

A  
DISSERTATION REPORT  
ON  
PROCESS MODELING AND SIMULATION OF SOLVENT  
EXTRACTION COLUMN FOR EXTRACTION OF  
AROMATICS

PROJECT DISSERTATION SUBMITTED IN PARTIAL  
FULFILLMENT  
OF THE REQUIREMENT  
FOR  
BACHELOR DEGREE IN APPLIED PETROLEUM ENGINEERING  
By

Vineet Chawla

R010103050

Under the guidance of

Mr. T. Chandrashekhar



UNIVERSITY OF PETROLEUM AND ENERGY STUDIES, DEHRADUN

UPES - Library



D1884

CHA-2007BT



## UNIVERSITY OF PETROLEUM & ENERGY STUDIES

### CERTIFICATE

*This is to certify that the project report on “Modeling and Simulation of Solvent Extraction Column for the Extraction of Aromatics” submitted to UPES, Dehradun by Mr. Vineet Chawla in partial fulfillment of the requirements for the degree of Applied Petroleum Engineering & academic session (2003-2007) is a bonafide work carried out by him under my supervision & guidance.*

Date:

*T. Chandrashekhar*  
*3/05/07*

Mr. T. Chandrashekhar  
(Lecturer- COE, UPESDDN)

Corporate Office :  
Hydrocarbons Education & Research Society  
3rd Floor, PHD House 4/2, Siri Institutional Area  
August Kranti Marg, New Delhi-11001 India  
Ph : + 91-11-41730151-53 Fax : +91-11 1730154

Main Campus :  
Energy Acres, PO Bidholi, Via Prem Nagar,  
Dehradun-248 007 (Uttaranchal) India  
Ph : +91-135-2261090-91, 2694201/203/208  
Fax : +91-135-2694204

Regional Centre (NCR) :  
SCO 9-12, Sector-14, Gurgaon 122 007  
(Haryana), India  
Ph : + 91-124-4540300  
Fax : +91 124 4540 330

## INDEX

1. Introduction	01
a. Aromatics Extraction	01
2. Applications	02
3. Solvent Extraction and its Recovery Process	03
a. Characteristics of the Solvent	05
b. Comparison of Furfural, NMP and Phenol	06
4. Different type of Extraction Processes	08
a. Edeleanu Process	08
b. Udex Process	09
c. Sulfolane Process	09
5. Types of Extractors	10
a. DIFFERENTIAL (CONTINUOUS-CONTACT) EXTRACTORS	10
b. SPRAY TOWERS	12
c. PACKED TOWERS	13
d. MECHANICALLY AGITATED COUNTERCURRENT EXTRACTORS	16
e. MIXED LIGHTNING CONTACTOR	16
f. ROTATING DISK CONTACTOR	18
g. SCHEIBEL EXTRACTOR	19
h. KARR EXTRACTOR	20
i. TREYBAL EXTRACTOR	20

j. GRAESSER EXTRACTOR	20
k. PULSED COLUMNS	21
l. CENTRIFUGAL EXTRACTOR	22
6. Models of Extractors	23
7. Process modeling and Simulation	29
8. Simulation	31
9. Model for counter – current extraction	35
10. CASE STUDY 1	40
11. C++ Computer Program	42
12. CASE STUDY 2	45
13. Literature Survey	49
14. Bibliography	58

## ACKNOWLEDGEMENT

We the Students of 8<sup>th</sup> Semester of B.Tech (Applied Petroleum Engineering). University of Petroleum and Energy Studies, Dehradun. would like to take this opportunity to thank Mentor **MR. T.CHANDRASHEKHAR** for giving us valuable inputs without which this project would not have been such a success.

We are really indebted to the constant motivation provided by my respected **Dean Dr. B.P. Pandey** who has been a torchbearer and a driving force in bringing up this uphill task.

We would specially like to thank **Mr. Kamal Bansal** our project coordinator for allowing us to join the major project program.

We are also indebted to all the lecturers of my class whose constant inspiration and unwaning enthusiasm made me intrepid to face all the crests and troughs of life. The university has also been a great help in making of this project especially the library.

Above all, we are indebted to my parents whose moral guidance and support helped me reach to this great position.

# INTRODUCTION

## AROMATICS EXTRACTION

Aromatics (Benzene, Toluene, Xylenes) are high value petrochemicals produced by the catalytic reforming of naphthas, and recovered from the "reformate" stream by extraction. The reformate may be produced specifically as a source of BTX, or as a high-octane gasoline blending component. Whether or not other aromatics are recovered, it is sometimes necessary to remove benzene from reformate in order to meet US Environmental Protection Agency (EPA) mandated specifications on gasoline composition.

HEA's experience includes both the principles and operating practice of liquid-liquid extraction and extractive distillation, proper operating techniques for maintenance of solvent purity, and BTX separations and product specifications. HEA is familiar with the major proprietary licensed extraction processes and solvents including the Udex, Sulfolane, and Carom processes, and glycol (di-, tri-, and tetra-ethylene), and sulfolane solvents.

## APPLICATIONS

Removal of aromatic compounds can be desirable for two different reasons. Either the aromatics have detrimental effects on the quality of the mixture they're in, or the aromatics are worth more if they are separated than if they're not.

- For example now a days benzene composition is limited in the gasoline up to a certain % so removal of benzene from gasoline has become necessary to meet the specifications.
- Aromatic compounds in kerosene cause unacceptable smoke points.
- Kerosene range solvents that are aromatics free or aromatics-laden have various industrial applications
- Separated benzene, xylene, and toluene have numerous chemical applications
- Removing aromatics from heavy gas oil stocks can improve the lubricating oil characteristics

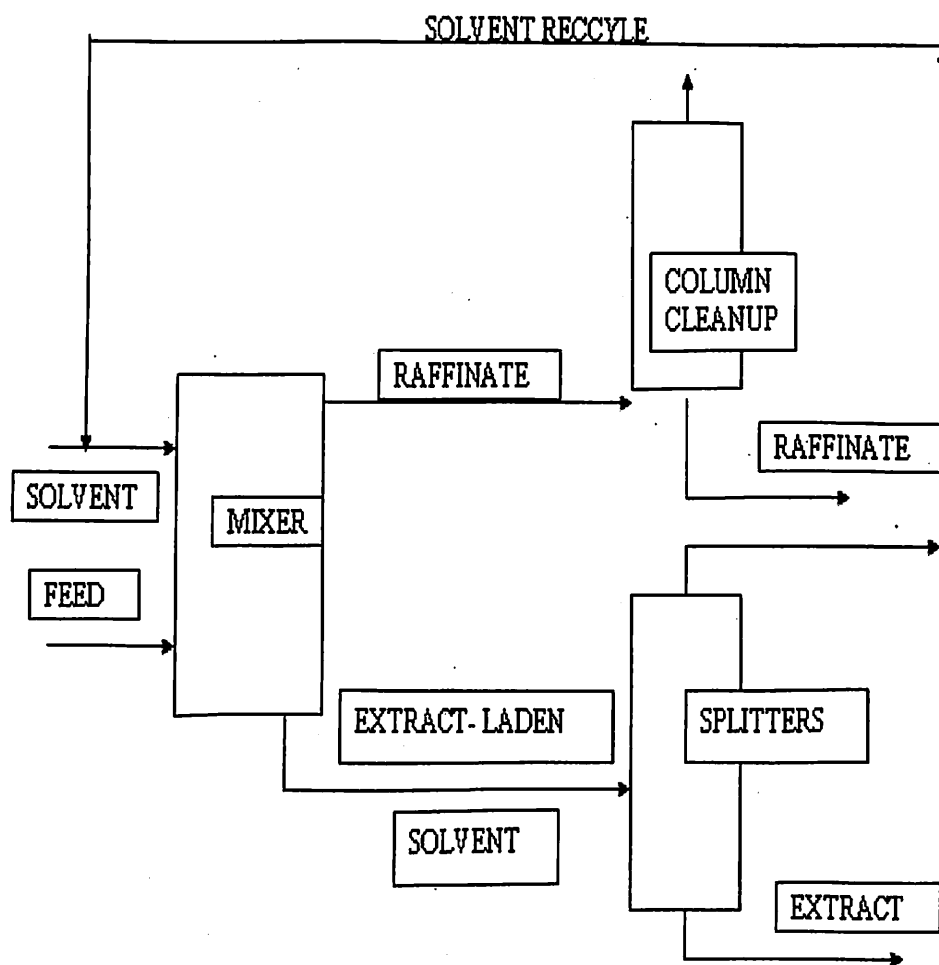
## **Solvent extraction and its Recovery process**

The solvent recovery is based upon the ability of certain compounds to dissolve certain classes of other compounds to dissolve certain classes of other compounds selectively. In this case certain solvents will dissolve aromatics but not paraffins, olefins, or naphthenes.

The first co-requisite that makes this approach successful is that the solvent with the extracted compounds dissolved in it readily separating itself from the starting hydrocarbon mixture. The second co-requisite is that the solvent and the dissolved extract can easily be split in a Fractionator.

Knowing how a simple batch process works, a continuous flow process is easy to conceptualize. In fig- a three-column system is shown. The feed is introduced as a vapour into the lower part of a vessel or column with a labyrinth of mixers inside. Some times the mixers are mechanically moved, such as in rotating disc contractor. The solvent is introduced as a liquid near the top. The solvent works its way towards the bottom of the vessel, dissolving the extract as it goes along the rest of the hydrocarbon, which rises to the top, is called the raffinate.





SOLVENT EXTRACTION AND RECOVERY PROCESS

## **Characteristics of the solvent**

The following characteristics are to be considered in the selection of a solvent for use in commercial extraction process: -

1. Solvent should possess high selectivity for undesirable components.
2. Solvent should have good solvent power to keep low solvent to feed ratio.
3. Solvent should be such that can employ high extraction temperature for good mass transfer.
4. Solvent must be easy to recover from extract and raffinate streams by simple flash distillation.
5. Solvent should have low vapour pressure in order to avoid use of pressure equipment.
6. Solvent should have high density so that rapid separation of oil and solvent phases can take place.
7. Solvent should not show emulsification so that rapid separation of oil and solvent phase can take place.
8. Solvent must be stable to avoid its chemical or thermal degradation.
9. Solvent must be adaptable to a wide range of feed stocks.
10. Solvent must be adaptable at low cost.
11. Solvent must be non-corrosive to conventional material of construction.
12. Solvent must be non-toxic, i.e. environmentally safe.

The most common solvents used today in commercial solvent extraction processes are furfural, phenol and N-methyl-2-pyrrolidone (NMP).

## **Comparison of Furfural, NMP and Phenol**

Some information indicates that there are economical and technical advantages. For example, solvent cost is lower for phenol, but physical properties and selectivity are best for furfural. However, NMP exhibits better solvent power, better chemical and thermal stabilities and lower toxicity than either furfural or phenol.

Also some information indicates that furfural is adaptable to a wider range of feed stocks, emulsifies less or separates from the oil more easily, and in some cases provides a better yield of refined oil. On the other hand, NMP is the best in the areas of solvent circulation and it requires less corrosion protection. This results in the lowest requirements in energy, investment and operating costs.

Although there are technical advantages of each of these solvents for use in the extraction of lube stocks, furfural remains the solvent of choice in many parts of the world. The major factors favoring its use are low toxicity, low cost availability, history of commercial experience, adaptability to extraction of gas oils and better selectivity in the extraction of those lube stocks which exhibit excellent refining response at low solvent to oil ratios. For these reason furfural is at present most widely used solvent for the extraction of both paraffinic and naphthenic lube stocks.

Phenol is considered to be suitable for the extraction of paraffinic lube stocks which require high extraction temperatures and is in general less suitable than furfural for the extraction of naphthenic lube stocks. The yield of refined oil is usually somewhat lower with phenol than that obtained with either furfural or NMP. The selectivity of phenol is improved by inclusion of water in the solvent

or by the injection of water into the feed or lower stages of extractor. The main disadvantages of phenol are its limited adaptability to different type of feed stocks and high toxicity which requires special handling precautions and special facilities to protect employees and the environment. For these reasons petroleum refiners are converting phenol extraction units to use either furfural or NMP.

The non-toxic nature, high solvent power, good selectivity and adaptability to the extraction of both paraffinic and naphthenic feed stocks, make NMP an attractive to, or replacement for phenol. When available, NMP is an attractive alternative to furfural for extraction of both high viscosity feed stocks and certain feed stocks, of both high and low viscosity, which have poor refining response or which require high solvent to oil ratios. The yield of refined oil is, in general, higher with NMP than with phenol, but is slightly lower than the yield obtained with furfural. In the refining of certain feed stocks the selectivity of NMP, like that of phenol can be improved through the use aqueous solvent. The major disadvantages to the use of NMP are its cost and limited availability in certain parts of the world. In addition, the high boiling point and non-azeotropic nature of NMP limits its use to lube stocks or gas oils with initial boiling points.

