMI(2,3).GT.0.01)  GO TO 4
      ENTHI2 = 0.0
      ENTHO3 = 0.0
      GO TO 8
    4 X = STRMI(2,4)
      NOPP = ENC(NE,7)
      DO 6 J=1,NOCOMP
    6 XMOLE(J) = STRMI(2,J+5)
      CALL PROMIX(1)
      ENTHI2 = PPMX(NOPP)*(STRMI(2,4)-32.)
    8 HIN = ENTHI1 + ENTHI2 + EN(NE,5)
C     HIN IS THE TOTAL INPUT ENTHALPY ABOVE 32 DEGREES F. INCLUDING
C     ANY ADDITIONAL HEAT IN FROM EN(NE,5)
C
C     CALCULATE THE OUTPUT STREAMS FOR A GIVEN TEMPERATURE
C     THE FIRST TEMPERATURE GUESS FOR THE CURVE FIT IS EN(NE,6)
      TFLASH=EN(NE,6)
      TDIF(1)=TFLASH
      DO 10 J=1,NOCOMP
   10 XX(J) = STRMI(1,J+5)/STRMI(1,3)
C     XX(J) IS THE MOLE FRACTION OF J IN THE STREAM WHICH IS FLASHED
      ADJUST = EN(NE,4)/EN(NE,3)
      NTEMP=0
   20 NTEMP = 1 + NTEMP
      X = TFLASH
      NOPP = ENC(NE,6)
      CALL PROCAL
      DO 23 J = 1,NOCOMP
   23 PPSC(NOPP,J) = PPSC(NOPP,J)*ADJUST
C     PSI=(MOLAL LIQUID FLOW RATE AFTER FLASHING)/(MOLAL FEED FLOW RATE)
C     FPSI=FUNCTION OF PSI
C     FPPSI=FIRST DERIVATIVE OF FPSI
      PSI=1.0
      DO 40 K=1,40
      FPSI=-1.0
      FPPSI=0.0
      DO 35 J=1,NOCOMP
      A = 1.-1./PPSC(NOPP,J)
      B = 1.-A*PSI
      FPSI = XX(J)/B + FPSI
   35 FPPSI = XX(J)*A/(B*B) + FPPSI
      PSIN=PSI-FPSI/FPPSI
      IF(PSIN.LT.0.0)   PSIN = 0.0
      IF(PSIN.GT.1.0)   PSIN = 1.0
      IF(ABS(PSIN-PSI).LE.0.001)  GO TO 45
      PSI = PSIN
   40 CONTINUE
   45 V=STRMI(1,3)*(1.-PSIN)
      FLOWLL=STRMI(1,3)-V
      IF(EN(NE,8).GT.0.5)  WRITE(6,988) FLOWLL, V, X
C     V = TOTAL MOLES OF VAPOUR AFTER FLASHING
C     FLOWLL= TOTAL MOLES OF LIQUID AFTER FLASHING
C     CALCULATE COMP. OF OUT VAPOUR STREAM(1) AND OUT LIQUID STREAM(2)
      SUM = 0.0
      DO 50 J=1,NOCOMP
      STRMO(1,J+5) = V*XX(J)/(1.-PSIN*(1.-1./PPSC(NOPP,J)))
```

```
      SUM=SUM+STRMO(1,J+5)
   50 STRMO(2,J+5)= STRMI(1,J+5)- STRMO(1,J+5)
C     STRMO(2,J) IS THE LIQUID OUT AFTER FLASHING
      STRMO(1,3)=SUM
      STRMO(2,3)= STRMI(1,3)- STRMO(1,3)
      STRMO(1,4)=TFLASH
      STRMO(2,4)=TFLASH
      STRMO(1,5) = EN(NE,3)
      STRMO(2,5) = EN(NE,3)
      JJ = NOCOMP+5
      DO 55 J=5,JJ
   55 STRMO(3,J)= STRMI(2,J)
      STRMO(3,3)= STRMI(2,3)
C
C     NOW CALCULATE THE TUBE TEMPERATURE FOR THIS FLASH TEMPERATURE
      IF(STRMI(2,3).LT.0.01)  GO TO 65
      UA=EN(NE,2)
      X = STRMI(2,4)
      ICOUNT=0
   60 ICOUNT = ICOUNT+1
C     CALCULATE THE HEAT CAPACITY OF THE MIXTURE TO THE EXCHANGER TUBES
      NOPP = ENC(NE,7)
      DO 62 J=1,NOCOMP
   62 XMOLE(J) = STRMI(2,J+5)
      CALL PROMIX(1)
C     EFFECTIVINESS FACTOR CALCULATION
      Z = 1. - EXP(-UA/PPMX(NOPP))
      STRMO(3,4) = STRMI(2,4)- Z*(STRMI(2,4)-TFLASH)
      IF(ICOUNT.EQ.2) GO TO 63
      X =  (STRMO(3,4)+STRMI(2,4))/2.0
C     THIS GIVES THE HEAT CAPACITY AT AN AVERAGE OF THE INPUT AND
C      OUTLET TEMPERATURE
      GO TO 60
   63 X = STRMO(3,4)
      CALL PROMIX(1)
      ENTHO3 = PPMX(NOPP)*(STRMO(3,4)-32.)
C
C     CALCULATE THE ENTHALPY OF THE OUTPUT STREAMS
C     ENTHO1 IS THE OUTPUT ENTHALPY OF STRMO(1) ABOVE 32 DEGREES F.
   65 X = STRMO(1,4)
      NOPP = ENC(NE,4)
      DO 68 J=1,NOCOMP
   68 XMOLE(J) = STRMO(1,J+5)
      CALL PROMIX(2)
      CPL = PPMX(NOPP)
      TTT = ((STRMO(1,4)-32.)/1.8)+273.
      H2OLAM = (1187.219-0.0015735*TTT*TTT)*18.
      NOPP = ENC(NE,5)
      CALL PROMIX(2)
      ZZ = PPMX(NOPP)*H2OLAM
      ENTHO1 = STRMO(1,3)*(ZZ+CPL*(STRMO(1,4)-32.))
      X = STRMO(2,4)
      NOPP = ENC(NE,4)
      DO 70 J=1,NOCOMP
   70 XMOLE(J) = STRMO(2,J+5)
      CALL PROMIX(1)
      ENTHO2 = PPMX(NOPP)*(STRMO(2,4)-32.)
      HOUT=ENTHO1+ENTHO2+ENTHO3
```

```
C     HOUT IS THE TOTAL OUTPUT ENTHALPY ABOVE 32 DEGREES F.
      DIF(NTEMP)=HIN-HOUT
C
C     IF COUNTER ''NTEMP'' EXCEEDS ''NITMAX'' THE PROGRAM EXITS
      IF(NTEMP.GE.NITMAX) GO TO 84
      IF(NTEMP.GE.2) GO TO 81
      IF(DIF(1).GT.0.0)  TDIF(2) = TDIF(1) + 2.0
      IF(DIF(1).LE.0.0)  TDIF(2) = TDIF(1) - 2.0
      TFLASH=TDIF(2)
      GO TO 20
C
C     CHECKS TO SEE IF HEAT BALANCE IS WITHIN SPECIFIED TOLERANCE LIMITS
   81 AA = ABS(DIF(NTEMP)/HIN)
      IF(AA.LE.TOL1) GO TO 90
C
C     HEAT BALANCE SEARCH  -  REGULI FALSI WITH CHANGING PIVOT POINT
      IF(DIF(1)*DIF(NTEMP).LT.0.0) GO TO 83
      SLOPE = (DIF(1) - DIF(NTEMP))/(TDIF(1) - TDIF(NTEMP))
      TDIF(NTEMP+1) = TDIF(1) - DIF(1)/SLOPE
      TFLASH=TDIF(NTEMP+1)
      IF(DIF(1)*DIF(1).LE.DIF(NTEMP)*DIF(NTEMP)) GO TO 20
      DIF(1) = DIF(NTEMP)
      TDIF(1) = TDIF(NTEMP)
      GO TO 20
   83 TDIF(NTEMP+1) = (TDIF(1)*DIF(NTEMP) - TDIF(NTEMP)*DIF(1))/
     1 (DIF(NTEMP) - DIF(1))
      TFLASH=TDIF(NTEMP+1)
      GO TO 20
C
   84 WRITE(6,987) TOL2,NITMAX,TDIF(NTEMP),DIF(NTEMP),DIF(NTEMP-1)
   90 EN(NE,6) = TFLASH
      EN(NE,7) = EN(NE,3)
C
C
C     ***************************************************************
C     THIS PART OF EXCH14 WAS ADDED FOR THE ALKYLATION STUDY TO SEPARATE
C     THE INPUT ACID, WATER AND SULPHATES INTO THE TWO OUTPUT STREAMS
C     ACCORDING TO APPROXIMATE SEPARATION FACTORS
C     HALF OF INPUT ACID, NA2SO4, AND ALKYL SULPHATE IS REMOVED THROUGH
C     ACID LEG, AND 0.8 OF REMAINING ACID PHASE GOES OUT THE BOTTOM
      STRMO(2,7) = 0.8*0.5*STRMI(1,7)
      STRMO(1,7) = 0.2*0.5*STRMI(1,7)
      STRMO(2,9) = 0.8*0.5*STRMI(1,9)
      STRMO(1,9) = 0.2*0.5*STRMI(1,9)
      STRMO(2,10) = 0.8*0.5*STRMI(1,10)
      STRMO(1,10) = 0.2*0.5*STRMI(1,10)
      STRMO(1,6) = 0.1 * STRMI(1,6)
      STRMO(2,6) = 0.9 * STRMI(1,6)
C
      RETURN
C
  987 FORMAT(1H0,4X,42HSOLUTION NOT CONVERGED WITHIN TOLERANCE OF
     1 F5.2,9H PER CENT/ 5X,57HSOLUTION TERMINATED BECAUS[illegible]
     2RATIONS EXCEEDED, I4//5X, 11HFLASH TEMP.,F9.3, 5X,14HENTHALPY DIF
     3., E11.4,5X, 23HPREVIOUS ENTHALPY DIFF., E11.4//
  988 FORMAT( 1X,22H TOTAL MOLES LIQUID IS,F12.4,10X,22H TOTAL MOLES VA
     1OUR IS,F12.4,8X,19H FOR TEMPERATURE OF,F[illegible].4  )
      END
```

