

# MEMBRANE SEPARATION : A CASE STUDY ON PURGE GAS SYSTEM

## A DISSERTATION

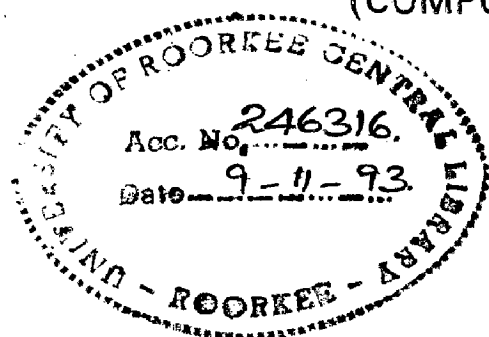
submitted in partial fulfilment of the  
requirements for the award of the degree  
of

MASTER OF ENGINEERING

in

CHEMICAL ENGINEERING

(COMPUTER AIDED PROCESS PLANT DESIGN)



By

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## CANDIDATE'S DECLARATION

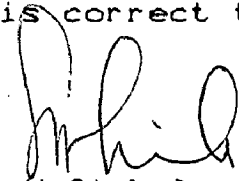
I hereby declare that the work which is being presented in the dissertation entitled " MEMBRANE SEPARATION : A CASE STUDY ON PURGE GAS SYSTEM " in partial fulfilment of the requirements for the award of the degree of MASTER OF ENGINEERING in CHEMICAL ENGINEERING with specialization in COMPUTER AIDED PROCESS PLANT DESIGN, submitted in the Department of Chemical Engineering, University of Roorkee, Roorkee, is an authentic record of my own work carried out for a period of seven months from July 1990 to January 1991, under the supervision of Dr. S.N. Sinha, Lecturer and Dr. A.K. Agarwal, Lecturer Department of Chemical Engineering, University of Roorkee, Roorkee.

The matter embodied in this dissertation has not been submitted by me for the award of any other degree or diploma.

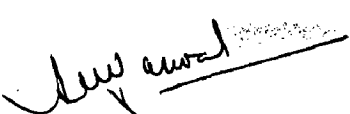
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This is certified that the above statement made by the candidate is correct to the best of my knowledge.

  
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Lastly I would like to thanks all those who directly or indirectly helped me in my dissertation.



( SANJIV KUMAR GUPTA )

## ABSTRACT

Membrane separation technologies are now widely used in chemical industries because of their lower costs, less maintenance, lower energy consumption and reduced pollution problems than other separation technologies. The mechanism of gas separation is based on the principle that certain gas permeates more rapidly than others. Membranes are now widely used in fertilizer plant for separation of hydrogen. The purge gas in ammonia plant contains approximately 65% of  $H_2$  and rest is  $N_2$  with Ar and  $CH_4$ . We can achieve hydrogen purity upto 99% using these membrane.

A mathematical model was developed considering counter current mode of flow for membrane configuration of flat sheet, hollow fiber feed outside mode and hollow fiber feed inside mode. The assumptions of steady state, no radial concentration gradient, permeability dependent of temperature only etc. were taken. The model equations were derived from mass balance equation along with Henry's law and Fick's law for molar flux relation and pressure drop relation of Hagen Poiseuille. Numerical integration was done using Fourth order Runge Kutta method. A computer program in Fortran was developed and the model was checked with reported data.

The comparison of mode of flow (co-current and counter current) and membrane configuration (flat sheet and hollow fiber) was done. Hollow fiber feed outside mode with counter current flow was found having highest permeate composition and was considered

for further study with purge gas system taking three membrane materials (cellulose acetate, polyimide and polystyrene).

The simulation study was done to see the effect of feed flow rate, pressure ratio and temperature on permeate composition for the separation of purge gas system ( $H_2 - N_2$ ).

Simulation studies showed that polyimide membrane is better than cellulose acetate and polystyrene for the separation of hydrogen from purge gas. Polystyrene was found to be most inferior for purge gas separation. The effect of temperature was insignificant in all cases. The permeate composition was found to increase with a increase in flow rate and a decrease in pressure ratio. It is advisable to use counter current hollow fiber feed outside mode permeator with polyimide membrane at high feed flow rate and at as high a feed pressure as permitted by the mechanical strength of membrane system for better hydrogen recovery from purge gas.

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## NOMENCLATURE

|            |   |
|------------|---|
| A          | Surface area of membrane, $\text{cm}^2$   |
| $D_i$      | Inside diameter of hollow fiber, cm   |
| $D'_i$     | Diffusivity of 'i' species, $\text{cm}^2/\text{sec}$  |
| $D_{LM}$   | Logarithmic mean of inside and outside diameter of hollow fiber, cm                         |
| d          | Thickness of membrane, cm   |
| $k_i$      | Henry's Constant  |
| l          | Length of hollow fiber, cm  |
| L          | Local feed flow rate, mol/sec   |
| $L_w$      | Feed flow rate at reject end, mol/sec   |
| $L_f$      | Feed flow rate at permeator entry, mol/sec  |
| $L^*$      | Normalized value of L.  |
| $P_1, P_2$ | Total pressure on two sides of membrane, Pa   |
| $P_f$      | Inlet feed pressure, Pa   |
| $P_i$      | Pressure inside the hollow fiber, Pa  |
| $P_o$      | Permeate pressure, Pa   |
| $q_i$      | Volumetric flow rate of 'i' species, $\text{cm}^3/\text{sec}$                               |
| R          | Universal gas constant, $\text{Pa}\cdot\text{cm}^3/\text{mol}\cdot\text{K}$                 |
| $R_w$      | Non dimensional membrane area.  |
| $S_i$      | Specific permeability of 'i' species, $\text{mol}/\text{sec}\cdot\text{cm}^2\cdot\text{Pa}$ |
| $S_1$      | Specific permeability of more permeable component.  |
| $S_2$      | Specific permeability of less permeable component.  |
| T          | Absolute temperature, K   |
| V          | Local permeate flow rate, mol/sec   |
| $V^*$      | Normalized value of V.  |
| $V_f$      | Permeate flow rate at feed side, mol/sec  |
| $V_w$      | Permeate flow rate at reject side, mol/sec  |



|                  |  |
|------------------|--|
| $x_{i1}, x_{i2}$ | Mole fraction of $i$ species on two side of membrane.                        |
| $x$              | Local mole fraction of more permeable component.                             |
| $x_f$            | Mole fraction of more permeable component on feed side                       |
| $x_w$            | Mole fraction of more permeable component in reject stream.                  |
| $y$              | Local mole fraction of more permeable component on permeate side.            |
| $y_w$            | Mole fraction of more permeable component in permeate stream at reject side. |
| $y_f$            | Mole fraction of more permeable component in permeate stream at feed side.   |

#### GREEK LETTERS

|          |                                   |
|----------|-----------------------------------|
| $\alpha$ | Separation factor ( = $S_1/S_2$ ) |
| $\beta$  | Constant given by equation 3.33a  |
| $\gamma$ | Pressure ratio ( = $P_o/P_f$ )    |
| $\mu$    | Viscosity of gas, cp              |
| $\phi$   | Pressure ratio ( = $P_v/P_f$ )    |

#### SUBSCRIPT

|     |  |
|-----|--|
| $f$ | pertaining to the permeator axial location where high feed enters. |
| $w$ | pertaining to the permeator axial location where high feed enters. |
| $T$ | Total value, used for permeator membrane area.                     |

#### SUPERSCRIPIT

|   |                  |
|---|------------------|
| * | Normalized value |
|---|------------------|

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## INTRODUCTION

It is for almost two hundred years that biologists have realized the membrane in living organism have extra ordinary power of creating and maintaining concentration differences among different substances. A hundred and twenty years ago Thomas Graham (1866) showed that synthetic membranes could do the same thing. He used rubber sheet through which air was permeated. Scientists later developed membrane dialysis as a means of purification in the laboratory and then it is used industrially to treat some waste streams.

Membranes are thin barriers that allow preferential passage of certain substance. They are predominantly based on polymeric materials but some ceramic glass and metallic membranes also exists [Haraya et al. (1986), Konno et al. (1988)]. Polymers commonly employed for gas separation membrane include cellulose acetate and its derivatives, polyamide, and polyimides.

Membrane separation processes have important advantages over other separation processes because no phase change is involved and therefore energy requirement of the system is low. Feed, product, and waste streams are totally contained and kept separate, so no uncontrolled pollution problem can arise.

Now membrane systems are replacing number of older, more

costly separation technologies such as distillation, cryogenics, pressure swing adsorption etc. Even though separation technology tends to be very site or application specific, membrane systems offer lower costs, less maintenance and more flexibility than the older technologies. Membrane systems are smaller in size and more modular in design than the equipment they replace and therefore, fit into existing plant structures without requiring any new construction, which results in lower capital investment and shorter construction time. Labor and maintenance costs are reduced because the membrane systems generally have fewer moving parts and require minimal operator attention. The modular system approach also offer more flexibility in design and operation. New units can be easily added or section can be turned on or off depending on plant efficiency.

Although gas membrane technology is still young, it is proving to be one of the most significant new operation to appear in the past two decades. The separation of gases by membrane is an energy efficient separation process, that is, simple and compact and can operate isothermally with no change of phase . Because of inability to perfect the process to produce uniformly good membranes in quantity, membranes were not commercially successful earlier. Later, Loeb and Souriranjan (1960) achieved a technical break through when they developed an asymmetric membrane. Figure 1.1 shows the asymmetric membrane. It consists of an ultra thin dense skin supported on a highly porous substructure having negligible resistance to gas flow. The skin which acts as a separation

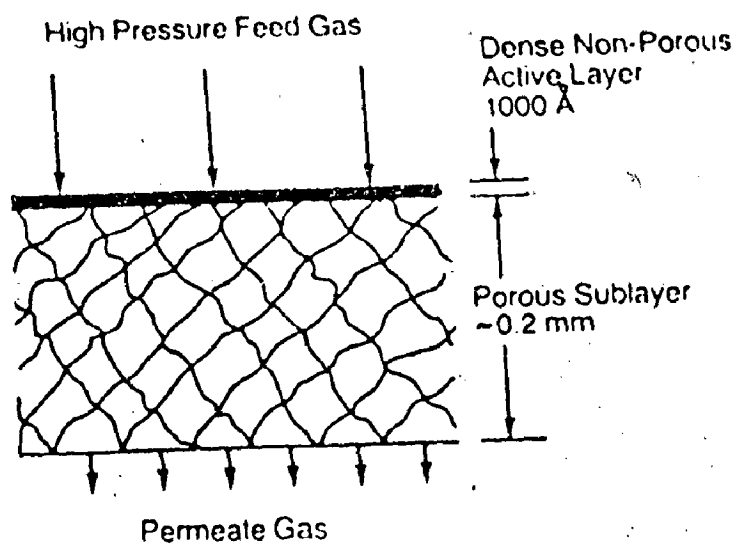


FIG.1.1: ASYMMETRIC MEMBRANE FOR GAS SEPARATION.

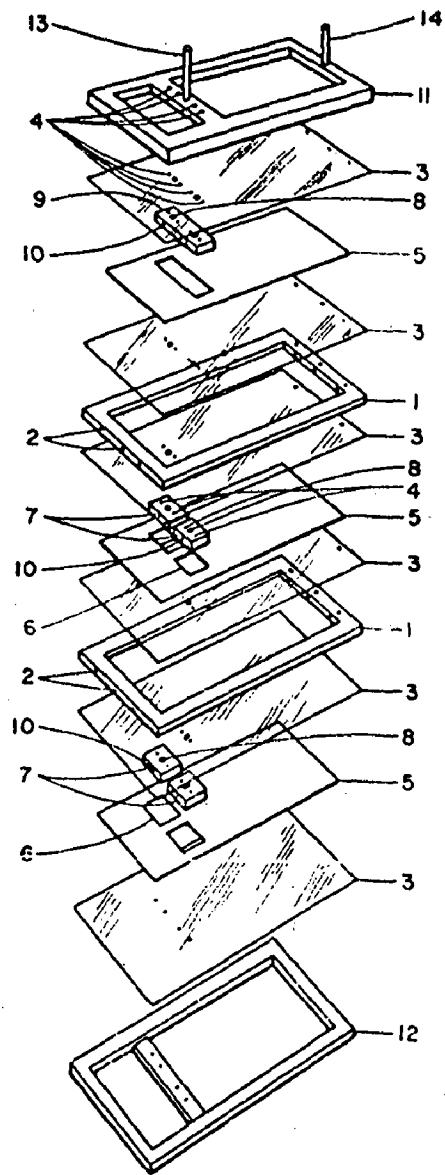
barrier is nonporous and is highly permeable due to its thinness. The porous support provides the mechanical strength to membrane to withstand high pressure. The presence of the porous supporting layer, renders the permeation behavior of the asymmetric membrane some what different from that of symmetric membranes. Asymmetric membranes have made it possible to have both high permeability and high selectivity for efficient gas separation.

Successful application of the membrane for gas separation depends upon discovery of economically competitive membrane with high selectivities and permeabilities. On the other hand, engineering considerations such as membrane configuration and flow pattern (co-current, counter current and cross flow) of the feed and permeate streams are also important in determining the performance of the separation system. The separation equipment is mainly of three types - Flat Sheet Permeator (Figure 1.2), Spiral Permeator (Figure 1.3) and Hollow Fiber Permeator (Figure 1.4). These equipment are simple, modular and easy to control.

Membrane separation technology has captured the attention of industries related to hydrocarbon processing, chemical purification, pharmaceutical and biotechnology processing, water desalination and liquid waste processing. One of the most recent development of membrane has been commercialization for separation and/or purification of mixed gas stream found in refineries, chemical plant and natural gas reservoirs.

The design of industrial processes for separating gases





1, Rectangular frame; 2, gas passages in frame; 3, membrane; 4, holes in membrane, frame, or collector blocks for bolting; 5, porous sheet; 6, cut-out portion in porous sheet; 7, collector blocks; 8, passages in collector blocks; 9, uppermost collector block; 10, lateral passages in collector blocks; 11, upper clamping frame; 12, lower clamping frame; 13, outlet for permeated gas; 14, outlet for unpermeated gas.

FIG. 1.2: FLAT SHEET PERMEATOR.

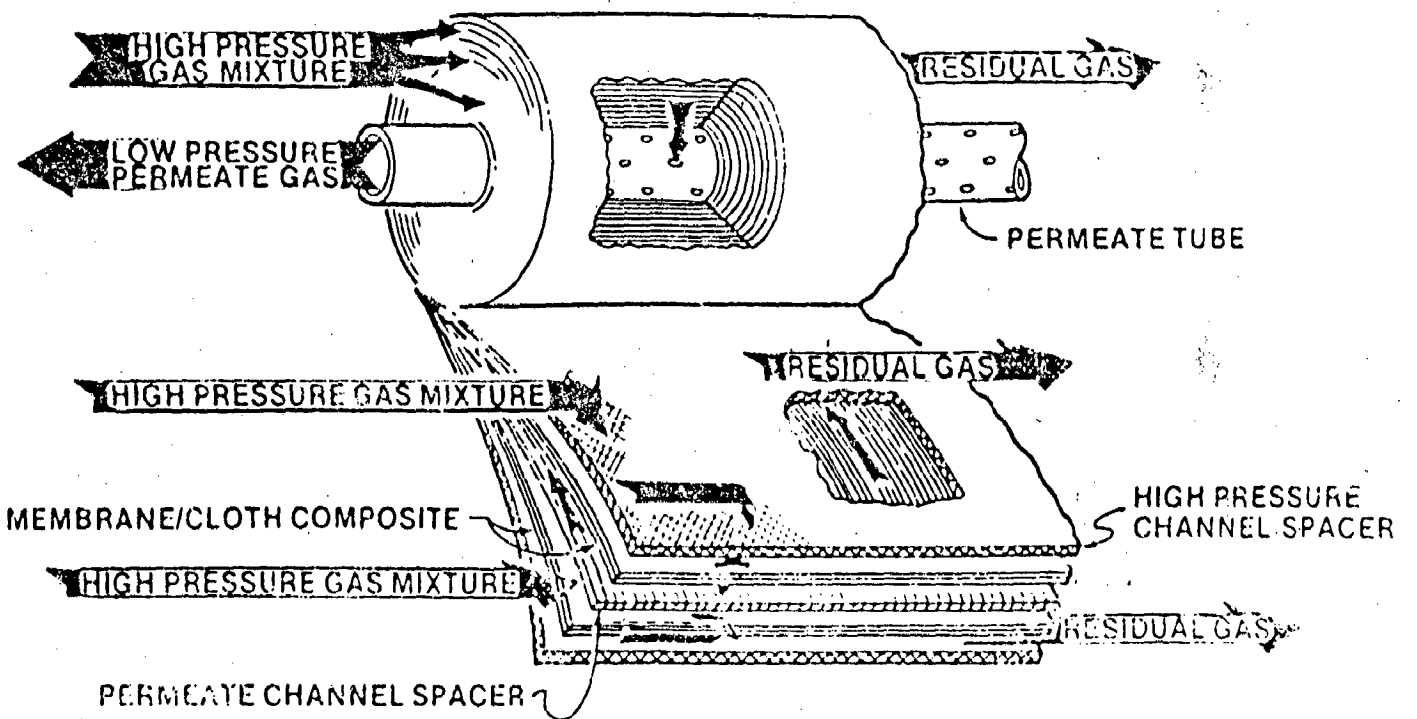


FIG. 1.3: SPIRAL WOUND PERMEATOR.