## Solvent Extraction Processes

### Edeleanu Process

The Edeleanu process is the oldest liquid-liquid extraction process used in the petroleum industry and uses liquid sulphur dioxide as the solvent. At the normal boiling point of sulfur dioxide of  $-10.0^{\circ}\text{C}$ , aromatic and unsaturated hydrocarbons are completely miscible with liquid sulphur dioxide but the paraffinic and naphthenic hydrocarbons are not. Sulphur dioxide treatment also removes cyclic sulphur compounds and nitrogen compounds.

The Edeleanu process has long been used in the manufacture of premium kerosene, which involves the removal of aromatics leading to enhanced burning properties. Straight-run kerosene cut ( $150-250^{\circ}\text{C}$ ) obtained from Assam crude as such is unsuitable for marketing purposes because of its high aromatic content. Kerosene with high aromatic content burns with a smoky flame. In order, therefore, to produce a superior quality of kerosene which will burn with a stipulated flame height without smoke, the straight-run kerosene is treated with liquid sulphur-dioxide to reduce its aromatic content. This process is also applied to selected naphthas for the recovery of high octane number blending stocks and for the recovery of lacquer diluents. Diesel oils of high diesel index and improved ignition quality can be made from selected gas oils. The operating conditions in the  $\text{SO}_2$  extraction process vary from  $-30^{\circ}\text{C}$  for kerosene and other light stocks to  $150^{\circ}\text{C}$  or higher pour point material. The high

solvent power and selectivity of sulphur dioxide permit solvent ratios of the order of 0.5 to 1.5 volumes of solvent per volume of oil.

### **Udex process**

Udex process developed by Universal Oil Products uses concentrated aq. solution of di- or tri-ethylene glycol for the extraction of benzene, toluene, xylenes, and heavy aromatics from straight-run naphthas or from reformed naphthas rich in aromatics. This process is used in Gujarat refinery for the manufacture of benzene and toluene from reformat. Benzene is used as raw material for the manufacture of caprolactum which is used as raw material for Nylon-6. Benzene is also used for the manufacture of styrene monomer, styrene resins, cyclohexane, phenol, phenolic resins, DDT and detergents. Toluene is mainly used for manufacturing TNT for defense purposes. Toluene is also used for the manufacture of various chemicals like benzoic acid, benzaldehyde, benzyl chloride, vinyl toluene for the manufacture of flexible and rigid foams

### **Sulfolane process**

Sulfolane process is reliable and efficient process for the production of high purity aromatics (benzene, toluene, and xylenes), high-octane aromatic concentrates, jet fuel components and specially solvents of closely controlled aromatics contents, by extraction of suitable feed stocks. This process is also applicable for de-aromatization of naphthas for producing food-grade hexane solvent or for making it suitable as feedstock for the fertilizer industry.

This process uses sulfolane as the extraction solvent. Sulfolane has extremely favorable combination of selectivity and solvent power. The additional features of sulfolane include its high specific gravity, low heat capacity, relatively high boiling point (2870 C) and good stability.

## **Different Types of Extractors**

### **DIFFERENTIAL (CONTINUOUS-CONTACT) EXTRACTORS**

When the liquids flow counter currently through a single piece of equipment, the equivalent of as many theoretical stages may he had as desired. In such devices, the countercurrent flow is produced by virtue of the difference in densities of the liquids, and if the motivating force is the force of gravity, the extractor usually takes the form of a vertical tower, the light liquid entering at the bottom, the heavy liquid at the top. As an alternative, a larger centrifugal force can be generated by rotating the extractor rapidly, in which case the counter flow is radial with respect to the axis of revolution.

There are several characteristics common to countercurrent extractors which have an important bearing upon their design and performance. It is typical that only one of the liquids can be pumped through the device at any desired rate. The maximum rate for the other will depend, among

other things, upon the density difference of the liquids. If an attempt is made to exceed this rate for the second liquid, the extractor will reject one of the liquids, and it is said to be *flooded*. The same is true, of course, for gas-liquid contactors, but since the density difference is much smaller than for a gas and liquid, the flooding velocities of extractors are much lower. For a given volumetric rate of liquids to be handled, the extractor cross section must be large enough to ensure that the flooding velocities are not reached. The more open the cross section, the greater the flow rates before flooding occurs. Internal structures, packing, mechanical agitators, and the like normally reduce the velocities at which flooding occurs.

The differential extractors are also subject to *axial mixing*; it severely reduces extraction rates because of the deterioration of the concentration differences between phases which is the driving force for mass transfer. This is illustrated in Fig. 1, where the real (axial-mixing) concentration profiles show a substantially smaller concentration difference than those for plug flow. If the flow ratio of the liquids is not unity, and it very rarely is, dispersing the liquid flowing at the lower rate will lead to small numbers of dispersed-phase 'drops, small interfacial areas, and small mass-transfer rates. On the other hand, if the majority liquid is dispersed, the axial-mixing problem is exacerbated. The problem becomes more acute the greater the flow ratio and this difficulty is common to all differential extractors.



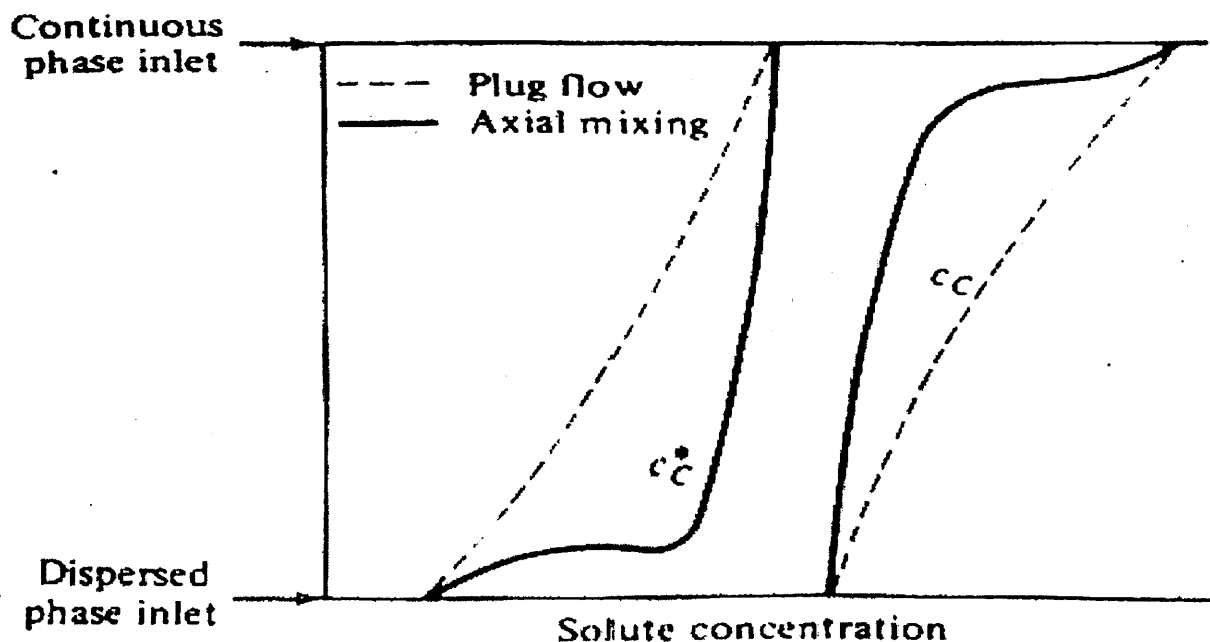


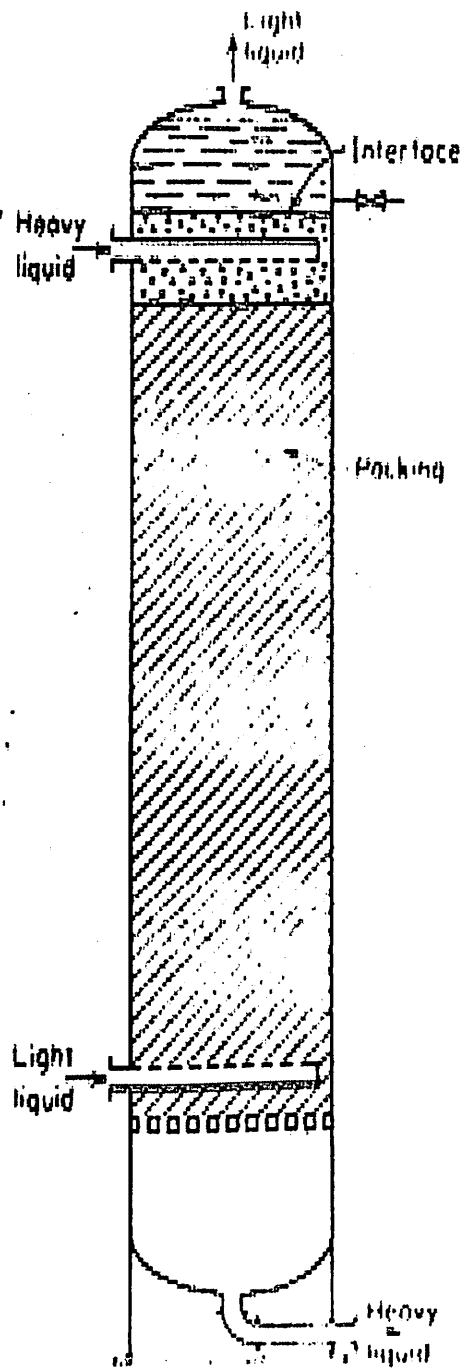
Figure 1 Effect of axial mixing on concentration profiles in towers subject to axial mixing.

## SPRAY TOWERS

These, the simplest of the differential-contact devices, consist merely of an empty shell with provisions at the extremities for introducing and removing the liquids. Because the shell is empty, the extreme freedom of liquid movement makes these towers the worst offenders as far as axial mixing is concerned, so much so that it is difficult to obtain much more than the equivalent of a single stage with them. It is not recommended that they be used. Horizontal baffles (both the segmental and the disk-and-doughnut type) have been used to reduce the axial mixing but with little improvement in results. Spray towers have also been fairly extensively studied for direct-contact heat exchange between two liquids, but the deleterious effects of axial mixing are just as severe in this service as for extraction.

## PACKED TOWERS

Towers filled with the same random packings used for gas-liquid contact have also been used for liquid extractors. The packing serves to reduce axial mixing somewhat and to jostle and distort the drops of dispersed phase. A typical packed tower is shown schematically in Fig. 2, arranged for light liquid dispersed. The void space in the packing is largely filled with the continuous heavy liquid, which flows downward. The remainder of the void space is filled with droplets of light liquid formed at the lower distributor, which rise through the heavy liquid and coalesce at the top into a bulk layer, forming an interface as shown. To maintain the interface in this position, the pressure of liquid in the tower at the bottom must be balanced by a corresponding pressure in the bottom outlet pipe, as set by a control valve. If the pressure drop through that valve is reduced, the weight of the contents of the tower adjusts to a lower value, the light liquid becomes continuous, the heavy liquid dispersed, and the interface falls to below the light-liquid distributor. The interface positions are best regulated by a liquid-level control instrument activating the bottom outlet valve. The valve just above the interface in Fig. 2 is for periodic removal of scum and dust particles (*rag*) which accumulate at the interface.



*Fig.2 Packed Extraction Tower*

The nature of the liquid flow in such towers requires that the choice of packing and arrangement of dispersed-phase distributor be given careful attention. If the dispersed liquid preferentially wets the packing, it will pass through in rivulets on the packing, not as droplets, and the interfacial area produced will be small. For this reason, the packing material should be preferentially wetted by the continuous phase. Usually, ceramics are preferentially wet by aqueous liquids and carbon and plastics by organic liquids. The packing should be sufficiently small, no greater than one-eighth the tower diameter, for the packing density to be fully developed yet larger than a certain critical size (see below). Where the material of the packing support is not wet by the dispersed droplets and the distributor is placed outside the packing, the drops will have difficulty in entering the packing and premature flooding results. For this reason it is always desirable to embed the dispersed-phase distributor in the packing, as in Fig. 2

Correlations for estimating flooding rates are available, and data for mass transfer coefficients and axial mixing have been summarized.