```
$IBFTC FSOL
      SUBROUTINE FSOL ( FSOLW )
C
C     SUBROUTINE WRITTEN FOR THE SHELL REFINERY, OAKVILLE ONT. CAN.
C     THIS PROGRAM CALCULATES THE FLOWRATE OF SOLUBLE WATER IN A.H.C.
C     STREAM GIVEN THE HYDROCARBON FLOWRATE , TEMP. , AND COMPOSITION
C     SOLUBILITY DATA OBTAINED FROM A.P.I. HANDBOOK -- PAGE 9A1.1
C
C     ********MACSIM COMMON DECK, FOR ALKYLATION.  APR.30,1968. T.T.****
      COMMON NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
      COMMON AEN(4,102),ENC(50,20),NOPP,X,XMOLE(26),PPSC(17,26),PPMX(17)
      DIMENSION D1(18),D2(18),Y(18)
C
      DATA D1 / 8.82,5.24,9.13,7.51,0.0,2.70,0.0,8.06,0.0,6.96,6.96,7.66
     1 ,7.66,7.66,-3.79,-3.79,-3.79,-3.79/
      DATA D2 / 9060.,6390.,9740.,8390.,0.0,5475.,0.0,8420.,0.0,7640.,
     1 7640.,7940.,7940.,7940.,2105.,2105.,2105.,2105./
C
      FSOLW = 0.0
      A = 1.0/(X+460.0)
      DO 10 J=7,24
      K = J-6
      Y(K) =  EXP(D1(K) - D2(K)*A)
      Y(5) = 0.0
      Y(7) = 0.0
      Y(9) = 0.0
   10 FSOLW = FSOLW + XMOLE(J)*Y(K)
C
      RETURN
      END
```

```
*IBFTC JUNC02
C
C     SUBROUTINE JUNC02  (MIXER - MASS AND/OR HEAT BALANCES)
C     REVISED BY T. TOONG      FEB.20,1968
C     *APPROXIMATE HEAT BALANCE  (THE OUTPUT TEMPERATURE IS CALCULATED
C     *ASSUMING THE HEAT COEFFICIENTS ARE CONSTANT WITHIN THE RANGE
C     *BETWEEN THE INPUT TEMPERATURES AND THE OUTPUT TEMPERATURE.)
C
C
C     *PHYSICAL PROPERTY SUBROUTINES REQUIRED.
C
C     *MAXIMUM VALUE OF NOCOMP, NUMBER OF FLOW COMPONENTS, IS 26
C     *         ,,             NIN,       ,,       INPUT STREAMS,     5
C     *         ,,            NOUT,       ,,      OUTPUT STREAMS,     5
C
C
C
C     EN VECTOR -
C     1. EQUIPMENT NUMBER
C     2. TEMPERATURE OF OUTPUT STREAMS, DEG F, IF 0., OUTPUT TEMPERATURE
C        WILL BE CALCULATED BY HEAT BALANCING.
C     3. PRESSURE OF OUTPUT STREAMS, PSIA, IF 0., OUTPUT PRESSURE
C        ARE SET EQUAL TO PRESSURE OF 1ST INPUT STREAM.
C     4. (BLANK)
C     5. (BLANK)
C     6. FRACTION OF TOTAL INPUT IN 1ST OUTPUT STREAM
C     7.                ,,             2ND        ,,
C     8.                ,,             3RD        ,,
C     9.                ,,             4TH        ,,
C     10.               ,,             5TH        ,,
C
C
C     ENC VECTOR (OPTIONAL, IF 2. OF EN VECTOR IS NOT 0.) -
C     1. EQUIPMENT NUMBER
C     2. FLAG
C     3. LENGTH OF EN LIST (FOR PRINTING)
C     4. PHYSICAL PROPERTY CODE FOR LIQUID SPECIFIC HEAT COEFFICIENTS
C        IN BTU/LBMOLE/DEG F,(FLOATING POINT NUMBER)
C
C     SN VECTOR -
C     1. STREAM NUMBER
C     2. STREAM FLAG
C     3. TOTAL FLOW IN LBMOLE/HR
C     4. TEMPERATURE IN DEGREE F
C     5. PRESSURE IN PSIA
C     6. FLOW OF COMPONENT 1 IN LBMOLE/HR
C     7.            ,,       2       ,,
C     8.            ,,       3       ,,
C     9.           ETC.
C
C
C     SNC VECTOR - NOT REQUIRED
C
C
C
      SUBROUTINE JUNC02
C     ********MACSIM COMMON DECK, FOR ALKYLATION.  APR.30,1968. T.T.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
      COMMON AEN(4,102),ENC(50,20),NOPP,X,XMOLE(26),PPSC(17,26),PPMX(17)
```

```
C       ****************************************************************
C TO CHECK IF INPUT STREAMS ARE NOT MORE THAN 5
      IF(NIN.LE.5) GOTO 10
      WRITE(6,90) NE
      NIN= 5
   10 JJ= NOCOMP+5
C
C
C MASS BALANCE
C (INPUT)
      DO 1 J=6,JJ
      STRMO(NOUT,J)=0.
      DO 1 I=1,NIN
    1 STRMO(NOUT,J)= STRMO(NOUT,J)+STRMI(I,J)
C (OUTPUT)
      DO 2 I=1,NOUT
      STRMO(I,4)= EN(NE,2)
      IF(EN(NE,2).EQ.0.) STRMO(I,4)=STRMI(1,4)
      STRMO(I,5)= EN(NE,3)
      IF(EN(NE,3).EQ.0.) STRMO(I,5)=STRMI(1,5)
      STRMO(I,3)=0.
      DO 2 J=6,JJ
      STRMO(I,J)= STRMO(NOUT,J)*EN(NE,I+5)
    2 STRMO(I,3)= STRMO(I,3)+STRMO(I,J)
C
C HEAT BALANCE
      IF(EN(NE,2).NE.0.) GOTO 24
      IF(NIN.EQ.1) GOTO 24
      CPTOT=0.
      ENTH= 0.
      NOPP= ENC(NE,4)
      DO 21 I=1,NIN
      X= STRMI(I,4)
      DO 22 J=1,NOCOMP
   22 XMOLE(J)= STRMI(I,J+5)
      CALL PROMIX(1)
      CPTOT= CPTOT+PPMX(NOPP)
   21 ENTH= ENTH+PPMX(NOPP)*X
      TOUT= ENTH/CPTOT
      DO 23 I=1,NOUT
   23 STRMO(I,4)= TOUT
   24 CONTINUE
C
C FORMATS
   90 FORMAT (////1X, 25H**ERROR**IN JUNC01 MODULE, I3,
     173H, NIN EXCEEDS 5, CALCULATION CONTINUES USING THE FIRST FIVE INP
     2UT STREAMS////)
C
      RETURN
      END
```

```
$IBFTC MSTEM1
      SUBROUTINE MSTEM1
C     ******* MACSIM COMMON DECK, FOR ALKYLATION.  T.T. APR.29.1968.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20
C
      JJ=NOCOMP+5
      STRMO(1,4)=STRMI(1,4)
      STRMO(1,5)=STRMI(1,5)
      STRMO(1,3)=0.0
      DO 20 J=6,JJ
      STRMO(1,J)=STRMI(2,J)
   20 STRMO(1,3)=STRMO(1,3)+STRMO(1,J)
      RETURN
      END
```