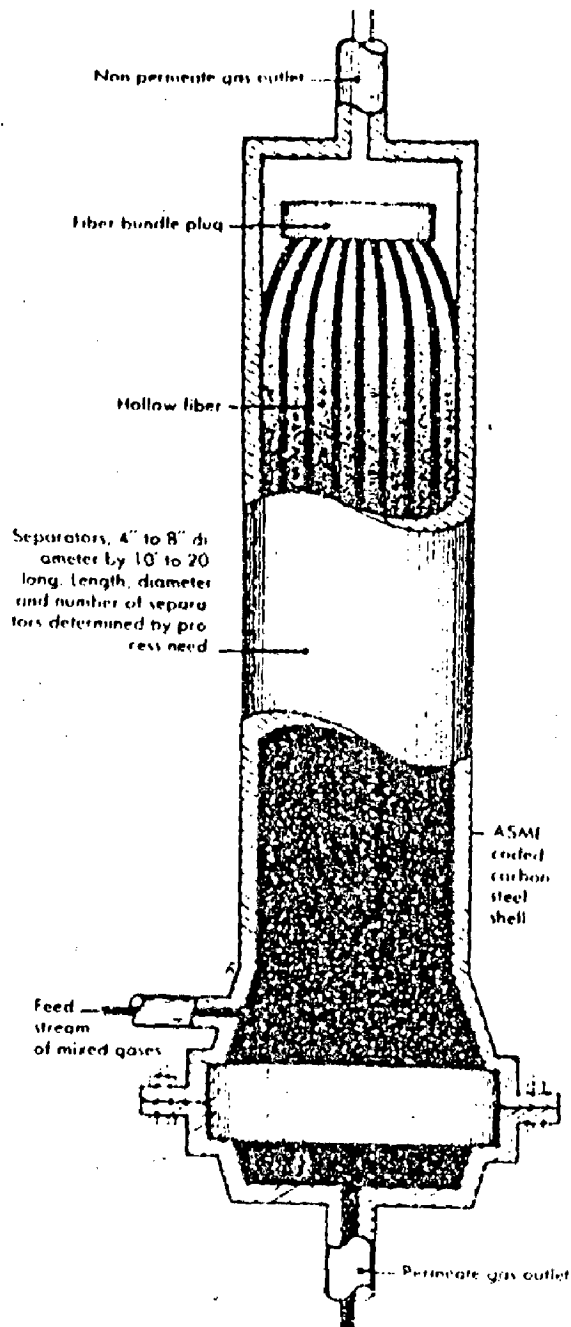


FIG. 1.4: HOLLOW FIBER PERMEATOR.

with membranes depend ultimately on relative rates of transport of components of a mixture through a membrane. The use of membranes to recover hydrogen is now widely spread in the ammonia and refinery industries. This area provides an excellent opportunity for membrane because these are cost effective and <sup>involve</sup> lesser risk to the user. Also, membrane failure would not affect the plant operation because they are recovery units added to increase efficiency.

In the modern and new ammonia plants, hydrogen is an expensive raw material which is produced by steam reforming of natural gas. Ammonia is produced in a recycle catalytic reactor. To overcome the built up of inert gases (such as argon and unreacted methane) in the closed loop of the reaction system a continuous gas purging is carried out to keep the level of inerts at a constant and tolerable limit. This purge gas contained valuable hydrogen but separation is considered expensive with traditional processes. Therefore an efficient process is required which could give good yield and also cheap and easy to operate. Membranes are now used to provide a cost effective separation process which result in energy saving.

The modelling and simulation of membrane separation system is essential for its proper control and good performance. Literature reveals that several workers have contributed significantly in the understanding and performance of membrane systems for several binary gas mixture by way of modelling the different membrane configurations. However there still exists a lot of scope for

future work in this direction.

The present work is aimed to study the performance of different membrane for enriching the hydrogen gas from the purge gas.

The main aims of present investigation is summarized as follows :

- (1) Analysis and modelling of gas separation system by membrane operating in counter current mode for Flat Sheet and Hollow Fiber.
- (2) Development of computation technique and simulation program.
- (3) Comparison of co-current and counter current mode.
- (4) A case study of hydrogen separation from purge gas by treating it as binary gas mixture of hydrogen and nitrogen.

## PERMEATOR ANALYSIS

At the early stage of gas separation, the porous membranes were used in which the permeation of the gas takes place due to pore size of the membrane, but it was found that these membranes were not very effective for industrial purposes.

In 50's several workers worked on nonporous homogeneous membrane. They consider the flat sheet membrane and developed the several models based on different assumptions [Weller and Steiner, 1950; Naylor and Backer, 1955; Blaisdell and Kammermeyer, 1973; Stern and Wang, 1978; Sirkar et al., 1984; Pan and Habgood, 1974]. It was found that permeation was not very good because of the thick membrane. In 60's gas permeation took a new turn when asymmetric membrane was developed. Several papers were published based on asymmetric membrane. [Antonson et al., 1977; Stern et al., 1977; Pan and Habgood, 1978; Pan, 1983; Sirkar et al., 1986; Sirkar et al., 1987; Sirkar et al., 1988; Singh, 1990].

The golden era for gas permeation was achieved when scientists got success in making hollow fiber. [Loeb and Sourirajan, 1960]. Now a days still lot of works are going on this field. This chapter reviews the development in the modelling of different gas permeators and their performance.

## 2.1 FLAT SHEET PERMEATOR

Weller and Steiner (1950) considered both single stage and multistage flat sheet permeator and developed the model for binary gas system based on the fact that number of nonporous organic membranes have a property of showing a much higher permeability toward some gases than others. The model equations consist of mass balance equation, Henry's Law and Fick's Law relation. They made following assumptions to simplify their model :

- (1) The system is operated at steady state.
- (2) Permeability of species are independent of pressure and composition.
- (3) Membrane is homogeneous in structure and fiber remains physically undeformed.
- (4) The flow is laminar on both side of the membrane.
- (5) Pressure drop is insignificant on each side of the membrane.

Permeability coefficients for <sup>a</sup> number of gases were determined for ethyl cellulose and polystyrene membrane and it was found that ethyl cellulose is suitable for fractionation of air, whereas polystyrene is suitable for separation of helium and oxygen from gas mixture. They observed that the total membrane area is approximately inversely proportional to the pressure used on the high pressure side. The theoretical result obtained agreed to the lab data within experimental error.

The major shortcoming of their model was non consideration of flow pattern of the gas. However, their equations were simple and easy to apply for single stage.

Naylor and Backer (1955) developed the general method of calculating number of stages requirement for separating gases of widely differing molecular weight. Following assumptions were different from Weller and Steiner's :

- (1) Plug flow on the high pressure side.
- (2) There exists a constant effective separation factor at any point along the membrane.

Their model equations were derived using Knudson's Law of Molecular Diffusion. The solution procedure was similar to the McCabe and Thiele diagram used in distillation. They showed that the separation of such gases depends on square-root of the molecular weight ratio.

Similar to Weller and Steiner they also did not consider the direction of the permeate flow.

Blaisdell and Kammermeyer (1973) modified the model given by Weller and Steiner by incorporating the flow pattern in it. They assume the plug flow on both side of the membrane for their model. The binary system of Oxygen and Helium was used for the investigation. The area requirement for a given separation was evaluated by a numerical integration.

They observed that the direction of flow pattern (that is, co-current or counter current flow) have an important role in permeate composition. They showed that the permeate composition varies with the direction of the flow and also showed that maximum separation can be achieved in counter current mode.

Stern and Wang (1978) compared the above two methods given by Walawender and Stern (1972) and Blaisdell and



Kammermeyer (1973) and showed that the computational time required for numerical solution was same in both cases. In fact, the nature of problem specification dictates the preferred method of formulation and their solution. For example, if mole fraction of permeate is specified it is better to formulate with mole fraction as the independent variable and if area is specified as in simulation problems, then area should be the independent variable.

The solution of differential equation for counter current flow had a convergence problem, therefore computer time required to solve it was more than that of co-current.

Sirkar *et al.* (1984) developed the series solution technique with assumption that there is no axial pressure drop on either side of the membrane and membrane thickness is constant and showed that analytical solution takes very less time with respect to numerical solution.

In DEC-10 computer counter current, numerical solution requires an average CPU time of 1min. 40sec, while the analytical solution requires only 2.6sec. Similarly for co-current the numerical solution requires 13.2sec, while analytical solution requires only 0.6sec. The result obtained through numerical solution and that by analytical solution were slightly different but within the tolerable limit. This method therefore can be used for preliminary process design.

A conventional membrane gas separator has only the high pressure feed stream entering the permeator. The permeate stream is produced strictly by permeation. Applications where purification of the feed stream is of interest could benefit

by having a purge or sweep stream entering the permeate side. The most important advantage is that the partial pressure difference could be significantly increased since the partial pressure of the permeating species is reduced.

*Pan and Habgood (1974)* analyzed a permeator having purge stream on the permeate side. The assumptions made for their model were similar to that of *Blaisdell and Kammermeyer*. The gas system taken by them was recovery of Helium from Natural gas. They observed that counter current is the most effective flow pattern followed by cross flow with co-current pattern having the worst performance. Purging implies a higher driving force which result in a significant reduction in membrane area requirement without diluting the permeate stream.

## 2.2 HOLLOW FIBER PERMEATOR

*Antonson et al. (1977)* studied the symmetric hollow fiber membrane system performance with flow on both side, that is, shell side flow and tube side flow of the high pressure feed. Following assumptions were made to develop the model:

- (1) Permeation involves three mass transfer step for each gas: Adsorption on the membrane surface, Diffusion in the membrane and Desorption from membrane surface.
- (2) Permeability coefficients for both gases depends on fiber characteristics and temperature.
- (3) Permeability coefficients for components of a permeating gas mixture are same as those for pure components

- (4) Pressure drop in fiber follows Poiseuille's equation for laminar flow.
- (5) Mixture viscosity is based on mole fractions.

They consider a binary gas system consisting of  $H_2$  and  $CH_4$  for their investigation. They showed the effect of flow rate and flow pattern and showed that as the flow rate of feed is increased the permeate composition increased. They also showed that whether the feed flow is shell side or fiber side counter current flow is superior to co-current flow.

*Stern et al.* (1977) also studied experimentally the separation of various gas mixtures. They have used the shell side flow of feed gas mixture for symmetric silicon capillary membranes. Since hollow fiber are in general pressurized from outside, the analysis had been done to shell side flow.

These permeators have very low productivity due to thick membrane, so they are not preferred. Now a days asymmetric membranes are used because of its high flux capabilities.

*Pan and Habgood* (1978) modeled the hollow fiber permeator with symmetric membrane. They consider shell side feed with assumptions similar to that of *Antonson et al.* for a binary gas mixture of Helium and Methane. *Pan* (1983) analyzed the same problem using asymmetric membrane with a dense skin on the outer side of the hollow fiber. *Pan* studied the behaviour of the co-current and counter current flow patterns and compared them with experimental data.

He obtained almost identical performance for both flow pattern ( with a difference of 4 % , which he considered as an experimental error ). Therefore he preferred co-current

flow rather than counter current for asymmetric membrane.

Sirkar et al. (1986) extended their series solution technique from flat sheet [Sirkar et al. (1984)] to hollow fiber membrane. In this paper they developed a series solution technique for both the permeate and reject composition. The error in the series solution for co-current flow was around 6% while that for counter current mode was around 4%. The counter current flow had produce a richer permeate and leaner reject than co-current flow.

Sirkar et al. (1987) investigated experimentally the oxygen enrichment of air by permeation through silicon capillary membrane, with partial or total recycle of the oxygen enriched permeate to the fresh air feed. The basic assumptions for the recycle permeator were plug flow, counter current, parallel plate silicone permeator with no axial pressure drop and no membrane deformation. They showed that the partial recycle of the oxygen enriched permeate to the feed side significantly enhance the oxygen enrichment of the permeate, and the oxygen enrichment increases with increase in recycle ratio. They further showed that if feed stream pressure drop and capillary deformation is also incorporated in it then the behaviour of the model was quite well.

Sirkar et al. (1988) studied the difference between the symmetric and asymmetric membrane models using a sweep gas technique. Two systems  $\text{CO}_2 - \text{N}_2$  and  $\text{O}_2 - \text{N}_2$  were studied with cellulose acetate membrane. They showed that for the feed outside mode, the symmetric model fits the experimental behaviour of the cellulose acetate membrane better than the

asymmetric model. Similar were the results obtained when operated in feed inside mode.

Singh (1990) developed the mathematical model in co-current mode for flat sheet and hollow fiber. He studied the effect of feed flow and feed pressure on permeate composition for two systems, bio-gas and air with three different membrane materials i.e. cellulose acetate, ethyl cellulose and polystyrene. Assumptions made for the modeling were similar to that of Sirkar et al. (1987). He showed that variation in feed flow does not effect the permeate composition while permeate composition increases with increase in feed pressure.

### 2.3 TWO MEMBRANE PERMEATOR

Two membrane permeator consists of two membrane in same permeator having reverse membrane selectivity i.e. one membrane is more permeable to one component while the other membrane is more permeable to second component.

The advantages of using two membrane in a permeator is that the extent of separation is increased and also it lowers the energy and capital investment costs of membrane separation process. These systems are useful for the separation of multi component gas mixtures.

Perrin and Stern (1985) developed the mathematical model for separation of binary gas mixture in permeator having two flat sheet membranes. The assumptions were similar to that of Blaisdell and Kammermeyer for flat sheet membrane. Based on that model they studied the effect of flow pattern on the

performance of two membrane permeator.

They showed that in general counter current is the most efficient flow pattern, followed by co current. In other words it can be said as, counter current flow yield the highest degree of separation and required the smallest membrane area for a given flow rate.

*Sirkar and Sengupta (1987)* studied the ternary gas mixture. The gas mixture consists of He, CO<sub>2</sub>, and N<sub>2</sub> and the two membranes were cellulose acetate and silicon rubber. The assumptions differed from Antonson et al. as follows :

- (1) Viscosity of gas mixture depend on the composition of mixture.
- (2) No axial dispersion in the bulk flow direction.

They showed that the selectivities of two membranes are coupled to each other i.e. the increase in selectivity of one membrane improves the performance of both membranes in the permeator and a decrease in the selectivity of undermines the performance of both. They further showed that increase in the relative permeation area of the more selective membrane of the two improves the performance of both membrane.

*Sirkar et al. (1989)* studied the internally staged permeator consisting of two hollow fiber membrane in same permeator. In this permeator permeation takes place in two stage. The high pressure feed gas enters the lumen of the first membrane, gas permeate from this fiber to the shell side and from there the gas permeate through second membrane. The membranes used were cellulose acetate membrane and the system studied were O<sub>2</sub> - N<sub>2</sub> (air) and CO<sub>2</sub> - N<sub>2</sub>.

It was shown that internal stage permeator in co current

mode performs better than counter current flow pattern. The performance of the internal stage permeator can be improved by recycling the intermediate shell side reject stream to the feed stream. The internal stage permeator produces a richer permeate without any additional energy expenditure.

## MATHEMATICAL MODELLING

The mathematical model, precisely defining the membrane separation process, may be written in form of mass balance, momentum balance, and heat balance equations. The equation for rate of gas permeation is given by Fick's Law and the pressure drop relation in hollow fiber is given by Hagen Poiseuille Law. The equations obtained are nonlinear and coupled ordinary differential equations. For the case of co-current flow model, equations and the simplifying assumptions have been presented by Singh (1990). For the counter current, the solution of these equations showed difficulties due to the convergence problem. Therefore in order to get a model which could give the inside and exit conditions of the permeator with reasonable accuracy, certain simplified assumption are to be made.

Usually two types of membrane configuration are used in gas separation, one is flat sheet and another is hollow fiber. In hollow fiber feed may flow from inside or outside the fiber. Therefore, models were developed for the above three cases, that is, for flat sheet membrane and hollow fiber feed outside mode and hollow fiber feed inside mode.

Following assumptions were made for the modelling of membrane system :

- (1) The permeator is operated at steady state.



- (2) Permeabilities of species are constant irrespective of pressure and composition.
- (3) Membrane is assumed to be homogeneous in structure.
- (4) Diffusion along flow pattern is insignificant as compared to bulk flow.
- (5) The flow pattern inside the permeator is counter current.
- (6) There is no radial concentration gradient in the gas phase.
- (7) Fibers are not physically deformed on pressurization.

The main laws for the gas permeation are Henry's Law and Fick's Law. Henry law relates the concentration  $x_i$  of the gaseous component  $i$  at the membrane surface to the partial pressure  $p_i$  of the component.

By applying the Henry's Law at membrane surface we get

$$x_i = k_i p_i \quad \dots\dots\dots(3.1)$$

Let the membrane thickness be  $t$ . So applying Fick's Law of diffusion we get

$$\frac{q_i}{A} = \frac{D_i(x_{i2} - x_{i1})}{t} \quad \dots\dots\dots(3.2)$$

where,  $D_i$  = Diffusibility of species  $i$  in the membrane.