Although axial mixing is less severe than in spray towers, mass-transfer rates are poor. It is recommended instead that sieve-tray towers be used for systems of low interfacial tension and mechanically agitated extractors for those of high interfacial tension.

## **MECHANICALLY AGITATED, COUNTERCURRENT EXTRACTORS**

The extraction towers previously described are very similar to those used for gas-liquid contact, where density differences between liquid and gas are of the order of  $800 \text{ kg/m}^3$  ( $50 \text{ lb/ft}^3$ ) or more, <sup>available</sup> to provide the energy for good dispersion of one fluid into the other. In liquid extractors, where density differences are likely to be one-tenth as large or less, good dispersion of systems of high interfacial tension is impossible in such towers, and mass-transfer rates are poor. For such systems, dispersion is best brought about by mechanical agitation of the liquids, whereupon good mass-transfer rates are developed.

Some examples of such extractors follow. Except for pulse columns, they are proprietary devices for which complete design procedures are not publicly available, and the manufacturers are best consulted.

### **Mixco Lightning CMContactor (Oldshue-Rushton Extractor)**

This device uses flat-blade disk turbine impellers to disperse and mix the liquids and horizontal compartmenting plates to reduce axial mixing. There have been a few mass-transfer and somewhat more extensive axial-mixing studies.

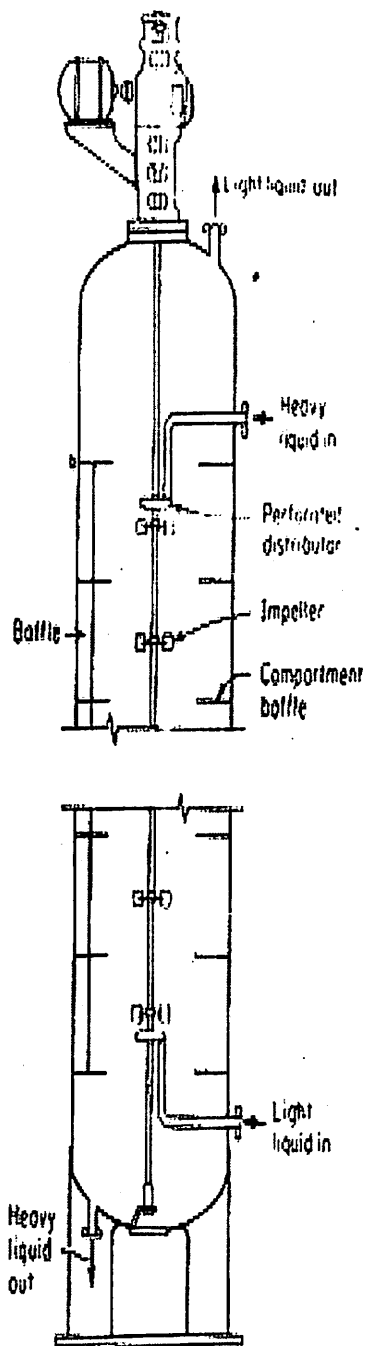
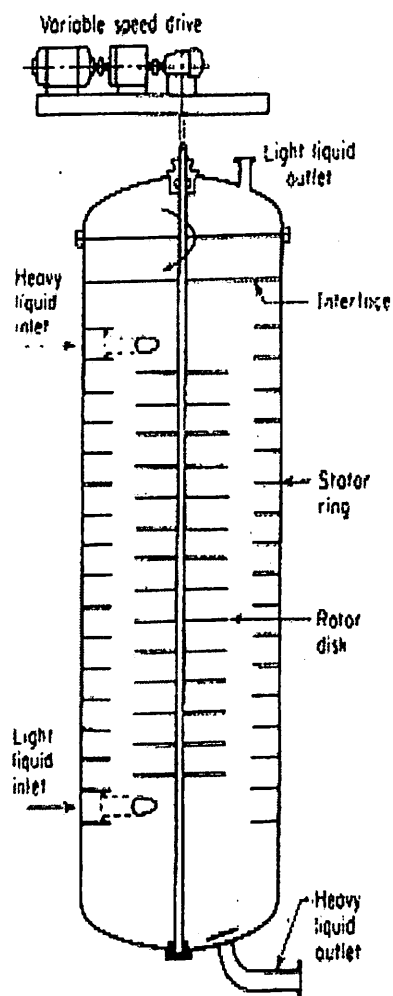


Fig. 3 Mixco Lightnin CMContractor

## ROTATING-DISK CONTACTOR (RDC)

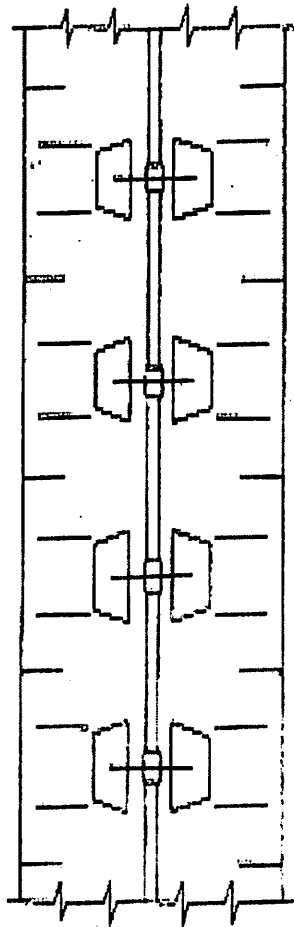
This (Fig.4) is a somewhat similar device, except that the vertical baffles are omitted and agitation results from rotating disks, which usually turn at much higher speeds than turbine-type impellers.



*Fig. 4 Rotating Disc Contactor*

## **SCHEIBEL EXTRACTOR**

There have been several designs, of which the most recent is shown in Fig. 5. The impellers are of the turbine type, and the doughnut-type baffles surrounding them are supported by vertical tie rods, not shown. Earlier designs included sections of knit, wire-mesh packing alternating with sections containing an impeller.



*Fig. 5 Scheibel Extractor*



## **KARR RECIPROCATING - PLATE EXTRACTOR**

This follows an early design of van Dijk, who suggested moving the plates of a perforated-plate extractor of the type shown in Fig. 6 up and down. The Karr design uses plates of much larger free area, fitting loosely in the tower shell and attached to a vertical, central shaft. They are moved vertically up and down over a short distance.

## **TREYBAL EXTRACTOR**

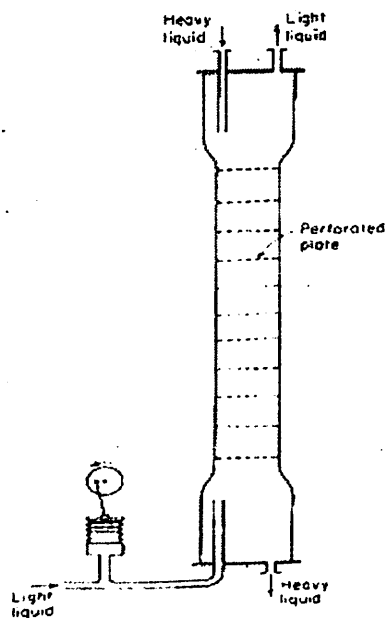
This is in reality a vertical stack of mixer-settlers. The mixers are in a vertical line, and the impellers for the stages on a common shaft. They not only mix but also pump, so that throughput rates are high. Since there is no axial mixing, mass-transfer rates are high.

## **GRAESSER EXTRACTOR**

This is a horizontal shell fitted with a series of rotating disks on a central horizontal shaft. C'-shaped buckets between the disks shower the liquids, one in the other, as they flow counter currently and horizontally through the extractor. It has been used especially in Europe.

## PULSED COLUMNS

A rapid (0.5 to 4 s<sup>-1</sup>) reciprocating pulse of short amplitude (5 to 25 mm) is hydraulically transmitted to the liquid contents. Since the extractors have no moving parts, they have found extensive (and exclusive) use in processing radioactive solutions in atomic-energy work, where they can be put behind heavy radiation shields without requiring maintenance. The most common arrangement is that of Fig. 10.55; the perforated plates, which have no downspouts, are drilled with very small holes so that ordinarily flow will not occur. The pulsing superimposed upon the liquids alternately forces light and heavy liquids through the perforations. Packed columns, indeed any type of extractor, can also be pulsed. Although the mass-transfer rates are thereby improved at the expense of substantial energy costs, the flow capacities become smaller.



*Fig 6 Pulsed Column*

## CENTRIFUGAL EXTRACTORS

The most important of these is the *Podbielniak extractor* (Fig. 7). The cylindrical drum containing perforated concentric shells is rapidly rotated on the horizontal shaft (30 to 85 r/s). Liquids enter through the shaft: heavy liquid is led to the center of the drum, light liquid to the periphery. The heavy liquid flows radially outward, displacing the light liquid inwardly, and both are led out through the shaft. These extractors are especially useful for liquids of very small density difference and where very short residence times are essential, as in some pharmaceutical applications, e.g., extraction of penicillin from nutrient broth.

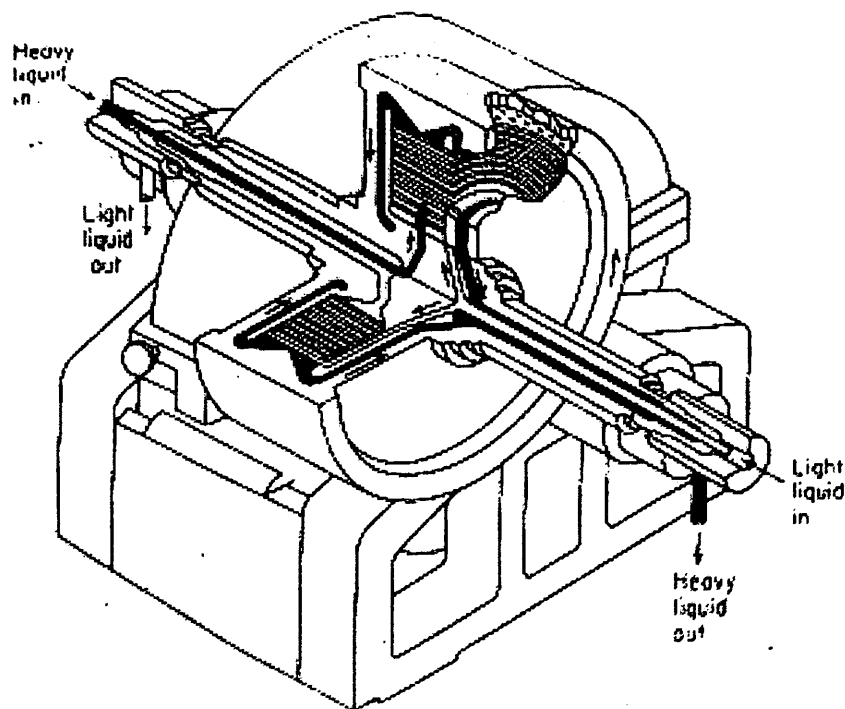


Fig.7 Podbielniak Centrifugal extractor

# MODELS OF EXTRACTORS

## Design

Since the change in concentration with height of either liquid as it passes through the extractor is differential, the height of the tower is expressed not in terms of stages or steps but in terms of transfer units.

Consider the continuous-contact tower of Fig.8. Although the raffinate is shown flowing downward as if it were denser, in some instances the solvent rich, or extract, phase will be denser and will enter at the top. In either case, in what follows subscript 1 will always represent that end of the tower where the raffinate enters and extract leaves, while subscript 2 will indicate where extract enters and raffinate leaves. We are presently unconcerned with which phase is dispersed and which is continuous. If the extractor is fed along the side, Fig.8 and the relationships which *follow apply* separately to each section above and below the feed inlet.

Throughout this discussion, *unless otherwise specified*  $x$  and  $y$  will refer to solute concentrations expressed as mole fractions in the raffinate and extract, respectively, and rates of flow of raffinate  $R$  and of extract  $E$  will be expressed - as mol/(cross-sectional area)(time). Except in special cases, the transfer of solute usually results in changes of mutual solubility of the contacted liquids, so that in general all components of the systems transfer from one phase to the other. The F-type mass-transfer coefficients are capable of handling this problem, but in reality our knowledge of mass-transfer rates in extractors is so poorly developed that we can ordinarily consider only the transfer of a single solute. This discussion is therefore

limited to cases where the liquids are insoluble, only solute is transferred, and mutual solubility unchanged. In practice, however, the expressions developed are used for all cases.