```
$IBFTC MAKEUP
      SUBROUTINE MAKEUP
C     WRITTEN BY I. SHAW  MAY 21 1968
C
C    -MODULE WRITTEN FOR SHELL ALKYLATION SIMULATION
C    -THE ACID MAKE-UP STREAM IS SPECIFIED FROM A MASS BALANCE
C
C     FIRST INPUT STREAM IS ACID RECYCLE
C     SECOND INPUT STREAM IS MAKE-UP ACID
C     FIRST EXIT STREAM IS ACID FEED TO REACTOR
C     SECOND EXIT STREAM IS WASTE ACID
C
C     EN VECTOR
C     1. EQUIPMENT NUMBER
C     2. WEIGHT FRACTION ACID IN MAKE-UP ACID (0.99 - 1.01)
C     3. WEIGHT FRACTION ACID REQUIRED IN FEED TO REACTOR (0.88 - 0.96)
C     4. VOLUME FRACTION OF REACTOR FEED THAT IS ACID (0.45 TO 0.50)
C     5. STREAM NUMBER OF ORGANIC FEED TO REACTOR
C     6. LOCATION OF PHYSICAL PROPERTY FOR LIQUID DENSITY (13)
C     7. LOCATION OF PHYSICAL PROPERTY FOR MOLECULAR WEIGHT (1)
C     8. LOCATION OF PHYSICAL PROPERTY FOR LIQUID SPECIFIC HEAT (7)
C     9. TEMPERATURE OF FRESH MAKE-UP ACID (45. - 70.)
C     10. COUNTER FOR CONVERGENCE PROMOTION (INITIALLY BLANK)
C     11. WEIGHT FRACTION WATER TO REACTOR (CALCULATED BY PROGRAM)
C     12. STORAGE FOR CONVERGENCE PROMOTION (CALCULATED BY THE PROGRAM)
C
C     *******MACSIM COMMON DECK, FOR ALKYLATION.  APR.30,1968. T.T.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
      COMMON AEN(4,102),ENC(50,20),NOPP,X,XMOLE(26),PPSC(17,26),PPMX(17)
      COMMON  SN(75,31),DELS(31), KPM(50,10),KUS(75),KPS(3)
      DIMENSION Y(3,4)
C
      NOPP = EN(NE,6)
      NEFEED = EN(NE,5)
      DO 20 J=1,5
   20 XMOLE(J) = 0.0
      DO 40 J=6,26
   40 XMOLE(J) = SN(NEFEED,J+5)
      CALL PROMIX(1)
C     ASSUME ACID TO THE REACTOR HAS A DENSITY OF 1.85
      F4 = (PPMX(NOPP)/(1.0-EN(NE,4)))*EN(NE,4)*62.4*1.85
      NOPP = EN(NE,7)
      F1 = STRMI(1,6)*PPSC(NOPP,1) + STRMI(1,7)*PPSC(NOPP,2) +
     1     STRMI(1,9)*PPSC(NOPP,4) + STRMI(1,10)*PPSC(NOPP,5)
      Y(1,1) = STRMI(1,6)*PPSC(NOPP,1)/F1
      Y(1,2) = STRMI(1,7)*PPSC(NOPP,2)/F1
      Y(1,3) = STRMI(1,9)*PPSC(NOPP,4)/F1
      Y(1,4) = STRMI(1,10)*PPSC(NOPP,5)/F1
      Y(2,1) = 1.0-EN(NE,2)
      Y(2,2) = EN(NE,2)
C
      F3 = (F1*Y(1,2)+(F4-F1)*EN(NE,2)-F4*EN(NE,3))/(Y(1,2)-EN(NE,2))
      F2 = F3 + F4 - F1
      Y(3,1) = ((F1-F3)*Y(1,1) + F2*Y(2,1))/F4
      Y(3,3) = ((F1-F3)*Y(1,3) +   0.0     )/F4
      Y(3,4) = ((F1-F3)*Y(1,4) +   0.0     )/F4
C
C     DEFINE FLOW OF INPUT ACID STREAM
      STRMI(2,4) = EN(NE,9)
```

```
      STRMI(2,6) = F2*(1.0-EN(NE,2))/PPSC(NOPP,1)
      STRMI(2,7) = F2*EN(NE,2)/PPSC(NOPP,2)
      STRMI(2,3) = STRMI(2,6) + STRMI(2,7)
C     DEFINE FLOWS OF TWO EXIT STREAMS
      STRMO(1,6) = F4*Y(3,1)/PPSC(NOPP,1)
      STRMO(1,7) = F4*EN(NE,3)/PPSC(NOPP,2)
      STRMO(1,8) = 0.0
      STRMO(1,9) = F4*Y(3,3)/PPSC(NOPP,4)
      STRMO(1,10) = F4*Y(3,4)/PPSC(NOPP,5)
      STRMO(2,6) = F3*Y(1,1)/PPSC(NOPP,1)
      STRMO(2,7) = F3*Y(1,2)/PPSC(NOPP,2)
      STRMO(2,8) = 0.0
      STRMO(2,9) = F3*Y(1,3)/PPSC(NOPP,4)
      STRMO(2,10) = F3*Y(1,4)/PPSC(NOPP,5)
      EN(NE,11) = Y(3,1)
C
C     CONVERGENCE PROMOTION SECTION FOR WATER AND ALKYL SULPHATE
      EN(NE,10) = EN(NE,10) + 1.0
      WATER = (EN(NE,12)-STRMO(1,6))*3.0
      ASO = -WATER*(18.016/198.0)
      IF(EN(NE,10).LT.5.9)  GO TO 150
      STRMO(1,6) = STRMO(1,6) - WATER
      STRMO(2,6) = STRMO(2,6) + WATER
      STRMO(1,10) = STRMO(1,10) - ASO
      STRMO(2,10) = STRMO(2,10) + ASO
  150 STRMO(1,3) = 0.0
      STRMO(2,3) = 0.0
      DO 160 J=6,10
      STRMO(1,3) = STRMO(1,3) + STRMO(1,J)
  160 STRMO(2,3) = STRMO(2,3) + STRMO(2,J)
      EN(NE,12) = STRMO(1,6)
C
C     HEAT BALLANCE
      CPTOT = 0.0
      ENTH = 0.0
      NOPP = EN(NE,8)
      DO 220 I=1,2
      X = STRMI(I,4)
      DO 210 J=1,NOCOMP
  210 XMOLE(J) = STRMI(I,J+5)
      CALL PROMIX(1)
      CPTOT = CPTOT + PPMX(NOPP)
  220 ENTH = ENTH + PPMX(NOPP)*X
      TOUT = ENTH/CPTOT
      STRMO(1,4) = TOUT
      STRMO(2,4) = TOUT
C
      RETURN
      END
```

```
$IBFTC PROCAL
C     PHYSICAL PROPERTY SUBROUTINE - COMPONENT CALCULATION
C     REVISED BY T. TOONG     JULY 29,1968
C
      SUBROUTINE PROCAL
C     ********MACSIM COMMON DECK, FOR ALKYLATION.  APR.30,1968. T.T.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
      COMMON AEN(4,102),ENC(50,20),NOPP,X,XMOLE(26),PPSC(17,26),PPMX(17)
C     ******************************************************************
      COMMON/PPDATA/NTPC(17),LOC(17),PROP(17,26,4)
C
C CHECK THAT NOPP LIES WITHIN 1 AND 17
      N= NOPP
      IF (N.GE.1.AND.N.LE.17) GOTO 90
      WRITE(6,1030) NE,N
      GOTO 2000
   90 NT= NTPC(N)
      IF(NT.EQ.0) GOTO 1000
C
C TABLE INTERPOLATION NOT SET UP YET
      IF(NT.GT.10) GOTO 100
C
C PARAMETER EQUATION-   NTPC=11 TO 20
C POLYNOMIAL-  Y= A0+A1*X+A2*X**2+A3*X**3+...........+A9*X**9
  100 IF(NT.GT.20) GOTO 200
      NT= NT-10
      DO 120 J=1,NOCOMP
      E= 0.
      DO 110 K1=1,NT
      K= NT+1-K1
  110 E= PROP(N,J,K)+E*X
  120 PPSC(N,J)= E
      GOTO 1000
C
C PARAMETER EQUATION-   NTPC= 21
C Y= EXP(A/X+B+C*X*X)  IF A IS NOT ZERO,   BUT Y= 0  IF A IS ZERO
  200 IF (NT.GT.21) GOTO 300
      X = X + 460.
      DO 210 J=1,NOCOMP
      PPSC(N,J)= 0.
  210 IF (PROP(N,J,1).NE.0.) PPSC(N,J)= EXP(PROP(N,J,1)/X+PROP(N,J,2)+
     1PROP(N,J,3)*X*X)
      X = X - 460.
      GOTO 1000
C
  300 CONTINUE
C PRINTING PPSC (IF KSETS IS GREATER THAN ONE)
 1000 IF(KSETS.LT.2) GOTO 2000
      WRITE (6,1010) N, X
      WRITE (6,1020) (PPSC(N,J),J=1,NOCOMP)
C
 1010 FORMAT (/ 9X, 23H*PHYSICAL PROPERTY NO.=, I2, 15H,     VARIABLE=,
     11PE10.3, 45H,     (PPSC(NOPP,J),J=1,NOCOMP) ARE AS FOLLOWS)
 1020 FORMAT (9X,1H*, 1P10E11.3)
 1030 FORMAT (/ 26H **ERROR**IN EQUIPMENT NO., I3,
     153 H, PHYSICAL PROPERTY SUBROUTINES ARE CALLED WITH NOPP=, I3,
     221 H.  PROCAL IS BYPASSED /)
 2000 RETURN
      END
```