$q_i$  = Volumetric flow rate of species  $i$ .

$A$  = Surface area of membrane.

$x_{i1}, x_{i2}$  = Mole fraction of species  $i$  on both side of membrane.

From Equation (3.1) and (3.2) we get

$$\frac{q_i}{A} = \frac{k_i D_i}{t} (p_{i2} - p_{i1})$$

Let  $\frac{k_i D_i}{t} = S_i$

$$\frac{q_i}{A} = S_i (P_{i2} - P_{i1})$$

$$= S_i (P_2 x_{i2} - P_1 x_{i1}) \dots\dots\dots (3.3)$$

where,  $P_1, P_2$  = Total pressure on two sides of membrane.

$S_i$  = Specific permeability of species i.

### 3.1 FLAT SHEET MEMBRANE :

Consider a permeation cell as shown in Figure 3.1 consisting of a rectangular flat sheet membrane which divide inside volume into two parts. Feed flows on one side of membrane and reject is withdrawn from the same side while permeate is withdrawn from the other side of membrane.

From Equation (3.3) we get

$$\frac{d(Lx)}{dA} = S_i (P_f x - P_o y)$$

$$= S_i P_f (x - (P_o/P_f) y)$$

$$= S_i P_f (x - \gamma y)$$

where,  $\gamma = P_o/P_f$

$$L_w \frac{d((L/L_w)x)}{dA} = S_i P_f (x - \gamma y)$$

$$\frac{d(L^*x)}{dR_w} = \alpha (x - \gamma y) \dots\dots\dots (3.4)$$

where,  $L^* = L/L_w$

$$R_w = \frac{AS_2 P_f}{L_w}$$

$$\alpha = S_1/S_2$$

Similarly for another component we get

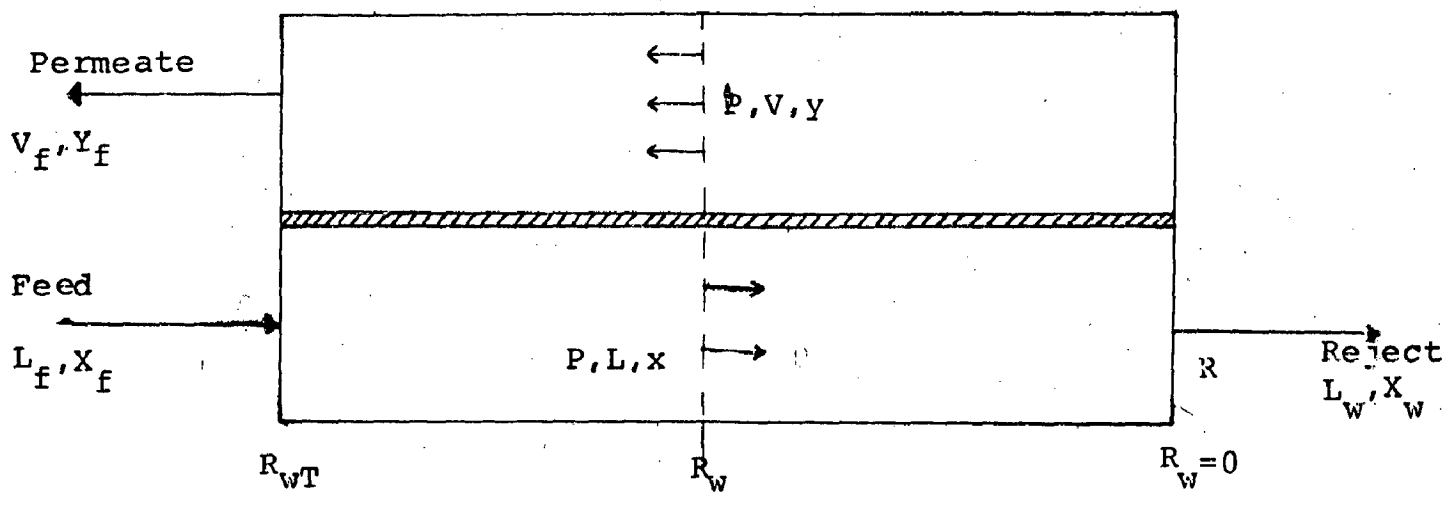


FIG. 3.1 : SCHEMATIC OF A FLAT SHEET PERMEATOR HAVING COUNTER CURRENT FLOW.

$$\frac{d(L^*(1-x))}{dR_w} = ((1-x) - \gamma(1-y)) \dots\dots\dots (3.5)$$

Expanding Equation (3.4) and (3.5) we get

$$L^* \frac{dx}{dR_w} + x \frac{dL^*}{dR_w} = \alpha(x - \gamma y) \dots\dots\dots (3.6)$$

$$L^* \frac{d(1-x)}{dR_w} + (1-x) \frac{dL^*}{dR_w} = ((1-x) - \gamma(1-y)) \dots (3.7)$$

Adding Equation (3.6) and (3.7) we get

$$\frac{dL^*}{dR_w} = \alpha(x - \gamma y) + ((1-x) - \gamma(1-y))$$

Substituting this value in Equation (3.6) we get

$$L^* \frac{dx}{dR_w} = \alpha(x - \gamma y)(1-x) - x((1-x) - \gamma(1-y))$$

or 
$$\frac{dx}{dR_w} = (\alpha(1-x)(x - \gamma y) - x((1-x) - \gamma(1-y))) / L^* \dots\dots (3.8)$$

Similarly for permeate composition we get

$$\frac{dy}{dR_w} = (\alpha(1-y)(x - \gamma y) - y(1-x) - \gamma(1-y)) / V^* \dots (3.9)$$

where  $V^* = V / L_w$

$L_w$  = Molar flow rate of the reject stream.

Taking the mass balance at feed outlet and at any point in a permeator we get

Total mass balance

$$L = V + L_w \dots\dots\dots (3.10)$$

Component mass balance

$$Lx = Vy + L_w x_w \dots\dots\dots (3.11)$$

From Equation (3.10) and (3.11) we get

$$L^* = \frac{y - x_w}{y - x} \dots\dots\dots (3.12)$$

$$V^* = \frac{x - x_w}{y - x} \dots\dots\dots (3.13)$$

Substituting the value of  $L^*$  and  $V^*$  from Equation (3.12) and (13) in Equation (8) and (9) respectively we get

$$\frac{dx}{dR_w} = \frac{(y-x)}{(y-x_w)} (\alpha(1-x)(x-\gamma y) - x((1-x) - \gamma(1-y))) \dots (3.14)$$

$$\frac{dy}{dR_w} = \frac{(y-x)}{(x-x_w)} (\alpha(x-\gamma y)(1-y) - y((1-x) - \gamma(1-y))) \dots (3.15)$$

The permeate concentration at reject end can be determined by assuming cross flow at that point. In that case permeate composition will depend only on flow of that component in feed side.

Hence from Equation (3.4) and (3.5) we get

$$\frac{d(L^*x)}{d(L^*(1-x))} = \frac{\alpha(x-\gamma y)}{(1-x) - \gamma(1-y)}$$

Since cross flow is assumed, hence the mole fraction of two component on permeate side will be proportional to the flow of respective components on the feed side and so the above equation will become

$$\frac{y}{1-y} = \frac{\alpha(x-\gamma y)}{(1-x) - \gamma(1-y)}$$

At  $x=x_w$ ,  $y=y_w$

$$\frac{y_w}{1-y_w} = \frac{\alpha(x_w - \gamma y_w)}{(1-x_w) - \gamma(1-y_w)}$$

Solving the above quadratic equation we get

$$y_w = \frac{1 + (\alpha - 1)(x_w + \alpha) - ((1 + (\alpha - 1)x_w))^2 - 4\alpha(\alpha - 1)\gamma x_w^{0.5}}{2(\alpha - 1)\gamma} \dots (3.16)$$

We see that at  $x=x_w$  Equation (3.15) becomes indeterminate. Hence its value is obtained by applying L'Hopital Rule.

Differentiating the numerator and denominator of Equation (3.12) with respect to  $R_w$  at point  $x_w, y_w$  we get

$$\begin{aligned} & (y_w - x_w)(\alpha(1 - y_w))((dx/dR_w)_w - \gamma(dy/dR_w)_w) - \alpha(x_w - \gamma y_w) \\ & (dy/dR_w)_w - y_w(\gamma(dy/dR_w)_w - (dx/dR_w)_w) - (1 - x_w - \gamma(1 - y_w)) \\ & (dy/dR_w)_w + (\alpha(1 - y_w)(x_w - \gamma y_w) - y_w(1 - x_w - \gamma(1 - y_w))) \\ & ((dy/dR_w)_w - (dx/dR_w)_w) \dots \dots \dots (3.17) \end{aligned}$$

$$\frac{dy}{dR_w} = \frac{\dots \dots \dots}{-(dx/dR_w)_w}$$

Solving for  $(dy/dR_w)_w$  and substituting  $(dx/dR_w)_w$  from Equation (3.14) with  $L^*$  equal to 1 we get

$$\left(\frac{dy}{dR_w}\right)_w = \frac{((y_w - x_w)(\alpha(1 - y_w) + y_w) - \alpha(1 - y_w)(x_w - \gamma y_w) + y_w(1 - x_w - \gamma(1 - y_w))) (\alpha(1 - x_w)(x_w - \gamma y_w) - x_w(1 - x_w - \gamma(1 - y_w)))}{2\alpha(x_w - \gamma y_w)(y_w - 1) + 2y_w(1 - x_w - \gamma(1 - y_w)) + \gamma(y_w - x_w)(\alpha(1 - y_w) + y_w)} \dots (3.18)$$

So the model equation for flat sheet membrane becomes

$$\frac{dx}{dR_w} = \frac{(y - x)}{(y - x_w)} (\alpha(1 - x)(x - \gamma y) - x((1 - x) - \gamma(1 - y))) \dots (3.19)$$

$$\frac{dy}{dR_w} = \frac{(y - x)}{(x - x_w)} (\alpha(1 - y)(x - \gamma y) - y((1 - x) - \gamma(1 - y))) \dots (3.20)$$

$$L^* = \frac{y - x_w}{y - x} \dots \dots \dots (3.21)$$

$$V^* = \frac{x - x_w}{y - x} \dots \dots \dots (3.22)$$

Initial Conditions

At  $R_w = 0$ ,  $x = x_w$ ,  $y = y_w$ , and  $\frac{dy}{dR_w} = \left(\frac{dy}{dR_w}\right)_w$

### 3.2 HOLLOW FIBER MEMBRANE :

In hollow fiber permeator membrane is tubular in shape and feed may flow outside or inside the tube.

#### (3.2.1) HOLLOW FIBER FEED OUTSIDE MODE

In hollow fiber feed outside mode feed is flowing outside the hollow fiber as shown in Figure 3.2. The general theory of permeation remains the same except that in hollow

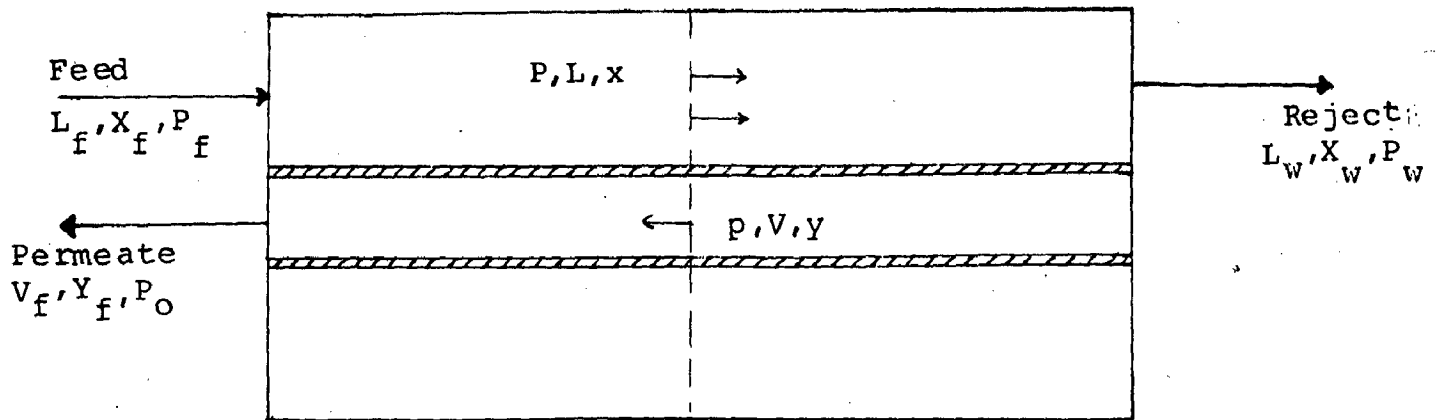


FIG. 3.2: SCHEMATIC OF A HOLLOW FIBER FEED OUTSIDE MODE GAS PERMEATOR HAVING COUNTER CURRENT FLOW.

$$\frac{P_f^2 Q_2}{L_w} \frac{dy}{dR_w} = - \frac{128\mu RTV^* L_w}{\pi^2 D_i^4 D_{LM} \gamma P_f N} \quad \dots (3.31)$$

$$\frac{dy}{dR_w} = - \frac{128\mu RTV^* L_w^2}{\pi^2 D_i^4 D_{LM} P_f^3 Q_2 \gamma N} \quad \dots (3.32)$$

$$= - \beta \frac{V^*}{\gamma} (L_w/L_f)^2 \quad \dots (3.33)$$

where,  $\beta = \frac{128\mu RT L_f^2}{\pi^2 D_i^4 D_{LM} Q_2 P_f^3 N} \quad \dots (3.33a)$

Substituting the value of  $V^*$  from Equation (3.13) in Equation (3.33) we get

$$\frac{dy}{dR_w} = - \frac{\beta(x-x_w)(L_w)^2}{\gamma(y-x)(L_f)^2} \quad \dots (3.34)$$

$$\frac{dy}{dR_w} = - \frac{\beta(x-x_w)(x_f-y_f)^2}{\gamma(y-x)(x_w-y_f)^2} \quad \dots (3.35)$$

Hence the model equations for hollow fiber feed outside mode are as follow :-

$$\frac{dx}{dR_w} = \frac{(y-x)}{(y-x_w)} (\alpha(1-x)(x-\gamma y) - x((1-x) - \gamma(1-y))) \quad \dots (3.36)$$

$$\frac{dy}{dR_w} = \frac{(y-x)}{(y-x_w)} (\alpha(1-y)(x-\gamma y) - y((1-x) - \gamma(1-y))) \quad \dots (3.37)$$

$$\frac{dy}{dR_w} = - \beta \frac{(x-x_w)(x_f-y_f)^2}{\gamma(y-x)(x_w-y_f)^2} \quad \dots (3.38)$$

$$L^* = \frac{(y-x_w)}{(y-x)} \quad \dots (3.39)$$

$$V^* = \frac{(x-x_w)}{(y-x)} \quad \dots (3.40)$$

Initial Conditions

At  $R_w = 0$ ,  $x = x_w$ ,  $y = y_w$ , and  $\frac{dy}{dR_w} = \left(\frac{dy}{dR_w}\right)_w$



### (3.2.2) HOLLOW FIBER FEED INSIDE MODE

In this case feed is flowing inside the fiber as shown in Figure 3.3, therefore pressure  $P_i$  will vary along the fiber. Let  $\phi$  be the ratio of  $P_i$  to  $P_f$ , then driving force for permeation will be " $\phi x - \gamma y$ " instead of " $x - \gamma y$ ". Hence the model equations will become as follows :

$$\frac{dx}{dR_w} = \frac{(y-x)}{(y-x_w)} (\alpha(1-x)(\phi x - \gamma y) - x(\phi(1-x) - \gamma(1-y))) \quad \dots (3.41)$$

$$\frac{dy}{dR_w} = \frac{(y-x)}{(x-x_w)} (\alpha(1-y)(\phi x - \gamma y) - y(\phi(1-x) - \gamma(1-y))) \quad \dots (3.42)$$

$$\frac{d\phi}{dR_w} = -\beta \frac{(y-x_w)(x_f - y_f)^2}{\phi(y-x)(x_w - y_f)^2} \quad \dots (3.43)$$

$$L^* = \frac{(y-x_w)}{(y-x)} \quad \dots (3.44)$$

$$V^* = \frac{(x-x_w)}{(y-x)} \quad \dots (3.45)$$

Initial Conditions

$$\text{At } R_w = 0, \quad x = x_w, \quad y = y_w, \quad \frac{dy}{dR_w} = \left( \frac{dy}{dR_w} \right)_w$$

fiber there is a pressure variation which is calculated by Hagen Poiseuille equation.

$$\frac{dP_o}{dl} = - \frac{32\mu u}{D_i^2} \dots\dots(3.23)$$

where,  $u$  = velocity of gas

$\mu$  = viscosity of gas

$D_i$  = Inside diameter of hollow fiber.