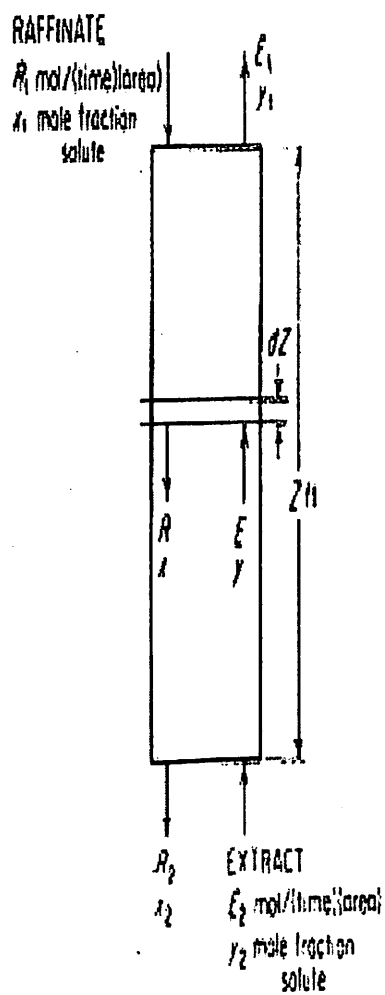


Fig. 8 Continuous Contact Tower

$$Z = \int_{x_2}^{x_1} \frac{R(1-x)_{iM} dx}{F_R a (1-x)(x-x_i)} = H_{iR} \int_{x_2}^{x_1} \frac{(1-x)_{iM} dx}{(1-x)(x-x_i)} = H_{iR} N_{iR}$$

$$H_{iR} = \frac{R}{F_R a} = \frac{R}{k_R a (1-x)_{iM}}$$

$$N_{iR} = \int_{x_2}^{x_1} \frac{(1-x)_{iM} dx}{(1-x)(x-x_i)} = \int_{x_2}^{x_1} \frac{dx}{x-x_i} + \frac{1}{2} \ln \frac{1-x_2}{1-x_1}$$

Where  $x_i$  = interface concentration of solute

$F_R, k_R$  = transfer coefficient for raffinate phase

$H_{iR}$  = raffinate height of transfer unit

$N_{iR}$  = number of raffinate transfer units

$(1-x)_{iM}$  = logarithmic mean of  $(1-x)$  &  $(1-x_i)$

The interface concentration corresponding to any bulk raffinate concentration  $x$  is found through adapted to the present situation.

$$\frac{1-x_i}{1-x} = \left( \frac{1-y}{1-y_i} \right)^{F_I/F_A}$$

This equation is plotted, for any value of  $(x, y)$  on the operating curve, to determine its intersection with the equilibrium curve at  $(x_i, y_i)$ , just as for gas absorption. As an approximation, a straight line of slope  $-k_R/k_E$  is plotted from  $(x, y)$  on the operating line to obtain the intersection at  $(x_i, y_i)$ .

Similarly, we have the corresponding expressions for the extract (corresponding to the liquid in gas absorption).

In reality, we know so little about the mass-transfer coefficients that the above expressions are of little use. For practical reasons, even though not strictly applicable unless the equilibrium curve is of constant slope, it is usually necessary to deal with overall coefficients and transfer units. These we can take from their gas-absorption counterparts:

$$Z = H_{IOR} N_{IOR} = H_{IOE} N_{IOE}$$

$$H_{IOR} = \frac{R}{F_{OR} a} = \frac{R}{K_R a (1-x)_{*M}}$$

$$H_{IOE} = \frac{E}{F_{OE} a} = \frac{E}{K_E a (1-y)_{*M}}$$

$$N_{IOR} = \int_{x_2}^{x_1} \frac{(1-x)_{*M} dx}{(1-x)(x-x^*)} = \int_{x_2}^{x_1} \frac{dx}{x-x^*} + \frac{1}{2} \ln \frac{1-x_2}{1-x_1}$$

$$N_{IOE} = \int_{y_2}^{y_1} \frac{(1-y)_{*M} dy}{(1-y)(y^*-y)} = \int_{y_2}^{y_1} \frac{dy}{y^*-y} + \frac{1}{2} \ln \frac{1-y_1}{1-y_2}$$

$$(1-x)_{*M} = \frac{(1-x^*)}{\ln[(1-x^*)/(1-x)]}$$

$$(1-y)_{*M} = \frac{(1-y) - (1-y^*)}{\ln[(1-y)/(1-y^*)]}$$

Where  $x^*$  is the concentration in equilibrium with  $y$  and  $y^*$  that in equilibrium with  $x$ .

Concentrations in above Eqs. are in mole fractions. If  $x$  and  $y$  are expressed as weight fractions, for convenience in use with the stage-calculation operating diagrams in terms of weight fractions,

$$N_{IOR} = \int_{x_2}^{x_1} \frac{dx}{x - x^*} + \frac{1}{2} \ln \frac{1 - x_2}{1 - x_1} + \frac{1}{2} \ln \frac{x_2(r - 1) + 1}{x_1(r - 1) + 1}$$

$$N_{IOE} = \int_{y_2}^{y_1} \frac{dy}{y^* - y} + \frac{1}{2} \ln \frac{1 - y_1}{1 - y_2} + \frac{1}{2} \ln \frac{y_1(r - 1) + 1}{y_2(r - 1) + 1}$$

where  $r$  is the ratio of molecular weights of non solute to solute. For weight-ratio concentrations,

$$N_{IOR} = \int_{x_2'}^{x_1'} \frac{dx'}{x' - x'^*} + \frac{1}{2} \ln \frac{1 + rx_2'}{1 + rx_1'}$$

$$N_{IOE} = \int_{y_2'}^{y_1'} \frac{dy'}{y'^* - y'} + \frac{1}{2} \ln \frac{1 + ry_1'}{1 + ry_2'}$$

### Dilute Solutions

For dilute solutions, only the integral terms of the above equations for  $N_{IOE}$  and  $N_{IOR}$  are important. If in addition the equilibrium curve and operating line are straight over the concentration range encountered.

$$N_{IOR} \approx \frac{x_1 - x_2}{(x - x^*)_M} \quad N_{IOE} \approx \frac{y_1 - y_2}{(y^* - y)_M}$$



The equivalent expressions in terms of mass-transfer coefficients are

$$R(x_1 - x_2) = E(y_1 - y_2) = K_R aZ(x - x^*)_M = K_E aZ(y^* - y)_M$$

If in addition the equivalent of Henry's law applies, so that the equilibrium distribution curve is a straight line passing through the origin ( $m = y'/x = y/x' = \text{const}$ ), a procedure exactly similar to that used previously in the case of gas absorption gives

$$N_{ODR} = \frac{\ln \left[ \frac{x_1 - y_2/m}{x_2 - y_2/m} \left( 1 - \frac{R}{mE} \right) + \frac{R}{mE} \right]}{1 - R/mE}$$

Similarly for the extract enriching section of a tower used with reflux, the same circumstances provide

$$N_{ODE} = \frac{\ln \left[ \frac{y_2 - mx_1}{y_1 - mx_1} \left( 1 - \frac{mE}{R} \right) + \frac{mE}{R} \right]}{1 - mE/R}$$

## **Process Modelling and Simulation**

Mathematical-modelling is an important component of all engineering sciences. Modelling involves representation of a process or a system in terms of equations, which best describe its physical nature and its working. In practice modelling, is very much an art requiring experience and practice, in addition to a thorough understanding of the physical principles involved.

Modelling of Chemical Engineering Systems can be transport phenomena based. population balance type or empirical. The transport phenomena approach encompasses three basics: mass, energy, and momentum balances applied in their time-varying form. Such a model is termed as an unsteady state model or dynamic model. A steady state model performs the balances over a system, when the properties do not change with time. A perfect steady state is difficult to achieve, but steady state is assumed to prevail if the system behavior does not change significantly with time.

The most important result of developing a mathematical model of a Chemical Engineering system is the understanding and insight gained into the functioning of the system. Models are useful in all phases of Chemical Engineering, From research and development to plant operations, and even in management decision making. In research and development, models can be used to explore the effect of different operating conditions for optimization and control studies and aid in scale-up studies. In the design phase, models can be used to: explore the sizing and arrangement of processing equipment for dynamic performance; study the interactions of various parts of the process in a

recycle system; evaluate alternative process and control structures and strategies; simulate start-up, shutdown, and emergency situations and procedures. In actual plant operation, models help in studying the effects of and the requirements for expansion projects, de-bottlenecking, and optimizing plant operations.

The bases for mathematical models are the fundamental physical and chemical laws, such as the law of conservation of mass, energy, and momentum. Models are based upon carefully chosen assumptions. Assumptions are necessary, as an extremely rigorous model that includes every phenomenon down to microscopic detail would be so complex that it would take a long time to develop and might be impractical to solve. Assumptions impose limitations on the model that should always be kept in mind when evaluating its predicted results. The most important part of model development is proving that the model describes the real-world situation. A model needs to be validated with experimental or plant operating data. Most often, the model predicted results do not match well with the measured values. The model then needs to be tuned to the plant performance by suitably, adjusting the parameters of the model equations. Such parameters are called tuning parameters. The model development is complete when it has been tuned to match the measured variables.

## What is Simulation?

Even if there is only one possible unified theory (of the universe) it is just a set of rules and equations. What is it that breathes fire into the equations and makes a universe for them to describe? The usual approach of science of constructing a mathematical model cannot answer the questions of why there should be a universe. for the model to describe. Why does the universe go to all the bother of existing? Is the unified theory so compelling that it brings about its own existence? Or does it need a creator, and if so, does he have any other effect on the universe? And who created him?

Stephen W Hawking

The word simulation is a term that has come into vogue more recently in a number of scientific disciplines to describe the ancient art of model building. A large variety of definitions have been put forward as different people take it to mean different things with no consensus in sight. Let us look at a few definitions:

A formal definition by Churchman:

'x simulates y' is true if and only if

- i) x and y are formal systems
- ii) y is taken to be the real system
- iii) x is taken to be an approximation to the real system
- iv) The rules of validity in x are non-error-free.

Another definition:

"Simulation model is a simplified representation of a real life which allows the understanding and solution of a problem to be achieved by a trial and error approach."

Another one:

"Simulation is essentially a technique that involves setting up a model of a real situation and then performing experiments on the model."

Models can be conceptual or physical and we restrict our discussion to the former. Conceptual models can be either mathematical or analog and here again we will concern ourselves with mathematical model.

Rutherford Aris has defined it thus:

A mathematical model is a representation, in mathematical terms, of certain aspects of a non-mathematical system. The arts and crafts of mathematical modeling are exhibited in the construction of the models that not only are consistent in themselves and mirror the behavior of their prototype but also serve some exterior purpose. From above it would appear that people have used modeling and simulation interchangeably and indeed it is so.

Let us try to understand the distinction between simulation and modeling.

For our purpose, "Process simulator is a computer based software package consisting of differential and /or algebraic equations which describe the model)

which simulates the performance of an actual process and responds to changes in the inputs in a similar way."

## DYNAMIC PROCESS SIMULATORS

The availability of differential equation simulation programs has led to the development of several higher-level programs that are designed to simulate the dynamic behavior of chemical process units, either singly or combined in a system. They are the dynamic equivalent of the steady-state material and energy-balance programs such as PACER, FLOWTRAN, CHESS, and others. Figure shows schematically the supporting structure for these programs and also demonstrates the fact that a process simulation problem can be programmed in any of the three levels.