```
$IBFTC PROMIX
C     PHYSICAL PROPERTY SUBROUTINE - MIXTURE CALCULATION
C     REVISED BY T. TOONG     FEB.20,1968
C
C
      SUBROUTINE PROMIX(M)
C     *******MACSIM COMMON DECK, FOR ALKYLATION.  APR.30,1968. T.T.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
      COMMON AEN(4,102),ENC(50,20),NOPP,X,XMOLE(26),PPSC(17,26),PPMX(17)
C     ******************************************************************
C
C CHECKING THE VALUE OF M
   10 IF(M.LT.0.OR.M.GT.2) GOTO 120
      N= NOPP
      IF(M.EQ.0) GOTO 100
      CALL PROCAL
C
C TYPE 1 CALCULATION (MOLE TOTAL)
      IF(M.GT.1) GOTO 20
      PPMX(N)= 0.
      DO 11 J=1,NOCOMP
   11 PPMX(N)= PPMX(N)+PPSC(N,J)*XMOLE(J)
      GOTO 100
C
C TYPE 2 CALCULATION (MOLE FRACTION)
   20 TMOLE= 0.
      DO 21 J=1,NOCOMP
   21 TMOLE= TMOLE+XMOLE(J)
      PPMX(N)= 0.
      DO 22 J=1,NOCOMP
      XMOLE(J)= XMOLE(J)/TMOLE
   22 PPMX(N)= PPMX(N)+ PPSC(N,J)*XMOLE(J)
      GOTO 100
C
C PRINTING PPMX (IF KSETS IS GREATER THAN ONE)
  100 IF(KSETS.LT.2) GOTO 200
      WRITE(6,150) PPMX(N)
      GOTO 200
C
C PRINTING ERROR IN 'M'
  120 WRITE (6,151) NE,M
      M=1
      GOTO 10
C
C FORMATS
  150 FORMAT(9X, 12H*PPMX(NOPP)=, 1PE15.7/)
  151 FORMAT (/1X, 21H**ERROR**IN EQUIPMENT, I3,
     129H, PROMIX(M) IS CALLED WITH M=, I2,
     262H, WHICH IS NOT PROVIDED, CALCULATION CONTINUES WITH M SET TO 1,
     3/)
C
  200 RETURN
      END
```

```
$IBFTC REAC25
      SUBROUTINE REAC25
C     WRITTEN BY H. CANNING AND J. GATES
C     REVISED BY I. SHAW    MAY 1968
C     THIS MODEL PERFORMS A MASS AND HEAT BALANCE ON THE STRATCO
C     REACTOR AT SHELL OAKVILLE
C
C     EN VECTOR
C     1. EQUIPMENT NUMBER
C     2. SET TO 0.0 TO SUPRESS MASS BALANCE PRINTOUT
C     3. SET AT 0.0 TO SUPRESS HEAT BALANCE PRINTOUT
C     4. SET TO 1.0 TO SUPRESS LIMIT OF CORRELATION CHECK AND PRINTOUT
C     5. EQUIPMENT NUMBER OF PRODUCT SEPARATOR
C     6. LOCATION OF MOLECULAR WEIGHT IN PHYSICAL PROPERTIES
C     7. LOCATION OF LIQUID SPECIFIC HEATS IN PHYSICAL PROPERTY PACKAGE
C     8. IMPELLER POWER IN KW WHICH IS A CONSTANT
C
C     **********************************************************************
C    -MODEL USES CORRELATION EQUATIONS TO PREDICT OUTPUTS FROM INPUTS
C    -ACID DILUTUON IS CAUSED BY WATER IN THE FEED AND BY THE PRODUCTION
C     OF ALKYL SULPHATES
C    -PRODUCTION OF ALKYL SUPHATES CALCULATED BY EQUATIONS BASED ON
C     MASS BALANCES AND FACTORS BELIEVED TO EFFECT ACID CONSUMPTION
C    -ANY NAOH ASSUMED TO GO TO NA2SO4
C    -N-C3 AND N-C4 ARE ASSUMED INERT AND UNCHANGED ACROSS THE REACTOR
C    -I-C4 USAGE IS CALCULATED FROM I-C4 TO OLEFIN USAGE FACTORS
C    -OLEFINS ASSUMED COMPLETELY REACTED
C    -ALL OTHER OUTPUTS CALCULATED BY REGRESSION EQUATIONS
C
C     STRMI(1,J) IS THE ORGANIC FEED TO THE REACTOR
C     STRMI(2,J) IS THE ACID RECYCLE TO THE REACTOR
C
C     ******* MACSIM COMMON DECK, FOR ALKYLATION.  T.T. APR.29,1968.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
      COMMON AEN(4,102),FNC(50,20),NOPP,X,XMOLE(26),PPSC(17,26),PPMX(17)
      DIMENSION B(9), C(9), D(9), E(9), F(9), G(9), H(9), R(9)
      DIMENSION HIHLMT(9), BTMLMT(9)
C
C     **********************************************************************
C     DEFINE CONSTANTS AND CORRELATION COEFFICIENTS
      DATA B /33.0341, -0.0671101, 0.0, -0.02202443, 0.0, 0.668633,
     1        -0.328644, -0.927387, 0.104107 /
      DATA C /15.1189, -0.0292867, 0.0830969, -0.0109155, 0.00763949,
     1        0.300093, -0.177285, -0.130126, 0.0133338 /
      DATA D /4.99554, -0.0351862, 0.0445619, 0.119407E-03, 0.00323341,
     1        0.139254, -0.168913, -0.102607, 0.294273 /
      DATA E /28.2760, -0.0483364, 0.251499, 0.00487267, -0.0116686,
     1        -0.182781, -0.341756, -0.0546192, 0.286463 /
      DATA F /-8.44706, 0.00144266, -0.140933, 0.0223955, -0.00217905,
     1        -0.0724850, -0.0237373, -0.0965011, 0.617014 /
      DATA G /2.45950, -0.0105513, -0.00913172, -0.00276322, 0.00446359,
     1        0.176672, -0.0644604, -0.0462004, 0.0956723 /
      DATA H /18.9267, -0.0175973, 0.0270972, 0.0133159, -0.739504E-03,
     1        -0.214328, 0.0827224, -0.119846, 0.150898 /
      DATA R /7.17834, -0.0146893, -0.0345164, -0.0144946, 0.00835222,
     1        0.337128, -0.205448, -0.150647, 0.263569 /
      DATA HIHLMT / 245.6, 91.4, 609.1, 989.0, 52.5, 62.9, 100.0, 25.1,
     1              100.0 /
      DATA BTMLMT / 92.6, 59.6, 190.6, 634.2, 28.1, 39.1, 0.0, 6.7, 0.0/
```