If 'q' be volumetric flow rate then

$$u = \frac{q}{(\pi/4)D_i^2 N} \dots\dots(3.24)$$

substituting the value of 'u' in Equation (3.23) we get

$$\frac{dP_o}{dl} = \frac{128\mu q}{\pi D_i^4 N} \dots\dots(3.25)$$

From ideal gas law molar volume of gas is  $RT/P_o$ . If 'V' is molar flow rate of gas in permeate side then volumetric flow rate can be expressed in terms of molar flow rate as

$$q = \frac{VRT}{P_o} \dots\dots(3.26)$$

Substituting the value of 'q' in Equation (3.25) we get

$$\frac{dP_o}{dl} = - \frac{128\mu TRV}{D_i^4 P_o N \pi} \dots\dots(3.27)$$

$$A = \pi D_{LM} l \dots\dots(3.28)$$

$$\frac{dP_o}{dA} = - \frac{128\mu RTV}{\pi^2 D_i^4 D_{LM} P_o N} \dots\dots(3.29)$$

Converting  $P_o$  and A into dimensionless form we get

$$\frac{P_f dy}{(L_w/P_f Q_2) dR_w} = - \frac{128\mu RT(V/L_w) L_w}{\pi^2 D_i^4 D_{LM} (P_o/P_f) P_f N} \dots\dots(3.30)$$

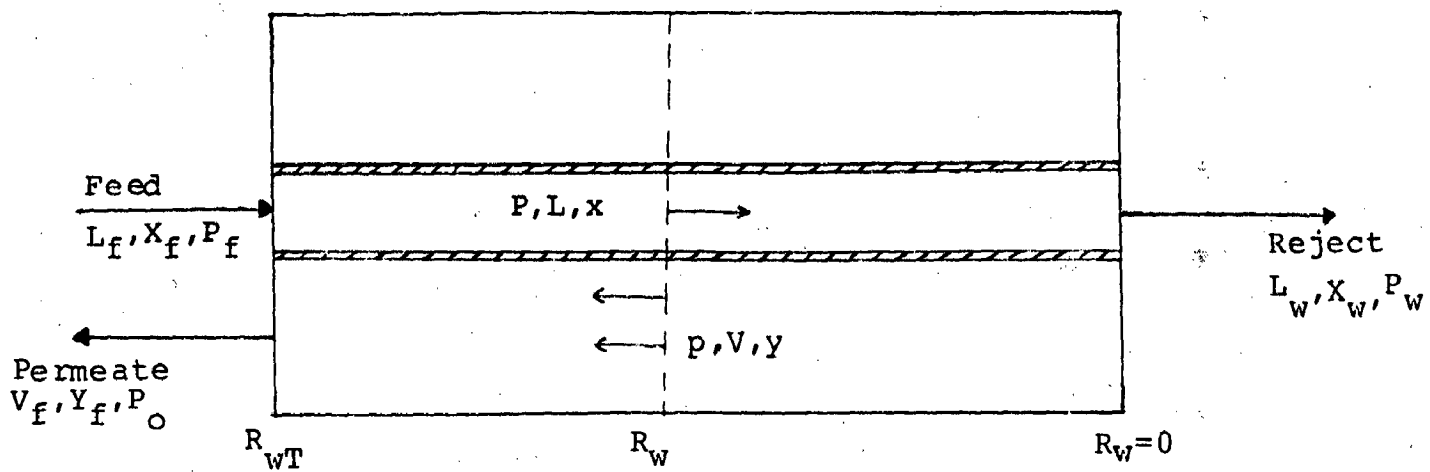


FIG. 3.3: SCHEMATIC OF A HOLLOW FIBER FEED INSIDE MODE GAS PERMEATOR HAVING COUNTER CURRENT FLOW.

## COMPUTATION TECHNIQUE

Equations obtained are the coupled first order ordinary differential equations and are solved by using fourth order Runge Kutta method. The computation procedure begins with by assuming a value of  $x_w$ . The set of differential equations are than solved to obtain the value of  $x$  and is compared with the value of  $x_f$ . If the value of  $x$  matches with the value of  $x_f$  within the given tolerance otherwise, another value of  $x_w$  is assumed and iteration continued till the value of  $x$  matches with  $x_f$  within the tolerance limit. The value of  $x_w$  was approximated by using the co-current flow.

The fourth order Runge Kutta method used for the solution of differential equation for flat sheet and hollow fiber membrane are as follows :

### 4.1 FLAT SHEET MEMBRANE :

For flat sheet membrane the differential equations are

$$f_1(x, y) = \frac{(y-x)}{(y-x_w)} (\alpha(1-x)(x-\gamma y) - x((1-x) - \gamma(1-y)))$$

$$f_2(x, y) = \frac{(y-x)}{(x-x_w)} (\alpha(1-x)(x-\gamma y) - y((1-x) - \gamma(1-y)))$$

If  $h$  be the increment given to the dimensionless area than the values of four constants of Runge Kutta method are calculated using the following expressions :

$$k_1 = h * f_1(x, y)$$

$$l_1 = h * f_2(x, y)$$

$$k_2 = h * f_1(x + 0.5 * k_1, y + 0.5 * l_1)$$

$$l_2 = h * f_2(x + 0.5 * k_1, y + 0.5 * l_1)$$

$$k_3 = h * f_1(x + 0.5 * k_2, y + 0.5 * l_2)$$

$$l_3 = h * f_2(x + 0.5 * k_2, y + 0.5 * l_2)$$

$$k_4 = h * f_1(x + k_3, y + l_3)$$

$$l_4 = h * f_2(x + k_3, y + l_3)$$

The next increment in the value of  $x$  and  $y$  are calculated by the following expressions :

$$x' = x + (k_1 + 2k_2 + 2k_3 + k_4) / 6$$

$$y' = y + (l_1 + 2l_2 + 2l_3 + l_4) / 6$$

#### 4.2 HOLLOW FIBER MEMBRANE :

The differential equations for hollow fiber membrane are as follow :

$$f_1(x, y, \gamma) = \frac{(y-x)}{(y-x_w)} (\alpha(1-x)(x-\gamma y) - x((1-x) - \gamma(1-y)))$$

$$f_2(x, y, \gamma) = \frac{(y-x)}{(x-x_w)} (\alpha(1-x)(x-\gamma y) - y((1-x) - \gamma(1-y)))$$

$$f_3(x, y, \gamma) = -\beta \frac{(x+x_w)(x_f - y_f)^2}{\gamma(y-x)(x_w - y_f)^2}$$

If  $h$  be the increment given to the dimensionless area than the constants of Runge Kutta method are calculated by the following expression :

$$k_1 = h * f_1(x, y, \gamma)$$

$$l_1 = h * f_2(x, y, \gamma)$$

$$m_1 = h * f_3(x, y, \gamma)$$

$$k_2 = h * f_1(x + 0.5 * k_1, y + 0.5 * l_1, \gamma + 0.5 * m_1)$$

$$l_2 = h * f_2(x + 0.5 * k_1, y + 0.5 * l_1, \gamma + 0.5 * m_1)$$

$$m_2 = h * f_3(x + 0.5 * k_1, y + 0.5 * l_1, \gamma + 0.5 * m_1)$$

$$k_3 = h * f_1(x + 0.5 * k_2, y + 0.5 * l_2, \gamma + 0.5 * m_2)$$

$$l_3 = h * f_2(x + 0.5 * k_2, y + 0.5 * l_2, \gamma + 0.5 * m_2)$$

$$m_3 = h * f_3(x + 0.5 * k_2, y + 0.5 * l_2, \gamma + 0.5 * m_2)$$

$$k_4 = h * f_1(x + k_3, y + l_3, \gamma + m_3)$$

$$l_4 = h * f_2(x + k_3, y + l_3, \gamma + m_3)$$

$$m_4 = h * f_3(x + k_3, y + l_3, \gamma + m_3)$$

The next increment in the value of  $x$ ,  $y$  and  $\gamma$  are calculated by the following expressions :

$$x' = x + (k_1 + 2k_2 + 2k_3 + k_4) / 6$$

$$y' = y + (l_1 + 2l_2 + 2l_3 + l_4) / 6$$

$$\gamma' = \gamma + (m_1 + 2m_2 + 2m_3 + m_4) / 6$$

### 4.3 ALGORITHM OF COMPUTER PROGRAM

The algorithm of the computer program is as follows :

- Step 1 Read the operating and design data.
- Step 2 Compute the values of constants.
- Step 3 Calculate values of  $x$ ,  $y$ , and  $\gamma$ , by solving differential equation with fourth order Runge Kutta method.
- Step 4 Calculate  $L^*$  and  $V^*$ .
- Step 5 If the values of dimensionless area reaches the given value then go to Step 6 otherwise go to Step 3
- Step 6 If the value of " $x$ " obtained is equal to " $x_f$ " then stop and print the result otherwise go to Step 7.
- Step 7 Assume new value of " $x_w$ " and go to Step 3.

Figure 4.1 shows the flow chart of the computer program.

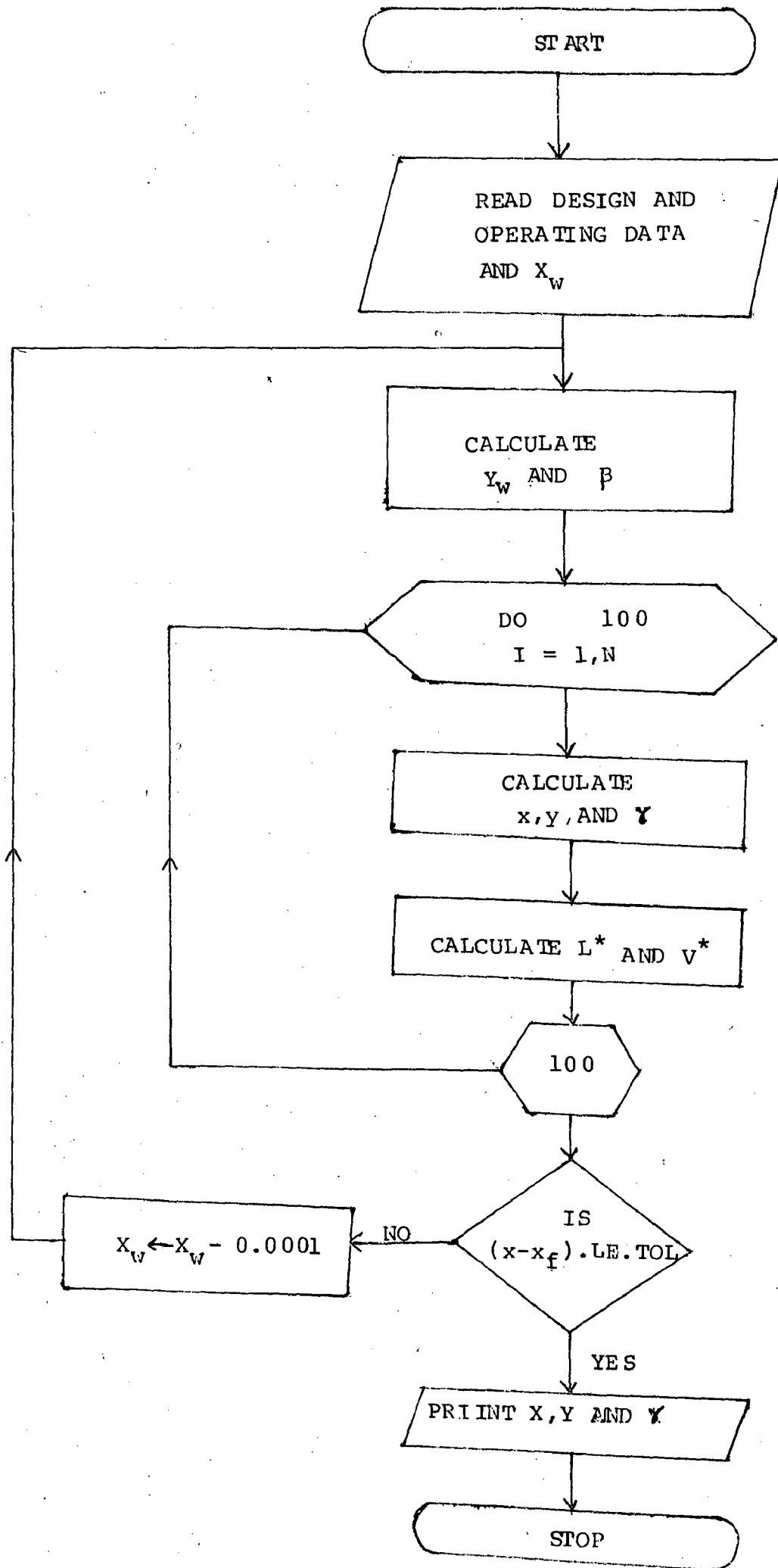


FIG. 4.1: BLOCK DIAGRAM FOR COMPUTATION ALGORITHM.

## RESULT AND DISCUSSION

This chapter describes the results and discussion of two studies. Firstly, the configuration of the membrane was established based on the mode of flow (that is, co-current and counter current). The established mode of flow and the membrane configuration was used in the simulation studies to obtain the performance of difference type of membrane for the purge gas system.

### 5.1 Computer Program :

Computer programs was developed for the different configuration of the membrane and the flow modes. Appendix A gives the listing of these programs.

The functions of the program were checked for the permeate composition obtained using the counter current flow in a flat sheet membrane. A permeate composition of 0.625 was obtained for a non-dimensional area of 0.024, under the following operating conditions :  $x_f = 0.05$ ,  $\gamma = 0.01$ , and  $\alpha = 80$ . The value matched with the reported value given in the Figure 12 of Sirkar et al.(1984). Therefore, it was concluded that the methodology and function of the developed program is right and was extended to the other membrane configuration.



## 5.2 Comparison of Mode of Flow :

Flow mode of the binary gas mixture was compared for different membrane configurations. Table 5.1 shows the data used for this comparison. These binary gas mixture data were used by Sirkar et al.(1986) for a series solution technique developed to express each product composition and pressure ratio (for hollow fiber only) as a power series in terms of a dimensionless membrane area.

The data were used to find the best mode of gas flow (that is, co-current and counter current) and the best membrane configuration (that is, flat sheet , hollow fiber feed outside, and hollow fiber feed inside mode).

Figure 5.1 to 5.3 compare the permeate composition obtained in the co-current and counter current flow for flat sheet hollow fiber feed outside and hollow fiber feed inside membrane respectively. It is evident from these figures that the permeate composition decreases as the non-dimensional membrane area increases. The decrease in the permeate composition is due to increase in the permeate flow rate. It is also evident from these figures that for a given non-dimensional membrane area, the permeate composition is higher for the counter current flow compared to the co-current flow. Figures 5.1 to 5.3 demonstrate that the counter current flow mode gives the better permeation.

Tables 5.2 to 5.4 show that the permeate composition for non-dimensional membrane area of 0.024 are 0.3979, 0.3991, and 0.3969 for flat sheet, hollow fiber feed outside and hollow fiber feed inside respectively. Similar observations have

**TABLE 5.1**  
Data for comparison of permeator

| S. No. | Parameter                        | Unit                     | Range                  |
|--------|----------------------------------|--------------------------|------------------------|
| 1      | Feed Composition (mole fraction) |                          | 0.08                   |
| 2      | Temperature                      | °K                       | 298                    |
| 3      | Separation Factor                |                          | 80                     |
| 4      | Permeability of Second Component | mol/s.m <sup>2</sup> .Pa | 5.66×10 <sup>-10</sup> |
| 5      | Feed Pressure                    | Pa                       | 40×10 <sup>5</sup>     |
| 6      | Pressure Ratio                   |                          | 0.1                    |
| 7      | Flow Rate                        | mol/sec                  | 4.14×10 <sup>-5</sup>  |
| 8      | Viscosity                        | Pa.sec                   | 1.5×10 <sup>-5</sup>   |

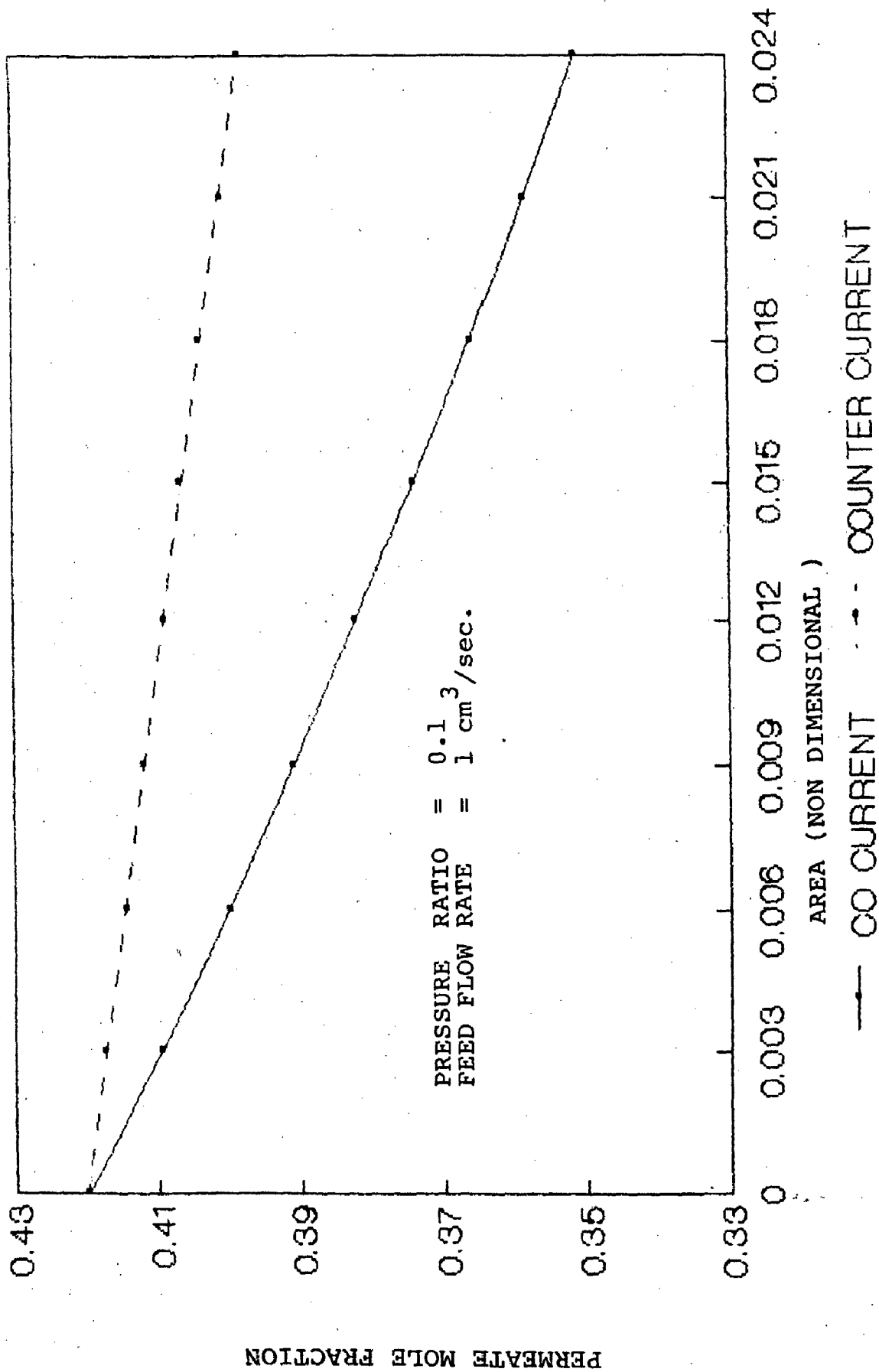


FIG. 5.1: COMPARISON OF CO-CURRENT AND COUNTER CURRENT FLOW FOR FLAT SHEET PERMEATOR.