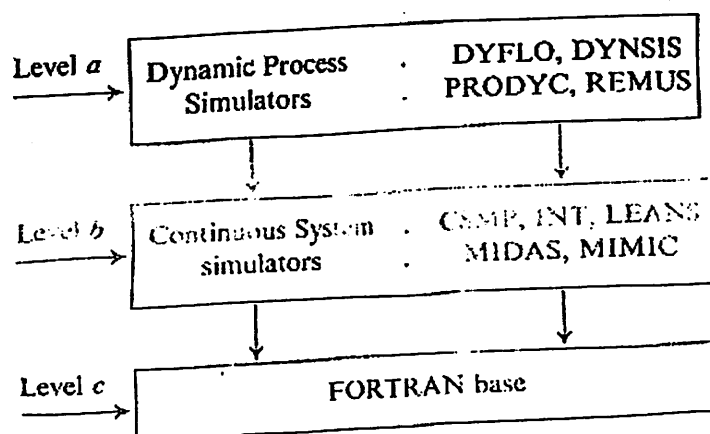


Fig. Structure for Simulation Programs

Use of a higher level merely facilitates the coding effort required; for example, programming at the continuous system level (b):eliminates coding most of the numerical procedures required for integrating differential equations, generating arbitrary functions, and converging algebraic equations. Programming at level c, using an available dynamic process simulator, in addition to eliminating the coding of numerical procedures, offered by level b, also greatly simplifies the effort for defining the system to be simulated. This is accomplished by the use of subprograms that simulate entire unit operations such as fractionation columns, heat exchangers, reactors, and so on. This project provides the listing and describes the use of one of these programs, called "DYFLO," that offers a library of several dozen unit operation subroutines. It has been in use for several years, and although it was originally conceived for use in schools at the undergraduate level, it has been used successfully for the solution of large, complex industrial problems

## Model for Countercurrent Extraction

The example consists of a series of agitated vessels, each containing a settling section that allows two solvents to flow countercurrent to each other while mixing intimately at each stage. (Fig. 9) The purpose of this liquid-liquid extraction is to concentrate a solute from a concentration  $X_{aF}$  in solvent a to a concentration  $X_{bF}$  in solvent  $\beta$  to reduce the solute in solvent a to as low a concentration possible. Each stage is numbered 1 to N; the general stage is n. This notation is shown as a subscript for the compositions. (Fig. 10)

In the general dynamic case being considered the flows and compositions at any stage may vary with time. Also, it is assumed that each stage achieves equilibrium between the two solvents according to the distribution coefficient D

$$D = X_{bn} / X_{an}$$

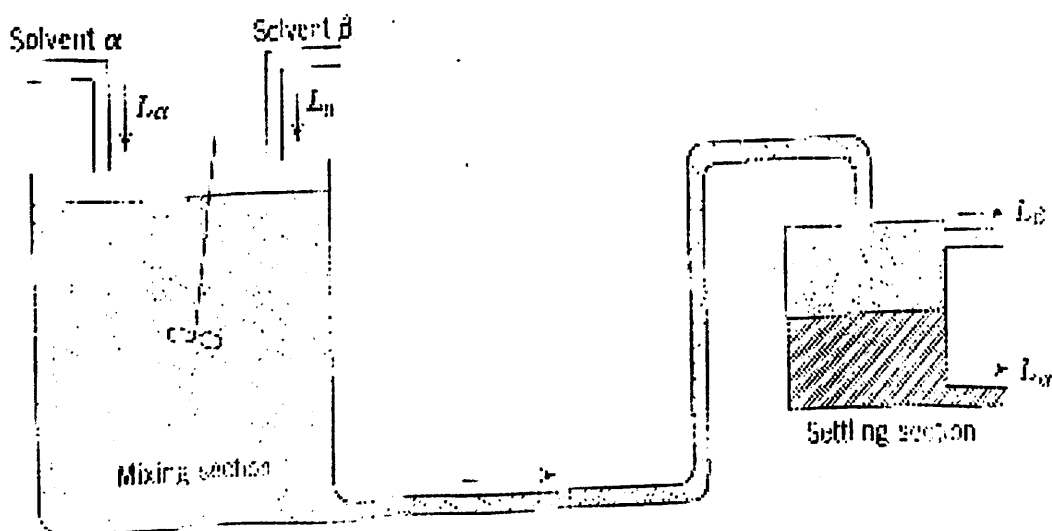


Fig.9 Single Stage for Countercurrent Extraction



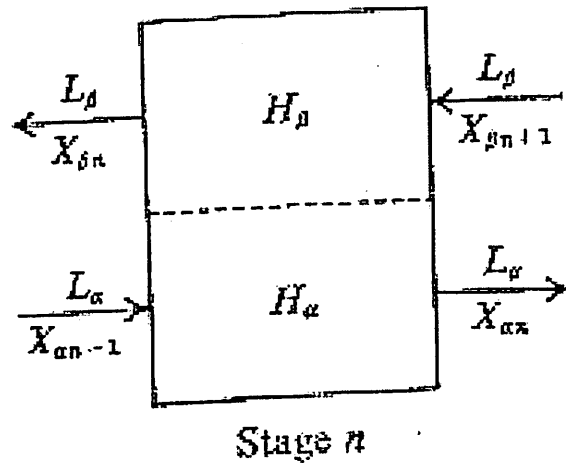


Fig 10 Extraction Stage n

Only, two equations are required for this case; the first is a component mass balance for both phases:

$$\text{Rate of change of holdup} = [\text{inflow}] - [\text{outflow}]$$

$$d/dt [(H_{\alpha n} X_{\alpha n}) + (H_{\beta n} X_{\beta n})] = (L_{\alpha} X_{\alpha n-1} + L_{\beta} X_{\beta n+1}) - (L_{\alpha} X_{\alpha n} + L_{\beta} X_{\beta n})$$

The second is the equilibrium equation

$$X_{\beta n} = D \cdot X_{\alpha n}$$

The component mass balance equation should be used to solve for either  $X_{\alpha n}$  or  $X_{\beta n}$ , whichever is larger. If they are of the same order of magnitude, it does not matter which one is selected. In this case it is assumed to be  $X_{\beta n}$ . The equilibrium equation is then used to solve for the other variable  $X_{\alpha n}$ .

For the simple steady state operation the differentials in the differential equation can be equated to zero and the equation reduces to

$$L_a X_{an-1} + L_\beta X_{\beta n+1} = L_{aa} X_{an} + L_\beta X_{\beta n}$$

For N stages of steady state operation, the overall relationship of  $X_{aF}$  to  $X_{B1}$  can be established by manipulating the equations that result in a single expression involving the ratio of the solvent flows  $L_a/L_\beta$ , the total number of stages N, and the distribution coefficient D. Such a regression to a simplified case is typical of the approach of conventional analysis. The technique of computerized model building, however, permits adding greater complexity to the system. For example, suppose that a component C is produced by the reaction

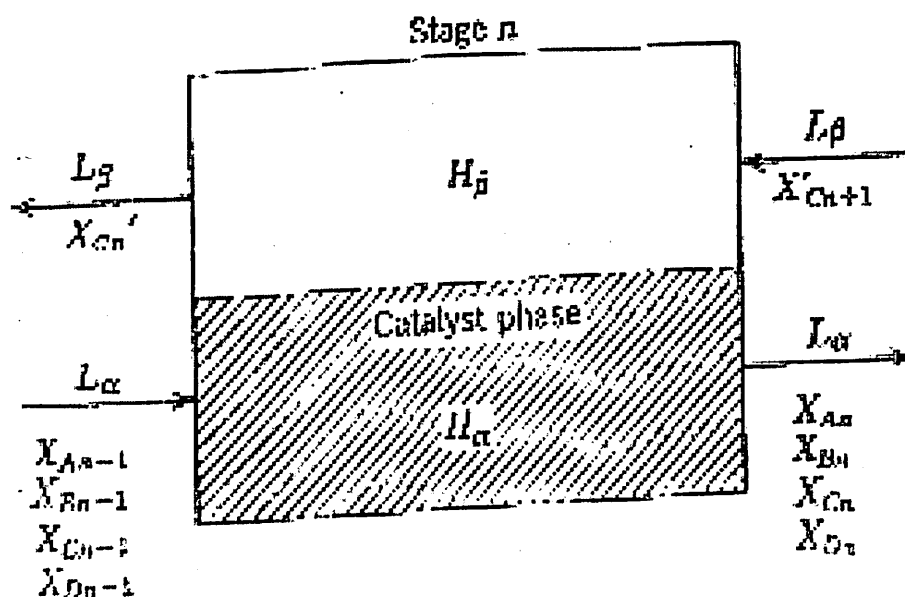
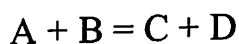


Fig 11 Signal Flow for Reaction Stage n

And that this reaction takes place in solvent a (containing the catalyst). Of the four components in the system, only component C is soluble in the  $\beta$  solvent with a distribution coefficient

$$D = X'_{Cn} / X_{Cn}$$

Where  $X'_{Cn}$  is the mole fraction of C in the  $\beta$  phase and  $X_{Cn}$  is the mole fraction in the a phase.

A model for a countercurrent staged system can be synthesized by considering a general section n (Fig. 11). The equations for this stage are as follows:

1. Reaction Rate in phase a

$$R = H_a(k_F X_A X_B - k_R X_C X_D) \quad 1$$

2. Mass Balance on Component A

$$\text{Accumulation} = \text{Inflow} - \text{Outflow} - \text{Reaction}$$

$$d/dt (H_a X_A) = L_a X_{An-1} - L_a X_{An} - R \quad 2$$

3. Mass Balance on component B

$$d/dt (H_a X_{Bn}) = L_a X_{Bn-1} - L_a X_{Bn} - R \quad 3$$

4. Mass Balance on component C (both phases a and B)

$$d/dt [(H_a X_{Cn}) + (H_B X'_{Cn})] = L_a X_{Cn-1} - L_a X_{Cn} + L_B X'_{Cn+1} - L_B X'_{Cn} + R \quad 4$$

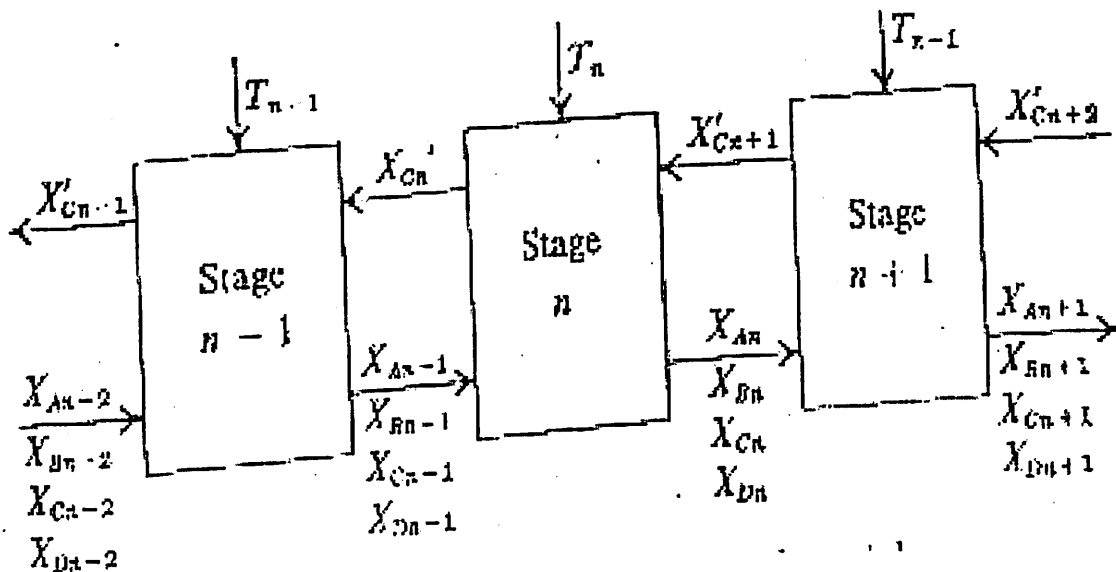


Fig. 12 Signal Flow for stages  $n-1$  to  $n+1$

5. Mass Balance on Component B

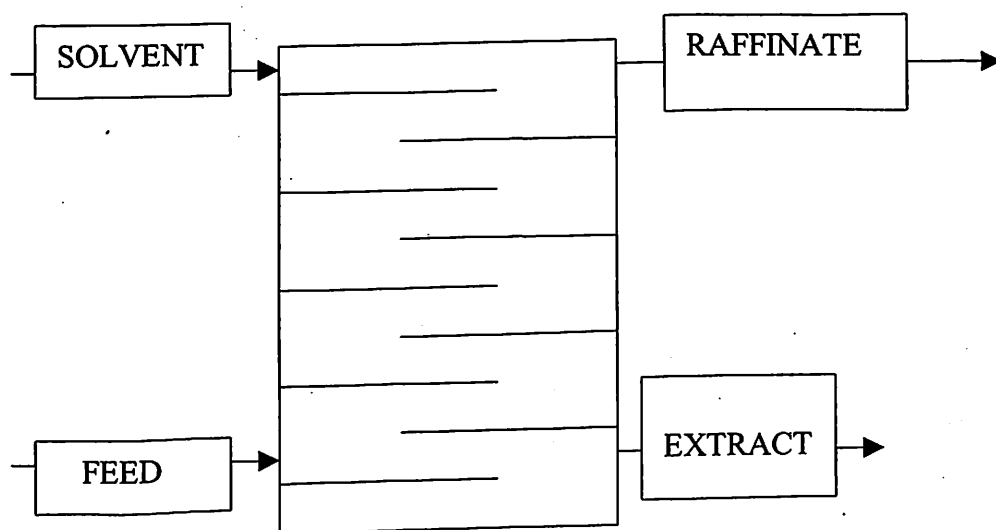
$$d/dt (H_a X_{Dn}) = L_a X_{Dn-1} - L_a X_{Dn} + R \quad 5$$

6. Equilibrium on component C

$$X'_{Cn} = DX_{Cn} \quad 6$$

## CASE STUDY 1

This is a simple case for a simple Counter-current solvent extraction column. In this case Benzene is separated from the feed with the help of sulfolane solvent.



$$dH / dt = XB_0 - XB_1 - YB_8' \quad (1)$$

At steady state

$$dH / dT = 0$$

From (1)

$$XB_0 - XB_1 - YB_8' = 0 \quad (2)$$

$$B_1 / B_8' = K \quad (3)$$

From (2) and (3)

$$B_8' = XB_0 / XK + Y$$

$$B_1 = KB_8'$$

Where B = Benzene in Feed from each tray

B' = Benzene in Solvent from each tray

Similarly we'll calculate the Benzene concentration for all stages.