```
C
C     ******************************************************************************
C     THIS CHECKS FOR INPUTS OUT OF CORRELATION LIMITS
      IF(EN(NE,4).GT.0.5)  GO TO 15
      DO 10 J=12,20
      LL = J-11
      IF(STRMI(1,J).LT.BTMLMT(LL)) WRITE(6,4446) BTMLMT(LL),J,STRMI(1,J)
   10 IF(STRMI(1,J).GT.HIHLMT(LL)) WRITE(6,4446) HIHLMT(LL),J,STRMI(1,J)
C
C     ******************************************************************************
C     USE REGRESSION EQUATIONS TO CALCULATE FLOWS IN ORGANIC PHASE
   15 STRMO(1,4) = STRMI(1,4) + 8.0
      STRMO(1,5) = 85.0
      STRMO(1,6) = STRMI(1,6) + STRMI(2,6)
      STRMO(1,8) = 0.0
      STRMO(1,9) = STRMI(1,9) + STRMI(2,9) + 0.5*STRMI(1,8)
      NOPP = EN(NE,6)
      WEIGHT = 0.0
      DO 20 J=1,26
   20 WEIGHT = WEIGHT + STRMI(2,J+5)*PPSC(NOPP,J)
      ACID = STRMI(2,7)*PPSC(NOPP,2)/WEIGHT
      ACDOIL = ((STRMI(1,13)*2.0)*(1.0 + 2.5*(0.90-ACID)) +
     1         ((STRMI(1,16)+STRMI(1,17))*0.6)*(1.0 + 2.5*(0.90-ACID)) +
     2           STRMI(1,20)*1.0)*0.0035
      RATIO = STRMI(1,15)/(STRMI(1,13)+STRMI(1,16)+STRMI(1,17)+
     1                                                            STRMI(1,20))
      ACDOIL = ACDOIL*(1.0 + (5.5-RATIO)*0.114)
      ACDOIL = ACDOIL*(1.0 - (50.0-STRMO(1,4))*0.0145)
      STRMO(1,10) = STRMI(1,10) + STRMI(2,10) + ACDOIL
      STRMO(1,7) = STRMI(2,7) - STRMI(1,8)*0.5 - (STRMO(1,10) -
     1                                 (STRMI(1,10)+STRMI(2,10)))
      STRMO(1,11)= STRMI(1,11)
      STRMO(1,12) = STRMI(1,12)
      STRMO(1,13) = 0.0
      STRMO(1,14) = STRMI(1,14)
      STRMO(1,15)= STRMI(1,15) - (0.8760*STRMI(1,13)+1.030*STRMI(1,16)
     1                +1.001*STRMI(1,17)+ 0.9411*STRMI(1,20))*0.926
      STRMO(1,16) = 0.0
      STRMO(1,17) = 0.0
      C5PROD   =    B(1) + B(2)*STRMI(1,12) + B(3)*STRMI(1,13) + B(4)*
     1 STRMI(1,15) + B(5)*STRMI(1,14) + B(6)*STRMI(1,17) + B(7)*
     2 STRMI(1,16) + B(8)*STRMI(1,19) + B(9)*STRMO(1,4)
      STRMO(1,18) = STRMI(1,18) + 0.10*C5PROD
      STRMO(1,19) = STRMI(1,19) + 0.90*C5PROD
      STRMO(1,20) = 0.0
      STRMO(1,21) = STRMI(1,21)
      STRMO(1,22) = C(1) + C(2)*STRMI(1,12) + C(3)*STRMI(1,13) + C(4)*
     1 STRMI(1,15) + C(5)*STRMI(1,14) + C(6)*STRMI(1,17) + C(7)*
     2 STRMI(1,16) + C(8)*STRMI(1,19) + C(9)*STRMO(1,4)
      STRMO(1,22)=STRMO(1,22)    +    STRMI(1,22)
      STRMO(1,23) = STRMI(1,23)
      STRMO(1,24) = D(1) + D(2)*STRMI(1,12) + D(3)*STRMI(1,13) + D(4)*
     1 STRMI(1,15) + D(5)*STRMI(1,14) + D(6)*STRMI(1,17) + D(7)*
     2 STRMI(1,16) + D(8)*STRMI(1,19) + D(9)*STRMO(1,4)
      STRMO(1,24)=STRMO(1,24)    +    STRMI(1,24)
      STRMO(1,25) = E(1) + E(2)*STRMI(1,12) + E(3)*STRMI(1,13) + E(4)*
     1 STRMI(1,15) + E(5)*STRMI(1,14) + E(6)*STRMI(1,17) + E(7)*
     2 STRMI(1,16) + E(8)*STRMI(1,19) + E(9)*STRMO(1,4)
```

```
      STRMO(1,25)=STRMO(1,25)    +    STRMI(1,25)
      STRMO(1,26) = STRMI(1,26)
      STRMO(1,27) = F(1) + F(2)*STRMI(1,12) + F(3)*STRMI(1,13) + F(4)*
     1 STRMI(1,15) + F(5)*STRMI(1,14) + F(6)*STRMI(1,17) + F(7)*
     2 STRMI(1,16) + F(8)*STRMI(1,19) + F(9)*STRMO(1,4)
      STRMO(1,27)=STRMO(1,27)    +    STRMI(1,27)
      STRMO(1,28) = G(1) + G(2)*STRMI(1,12) + G(3)*STRMI(1,13) + G(4)*
     1 STRMI(1,15) + G(5)*STRMI(1,14) + G(6)*STRMI(1,17) + G(7)*
     2 STRMI(1,16) + G(8)*STRMI(1,19) + G(9)*STRMO(1,4)
      STRMO(1,28)=STRMO(1,28)    +    STRMI(1,28)
      STRMO(1,29) = H(1) + H(2)*STRMI(1,12) + H(3)*STRMI(1,13) + H(4)*
     1 STRMI(1,15) + H(5)*STRMI(1,14) + H(6)*STRMI(1,17) + H(7)*
     2 STRMI(1,16) + H(8)*STRMI(1,19) + H(9)*STRMO(1,4)
      STRMO(1,29)=STRMO(1,29)    +    STRMI(1,29)
      AA      =      R(1) + R(2)*STRMI(1,12) + R(3)*STRMI(1,13) + R(4)*
     1 STRMI(1,15) + R(5)*STRMI(1,14) + R(6)*STRMI(1,17) + R(7)*
     2 STRMI(1,16) + R(8)*STRMI(1,19) + R(9)*STRMO(1,4)
      STRMO(1,30) = 0.5*AA + STRMI(1,30)
      STRMO(1,31) = 0.5*AA + STRMI(1,31)
C
C     *************************************************************
C     NORMALIZATION SECTION
      NOPP = EN(NE,6)
      M = NOPP
      CALL PROCAL
C     SUM THE WEIGHT OF INPUT AND OUTPUT ORGANICS TO BE NORMALLIZED
      SUMIN = STRMI(1,13)*PPSC(M,8) + STRMI(1,16)*PPSC(M,11) +
     1        STRMI(1,17)*PPSC(M,12) + STRMI(1,20)*PPSC(M,15) -
     2        (STRMO(1,10)-(STRMI(1,10)+STRMI(2,10)))*0.516*PPSC(M,5) -
     3        (STRMO(1,15)-(STRMI(1,15)+STRMI(2,15)))*PPSC(M,10)
      SUMOUT = C5PROD*PPSC(M,14)
      DO 40 J=21,31
   40 SUMOUT = SUMOUT + (STRMO(1,J)-STRMI(1,J))*PPSC(NOPP,J-5)
      AA = SUMIN/SUMOUT
      STRMO(1,18) = STRMI(1,18) + AA*C5PROD*0.10
      STRMO(1,19) = STRMI(1,19) + AA*C5PROD*0.90
      DO 70 J=21,31
   70 STRMO(1,J) = STRMI(1,J) + AA*(STRMO(1,J)-STRMI(1,J))
      STRMO(1,3)=0.0
      DO 80 J=6,31
   80 STRMO(1,3)=STRMO(1,3)+STRMO(1,J)
      IF(EN(NE,2).LT.0.5)  GO TO 110
      DIFFPC = (SUMIN-SUMOUT)*100.0/SUMIN
      WRITE(6,1005) SUMIN, SUMOUT, DIFFPC
      WRITE(6,9997)
      DO 90 J=1,26
      AA = STRMI(1,J+5)*PPSC(1,J)
      BB = STRMI(2,J+5)*PPSC(1,J)
      CC = STRMO(1,J+5)*PPSC(1,J)
   90 WRITE(6,9999) AA,BB,CC
C
C     *************************************************************
C     CHECK OUTPUT FOR NEGATIVE FLOWS
  110 IF(STRMO(1,4).GT.60.0.OR.STRMO(1,4).LT.40.0)  WRITE(6,4448)
      IF(STRMO(1,15).GT.STRMI(1,15)) GO TO 200
      DO 150 J=6,31
      IF(STRMO(1,J).LT.0.0)  GO TO 200
  150 CONTINUE
```

```
      GO TO 260
  200 WRITE(6,252)
      WRITE(6,9998)  (STRMI(1,J),J=1,31)
      WRITE(6,9998)  (STRMI(2,J),J=1,31)
      WRITE(6,9998)  (STRMO(1,J),J=1,31)
      STOP
C
C     ***********************************************************************
C    -HEAT BALANCE CALCULATES THE HEAT THAT MUST BE REMOVED BY THE COILS
C      IN THE RACTOR AND TRANSFERS THIS AMOUNT TO THE PRODUCT SEPARATOR
C    -THE HEAT OF REACTION IS CALCULATED KNOWING THE FLOWS OF OLEFIN
C      AND USING VALUES FROM CULPIT ADJUSTED BY A PLANT FACTOR
C    -THE IMPELLER HEAT INPUT IS THE EQUIVALENT OF A 50 HP MOTOR
260   CONTINUE
      ENTHIN=0.0
      NOPP = EN(NE,7)
      DO 21 I=1,NIN
      X=STRMI(I,4)
      DO 22 J=1,NOCOMP
22    XMOLE(J)=STRMI(I,J+5)
      CALL PROMIX(1)
21    ENTHIN=ENTHIN+PPMX(NOPP)*X
      X = STRMO(1,4)
      DO 24 J=1,NOCOMP
   24 XMOLE(J)=STRMO(1,J+5)
      CALL PROMIX(1)
      ENTHO = PPMX(NOPP)*X
      HR = (35280.*STRMI(1,13) + 34440.*(STRMI(1,16)+STRMI(1,17)) +
     1                                  34960.*STRMI(1,20))*0.845
      HI=1260000.0
      HEATLD=ENTHIN-ENTHO+HR+HI
      IF(EN(NE,3).GT.0.5)  WRITE(6,5555) ENTHIN, ENTHO, HR, HI, HEATLD
      NNN = EN(NE,5)
      EN(NNN,5) = HEATLD
      ENC(NE,16) = EN(NE,8)
      RETURN
C
C
  252 FORMAT(///51H **** STOP BECAUSE FLOW IN REACTOR EXIT IS NEGATIVE//)
 1005 FORMAT(/37H ORGANIC INPUT TO BE NORMALIZED (LB.), F11.2, 6X, 25HOU
     1TPUT BEFORE NORMALIZING, F11.2, 6X, 18HPERCENT DIFFERENCE, F9.5/)
 4446 FORMAT( 25H *** CORRELATION LIMIT OF,F7.1, 23H  EXCEEDED FOR STRMI
     1(1,, I2, 10H) WHICH IS, F7.1,  27H  IN THE REACTOR MODULE ***)
 4448 FORMAT(/  43H *** REACTOR TEMPERATURE OUTSIDE LIMITS ***/)
5555  FORMAT(     5X,11HENTHALPY IN,F12.3,5X,12HENTHALPY OUT,F12.3,5X,16H
     1HEAT OF REACTION,F12.3,/,5X,13HIMPELLER HEAT,F12.3,5X,10HTOTAL LOA
     2D,F12.3)
 9997 FORMAT(/ 12X, 32HMASS FLOWS IN AND OUT OF REACTOR/)
 9998 FORMAT(5F20.5)
 9999 FORMAT(5F15.1)
      END
```