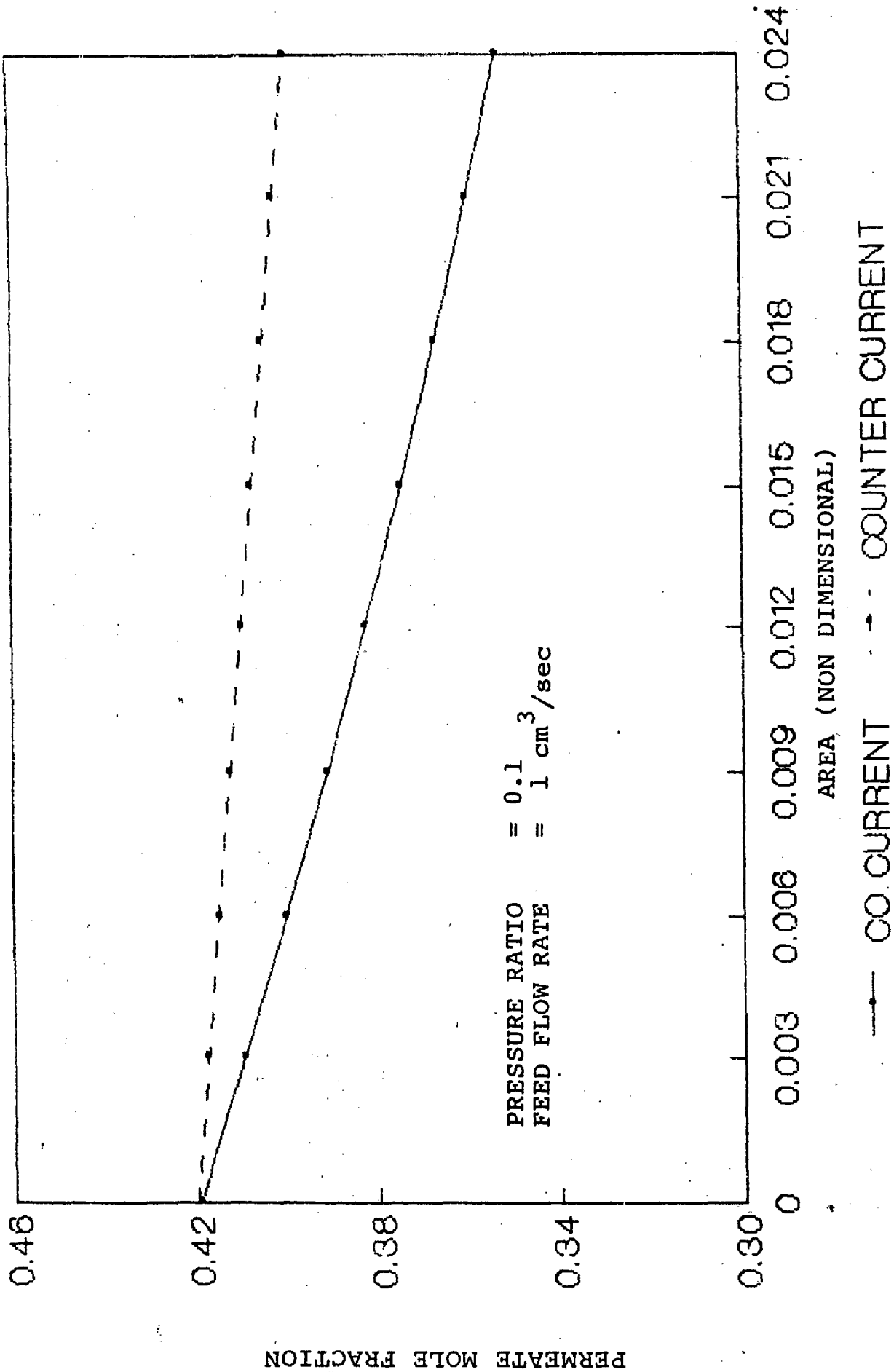


FIG. 5.2: COMPARISON OF CO-CURRENT AND COUNTER CURRENT FLOW FOR HOLLOW FIBER FEED OUTSIDE MODE.

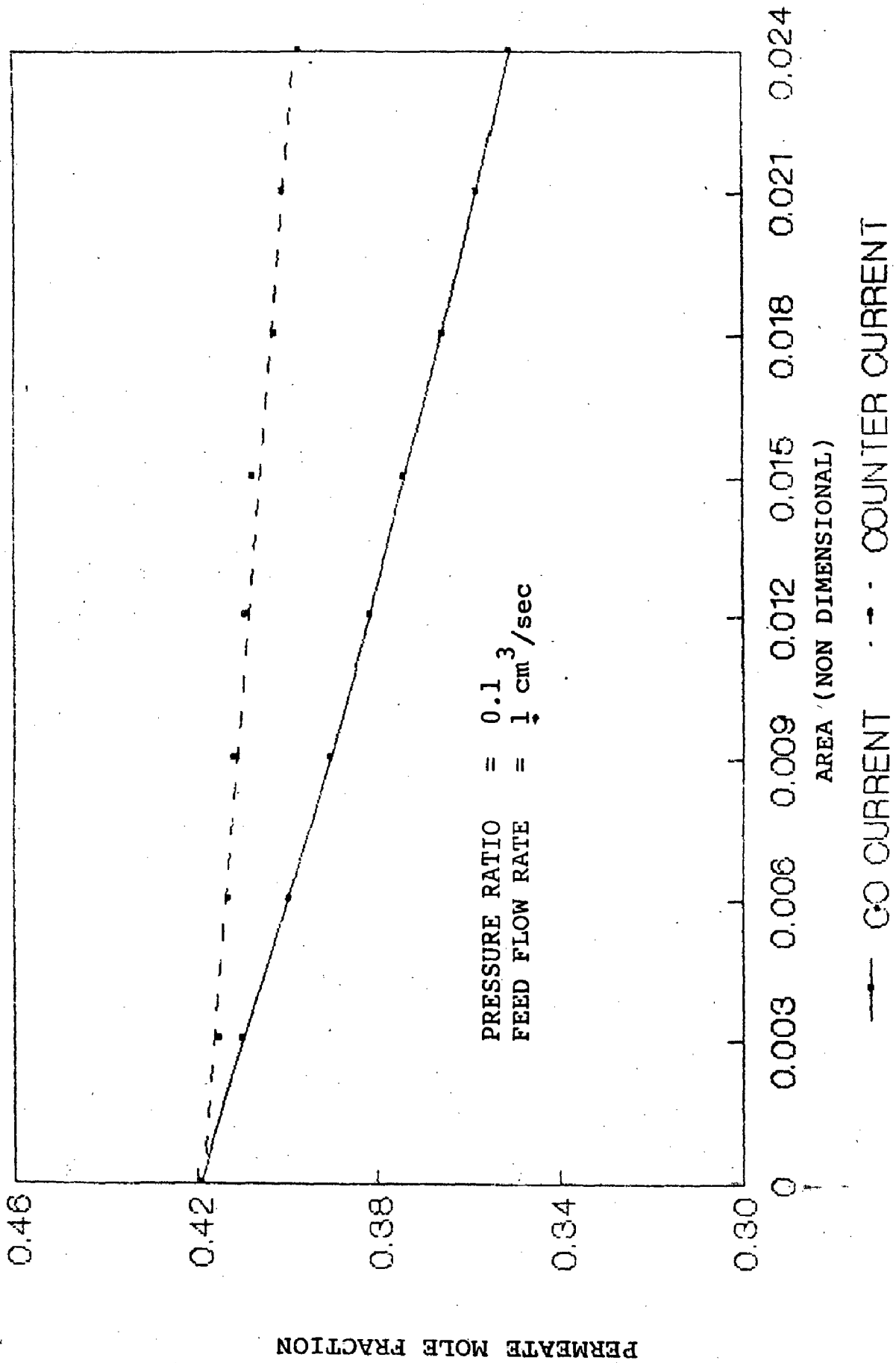


FIG. 5.3 : COMPARISON OF CO-CURRENT AND COUNTER CURRENT FLOW FOR HOLLOW FIBER FEED INSIDE MODE.

TABLE 5.2

Comparison of co current and counter current for flat sheet permeator

| S. No. | Non Dimensional Area | Permeate Composition |                 |
|--------|----------------------|----------------------|-----------------|
|        |                      | Co current           | Counter current |
| 1      | 0.000                | 0.419                | 0.419           |
| 2      | 0.003                | 0.4094               | 0.4175          |
| 3      | 0.006                | 0.3998               | 0.4145          |
| 4      | 0.009                | 0.3908               | 0.4120          |
| 5      | 0.012                | 0.3821               | 0.4090          |
| 6      | 0.015                | 0.3738               | 0.4066          |
| 7      | 0.018                | 0.3659               | 0.4038          |
| 8      | 0.021                | 0.3584               | 0.4006          |
| 9      | 0.024                | 0.3512               | 0.3979          |

TABLE 5.3

Comparison of co current and counter current flow for hollow fiber feed outside mode

| S.No. | Non Dimensional Area | Permeate Composition |                 |
|-------|----------------------|----------------------|-----------------|
|       |                      | Co current           | Counter current |
| 1     | 0.000                | 0.419                | 0.419           |
| 2     | 0.003                | 0.4094               | 0.4176          |
| 3     | 0.006                | 0.4000               | 0.4147          |
| 4     | 0.009                | 0.3910               | 0.4123          |
| 5     | 0.012                | 0.3825               | 0.4096          |
| 6     | 0.015                | 0.3775               | 0.4075          |
| 7     | 0.018                | 0.3669               | 0.4050          |
| 8     | 0.021                | 0.3596               | 0.4023          |
| 9     | 0.024                | 0.3528               | 0.3991          |

TABLE 5.4

Comparison of co-current and counter current flow for hollow fiber feed inside mode

| S.No. | Non Dimensional Area | Permeate Composition |                 |
|-------|----------------------|----------------------|-----------------|
|       |                      | Co current           | Counter current |
| 1     | 0.000                | 0.419                | 0.419           |
| 2     | 0.003                | 0.4092               | 0.4164          |
| 3     | 0.006                | 0.3995               | 0.4130          |
| 4     | 0.009                | 0.3903               | 0.4116          |
| 5     | 0.012                | 0.3815               | 0.4094          |
| 6     | 0.015                | 0.3773               | 0.4073          |
| 7     | 0.018                | 0.3652               | 0.4027          |
| 8     | 0.021                | 0.3576               | 0.4008          |
| 9     | 0.024                | 0.3504               | 0.3969          |



also been observed by Singh (1990).

It can be concluded from the above discussions that the counter current flow in hollow fiber feed, outside membrane configuration is better compared to the other membrane configuration for better permeation.

### 5.3 Simulation Studies of Purge Gas System :

The simulation study for purge gas was done to obtain the effect of flow rate, temperature and pressure ratio on the permeate composition. Three different membrane materials such as, cellulose acetate, polystyrene and polyimide were selected for the study. The membrane selected have wide range of the separation factor.

Purge gas consists of  $H_2$ ,  $N_2$ , Ar and  $CH_4$ . For the simulation study, the purge gas system was assumed to consist of  $H_2$  and  $N_2$  gases only (considering small fraction of  $CH_4$  and Ar having similar behaviour as  $N_2$ ).

The membrane configuration of hollow fiber feed outside mode having counter current flow was considered for this study because the permeate composition was found to be better as discussed in section 5.2. The range of operating variables studied in this investigation is given in table 5.5.

Figure 5.4 shows the permeate composition obtained for the three different types of membrane studied. It is evident from Figure 5.4 that for a given non-dimensional membrane area, the permeate composition is higher for polyimide membrane.

Table 5.6 shows that the permeate composition for 0.024

TABLE 5.5

Range of variables studied for purge gas system.

| S. No. | Parameter  | Unit                       | Range                   |
|--------|--|----------------------------|-------------------------|
| 1      | Feed Flow Rate                                   | cm <sup>3</sup> /sec       | 0.5 - 4.0               |
| 2      | Feed Pressure                                    | Pa                         | 25×10 <sup>3</sup>      |
| 3      | Pressure Ratio                                   |                            | 0.1 - 0.6               |
| 4      | Temperature                                      | °K                         | 298 - 773               |
| 5      | Viscosity  | Pa.sec                     | 2.4×10 <sup>-5</sup>    |
| 6      | Feed Composition (mole fraction)                 |                            |                         |
|        | Hydrogen   |                            | 0.65                    |
|        | Nitrogen and others                              |                            | 0.35                    |
| 7      | Separation factor                                |                            |                         |
|        | Polystyrene                                      |                            | 21.91                   |
|        | Cellulose Acetate                                |                            | 96.15                   |
|        | Polyimide  |                            | 255.68                  |
| 8      | Specific Permeability of<br>second component for | mol/sec.m <sup>2</sup> .Pa |                         |
|        | Polystyrene                                      |                            | 3.365×10 <sup>-11</sup> |
|        | Cellulose Acetate                                |                            | 2.953×10 <sup>-10</sup> |
|        | Polyimide  |                            | 6.078×10 <sup>-11</sup> |
| 9      | Inside diameter of<br>hollow fiber               | m                          | 1.5×10 <sup>-4</sup>    |
| 10     | Outside diameter of<br>hollow fiber              | m                          | 3.0×10 <sup>-4</sup>    |

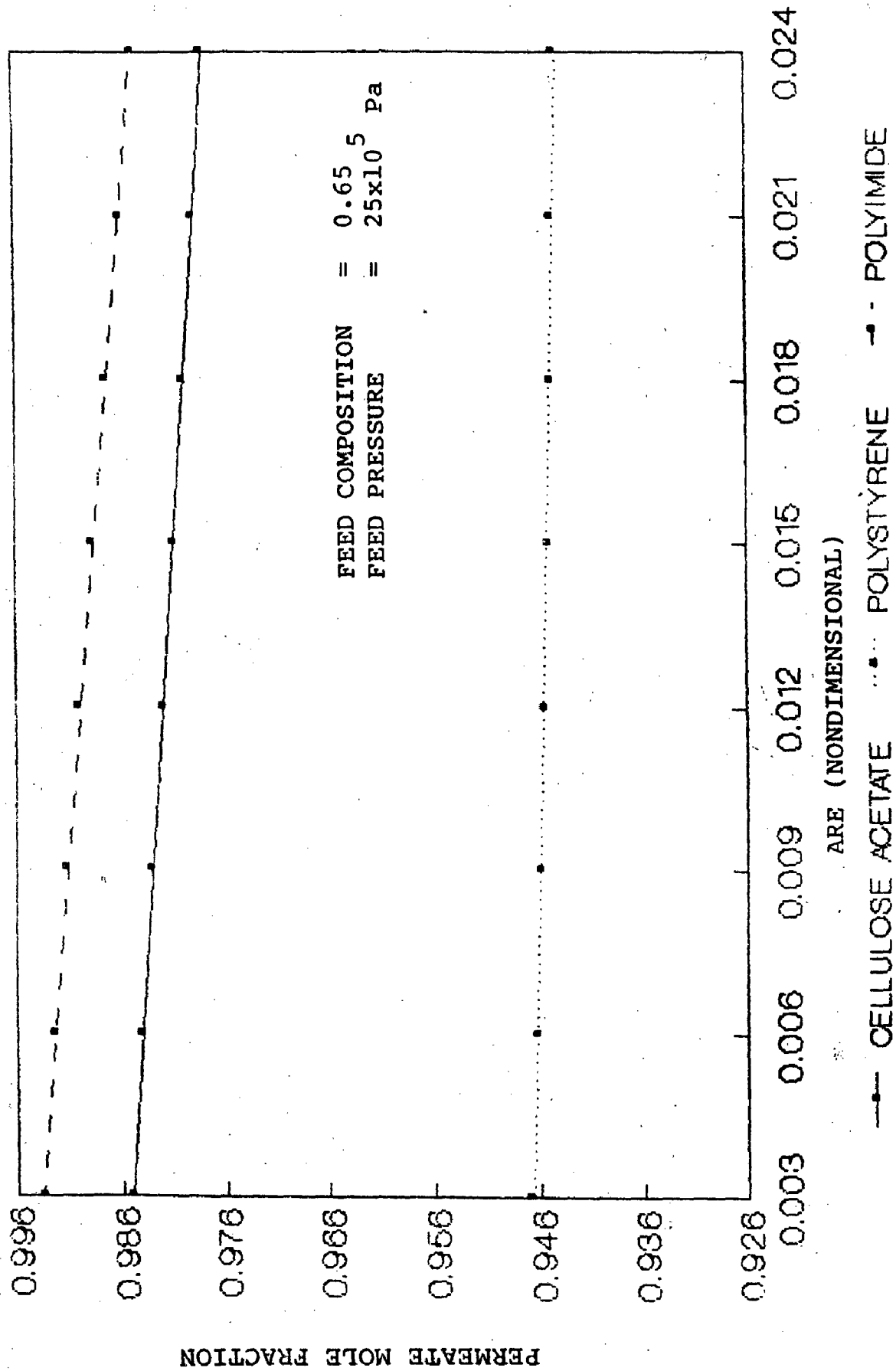


FIG. 5.4 : EFFECT OF MEMBRANE ON PERMEATE COMPOSITION FOR PURGE GAS SYSTEM.