## C++ Computer Program

```
#include <iostream.h>
#include <conio.h>
#include <stdio.h>
void main()
{
double b1[9],b2[9],k[9];
double x=0,y=0;
int j=0;
for(int i=0;i<9;i++)
{
b1[i]=0.00000;
b2[i]=0.00000;
k[i]=0.00000;
}
cout <<"\n\n\t\tEnter the flow rate of feed: ";
cin >>x;
cout <<"\n\n\t\tEnter the flow rate of solvent: ";
cin >>y;
cout <<"\n\n\t\tEnter the equilibrium constant values for each tray: ";
for(i=0;i<9;i++)
cin >>k[i];
```

```

cout << "\n\n\t\tEnter the initial concentration of benzene in feed: ";
cin >> b1[0];
cout << "\n\n\t\tTray No.\t\tFeed conc\t\tSolvent conc";
for(i=0;i<9;i++)
{
j=(8-i);
b2[j]=((x*b1[i]))/((x*k[i])+y);
b1[i+1]=(k[i]*b2[j]);
cout << "\n\t\t" << i+1 << "\t\t" << b1[i] << "\t\t" << b2[j];
}
getche();
}

```



## Solution

Enter the flow rate of feed: 30

Enter the flow rate of solvent: 60

Enter the value of K for each stage: - 50

50

50

50

50

50

50

50

50

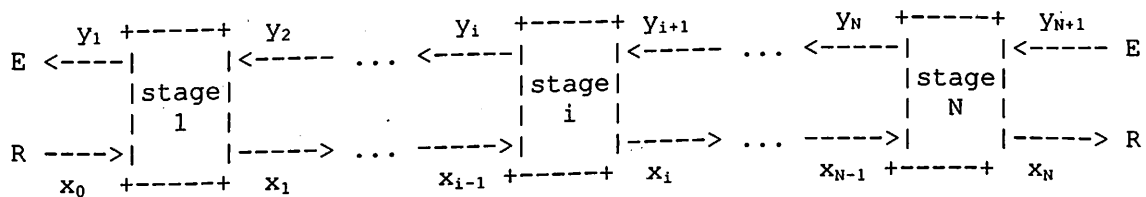
Enter the initial concentration of benzene in feed: .2

Tray No.	Feed conc	Solvent conc
1	0.2	0.00384615
2	0.192308	0.00369822
3	0.184911	0.00355599
4	0.177799	0.00341922
5	0.170961	0.00328771
6	0.164385	0.00316126
7	0.158063	0.00303967
8	0.151984	0.00292276
9	0.146138	0.00281035

## CASE STUDY 2

### Counter-Current Liquid-Liquid Extraction

**Problem Statement:** The following is a schematic diagram of an N-stage counter-current extraction operation, where E is the extract stream, R is the raffinate stream.



The following equations describe this counter-current extraction process.

$$x_{i-1} - (1+S)x_i + Sx_{i+1} = 0 \quad \text{for } i=1..N$$

$$y_i = Kx_i$$

where  $x$  = the composition of the raffinate phase,

R

$y$  = the composition of the extract phase, E

$K$  = the partition coefficient

$S = K \cdot E/R$

$N$  = the number of stages

Another equivalent form of the first equation is:

$$\frac{x_0 - x_N}{x_0 - x_{N+1}} = \frac{S^{N+1} - S}{S^{N+1} - 1}$$

Given  $E=200$  lb/hr,  $R=300$  lb/hr,  $K=3$ , and inlet raffinate and extract compositions of  $x_0=0.03$  and  $y_{N+1}=0$ , respectively, write a program to determine the number of stages,  $N$ , required for the process to achieve an exit raffinate composition of  $x_N=0.001$ . (Note that  $N$  is an integer -- you either have a stage or you don't.) Furthermore, output the composition of the raffinate phase at each stage.

## SOLUTION

Find the number of stages and composition in countercurrent liquid-liquid extraction.

Instructor: Nam Sun

Wang

Process Specification (Change the number in yellow cells. Other cells in this worksheet contain formula.)

R = 300	Flow rate of the raffinate phase
E = 200	Flow rate of the extract phase
$x_{in} = 0.03$	Inlet composition of the raffinate phase
$x_{out} = 0.001$	Outlet composition of the raffinate phase
$y_{in} = 0$	Inlet composition of the extract phase
K = 3	Partition coefficient

Calculated Variable:

$$S = 2 = K \cdot E / R$$

Find the number of equilibrium stages required by forcing the following  $f(N)=0$ .

$$f(xN) = 9E - 04 = (x_{in} - x_{out}) / (x_{in} - y_{in} / K) - (S^{xN+1} - S) / (S^{xN+1} - 1)$$

$xN = 3.916$  ← via |Goal Seek| by setting  $f(xN)$  to a value of 0 by changing  $xN$ .

Since a fractional stage does not make physical sense, set the number to be an integer.

$$N = 4$$

Find the raffinate composition. (We prepared a matrix A and a vector b to handle up to 14 stages.)

Define the yellow cells to be A and b. As N changes, we need to manually redefine A and b to match their size.

The following matrix A and vector b describe the material balance equation around each stage.

$$x_{i-1} - (1+S)x_i + Sx_{i+1} = 0 \quad \text{for } i=1,2,\dots,N$$

A =	<table style="border-collapse: collapse; text-align: center; width: 100%;"> <tr><td style="border: none;">-</td><td style="border: none;">3</td><td style="border: none;">2</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">1</td><td style="border: none;">3</td><td style="border: none;">2</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">1</td><td style="border: none;">3</td><td style="border: none;">2</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">1</td><td style="border: none;">3</td><td style="border: none;">2</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">1</td><td style="border: none;">3</td><td style="border: none;">2</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">1</td><td style="border: none;">3</td><td style="border: none;">2</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">1</td><td style="border: none;">3</td><td style="border: none;">2</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">1</td><td style="border: none;">3</td><td style="border: none;">2</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">1</td><td style="border: none;">3</td><td style="border: none;">2</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">1</td><td style="border: none;">3</td><td style="border: none;">2</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">1</td><td style="border: none;">3</td><td style="border: none;">2</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">1</td><td style="border: none;">3</td><td style="border: none;">2</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td><td style="border: none;">0</td></tr> </table>	-	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	3	2	0	0	0	0	0	b =	<table style="border-collapse: collapse; text-align: center; width: 100%;"> <tr><td style="border: none;">-</td><td style="border: none;">0.03</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td></tr> <tr><td style="border: none;">0</td><td style="border: none;">0</td></tr> </table>	-	0.03	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0																																																																																																																																																																																																																																				
1	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0																																																																																																																																																																																																																																				
0	1	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0																																																																																																																																																																																																																																				
0	0	1	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0																																																																																																																																																																																																																																				
0	0	0	1	3	2	0	0	0	0	0	0	0	0	0	0	0	0																																																																																																																																																																																																																																				
0	0	0	0	1	3	2	0	0	0	0	0	0	0	0	0	0	0																																																																																																																																																																																																																																				
0	0	0	0	0	1	3	2	0	0	0	0	0	0	0	0	0	0																																																																																																																																																																																																																																				
0	0	0	0	0	0	1	3	2	0	0	0	0	0	0	0	0	0																																																																																																																																																																																																																																				
0	0	0	0	0	0	0	1	3	2	0	0	0	0	0	0	0	0																																																																																																																																																																																																																																				
0	0	0	0	0	0	0	0	1	3	2	0	0	0	0	0	0	0																																																																																																																																																																																																																																				
0	0	0	0	0	0	0	0	0	1	3	2	0	0	0	0	0	0																																																																																																																																																																																																																																				
0	0	0	0	0	0	0	0	0	0	1	3	2	0	0	0	0	0																																																																																																																																																																																																																																				
-	0.03																																																																																																																																																																																																																																																				
0	0																																																																																																																																																																																																																																																				
0	0																																																																																																																																																																																																																																																				
0	0																																																																																																																																																																																																																																																				
0	0																																																																																																																																																																																																																																																				
0	0																																																																																																																																																																																																																																																				
0	0																																																																																																																																																																																																																																																				
0	0																																																																																																																																																																																																																																																				
0	0																																																																																																																																																																																																																																																				
0	0																																																																																																																																																																																																																																																				
0	0																																																																																																																																																																																																																																																				
0	0																																																																																																																																																																																																																																																				
0	0																																																																																																																																																																																																																																																				

0	0	0	0	0	0	0	0	0	0	0	0	1	3	2	0
0	0	0	0	0	0	0	0	0	0	0	0	0	1	3	0

Summary

Stage	Raffinate x	Extract y
0	0.03000	0.09000
1	0.01452	0.04355
2	0.00677	0.02032
3	0.00290	0.00871
4	0.00097	0.00290

=IF(A48>=N,"",A48+1)  
 There are formula up to the above row, but they are such that only blank is shown beyond N.

## Literature Survey

### Data Collected from different sources

TABLE 2  
Extraction runs in single stage mixer - settler unit  
Intermediate viscosity stock (P = 115 °C)

Feed source	Aghajari				Barab			
Solvent (Feed ratio = 1/ wt.)	1.5	2.5	3.1	4.0	1.5	2.5	3.2	4.0
Yield (% wt.)	61.8	55.3	50.0	42.8	67.1	55.0	50.6	43.7
<b>Raffinate Characteristics</b>								
Density ( $d_4^{20}$ )	0.9057	0.8960	0.8919	0.8872	0.9019	0.8960	0.8919	0.8890
Specific gravity (60/60°F)	0.9067	0.8965	0.8924	0.8876	0.9068	0.8965	0.8944	0.8898
Refractive index ( $n_D^{20}$ )	1.4475	1.4361	1.4335	1.4303	1.4486	1.4392	1.4362	1.4334
Pour point (°C)	43	45	45	45	45	45	45	45
Kinematic viscosity ( $m^2/s \times 10^{-6}$ )								
at 98.9 °C	10.3	9.6	9.4	9.2	11.1	10.4	10.1	9.98
75 °C	20.7	18.6	18.1	17.8	22.6	20.7	20.0	19.1
37.8 °C	100	62	71	73	113	103	96	89
Viscosity Index (VI)	91	103	107	109	84	89	96	100
ΔVI	36	48	52	54	22	27	34	38
VGC	0.9234	0.9154	0.9107	0.9053	0.9134	0.9162	0.9132	0.9060
<b>Ceppo Composition</b>								
% C <sub>1</sub>	30	27	26	25	29	27	26	24
% C <sub>2</sub>	41	42	42	41	42	42	42	42
% C <sub>3</sub>	28	31	32	34	28	31	32	33
<b>Dewaxing of Raffinates</b>								
Dewaxing solvent	Methyl Ethyl Ketone    Benzene    Toluene							
Composition (vol/vol)	50 : 35 : 15							
Dewaxing temperature (°C)	10							
Dilution and wash solvent (vol/vol)	1 : 1 and 2 : 1							
Yield:								
Raffinate loss (% wt.)	86.2	83.6	79.7	80.0	86.0	73.9	72.7	72.1
Feed loss (% wt.)	53.3	46.2	39.8	34.2	53.7	40.6	35.8	25.5
<b>Dewaxed Oil Characteristics</b>								
Density ( $d_4^{20}$ )	0.9174	0.9077	0.9038	0.8995	0.9180	0.9073	0.9033	0.8996
Specific gravity (60/60°F)	0.9179	0.9082	0.9043	0.9000	0.9185	0.9078	0.9038	0.9001
Refractive index ( $n_D^{20}$ )	1.4386	1.4271	1.4244	1.4218	1.4305	1.4247	1.4213	1.4168
Pour point (°C)	3	6	3	6	3	3	3	3
Kinematic viscosity ( $m^2/s \times 10^{-6}$ )								
at 98.9 °C	12.1	21.8	23.0	10.6	12.6	21.8	11.5	11.2
37.8 °C	156	133	134	112	155	128	122	113
Viscosity Index	64	72	76	8	76	85	88	91