```
$IBFTC READIN
      SUBROUTINE READIN
C     PHYSICAL PROPERTY SUBROUTINE - DATA READING
C     REVISED BY T. TOONG    MAR.28,1968
C     *PARAMETRIC DATA READING ONLY
C
C
C     *INPUT OR OUTPUT STREAMS ARE OPTIONAL
C     *IF CALCULATION ORDER IS SPECIFIED, CALCULATE THIS SUBROUTINE AS
C     *THE FIRST EQUIPMENT IN A DIRECT CALCULATION
C
C     *MAXIMUM NUMBER OF PHYSICAL PROPERTIES (CODES), NOPP, IS 17
C     *MAXIMUM NUMBER OF PARAMETRIC CONSTANTS PER COMPONENT, LOC, IS 4
C     *MAXIMUM NUMBER OF FLOW COMPONENTS, NOCOMP, IS 26
C
C
C
C     ********MACSIM COMMON DECK, FOR ALKYLATION.  APR.30,1968. T.T.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
C     ******************************************************************
      COMMON/PPDATA/NTPC(17),LOC(17),PROP(17,26,4)
      DIMENSION NO(17),NTYPE(17)
C
C READING PHYSICAL PROPERTY DATA
      READ(5,11) NPP
      DO 1 II=1,NPP
      READ(5,12) I,NTPC(I),LOC(I),NTYPE(I)
      NO(II)= I
      NTY= NTYPE(I)
      IF (NTPC(I).LT.10) GOTO 5
C
C PARAMETER READING
      L= LOC(I)
      GOTO(6,7),NTY
    6 DO 2 J=1,NOCOMP
    2 READ(5,13)  (PROP(I,J,K),K=1,L)
      GOTO 1
    7 DO 3 J=1,NOCOMP
    3 READ(5,14)  (PROP(I,J,K),K=1,L)
    1 CONTINUE
      GOTO 30
C
C TABLE READING NOT YET SET UP
    5 WRITE(6,19) I
      GOTO 31
C
C PRINTING PHYSICAL PROPERTY DATA (IF KSETS IS GREATER THAN ONE)
   30 IF(KSETS.LT.2) GOTO 40
   31 WRITE(6,15)
      WRITE(6,11) NPP
      DO 32 II=1,NPP
      I= NO(II)
      WRITE(6,12) I,NTPC(I),LOC(I),NTYPE(I)
      L= LOC(I)
      NTY= NTYPF(I)
      DO 32 J=1,NOCOMP
      GOTO(33,34),NTY
   33 WRITE(6,13) (PROP(I,J,K),K=1,L)
      GOTO 32
```

```
   34 WRITE(6,14) (PROP(I,J,K),K=1,L)
   32 CONTINUE
      WRITE(6,16)
C
C SUBROUTINE READIN IS USED AS A DUMMY EQUIPMENT
   40 JJ= 5+NOCOMP
      DO 41 J=3,JJ
   41 STRMO(1,J)= STRMI(1,J)
C
C FORMATS
   11 FORMAT(I15)
   12 FORMAT(4I15)
   13 FORMAT(5F15.6)
   14 FORMAT (1P5E15.6)
   15 FORMAT (1H1, 23H PHYSICAL PROPERTY DATA, ///)
   16 FORMAT (1H1)
   19 FORMAT (1H1,30(/),22H PHYSICAL PROPERTY NO.,I3,66H REQUIRES TABLE
     1READIN WHICH IS NOT PROVIDED YET. READING STOPPED.)
C
      RETURN
      END
```

```
$IBFTC REPORT
      SUBROUTINE REPORT
C
C     EN VECTOR
C     1. EQUIPMENT NUMBER
C     2. STREAM NUMBER OF REACTOR ORGANIC FEED
C     3. PRINT SUPRESSION FOR PRINTER IF EQUAL TO 1.0
C
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
      COMMON AEN(4,102),FNC(50,20),NOPP,X,XMOLE(26),PPSC(17,26),PPMX(17)
      COMMON SN(75,31), AA(1336), TITLE(24), BP(477), LOOP
C
      NFEED = EN(NE,2) + 0.1
      IF(EN(NE,9).EQ.0.0)  WRITE(7,9999) TITLE
      EN(NE,4) = EN(NE,7)
      EN(NE,5) = EN(NE,8)
      EN(NE,6) = EN(NE,9)
      EN(NE,7) = SN(NFEED,12)
      EN(NE,8) = SN(NFEED,14)
      EN(NE,9) = SN(NFEED,15)
      DIF12 = EN(NE,9) - EN(NE,6)
      DIF14 = EN(NE,8) - EN(NE,5)
      DIF15 = EN(NE,7) - EN(NE,4)
      WRITE(7,9998) LOOP, DIF12, DIF14, DIF15
      IF(EN(NE,3).LT.0.5)  WRITE(6,9997) LOOP, SN(9,12), SN(9,14),
     1    SN(9,15), SN(9,4), SN(17,3), SN(15,4), SN(15,5)
C
      RETURN
 9997 FORMAT(I6, 8F12.6)
 9998 FORMAT(I5, 3F15.6)
 9999 FORMAT(1X, 12A6, / 1X, 12A6//)
      END
```

```
$IBFTC SETL01
      SUBROUTINE SETL01
C
C     -MODEL FOR THE ACID DECANTER IN THE SHELL ALKYLATION PLANT
C     -THE NUMBER OF BARRELS OF ACID CARRIED OVER PER DAY IS READ IN AND
C      THE ACID PHASE IS SPLIT ACCORDINGLY
C     -NO ORGANICS ARE RECYCLED IN THE MAIN ACID RECYCLE
C     -FIRST OUTPUT STREAM IS THE HYDROCARBON
C
C      EN VECTOR
C      1. EQUIPMENT NUMBER
C      2. ACID CARRYOVER IN BBL./DAY (ABOUT 3.6)
C
C      ******* MACSIM COMMON DECK, FOR ALKYLATION.  T.T. APR.29,1968.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
C
      JJ=NOCOMP+5
C     SEND ALL HYDROCARBON OVERHEAD
      DO 10 J = 11,JJ
      STRMO(1,J) = STRMI(1,J)
   10 STRMO(2,J) = 0.0
C
C     SPLIT ACID PHASE
C     ONE BARREL PER DAY IS 0.268 LB. MOLE PER HOUR OF ACID
      RAT = EN(NE,2)*0.268/STRMI(1,7)
      DO 11 J = 6,10
      STRMO(1,J) = STRMI(1,J) * RAT
   11 STRMO(2,J) = STRMI(1,J) - STRMO(1,J)
C
C     SUM FLOWS AND TRANSFER TEMPERATURE AND PRESSURE
      DO 12 J = 4,5
      STRMO(1,J) = STRMI(1,J)
   12 STRMO(2,J) = STRMI(1,J)
      STRMO(2,3) = 0.0
      STRMO(1,3) = 0.0
      DO 13 J = 6,JJ
      STRMO(1,3) = STRMO(1,J) + STRMO(1,3)
   13 STRMO(2,3) = STRMO(2,J) + STRMO(2,3)
C
      RETURN
      END
```