TABLE 5.6

Effect of membrane on permeate composition for purge gas

| S. No. | Non Dimensional<br>Area | Permeate Composition |                      |           |
|--------|-------------------------|----------------------|----------------------|-----------|
|        |                         | Polystyrene          | Cellulose<br>Acetate | Polyimide |
| 1      | 0.003                   | 0.9469               | 0.9851               | 0.9935    |
| 2      | 0.006                   | 0.9463               | 0.9841               | 0.9924    |
| 3      | 0.009                   | 0.9459               | 0.9831               | 0.9912    |
| 4      | 0.012                   | 0.9454               | 0.9820               | 0.9900    |
| 5      | 0.015                   | 0.9451               | 0.9810               | 0.9887    |
| 6      | 0.018                   | 0.9448               | 0.9800               | 0.9874    |
| 7      | 0.021                   | 0.9446               | 0.9790               | 0.9860    |
| 8      | 0.024                   | 0.9444               | 0.9780               | 0.9846    |

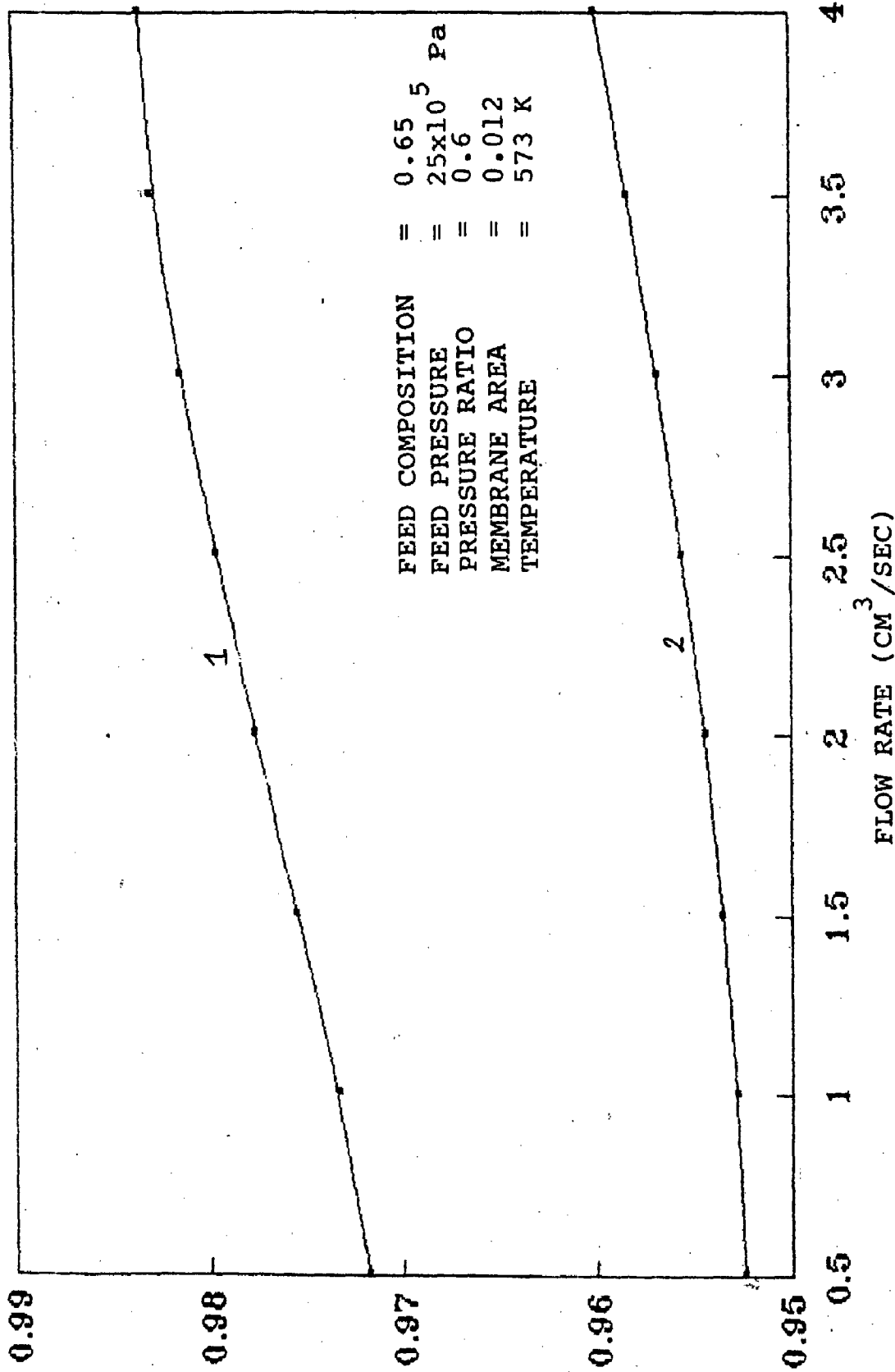
non-dimensional membrane area is 0.9444 for polystyrene whereas 0.9780 and 0.9846 for cellulose acetate and polyimide membrane respectively.

It can be concluded from the above discussion that polystyrene membrane is inferior to cellulose acetate and polyimide membrane. Therefore, the performance of cellulose acetate and polyimide membrane was studied for different variable such as, feed flow rate, gas, temperature and pressure ratio.

### 5.2.1 EFFECT OF FEED FLOW RATE

The performance of cellulose acetate and polyimide membranes was studied by varying the feed flow rate while keeping the other operating parameters constant. The range of flow rate varied between 0.5 to 4.0 cm<sup>3</sup>/sec. Figure 5.5 and Table 5.7 show the effect of feed flow rate on the permeate composition for cellulose acetate and polyimide membrane.

It is evident from Figure 5.5 that for the cellulose acetate membrane, there is a marginal increase in the permeate composition upto 2 cm<sup>3</sup>/sec feed flow rate while a gradual increase in the permeate composition is observed from the feed flow rate higher than 2 cm<sup>3</sup>/sec. On the other hand, for the polyimide membrane there is a gradual increase in the permeate composition upto 2.5 cm<sup>3</sup>/sec feed flow rate and there after the permeate composition have marginal effect with the increase in the feed flow rate. This phenomenon could be due to the material of the membrane.



1 — CELLULOSE ACETATE    2 — POLYIMIDE  
 FIG. 5.5 : EFFECT OF FLOW RATE ON PERMEATE COMPOSITION FOR PURGE GAS SYSTEM.

PERMEATE MOLE FRACTION

246316



TABLE 5.7

Effect of flow rate on permeate composition for purge gas system.

| S. No. | Flow Rate<br>(cm <sup>3</sup> /sec) | Permeate Composition |           |
|--------|-------------------------------------|----------------------|-----------|
|        |                                     | Cellulose acetate    | Polyimide |
| 1      | 0.5                                 | 0.9524               | 0.9718    |
| 2      | 1.0                                 | 0.9528               | 0.9733    |
| 3      | 1.5                                 | 0.9535               | 0.9755    |
| 4      | 2.0                                 | 0.9544               | 0.9776    |
| 5      | 2.5                                 | 0.9556               | 0.9796    |
| 6      | 3.0                                 | 0.9568               | 0.9814    |
| 7      | 3.5                                 | 0.9583               | 0.9829    |
| 8      | 4.0                                 | 0.9599               | 0.9834    |

### 5.2.2 EFFECT OF TEMPERATURE

The effect of temperature on the permeate composition has been studied for cellulose acetate and polyimide membrane by keeping all other parameter constant (that is, feed flow rate and pressure ratio). The range of temperature varied from 323 K to 773 K. Figure 5.6 and Table 5.8 show the effect of temperature on the permeate composition for cellulose acetate and polyimide membranes. It is evident from the Figure 5.6 that there is no effect of temperature on the permeate composition for both membranes. However, Table 5.8 shows the marginal increase in values of the permeate composition for both membranes.

This could be due to the fact that the permeability of both the gases will increase with rise in temperature and this will give a marginal effect on the separation factor because separation factor is the ratio of permeabilities.

### 5.2.3 EFFECT OF PRESSURE RATIO

The effect of pressure ratio has been studied for cellulose acetate and polyimide membrane by keeping all other parameters constant. The pressure ratio was varied from 0.1 to 0.6. Figure 5.7 and Table 5.9 shows the effect of pressure ratio on the permeate composition for both the membranes. It is evident from the Figure 5.7 that the permeate composition decreases as pressure ratio increases for both the membranes. However, there is a steep fall in the permeate composition after the pressure ratio of 0.4.

It is evident from Figures 5.4 to 5.7 that the performance of polyimide membrane is better than the



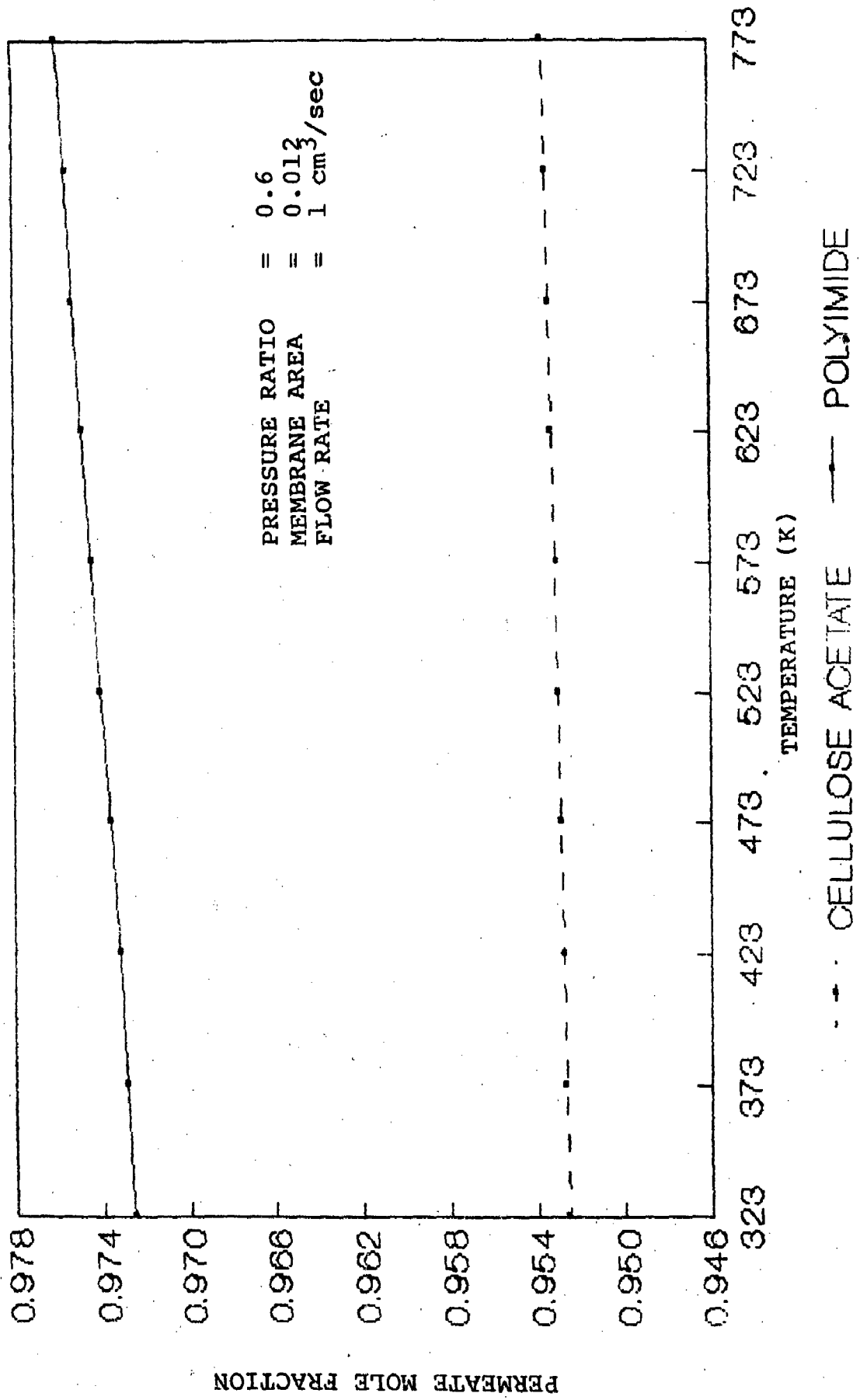
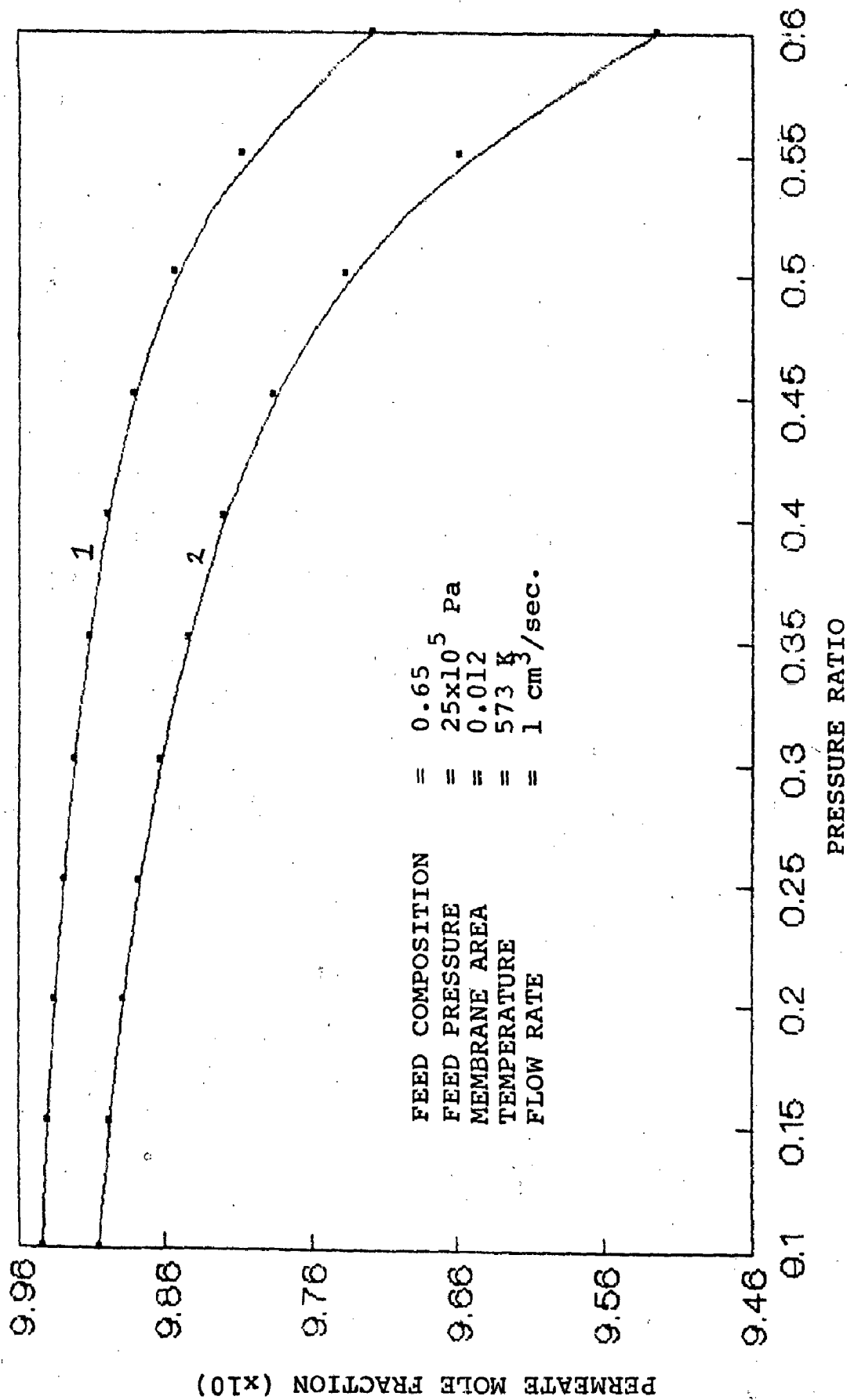


FIG. 5.6 : EFFECT OF TEMPERATURE ON PERMEATE COMPOSITION FOR PURGE GAS SYSTEM.