TABLE 1  
 Extraction runs in single stage mixer - neither used  
 Heavy viscosity stocks (T = 105°C)

Feed source	Agbajali Heavy				Bajrah Heavy			
	1.5	2.5	3.2	4.0	1.5	2.5	3.2	4.0
Solvent/Feed ratio (wt./wt.)	1.5	2.5	3.2	4.0	1.5	2.5	3.2	4.0
Yield (% wt.)	61.9	60.1	51.1	49.2	69.0	55.7	50.0	44.6
<b>Raffinate Characteristics</b>								
Density ( $d_4^{15}$ )	0.9174	0.9283	0.9032	0.8899	0.9111	0.9105	0.9054	0.9029
Specific gravity (60/60°F)	0.9179	0.9086	0.9037	0.9004	0.9216	0.9108	0.9059	0.9014
Refractive Index ( $n_D^{20}$ )	1.4590	1.4645	1.4612	1.4769	1.4926	1.4860	1.4840	1.4802
Pour point (°C)	54	57	57	53	54	54	51	51
Kinematic Viscosity ( $m^2/s \times 10^{-6}$ )								
at 98.9°C	18.7	17.0	16.5	16.1	19.9	17.9	17.5	16.7
35°C	43.3	33.0	35.8	34.8	46.1	39.6	36.8	35.0
37.8°C (1)	295	215	200	185	330	250	220	190
Viscosity Index (VI)	71	82	93	97	78	84	93	100
$\Delta VI$	24	37	48	52	17	28	37	64
VGC	0.9270	0.9174	0.9134	0.9078	0.9309	0.9187	0.9136	0.9082
<b>Crude Composition</b>								
% C <sub>A</sub>	30	29	28	27	30	28	27	26
% C <sub>H</sub>	39	38	38	38	44	43	42	41
% C <sub>P</sub>	31	33	34	35	26	29	31	33
<b>Dewaxing of raffinates</b>								
Dewaxing solvent	Methyl Ethyl Ketone - Benzene - Toluene							
Composition (vol/vol)	50 : 35 : 15							
Dewaxing Temperature (°C)	12 to 13				15			
Dilution and Wash solvent (vol/vol)	4 : 1 and 2 : 1							
<b>Yield</b>								
Raffinate, basis (% wt.)	83.3	81.6	80.3	79.2	81.9	83.6	79.8	82.3
Feed basis (% wt.)	56.4	49.1	41.4	38.9	56.5	46.1	39.4	36.7
<b>Dewaxed Oil Characteristics</b>								
Density ( $d_4^{15}$ )	0.9114	0.9216	0.9163	0.9127	0.9132	0.9222	0.9163	0.9125
Specific gravity (60/60°F)	0.9119	0.9221	0.9166	0.9132	0.9137	0.9227	0.9168	0.9131
Refractive Index ( $n_D^{20}$ )	1.4976	1.4910	1.4870	1.4847	1.4998	1.4921	1.4886	1.4856
Pour point (°C)	-9	9	-6	6	9	-9	-9	0
Kinematic viscosity ( $m^2/s \times 10^{-6}$ )								
at 98.9°C	23.9	21.9	20.5	19.8	23.7	21.1	20.6	20.2
37.8°C	517	468	339	311	466	364	320	302
Viscosity Index	57	66	74	79	69	75	81	84

TABLE 1

Comparison of the results of the present study with the results of the study by [Name] and [Name] (1977)

Description of the study	Present study					[Name] and [Name] (1977)				
	11	22	33	44	55	11	22	33	44	55
1. [Description]	11	22	33	44	55	11	22	33	44	55
2. [Description]	11	22	33	44	55	11	22	33	44	55
3. [Description]	11	22	33	44	55	11	22	33	44	55
4. [Description]	11	22	33	44	55	11	22	33	44	55
5. [Description]	11	22	33	44	55	11	22	33	44	55
6. [Description]	11	22	33	44	55	11	22	33	44	55
7. [Description]	11	22	33	44	55	11	22	33	44	55
8. [Description]	11	22	33	44	55	11	22	33	44	55
9. [Description]	11	22	33	44	55	11	22	33	44	55
10. [Description]	11	22	33	44	55	11	22	33	44	55



TABLE 3

Comparison of the results of the two methods of determining the critical point of a mixture

Mixture	Method 1					Method 2				
	Temp	Pressure	Phase	Phase	Phase	Temp	Pressure	Phase	Phase	Phase
Methane	100	1000	1000	1000	1000	100	1000	1000	1000	1000
	100	1000	1000	1000	1000	100	1000	1000	1000	1000
Ethane	100	1000	1000	1000	1000	100	1000	1000	1000	1000
	100	1000	1000	1000	1000	100	1000	1000	1000	1000
Propane	100	1000	1000	1000	1000	100	1000	1000	1000	1000
	100	1000	1000	1000	1000	100	1000	1000	1000	1000
n-Butane	100	1000	1000	1000	1000	100	1000	1000	1000	1000
	100	1000	1000	1000	1000	100	1000	1000	1000	1000
i-Butane	100	1000	1000	1000	1000	100	1000	1000	1000	1000
	100	1000	1000	1000	1000	100	1000	1000	1000	1000
n-Pentane	100	1000	1000	1000	1000	100	1000	1000	1000	1000
	100	1000	1000	1000	1000	100	1000	1000	1000	1000
i-Pentane	100	1000	1000	1000	1000	100	1000	1000	1000	1000
	100	1000	1000	1000	1000	100	1000	1000	1000	1000
n-Hexane	100	1000	1000	1000	1000	100	1000	1000	1000	1000
	100	1000	1000	1000	1000	100	1000	1000	1000	1000
i-Hexane	100	1000	1000	1000	1000	100	1000	1000	1000	1000
	100	1000	1000	1000	1000	100	1000	1000	1000	1000
n-Heptane	100	1000	1000	1000	1000	100	1000	1000	1000	1000
	100	1000	1000	1000	1000	100	1000	1000	1000	1000
i-Heptane	100	1000	1000	1000	1000	100	1000	1000	1000	1000
	100	1000	1000	1000	1000	100	1000	1000	1000	1000
n-Octane	100	1000	1000	1000	1000	100	1000	1000	1000	1000
	100	1000	1000	1000	1000	100	1000	1000	1000	1000
i-Octane	100	1000	1000	1000	1000	100	1000	1000	1000	1000
	100	1000	1000	1000	1000	100	1000	1000	1000	1000
n-Nonane	100	1000	1000	1000	1000	100	1000	1000	1000	1000
	100	1000	1000	1000	1000	100	1000	1000	1000	1000
i-Nonane	100	1000	1000	1000	1000	100	1000	1000	1000	1000
	100	1000	1000	1000	1000	100	1000	1000	1000	1000
n-Decane	100	1000	1000	1000	1000	100	1000	1000	1000	1000
	100	1000	1000	1000	1000	100	1000	1000	1000	1000
i-Decane	100	1000	1000	1000	1000	100	1000	1000	1000	1000
	100	1000	1000	1000	1000	100	1000	1000	1000	1000

TABLE 1: CHARACTERISTICS OF FEEDSTOCK (IN DISTILLATE)

Characteristics	Values
Density gm/ml at 15°C	0.9332
Sp Gravity 60/60°F	0.9337
Degree API, gravity	20.05
Refractive Index at 70°C	1.5020
Pour Point, °C	42
Kin. Visc. Cst at 100°C	11.07
at 70°C	28.68
CCR % wt	0.25
Distillation ASTM D-1160	
IBP, °C	380
5%	-
50% "	483
90% "	535
Molecular Weight (VPO)	450
Aniline point, °C	83.2
Flash point, °C (Seta)	241.5
Sulfur, % wt	2.94
Wax content, % wt (EH)	11.8

FIG 1 EFFECT OF INTERPHASE POSITION ON RAFFINATE YIELD FOR SAME TREATMENT

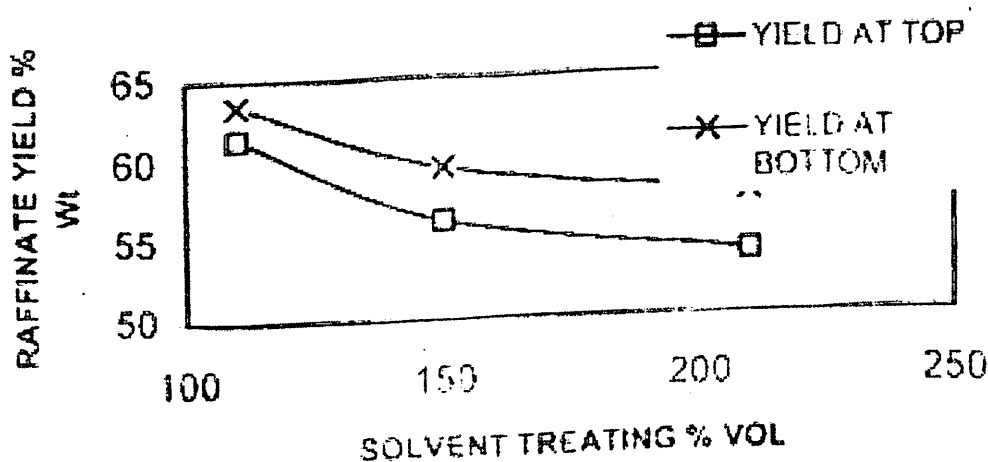
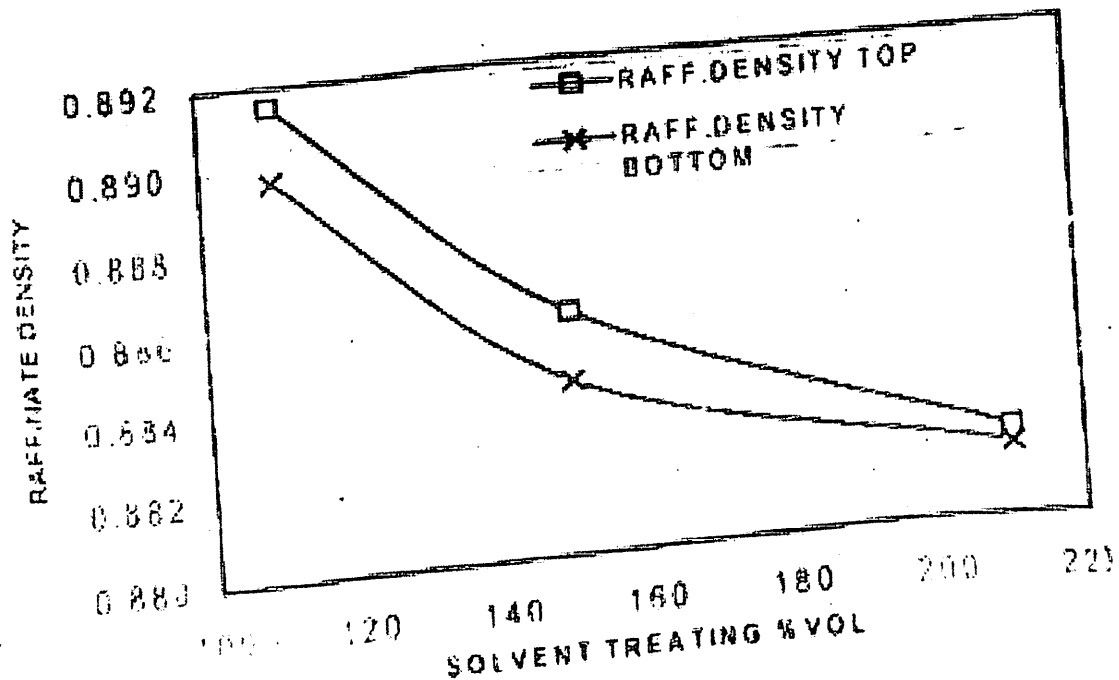