```
$IBFTC SETST2
      SUBROUTINE SETST2
C     TEMPERATURE SETTER  -  CALCULATION OF UTILITY USAGE
C     UTILITY USAGE IS OBTAINED FROM A HEAT BALANCE KNOWING THE INLET
C      AND THE REQUIRED OUTLET TEMPERATURE OF THE STREAM
C     WRITTEN BY I. SHAW     MARCH 1968
C
C     EN VECTOR
C     1. EQUIPMENT NUMBER
C     2. REQUIRED OUTLET TEMPERATURE
C     3. CODE FOR UTILITY USAGE
C       - NO UTILITY USAGE TO BE CALCULATED                    0.
C       - 1000 POUNDS PER HOUR OF LOW PRESSURE STEAM           1.
C       - 1000 POUNDS PER HOUR OF MEDIUM PRESSURE STEAM        2.
C       - 1000 POUNDS PER HOUR OF HIGH PRESSURE STEAM          3.
C       - M.M.  B.T.U. OF FIRST TYPE OF FUEL GAS               4.
C       - M.M.  B.T.U. OF SECOND TYPE OF FUEL GAS              5.
C       - K.W. OF ELECTRICITY                                  6.
C       - 1000 IMPERIAL GALLONS OF COOLING WATER               7.
C       - 1000 IMPERIAL GALLONS OF PROCESS WATER               8.
C     4. UTILITY USAGE PARAMETER
C       - IF STEAM,  B.T.U. PER POUND OF STEAM
C       - IF FUEL GAS,  FRACTIONAL EFFICIENCY
C       - IF ELECTRICY,  FRACTIONAL EFFICIENCY
C       - IF WATER COOLING,  OUTLET WATER TEMPERATURE
C     5. EQUIPMENT NUMBER OF COST MODULE (TO LOCATE INLET WATER TEMP.)
C     6. LOCATION OF HEAT CAPACITY COEFFICIENTS FOR THE FLUID
C
C     ******* MACSIM COMMON DECK, FOR ALKYLATION.  T.T. APR.29,1968.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
      COMMON AEN(4,102),ENC(50,20),NOPP,X,XMOLE(26),PPSC(17,26),PPMX(17)
C     *******************************************************************
C
      JJ = NOCOMP + 5
      DO 10 J=3,JJ
   10 STRMO(1,J) = STRMI(1,J)
      STRMO(1,4) = EN(NE,2)
C
      NTYPE = EN(NE,3)+0.001
      IF(NTYPE.LE.0.OR.NTYPE.GT.8)  GO TO 100
      X = (STRMI(1,4)+STRMO(1,4))*0.5
      NOPP = EN(NE,6)
      DO 20 J=1,NOCOMP
   20 XMOLE(J) = STRMI(1,J+5)
      CALL PROMIX(1)
      BTU = PPMX(NOPP)*ABS(STRMI(1,4)-STRMO(1,4))
      NCOST = NTYPE + 10
      GO TO (40,40,40,50,50,60,70,70), NTYPE
C
   40 ENC(NE,NCOST) = BTU/(EN(NE,4)*1000.)
      GO TO 100
   50 ENC(NE,NCOST) = BTU/(1.0E+06*EN(NE,4))
      GO TO 100
   60 ENC(NE,NCOST) = BTU*0.0002930/EN(NE,4)
      GO TO 100
   70 NECOST = EN(NE,5)
      ENC(NE,NCOST) = BTU/(1000.*10.*ABS(EN(NECOST,4)-EN(NE,4)))
  100 RETURN
      END
```

```
$IBFTC SEPA01
C      SUBROUTINE SEPA01  (SEPARATOR - SIMPLE MODULE)
C      REVISED BY T. TOONG      FEB.20,1968
C      *THIS MODULE SETS FRACTIONS OF FEED COMPONENTS INTO TWO STREAMS
C
C      *ONE INPUT STREAM AND TWO OUTPUT STREAMS
C
C      EQUIPMENT VECTOR -
C      1. EQUIPMENT NUMBER
C      2. DESIRED 1ST OUTPUT STREAM TEMPERATURE, DEG F
C      3. DESIRED 2ND OUTPUT STREAM TEMPERATURE, DEG F
C      4. DESIRED 1ST OUTPUT STREAM PRESSURE, PSIA
C      5. DESIRED 2ND OUTPUT STREAM PRESSURE, PSIA
C
C      EQUIPMENT CONTROL VECTOR - OPTIONAL
C
C      STREAM VECTOR -
C      1. STREAM NUMBER
C      2. STREAM FLAG
C      3. TOTAL FLOW,LB MOLES/HR
C      4. TEMPERATURE,DEGREES F
C      5. PRESSURE,PSIA
C      6. FLOW OF COMPONENT 1, LB MOLE/HR
C      7. ETC.
C
C      STREAM CONTROL VECTOR - NOT REQUIRED
C
C      ADDITIONAL EQUIPMENT VECTOR -
C      1. EQUIPMENT NUMBER
C      2. LENGTH OF AEN VECTOR
C      3. TO 5. (BLANK)
C      6.,7.,8.,.... FRACTIONS OF FEED COMPONENTS IN THE 1ST OUTPUT STREAM
C
C
C
C
C
      SUBROUTINE SEPA01
C     ********MACSIM COMMON DECK, FOR ALKYLATION.  APR.30,1968. T.T.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
      COMMON AEN(4,102),ENC(50,20),NORP,X,XMOLE(26),PRSC(17,26),PRMX(17)
C     ******************************************************************
      CALL XDATA
C     CALCULATING FLOWS IN THE OUTPUT STREAMS
      DO 1 I = 1,NOUT
    1 STRMO(I,3)= 0.
      JJ= 5+NOCOMP
      DO 2 J= 6,JJ
      STRMO(1,J)= STRMI(1,J)*AEN(1,J)
      STRMO(2,J)= STRMI(1,J)-STRMO(1,J)
      DO 2 I=1,NOUT
    2 STRMO(I,3)= STRMO(I,3)+STRMO(I,J)
C     SETTING TEMPERATURES AND PRESSURES OF OUTPUT STREAMS
      DO 10 I=1,NOUT
      STRMO(I,4)= EN(NE,I+1)
   10 STRMO(I,5)= EN(NE,I+3)
      RETURN
      END
```

```
$IBFTC STIR01
      SUBROUTINE STIR01
C     SUBROUTINE STIR01 (ALKYLATION STRATCO REACTOR - SIMPLE MODULE)
C     WRITTEN BY O. ORBACH      NOV.,1967
C     REVISED BY T. TOONG       MAR.28,1968
C
C     *THE 1ST INPUT STREAM IS THE HYDROCARBON FEED.
C     *THE 2ND INPUT STREAM IS AN ACID STREAM.
C     *THE 3RD INPUT STREAM IS THE CRUDE ALKYLATE.
C     *THE 1ST OUTPUT STREAM IS ACID AND ALKYLATE TWO PHASE MIXTURE.
C     *THE 2ND OUTPUT STREAM IS THE FLASHED ALKYLATE.
C
C     EN VECTOR -
C     1. EQUIPMENT NUMBER
C     2. TEMP OF FIRST OUTPUT STREAM DEG F
C     3. PRES OF FIRST OUTPUT STREAM PSIA
C     4. TEMP OF SECOND OUTPUT STREAM DEG F
C     5. PRES OF SECOND OUTPUT STREAM PSIA
C     6. MOLE FRACTION OF PROPENE REACTED
C     7. MOLE FRACTION OF ISOBUTENE REACTED
C     8. MOLES IC4 REACTED / MOLE PROPENE REACTED
C     9. MOLES IC4 REACTED / MOLE ISOBUTENE REACTED
C
C
C     ********MACSIM COMMON DECK, FOR ALKYLATION.  APR.30,1968. T.T.****
      COMMON  NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
C     *****************************************************************
C
      JJ= NOCOMP+5
      DO 1  J=6,JJ
      STRMO(1,J)  = STRMI(1,J)+STRMI(2,J)
    1 STRMO(2,J)  = STRMI(3,J)
      STRMO(1,4)  = EN(NE,2)
      STRMO(1,5)  = EN(NE,3)
      STRMO(2,4)  = EN(NE,4)
      STRMO(2,5)  = EN(NE,5)
C
      EC3= STRMO(1,13)*EN(NE,6)
      STRMO(1,13)= STRMO(1,13)-EC3
      STRMO(1,23)= STRMO(1,23)+EC3
      EC4= STRMO(1,17)*EN(NE,7)
      STRMO(1,17)= STRMO(1,17)-EC4
      STRMO(1,26)= STRMO(1,26)+EC4
      STRMO(1,15)= STRMO(1,15)-EC3*EN(NE,8)-EC4*EN(NE,9)
C
      STRMO(1,3)= 0.
      DO 2  J=6,JJ
    2 STRMO(1,3)  = STRMO(1,3)+STRMO(1,J)
      STRMO(2,3)  = STRMI(3,3)
      RETURN
      END
```