TABLE 5.8

Effect of temperature on permeate composition for purge gas system.

| S. No. | Temperature<br>(°K) | Permeate Composition |           |
|--------|---------------------|----------------------|-----------|
|        |                     | Cellulose acetate    | Polyimide |
| 1      | 323                 | 0.9526               | 0.9726    |
| 2      | 373                 | 0.9527               | 0.9729    |
| 3      | 423                 | 0.9528               | 0.9732    |
| 4      | 473                 | 0.9529               | 0.9736    |
| 5      | 523                 | 0.9530               | 0.9741    |
| 6      | 573                 | 0.9531               | 0.9745    |
| 7      | 623                 | 0.9533               | 0.9749    |
| 8      | 673                 | 0.9534               | 0.9753    |
| 9      | 723                 | 0.9535               | 0.9756    |
| 10     | 773                 | 0.9537               | 0.9760    |



2 ——— CELLULOSE ACETATE    1 ——— POLYIMIDE

FIG. 5.7 : EFFECT OF PRESSURE RATIO ON PERMEATE COMPOSITION FOR PURGE GAS SYSTEM.

TABLE 5.9

Effect of pressure ratio on permeate composition for purge gas system.

| S. No. | Pressure Ratio | Permeate Composition |           |
|--------|----------------|----------------------|-----------|
|        |                | Cellulose acetate    | Polyimide |
| 1      | 0.10           | 0.9905               | 0.9944    |
| 2      | 0.15           | 0.9897               | 0.9940    |
| 3      | 0.20           | 0.9888               | 0.9935    |
| 4      | 0.25           | 0.9877               | 0.9929    |
| 5      | 0.30           | 0.9863               | 0.9922    |
| 6      | 0.35           | 0.9844               | 0.9912    |
| 7      | 0.40           | 0.9820               | 0.9899    |
| 8      | 0.45           | 0.9786               | 0.9881    |
| 9      | 0.50           | 0.9737               | 0.9854    |
| 10     | 0.55           | 0.9658               | 0.9807    |
| 11     | 0.60           | 0.9524               | 0.9718    |

cellulose acetate membrane. Also, to achieve the better performance, polyimide membrane should be operated at low pressure ratio (that is, below 0.25) and high feed flow rate.

## CONCLUSIONS AND RECOMMENDATIONS

## 6.1 CONCLUSIONS :

The present work was divided into two different simulation studies. Firstly, the simulation studies was carried out to find the better mode of feed flow and the better membrane configuration. These studies were based on the data taken from the Sirkar et al. (1986) and was concluded that the counter current mode of the feed in the hollow fiber feed outside membrane configuration was better in all situations.

Secondly, these findings were utilized to study the performance of three membranes namely, polystyrene, cellulose acetate and polyimide for separating (or enriching) the hydrogen from the purge gas. It was observed that for a fixed non-dimensional membrane area, polystyrene membrane showed the poorest permeate composition compared to cellulose acetate and polyimide membrane.

The performance of the cellulose acetate and polyimide membrane were studied for the three operating variable such as, feed flow rate, temperature and the pressure ratio and following conclusions were drawn :

- (1) Permeate composition depends on the feed flow rate and it increases with increase in feed flow rate.
- (2) No temperature effect was observed on permeate composition. Increase in temperature from 323 K to 773 K increases the

permeate composition from 0.1 to 0.3 %.

- (3) The permeate composition decreases with increase in pressure ratio and the effect is more significant in the range of 0.4 to 0.6.

The performance of the polyimide membrane was better than the cellulose acetate membrane under all the circumstances.

## 6.2 RECOMMENDATIONS :

- (1) In present work the purge gas system has been modeled as binary gas system however the actual system is a multi component gas system consisting of  $H_2$ ,  $N_2$ , Ar and  $CH_4$ . So further work should be carried out to analyze the effect of other component on the accuracy of the result.
- (2) The study of multistage membrane separation system should be done using the model developed for single stage in the present work.
- (3) The work should be extended for the study of two membrane system for increase in hydrogen recovery.
- (4) Effect of pressure on membrane structure should be considered for further study.
- (5) Unsteady state behaviour of the membrane system should also be done for development of proper control strategy.

# APPENDIX - A



```

C THIS PROGRAM IS FOR FLAT SHEET MEMBRANE OPERATING IN
C CO CURRENT MODE.
DIMENSION X(110), Y(110), U(110), V(110), RZ(110)
EXTERNAL F1, F2, F3, F4
OPEN(1, FILE='RCOFLT.DAT', STATUS='OLD')
OPEN(2, FILE='RCOFLT.OUT', STATUS='NEW')
READ(1, *) SF, XF, PRO
READ(1, *) N, RXL, RLAST
RZ0=0.0
AN=N
H=RXL/AN
WRITE(2, *) H
X(1)=XF
XI=X(1)
CALL FIND (SF, PRO, XI, Y1)
Y(1)=Y1
Y0=Y(1)
WRITE(2, 4) Y(1)
4 FORMAT(4X, 'Y0=', F8.4 //)
WRITE(2, 23)
23 FORMAT(/4X, '*****CURRENT*****')
WRITE(2, 5)
5 FORMAT(10X, 'RXL', 9X, 'X', 9X, 'Y', 9X, 'U', 9X, 'V', //)
KI=(N/10)-1
DO 10 I=2, N+1
K=I-1
IF(K.NE.1) GO TO 11
XK=X(K)
YK=Y(K)
CALL RKA(SF, PRO, XK, YK, H, XI, Y1)
X(I)=XI
Y(I)=Y1
GO TO 10
11 XK=X(K)
YK=Y(K)
CALL RKB(SF, PRO, XK, YK, H, XI, Y1, XF)
X(I)=XI
Y(I)=Y1
U(I)=Y(I)-X(I)/(Y(1)-X(1))
V(I)=(X(I)-X(1))/(Y(1)-X(1))
IF(I.NE.N) GO TO 10
RX0=RX0+0.1*RXL
WRITE(2, 12) RX0, X(I), Y(I), U(I), V(I)
12 FORMAT(11X, 5(2X, F8.4))
KI=KI+(N/10)
CONTINUE
IF(ABS(RXL-RLAST).LE.0.0001) GO TO 50
RXL=RXL*0.003
GO TO 25
50 STOP
END
C
C SUBROUTINE TO FIND Y0
C
SUBROUTINE FIND(S, F, XI, Y1)
A=F*(S-1.)
B=1.+(S-1.)*(XI+P)
C=XI*S
Y1=(B-SQRT(B**2-4.*A*C))/(2.*A)
RETURN
END
C
C SUBROUTINE RKA(S, F, X, Y, H, T1, T2)
A1=H*F1(X, Y, S, F)
A2=H*F2(X+0.5*A1, Y+0.5*B1, S, F)
A3=H*F1(X+0.5*A2, Y+0.5*B2, S, F)
A4=H*F2(X+0.5*A3, Y+0.5*B3, S, F)
T1=X+(A1+A4+2.*(A2+A3))/6.
T2=Y+(B1+B4+2.*(B2+B3))/6.
RETURN
END
C
SUBROUTINE RKB(S, F, X, Y, H, T1, T2, XF)
A1=H*F3(X, Y, S, P, XF)
A2=H*F4(X, Y, S, P, XF)
A3=H*F3(X+0.5*A1, Y+0.5*B1, S, P, XF)
A4=H*F4(X+0.5*A2, Y+0.5*B2, S, P, XF)
A5=H*F3(X+0.5*A3, Y+0.5*B3, S, P, XF)
A6=H*F4(X+0.5*A4, Y+0.5*B4, S, P, XF)
T1=X+(A1+A6+2.*(A2+A5))/6.
T2=Y+(B1+B6+2.*(B2+B5))/6.
RETURN
END
C
FUNCTION F1(X, Y, S, F)
F1=S*(1.-X)*(X-P*Y)-X*((1.-X)-P*(1.-Y))
RETURN
END
FUNCTION F2(X, Y, S, P)
F2=((Y-X)*(S-(S-1.)*Y)*(S*(X-P*Y)+(1.-X)-X*((1.-X)-P*(1.-Y))))/
1*((S*(1.-X))*(X-P*Y)-X*((1.-X)-P*(1.-Y))-(Y-X)*(S-1.))*
2(2.*P*Y-X-P-1.)
RETURN
END
SUBROUTINE RKB(S, F, X, Y, H, T1, T2, XF)
A1=H*F3(X, Y, S, P, XF)
A2=H*F4(X, Y, S, P, XF)
A3=H*F3(X+0.5*A1, Y+0.5*B1, S, P, XF)
A4=H*F4(X+0.5*A2, Y+0.5*B2, S, P, XF)
A5=H*F3(X+0.5*A3, Y+0.5*B3, S, P, XF)
A6=H*F4(X+0.5*A4, Y+0.5*B4, S, P, XF)
T1=X+(A1+A6+2.*(A2+A5))/6.
T2=Y+(B1+B6+2.*(B2+B5))/6.
RETURN
END
FUNCTION F3(X, Y, S, P, XF)
F3=((Y-X)*(S*(1.-X)*(X-P*Y)-X*((1.-X)-P*(1.-Y))))/(XF-Y)
RETURN
END
FUNCTION F4(X, Y, S, P, XF)
F4=((Y-X)*(S*(X-P*Y)*(1.-Y)-Y*((1.-X)-P*(1.-Y))))/(XF-X)
RETURN
END

```

```

C THIS PROGRAM IS FOR FLAT SHEET MEMBRANE OPERATING IN
C COUNTER CURRENT MODE.
DIMENSION K(110),Y(110),U(110),V(110),RX(110)
EXTERNAL F5,F6,F7,F8
OPEN(1,FILE='RCNFILT.DAT',STATUS='OLD')
OPEN(2,FILE='RCNFILT.OUT',STATUS='NEW')
HEAD(1,*)SF,XF,PRO,TOL
READ(1,*)N,XW,RXL,RLAST
WRITE(2,22)
22 FORMAT(/4X, '*****COUNTER CURRENT*****')
WRITE(2,15)
15 FORMAT(18X, 'RXL', '2X', 'X', '2X', 'Y', '2X', 'U', '2X', 'V', 'V')
30 RX0=0.0
AN=N
H=RXL/AN
X(1)=XW
X1=X(1)
CALL FIND(SF,PRO,X1,Y1)
Y(1)=Y1
Y0=Y(1)
YW=Y(1)
14 FORMAT(4X, 'YW=', 'F6.5/', 'XW=', 'F8.5/')
DO 20 J=2, N+1
L=J-1
IF(L.NE.1)GO TO 21
XL=X(L)
YL=Y(L)
CALL RKD(SF,PRO, XL, YL, H, XJ, YJ)
X(J)=XJ
Y(J)=YJ
GO TO 20
21 XL=X(L)
YL=Y(L)
CALL RKD(SF,PRO, XW, XL, YL, H, XJ, YJ)
X(J)=XJ
Y(J)=YJ
U(J)=(Y(J)-X(1))/(Y(J)-X(J))
V(J)=(X(J)-X(1))/(Y(J)-X(J))
IF(J.NE.K1)GO TO 20
RX0=RX0+0.1*RXL
24 FORMAT(11X,5(2X,F8.4))
K1=K1+(N/10)
20 CONTINUE
WRITE(*,24)RXL,X(N+1),Y(N+1),U(N+1),V(N+1)
IF(ABS(XF-X(N+1)).LE.TOL)GO TO 50
XW=XW-0.0001
GO TO 30
50 WRITE(*,24)RXL,X(N+1),Y(N+1),U(N+1),V(N+1)
WRITE(2,24)RXL,X(N+1),Y(N+1),U(N+1),V(N+1)
IF(ABS(EXL-RLAST).LE.0.0001)GO TO 40
RXL=RXL*0.003
GO TO 30
40 STOP
END
C SUBROUTINE TO FIND Y0
C
C SUBROUTINE FIND(S,F,X1,Y1)
A=P*(S-1)
B=1.+(S-1.)*(X1+P)
C=X1*S
V1=(B-SQRT(B**2-4.*A*C))/(2.*A)
RETURN
END

```

```

SUBROUTINE RKC(S,P,XW,X,Y,H,T1,T2)
A1=H*F5(X,Y,S,P,XW)
B1=H*F6(X,Y,S,P,XW)
A2=H*F5(X+0.5*A1,Y+0.5*B1,S,P,XW)
B2=H*F6(X+0.5*A1,Y+0.5*B1,S,P,XW)
A3=H*F5(X+0.5*A2,Y+0.5*B2,S,P,XW)
B3=H*F6(X+0.5*A2,Y+0.5*B2,S,P,XW)
A4=H*F5(X+A3,Y+B3,S,P,XW)
B4=H*F6(X+A3,Y+B3,S,P,XW)
T1=X+(A1+A4+2.*(A2+A3))/6.
T2=Y+(B1+B4+2.*(B2+B3))/6.
RETURN
END

```

```

FUNCTION FS(X,Y,S,P,XW)
F5=((Y-X)*(S*(1.-X)*(X-P+Y)-X*((1.-X)-P*(1.-Y))))/(Y-XW)
RETURN
END

```

```

FUNCTION F6(X,Y,S,P,XW)
F6=((Y-X)*(S*(X-P*Y)*(1.-Y)-Y*((1.-X)-P*(1.-Y))))/(X-XW)
RETURN
END

```

```

SUBROUTINE RKD(S,P,X,Y,H,T1,T2)

```

```

A1=H*F7(X,Y,S,P)
B1=H*F8(X,Y,S,P)
A2=H*F7(X+0.5*A1,Y+0.5*B1,S,P)
B2=H*F8(X+0.5*A1,Y+0.5*B1,S,P)
A3=H*F7(X+0.5*A2,Y+0.5*B2,S,P)
B3=H*F8(X+0.5*A2,Y+0.5*B2,S,P)
A4=H*F7(X+A3,Y+B3,S,P)
B4=H*F8(X+A3,Y+B3,S,P)
T1=X+(A1+A4+2.*(A2+A3))/6.
T2=Y+(B1+B4+2.*(B2+B3))/6.
RETURN
END

```

```

FUNCTION F7(X,Y,S,P)
F7=S*(1.-X)*(X-P*Y)-X*((1.-X)-P*(1.-Y))
RETURN
END

```

```

FUNCTION F8(X,Y,S,P)
F8=((Y-X)*(S-(S-1.)*Y)*(S*(X-P*Y)*(1.-X)-X*((1.-X)-P*(1.-Y))))/
1*((S*(1.-X)*(X-P*Y)-X*((1.-X)-P*(1.-Y)))-(Y-X)*(S-1.))
2(2.*P*Y-X-P-1.))
RETURN
END