TABLE 2 SOLVENT EXTRACTION STUDIES

Index	Run No	Inter Phase at Top			Inter Phase at Bottom		
		1	2	3	4	5	6
Feed Stock		Inter Neutral Distillate					
Solvent		NMP + 1.5% Water					
Temperature, Top/Bottom, °C		75 / 65					
Solvent treat, % vol of feed		110	150	210	110	150	210
Solvent in Extract Phase, % wt		73.6	77.9	83.3	73.9	78.2	84.1
Solvent in Raff. Phase, % wt		17.3	15.9	13.7	17.4	16.0	13.6
Raffinate yield, % wt		61.3	56.1	53.9	63.4	59.4	57.6
RAFFINATE		0.8915	0.8859	0.8821	0.8897	0.8842	0.8817
Density g/ml at 15°C		0.8920	0.8864	0.8826	0.8902	0.8847	0.8822
Specific gravity, 60/60°F		27.13	28.13	28.82	27.45	28.44	28.89
API gravity, degree		1.4725	1.4693	1.4662	1.4701	1.4678	1.4651
Refractive Index at 70°C		45	45	45	45	45	48
Pour Point, °C		9.35	8.95	8.85	9.30	8.93	8.82
Kin. Viscosity cSt at 100°C		21.40	20.57	20.24	21.05	20.42	20.03
Kin. Viscosity cSt at 70°C							
EXTRACT		1.0116	1.0024	1.0000	1.0188	1.0150	1.0128
Density g/ml at 15°C		1.0122	1.0030	1.0006	1.0194	1.0156	1.0134
Specific gravity, 60/60°F		8.29	9.63	9.92	7.31	7.83	8.3
API gravity, degree		24	27	27	21	24	24
Pour Point, °C		21.67	20.77	19.87	23.18	22.95	22.71
Kin. Viscosity cSt at 100°C		87	83	82	90	89	87
BMCI							

FIG 2 EFFECT OF INTERPHASE POSITION ON RAFFINATE QUALITY



(1) C7H16      HEPTANE  
 (2) C6H6      BENZENE  
 (3) C4H8O2    BUTYRONE, TETRAMETHYLENE

FACONIS G.M., HODD G.C., WATCOCK R.L.  
 J. PHYS. CHEM. 59(1955)152

TEMPERATURE : 25.0 DEG C      TYPE OF SYSTEM : 1

EXPERIMENTAL TIE LINES ON HOLE POT

LEFT PHASE			RIGHT PHASE		
(1)	(2)	(3)	(1)	(2)	(3)
09.553	10.284	0.163	0.794	5.560	03.427
22.795	15.871	0.402	1.155	7.897	29.316
77.590	21.757	0.515	1.353	14.825	29.287
22.251	35.459	1.307	2.070	29.048	58.312
10.611	55.070	1.221	4.235	42.482	50.323
24.052	59.143	7.619	5.703	49.155	65.037

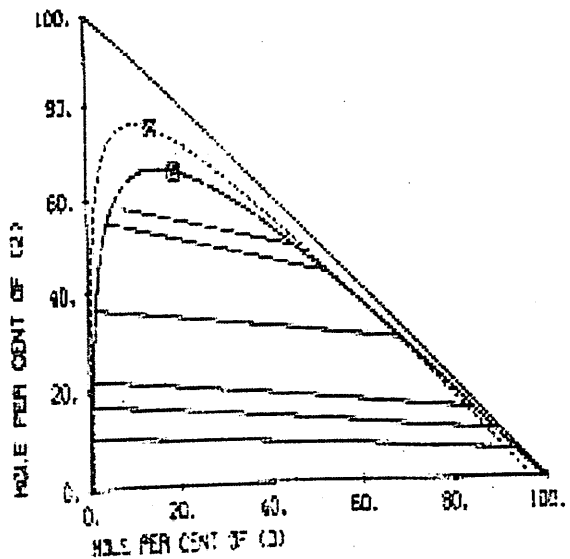
SPECIFIC MODEL PARAMETERS IN MOL%:

I, J	UNIQUAC		NRTL (PARAM. 2)	
	A1J	A2J	A1J	A2J
1, 2	151.52	-151.49	-245.21	105.94
1, 3	480.57	93.697	1822.3	347.29
2, 3	157.45	-93.251	580.26	-197.22

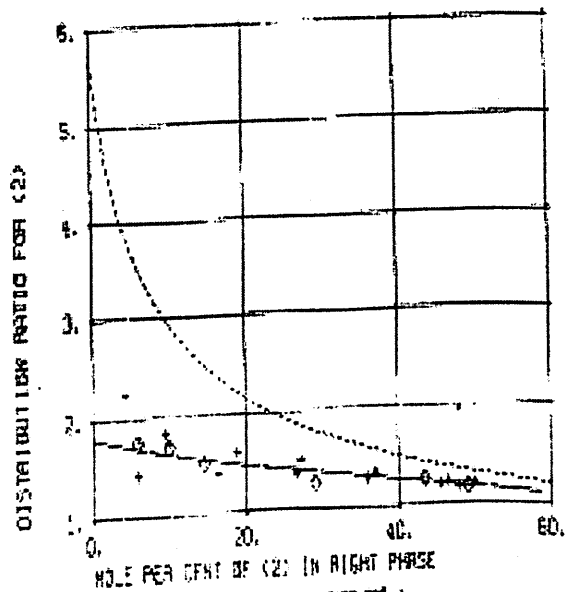
$\theta_1 = 5.1702$      $\theta_2 = 1.1373$      $\theta_3 = 4.0355$   
 $\sigma_1 = 1.396$      $\sigma_2 = 2.400$      $\sigma_3 = 1.200$

MEAN DEV. BETWEEN CALC. AND EXP. CONC. IN HOLE POT

UNIQUAC (SPECIFIC PARAMETERS)	0.78
NRTL (SPECIFIC PARAMETERS)	0.77
UNIQUAC (COMMON PARAMETERS)	1.99



EXP. TIE LINE  
 CALC. USING  
 UNIQUAC    NRTL (SP)    UNIQUAC  
 O    +    X



EXP. DISTR. RATIOS    THIS REF.    OTHER REF.    UNIQUAC  
 O    +    X    O    X    O

11) C6H6      HEXANE  
 -----  
 12) C8H18     BENZENE  
 -----  
 13) C10H16    SURFONE, TETRAMETHYLENE  
 -----

HANSON O., PATEL A.H., CHANDRASEKAR S.S.  
 J. APPL. CHEM. 15(1969)123

TEMPERATURE = 20.5 DEG C      TYPE OF CYCLE = 1

EXPERIMENTAL TOE CENTER IN MOLE PER CENT

LEFT PHASE			RIGHT PHASE		
(1)	(2)	(3)	(4)	(5)	(6)
83.071	8.467	2.462	1.410	4.211	14.550
80.160	17.161	2.40	1.610	3.820	14.150
57.581	38.802	2.307	2.100	3.200	13.100
57.039	40.371	2.443	2.382	2.700	12.100
47.258	53.037	2.434	2.520	2.000	11.000
38.108	64.237	2.413	2.700	1.600	10.000
31.248	70.150	2.383	2.820	1.200	9.000

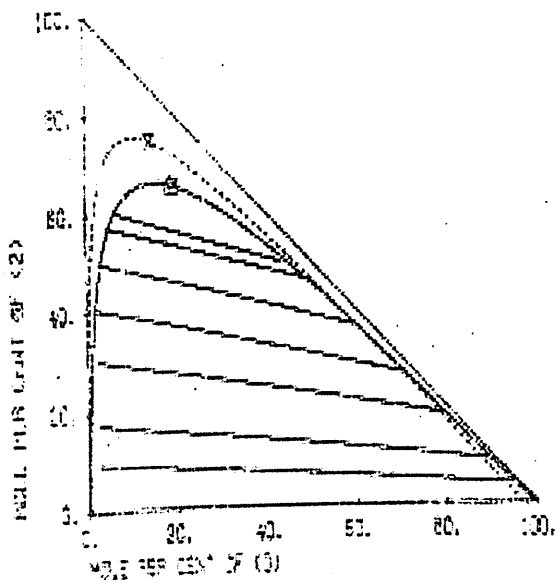
SPECIFIC MODEL PARAMETERS IN MOLE PER CENT

I	UNIQUE		TOTAL	
	ALL	100	100	100
1	101.34	-1.120	-100.00	100.00
2	40.17	1.120	100.00	100.00
3	43.17	-1.120	100.00	100.00

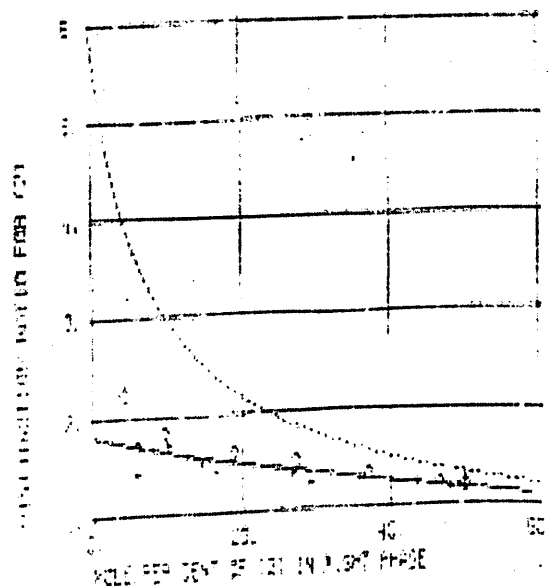
11 = 5.1740    12 = 1.1173    13 = 1.1173  
 21 = 4.1174    22 = 1.1173    23 = 1.1173

MEAN DEV. BETWEEN CALC. AND EXP. DATA IN MOLE PER CENT

UNIQUE (SPECIFIC PARAMETERS)	0.6%
TOTAL (SPECIFIC PARAMETERS)	1.0%
UNIQUE (COMMON PARAMETERS)	0.3%



11 = 5.1740    12 = 1.1173    13 = 1.1173  
 21 = 4.1174    22 = 1.1173    23 = 1.1173



11 = 5.1740    12 = 1.1173    13 = 1.1173  
 21 = 4.1174    22 = 1.1173    23 = 1.1173

TABLE 3 EXTRACTION OF LIGHT DISTILLATES

	Feedstock A		Feedstock B	
	Design	Actual	Design	Actual
<b>Feed</b>				
Benzene, %	1.0	0.7	0.5-1.0	0.07
Total aromatics, %	3.0	1.1	12.5	9.7
ASTM boiling range, °C	20-95	20-100	85-160	81-163
<b>Raffinate</b>				
Benzene, ppm	150	< 10	150	< 5
Total aromatics, %	0.1	< 0.01	0.3	0.2
Sulfolane, ppm		< 5		5.3
<b>Extract</b>				
Total aromatics, %		55-60 <sup>b</sup>	95	95
Sulfolane, ppm		< 5		< 5

	Feedstock C		Feedstock D		Feedstock E		Feedstock F	
	Design	Actual	Design	Actual	Design	Actual	Design	Actual
<b>Feed</b>								
ASTM distillation, °C	110-115	110-115	100-140	100-140	40-90	10-100	60-90	60-90
Total aromatics, %	7.7	7.6	12.0	11	0.8	1	0.8	0.7
<b>Raffinate</b>								
Total aromatics, %	5-10	7	< 1	< 1	< 0.1	0.005	< 0.1	< 0.01
<b>Extract</b>								
Total aromatics, %	99.9	99.9 <sup>a</sup>		99.9	-	5		5

Sulfolane, Aromatics and Benzene

No. of Stages – 9

Mass Flow Rate of Feed = 30 tonne/hr.

Mass Flow Rate of Solvent = 60 tonne/hr.

Temp. at Top = 80 C

Temp. at Bottom = 60 C

Column Pressure = 9 atm

## BIBLIOGRAPHY

- Robert E Treybal, Mass Transfer Operations, Tata Mc Graw Hill International Edition 1981, Pg 541-552.
- Dr. Ram Prasad, Petroleum Refining Technology, Khanna Publishers, Second Reprint Edition 2004, Pg 285-292, 303-305.
- Roger G.E Franks, Modeling & Simulation in Chemical Engineering, John Wiley and Sons INC., Copyright 1972, Pg 214-219
- Seader, J.D. and Henley, E.J. Separation Process Principles. John Wiley and Sons. New York, 1999
- Sandler, S.I. Chemical and Engineering Thermodynamics. John Wiley and Sons. New York, 1998.
- Douglas, J.M. Conceptual Design of Chemical Processes. McGraw-Hill. New York, 1988.
- Hanson, C., Baird, M.H.I., Lo, T.C. Handbook of Solvent Extraction. John Wiley and Sons. New York, 1983.
- [www.rccostello.com](http://www.rccostello.com)

- [www.chemstations.net](http://www.chemstations.net)
- [www.cheresources.com](http://www.cheresources.com)
- [www.prosim.net](http://www.prosim.net)
- [www.glue.umd.edu](http://www.glue.umd.edu)
- [www.google.com](http://www.google.com)