```
@IPETC WASH01
      SUBROUTINE WASH01
C     REVISED FEB 25 , 1968                           A.J. ORLICKAS
C     CAUSTIC WASH SETTLER MODEL
C     GIVEN A CAUSTIC SOLUTION FLOW RATE OF KNOWN WEIGHT PERCENT
C     AND A HYDROCARBON STREAM OF KNOWN CONCENTRATION.
C     THIS MODEL PREDICTS NEUTRALIZATION PRODUCTS AND THE SPLIT
C     OF THESE PRODUCTS INTO THE HYDROCARBON STREAM AND THE SEWER STREAM
C     BY USING SOLUBILITY AND ENTRAINMENT FACTORS
C
C     EQUIPMENT VECTOR
C     1. EQUIPMENT NO.
C     2. FRACTION OF TOTAL UNDISSOLVED WATER LEAVING IN THE HYDROCARBON
C           STREAM (ABOUT 0.1)
C     3. PHYSICAL PROPERTIES CODE FOR LIQUID SPECIFIC HEATS
C
C     STRMI(1,J) IS THE HYDROCARBON INPUT STREAM
C     STRMI(2,J) IS CAUSTIC INPUT STREAM
C     STRMO(1,J) IS THE HYDROCARBON OUTPUT STREAM
C     STRMO(2,J) IS THE EXIT STREAM TO THE SEWER
C
C     ********MACSIM COMMON DECK, FOR ALKYLATION.  APR.30,1968. T.T.****
      COMMON NOCOMP,KSETS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
      COMMON AEN(4,102),ENC(50,20),NOPP,X,XMOLE(26),PPSC(17,26),PPMX(17)
C
      JJ = NOCOMP + 5
C     MOLAR FLOW RATES OF BASE AND WATER IN CAUSTIC
      FMOLT = STRMI(2,8) + STRMI(2,6)
      IF (STRMI(1,7) .GT.(0.5*STRMI(2,8))) GO TO 20
C
C     CASE 1       MORE CAUSTIC THAN ACID ENTERS
C     FBASE -- INLET BASE FLOW RATE AFTER REACTION
      FBASE = STRMI(2,8) - 2.0*STRMI(1,7)
      FRECW = 2.0 * STRMI(1,7)
      STRMO(1,7) = 0.0
      STRMO(2,7) = 0.0
      Z = 2.0
      GO TO 22
C
C     CASE 2.   MORE ACID THAN CAUSTIC ENTERS SETTLER
C     FACID -- INLET ACID FLOW RATE AFTER REACTION
20    FACID = STRMI(1,7) - 0.5*STRMI(2,8)
      WRITE(6,9999) NE
 9999 FORMAT( 43H *** NOT ENOUGH CAUSTIC IS FED TO EQUIPMENT, I5)
      FRECW = STRMI(2,8)
      STRMO(1,8) = 0.0
      STRMO(2,8) = 0.0
      Z = 1.0
22    FSALTS = STRMI(1,7) + STRMI(1,9)
C
C     WATER OUT IN HYDROCARBON STREAM
      X = STRMI(1,4)
      DO 12 J=1,NOCOMP
   12 XMOLE(J) = STRMI(1,J+5)
      CALL FSOL ( FSOLW )
C     FENTW = FLOWRATE OF ENTRAINED WATER
C     FINW -- TOTAL INPUT WATER FLOW RATE
      FINW = FRECW + STRMI(1,6) + STRMI(2,6)
      FENTW = (FINW-FSOLW)*EN(NE,2)
```

```
      STRMO(1,6) = FENTW + FSOLW
      IF ( STRMO(1,6) .LE. FINW ) GO TO 23
      STRMO(1,6) = FINW
23    STRMO(2,6) = FINW - STRMO(1,6)
C
      DO 8 J = 11 , JJ
      STRMO(1,J)= STRMI(1,J)
8     STRMO(2,J) = 0.0
C
      RAT = (STRMO(1,6)-FSOLW) / ( FINW - FSOLW)
      STRMO(1,10) = STRMI(1,10) * RAT
      STRMO(2,10) = STRMI(1,10) - STRMO(1,10)
      IF ( Z .EQ. 1.0 ) GO TO 37
      STRMO(1,8)=(FBASE*RAT)
      STRMO(2,8)=FBASE - STRMO(1,8)
      GO TO 36
37    STRMO(1,7) = FACID*RAT
      STRMO(2,7) = FACID - STRMO(1,7)
      STRMO(1,9) = FSALTS * RAT
      STRMO(2,9) = FSALTS - STRMO(1,9)
C
36    STRMO(1,5) = STRMI(1,5)
      STRMO(2,5) = STRMI(1,5)
      STRMO(1,3) = 0.0
      STRMO(2,3) = 0.0
      DO 35 J = 6,JJ
      STRMO(1,3) = STRMO(1,J) + STRMO(1,3)
35    STRMO(2,3) = STRMO(2,J) + STRMO(2,3)
C
C     HEAT BALANCE
      CPTOT = 0.0
      ENTH = 0.0
      NOPP = EN(NE,3)
      DO 26 I = 1,NIN
      X = STRMI(I,4)
      DO 27 J = 1,NOCOMP
27    XMOLE(J) = STRMI(I,J+5)
      CALL PROMIX(1)
      CPTOT = CPTOT + PPMX(NOPP)
26    ENTH = ENTH + PPMX(NOPP)*X
      TOUT = ENTH/CPTOT
      STRMO(1,4) = TOUT
      STRMO(2,4) = TOUT
C
      RETURN
      END
```

```
$IBFTC WASH02
      SUBROUTINE WASH02
C
C     WATER WASH SETTLER
C     REVISED FEB 25 , 1968                          A.J. ORLICKAS
C     THIS MODEL WASHES THE HYDROCARBON STREAM
C     WATER DISOLVED IN THE HYDROCARBON AND ENTRAINED WATER LEAVE BY THE
C     EXITING HYDROCARBON STREAM, THE REMAINDER OF THE WATER LEAVES BY
C     SEWER. THE SPLIT OF THE CAUSTIC, ALKYL SULFATES AND THE SALT ARE
C     PROPORTIONAL TO THE SPLIT OF THE WATER
C
C     STRMI(1,J) IS THE INPUT HYDROCARBON STREAM
C     STRMI(2,J) IS THE INPUT WATER WASH STREAM
C     STRMO(1,J) IS THE OUTPUT HYDROCARBON STREAM
C      STRMO(2,J) IS THE OUTPUT STREAM TO THE SEWER
C
C     EN VECTOR
C     1. EQUIPMENT NO.
C     2. FRACTION OF TOTAL UNDISSOLVED WATER LEAVING IN THE HYDROCARBON
C          STREAM (ABOUT 0.1)
C     3. PHYSICAL PROPERTIES CODE FOR LIQUID SPECIFIC HEATS
C
C     ********MACSIM COMMON DECK, FOR ALKYLATION.  APR.30,1968. T.T.****
      COMMON NOCOMP,KSFTS,NIN,NOUT,NE,STRMI(5,31),STRMO(5,31),EN(50,20)
      COMMON AEN(4,102),ENC(50,20),NOPP,X,XMOLE(26),PPSC(17,26),PPMX(17,
C
C     FWAT --- WASH WATER FEED RATE
C     FWATT --- TOTAL INPUT WATER FLOWRATE
C     FENTW --- ENTRAINED WATER IN H.C. STREAM
      FWAT = STRMI(2,6)
      JJ = NOCOMP + 5
C
      X = STRMI(1,4)
      DO 12 J=1,NOCOMP
   12 XMOLE(J) = STRMI(1,J+5)
      CALL FSOL ( FSOLW )
      FWATT = FWAT + STRMI(1,6)
C
      IF ( FSOLW .GE. FWATT ) GO TO 20
      FENTW = (FWATT - FSOLW ) * EN(NE,2)
      STRMO(1,6) = FENTW + FSOLW
      IF ( STRMO(1,6) .GE. FWATT ) GO TO 20
      STRMO(2,6) = FWATT - STRMO(1,6)
      GO TO 21
20    STRMO(1,6) = FWATT
      STRMO(2,6) = 0.0
21    RAT = (STRMO(1,6) - FSOLW)/(FWATT - FSOLW)
      STRMO(1,3) = STRMO(1,6)
      STRMO(2,3) = STRMO(2,6)
      DO 25 J = 7,10
      STRMO(1,J) = STRMI(1,J)*RAT
      STRMO(2,J) = STRMI(1,J) - STRMO(1,J)
      STRMO(1,3) = STRMO(1,3) + STRMO(1,J)
25    STRMO(2,3) = STRMO(2,3) + STRMO(2,J)
      DO 10 J = 11 , JJ
      STRMO(2,J) = 0.0
      STRMO(1,J) = STRMI(1,J)
10    STRMO(1,3) = STRMO(1,3) + STRMO(1,J)
C
```

```
C
C       TRANSFER PRESSURES
        STRMO(1,5) = STRMI(1,5)
        STRMO(2,5) = STRMI(1,5)
C
C       HEAT BALANCE
        CPTOT = 0.0
        ENTH = 0.0
        NOPP = EN(NE,3)
        DO 26 I = 1,NIN
        X = STRMI(I,4)
        DO 27 J = 1,NOCOMP
 27     XMOLE(J) = STRMI(I,J+5)
        CALL PROMIX(1)
        CPTOT = CPTOT + PPMX(NOPP)
 26     ENTH = ENTH + PPMX(NOPP)*X
        TOUT = ENTH/CPTOT
        DO 28 I = 1,2
 28     STRMO(I,4) = TOUT
C
        RETURN
        END
```