```

```

R=1*(S-1.)*(P+X)
C=X*S
Y=(B-SORT(B**2-4.*A*C))/(2.*A)
RETURN
END

SUBROUTINE RKA(S,P,K,X,Y,R,I1,I2)
A1=H*F1(X,Y,S,P)
B1=H*F2(X,Y,S,P)
A2=H*F1(X+0.5*A1,Y+0.5*B1,S,P)
B2=H*F2(X+0.5*A1,Y+0.5*B1,S,P)
A3=H*F1(X+0.5*A2,Y+0.5*B2,S,P)
B3=H*F2(X+0.5*A2,Y+0.5*B2,S,P)
A4=H*F1(X+A3,Y+B3,S,P)
B4=H*F2(X+A3,Y+B3,S,P)
T1=X*(A1+A4+2.*(A2+A3))/6.
T2=Y*(B1+B4+2.*(B2+B3))/6.
RETURN
END

FUNCTION F(X,Y,S,P)
F1=-S*(1.-X)*(X-P*Y)-X*((1.-X)-P*(1.-Y))
RETURN
END

FUNCTION F2(X,Y,S,P)
F2=((Y-X)*(S-(S-1.)*Y)*(X-P*Y)-X*((1.-X)-P*(1.-Y))-P*(1.-Y))/
1*(S*(1.-X)*(X-P*Y)-X*((1.-X)-P*(1.-Y))-(Y-X)*(S-1.))
2*(2.*Y-X-P-1.)
RETURN
END

SUBROUTINE RKB(S,BE,X,Y,P,H,T1,T2,Y3,XF)
A1=H*F3(X,Y,P,S,XF)
B1=H*F4(X,Y,P,S,XF)
C1=H*F5(X,Y,P,XF,BE)
A2=H*F3(X+0.5*A1,Y+0.5*B1,P+0.5*C1,S,XF)
B2=H*F4(X+0.5*A1,Y+0.5*B1,P+0.5*C1,S,XF)
C2=H*F5(X+0.5*A1,Y+0.5*B1,P+0.5*C1,S,XF,BE)
A3=H*F3(X+0.5*A2,Y+0.5*B2,P+0.5*C2,S,XF)
B3=H*F4(X+0.5*A2,Y+0.5*B2,P+0.5*C2,S,XF)
C3=H*F5(X+0.5*A2,Y+0.5*B2,P+0.5*C2,S,XF,BE)
A4=H*F3(X+A3,Y+B3,P+C3,S,XF)
B4=H*F4(X+A3,Y+B3,P+C3,S,XF)
C4=H*F5(X+A3,Y+B3,P+C3,S,XF,BE)
T1=X*(A1+A4+2.*(A2+A3))/6.
T2=Y*(B1+B4+2.*(B2+B3))/6.
T3=P*(C1+C4+2.*(C2+C3))/6.
RETURN
END

FUNCTION F3(X,Y,P,S,XF)
F3=((Y-Y)*(S*(X-P*Y)*(1.-X)-X*((1.-X)-P*(1.-Y))))/(XF-Y)
RETURN
END

FUNCTION F4(X,Y,P,S,XF)
F4=((Y-X)*(S*(X-P*Y)*(1.-Y)-Y*((1.-X)-P*(1.-Y))))/(XF-X)
RETURN
END

FUNCTION F5(X,Y,P,S,XF,BE)
F5=-((BE*(XF-X1))/(2.*P*(Y-X))
RETURN
END

```

```

C C
THIS PROGRAM IS FOR HOLLOW FIBER FEED OUTSIDE
OPERATING IN CO CURRENT MODE.
PROGRAM FOR HOLLOW FIBRE MEMBRANE.
DIMENSION X(110),Y(110),U(110),V(110),FR(110),RX(110)
EXTERNAL F1,F2,F3,F4,F5,F6,F7,F8,F9,F10
OPEN(1,FILE='CORHL.DAT',STATUS='OLD')
OPEN(2,FILE='CORHL.OUT',STATUS='NEW')
READ(1,*)DO,DI,VIS,R,TEMP,FL,INF
READ(1,*)Q2,PF,SF,XF
READ(1,*)PRO,N,RXL
WRITE(2,*)DO,DI,VIS,R,TEMP,FL,INF
WRITE(2,*)Q2,PF,SF,XF
WRITE(2,*)PRO,N,RXL
DLM=(DO-DI)/ALOG(DO/DI)
A1=256*VIS*TEMP*(FL*2)
A2=(S.14**2)*Q2*DLM*(DI**4)*(PF**3)*INF
BE=A1/A2
WRITE(2,96)BE
FORMAT(4X,'BE=',F8.4/)
26 WRITE(15X,'*****OCURRENT*****')
AN=N
H=RXL/AN
RX0=0.0
X(1)=XF
X1=X(1)
CALL FIND(SF,PRO,XF,Y1)
Y(1)=Y1
Y0=Y(1)
PR(1)=PRO
WRITE(2,5)Y(1)
FORMAT(4X,'Y0=',F8.4)
K1=(N/10)+1
WRITE(2,14)
FORNAT(12X,'RKL',9X,'X',9X,'Y',9X,'U',9X,'V',9X,'PR')
DO 10 I=2,N+1
K=I-1
IF(K.NE.1)GO TO 11
XK=X(K)
YK=Y(K)
CALL RKA(SF,PRO,XK,YK,H,XI,YI)
X(I)=XI
Y(I)=YI
GO TO 10
PR(2)=PR(1)
XK=X(K)
YK=Y(K)
PRK=PR(K)
CALL RKB(SF,BE,XK,YK,PRK,H,XI,YI,PR1,XF)
X(I)=XI
Y(I)=YI
PR(I)=PR1
U(I)=(Y(I)-XF)/(Y(I)-X(I))
V(I)=(XF-X(I))/(Y(I)-X(I))
IF(I.NE.K1)GO TO 10
RX0=X0+0.1*RXL
WRITE(2,15)RX0,X(I),Y(I),U(I),V(I),PR(I)
FORMAT(4X,6(2X,F8.4))
K1=K1+(N/10)
CONTINUE
10 STOP
END
C C
SUBROUTINE TO FIND Y0
SUBROUTINE FIND(S,P,X,Y)
A=F*(S-1.)

```

```

X(J)=XJ
Y(J)=YJ
GO TO 20
PR(2)=PR(1)
PRL=PR(L)
XL=X(L)
YL=Y(L)
CALL RKC(SF,XV,XF,YF,BE,XL,YL,PRL,H,XJ,YJ,PRJ)
X(J)=XJ
Y(J)=YJ
PR(J)=PRJ
U(J)=(Y(J)-X(J))/(Y(J)-X(J))
V(J)=(X(J)-Y(J))/(Y(J)-X(J))
CONTINUE
WRITE(*,16)RXL,X(N+1),Y(N+1),U(N+1),V(N+1),PR(N+1),XW
YF=Y(N+1)
IF (ABS(XF-X(N+1))).LE.TOL)GO TO 40
XW=XW-.0001
GO TO 25
WRITE(*,16)RXL,X(N+1),Y(N+1),U(N+1),V(N+1),PR(N+1),XW
WRITE(2,16)RXL,X(N+1),Y(N+1),U(N+1),V(N+1),PR(N+1),XW
FORMAT(4X,7(2X,F8.4))//
IF(ABS(RXL-RLAST).LE.0.0001)GO TO 13
RXL=RXL+.0003
GO TO 25
STOP
END
C
C
SUBROUTINE TO FIND Y0
SUBROUTINE FIND(S,P,X,Y)
A=P*(S-1)
B=1.+(S-1.)*(P+X)
C=X*S
Y=(B-SQRT(B**2-4.*A*C))/(2.*A)
RETURN
END
C
C
SUBROUTINE RKB(S,P,XW,X,Y,KX,H,T1,T2,T3)
A1=H*F1(X,Y,S,P,XW)
R1=H*F2(X,Y,S,P,XW)
A2=H*F1(X+0.5*A1,Y+0.5*B1,S,P,XW)
B2=H*F2(X+0.5*A1,Y+0.5*B1,S,P,XW)
A3=H*F1(X+0.5*A2,Y+0.5*B2,S,P,XW)
B3=H*F2(X+0.5*A2,Y+0.5*B2,S,P,XW)
A4=H*F1(X+A3,Y+B3,S,P,XW)
B4=H*F2(X+A3,Y+B3,S,P,XW)
T1=X*(A1+A4+2.*(A2+A3))/6.
T2=Y*(B1+B4+2.*(B2+B3))/6.
T3=RX+H
RETURN
END
C
C
FUNCTION F1(X,Y,S,P,XW)
F1=((Y-X)*(S*(1.-X)*(X-P+Y)-X*((1.-X)-P*(1.-Y))))/(Y-XW)
RETURN
END
C
C
FUNCTION F2(X,Y,S,P,XW)
F2=((Y-X)*(S*(1.-Y)*(X-P+Y)-Y*((1.-X)-P*(1.-Y))))/(X-XW)
RETURN
END

```

```

C
C
THIS PROGRAM IS FOR HOLLOW FIRER FEED OUTSIDE MODE
OPERATING IN COUNTER CURRENT FLOW.
DIMENSION X(110),Y(110),U(110),V(110),PR(110),RX(110)
EXTERNAL F1,F2,F3,F4,F5,F6,F7,F8,F9,F10
OPEN(1,FILE='CNRHL.DAT',STATUS='OLD')
OPEN(2,FILE='CNRHL.OUT',STATUS='NEW')
READ(1,*)DO,DI,VIS,R,TEMP,FL,INF
READ(1,*)Q2,PF,SF,XF,XW
READ(1,*)PRO,N,RXL,RLAST,TOL
WRITE(2,*)DO,DI,VIS,R,TEMP,FL,INF
WRITE(2,*)Q2,PF,SF,XF,XW
WRITE(2,*)PRO,N,RXL,RLAST,TOL
DLM=(DO-DI)/ALOG(DO/DI)
A1=256*VIS*R*TEMP*(FL**2)
A2=(3.14**2)*Q2*DLM*(DI**4)*(PF**3)*TWF
BE=A1/A2
WRITE(2,98)BE
FORMAT(4X,'BE=',F8.4/)
AN=N
H=RXL/AN
RX0=0.0
X(1)=XW
PR(1)=PRO
RX(1)=RX0
X1=X(1)
CALL FIND(SF,PRO,X1,Y1)
Y(1)=Y1
DO 10 I=2,N+1
K=I-1
IF(K.NE.1)GO TO 11
CALL RKB(SF,PRO,XK,YK,KX,H,XI,YI,RX1)
Y(I)=YI
X(I)=XI
RX(I)=RX(1)+H
GO TO 10
XK=X(K)
YK=Y(K)
KX=KX(K)
CALL RKB(SF,PRO,XW,XK,YK,RXK,H,XI,YI,RX1)
X(I)=XI
Y(I)=YI
RX(I)=RXI
CONTINUE
WRITE(2,16)
FORMAT(16X,'*****COUNTER-CURRENT*****//)
WRITE(*,4)XW
FORMAT(4X,'XW=',F8.5/)
WRITE(2,17)
FORMAT(10X,'RXL',9X,'X',9X,'Y',9X,'U',9X,'V',9X,'PR',9X,'XW'//)
H=RXL/AN
X(1)=XW
X1=X(1)
PR(1)=PRO
CALL FIND(SF,PRO,X1,YW)
Y(1)=YW
K1=(N/10)+1
RX0=0.0
DO 20 J=2,N+1
I=J-1
IF(I.NE.1)GO TO 12
XL=X(L)
YL=Y(L)
CALL RKB(SF,PRO,XL,YL,H,XJ,YJ)

```

SUBROUTINE REC(S,XW,XF,YF,BE,X,Y,P,H,T1,T2,T3)

A1=H\*F6(X,Y,P,S,XW)
B1=H\*F7(X,Y,P,S,XW)
C1=H\*F8(X,Y,P,S,XW,XF,YF,BE)
A2=H\*F6(X+0.5\*A1,Y+0.5\*B1,P+0.5\*C1,S,XW)
B2=H\*F7(X+0.5\*A1,Y+0.5\*B1,P+0.5\*C1,S,XW)
C2=H\*F8(X+0.5\*A1,Y+0.5\*B1,P+0.5\*C1,S,XW,XF,YF,BE)
A3=H\*F6(X+0.5\*A2,Y+0.5\*B2,P+0.5\*C2,S,XW)
B3=H\*F7(X+0.5\*A2,Y+0.5\*B2,P+0.5\*C2,S,XW)
C3=H\*F8(X+0.5\*A2,Y+0.5\*B2,P+0.5\*C2,S,XW,XF,YF,BE)
A4=H\*F6(X+A3,Y+B3,P+C3,S,XW)
B4=H\*F7(X+A3,Y+B3,P+C3,S,XW)
C4=H\*F8(X+A3,Y+B3,P+C3,S,XW,XF,YF,BE)
T1=X\*(A1+A4+2.\*(A2+A3))/6.
T2=Y\*(B1+B4+2.\*(B2+B3))/6.
T3=P\*(C1+C4+2.\*(C2+C3))/6.
RETURN
END

FUNCTION F6(X,Y,P,S,XW)
F6=((Y-V)\*(S\*(1.-X)\*(X-P\*Y)-X\*((1.-X)-P\*(1.-Y)))/(Y-XW)
RETURN
END

FUNCTION F7(X,Y,P,S,XW)
F7=((Y-X)\*(S\*(1.-Y)\*(X-P\*Y)-Y\*((1.-X)-P\*(1.-Y)))/(X-XW)
RETURN
END

FUNCTION F8(X,Y,P,S,XW,XF,YF,BE)
F8=(-BE\*(X-XW)\*((XF-YF)\*\*2)/(2\*P\*(Y-X)\*((XW-YF)\*\*2))
RETURN
END

SUBROUTINE RAD(S,P,X,Y,H,T1,T2)
A1=H\*F9(X,Y,S,P)
B1=H\*F10(X,Y,S,P)
A2=H\*F9(X+0.5\*A1,Y+0.5\*B1,S,P)
B2=H\*F10(X+0.5\*A1,Y+0.5\*B1,S,P)
A3=H\*F9(X+0.5\*A2,Y+0.5\*B2,S,P)
B3=H\*F10(X+0.5\*A2,Y+0.5\*B2,S,P)
A4=H\*F9(X+A3,Y+B3,S,P)
B4=H\*F10(X+A3,Y+B3,S,P)
T1=X\*(A1+A4+2.\*(A2+A3))/6.
T2=Y\*(B1+B4+2.\*(B2+B3))/6.
RETURN
END

FUNCTION F9(X,Y,S,P)
F9=S\*(1.-X)\*(X-P\*Y)-X\*((1.-X)-P\*(1.-Y))
RETURN
END

FUNCTION F10(X,Y,S,P)
F10=((Y-X)\*(S\*(S-1.)\*Y)\*(S\*(1.-X)\*(X-P\*Y)-X\*((1.-X)-P\*(1.-Y)))/
1\*(S\*(1.-X)\*(X-P\*Y)-X\*((1.-X)-P\*(1.-Y))-(Y-X)\*(S-1.))
2\*(2.\*P\*Y-X-P)-1.))
RETURN
END





```

RETURN
END
FUNCTION F7(X,Y,Q,P,S,XW)
F7=((Y-X)*(S*(Q*X-P*Y)*(1.-Y)-Y*(Q*(1.-X)-P*(1.-Y))))/(X
RETURN
END

```

```

FUNCTION F1(X,Y,Q,S,P)
F1=S*(1.-X)*(Q*X-P*Y)-X*(Q*(1.-X)-P*(1.-Y))
RETURN
END
FUNCTION F2(X,Y,Q,S,P)
F2=-((Q*(Y-X)*(S*(1.-Y)+Y)-S*(1.-Y)*(Q*X-P*Y)+Y*(Q*(1.-X)-
P*(1.-Y)))+(S*(1.-X)*(Q*X-P*Y)-X*(Q*(1.-X)-P*(1.-Y)))/
Z(2.*S*(Q*X-P*Y)*(Y-1.))**2.*Y*(Q*(1.-X)-P*(1.-Y))+P*(Y-X)
S*(S*(1.-Y)+Y))
RETURN
END

```

C  
C  
C

```

SUBROUTINE KKC(S,EE,XW,XF,YF,P,X,Y,Q,H,T1,T2,T3)
A1=H*F3(X,Y,Q,P,S,XW)
B1=H*F4(X,Y,Q,P,S,XW)
C1=H*F5(X,Y,Q,XF,XW,YF,EE)
A2=H*F3(X+0.5*A1,Y+0.5*B1,Q+0.5*C1,P,S,XW)
B2=H*F4(X+0.5*A1,Y+0.5*B1,Q+0.5*C1,P,S,XW)
C2=H*F5(X+0.5*A1,Y+0.5*B1,Q+0.5*C1,XF,XW,YF,EE)
A3=H*F3(X+0.5*A2,Y+0.5*B2,Q+0.5*C2,P,S,XW)
B3=H*F4(X+0.5*A2,Y+0.5*B2,Q+0.5*C2,P,S,XW)
C3=H*F5(X+0.5*A2,Y+0.5*B2,Q+0.5*C2,XF,XW,YF,EE)
A4=H*F3(X+A3,Y+B3,Q+C3,P,S,XW)
B4=H*F4(X+A3,Y+B3,Q+C3,P,S,XW)
C4=H*F5(X+A3,Y+B3,Q+C3,XF,XW,YF,EE)
T1=X*(A1+A4+2.*(A2+A3))/6.
T2=Y*(B1+B4+2.*(B2+B3))/6.
T3=Q*(C1+C4+2.*(C2+C3))/6.
RETURN
END

```

```

FUNCTION F3(X,Y,Q,P,S,XW)
F3=((Y-X)*(S*(Q*X-P*Y)*(1.-X)-X*(Q*(1.-X)-P*(1.-Y))))/(Y-XW)
RETURN
END

```

```

FUNCTION F4(X,Y,Q,P,S,XW)
F4=((Y-X)*(S*(Q*X-P*Y)*(1.-Y)-Y*(Q*(1.-X)-P*(1.-Y))))/(X-XW)
RETURN
END

```

```

FUNCTION F5(X,Y,Q,XF,XW,YF,EE)
F5=-((B*(Y-XW)*(XF-YF)**2)/(2.*Q*(Y-X)*(XW-YF)**2))
RETURN
END

```

```

SUBROUTINE KKB(S,XW,Q,P,X,Y,H,T1,T2)
A1=H*F6(X,Y,Q,P,S,XW)
B1=H*F7(X,Y,Q,P,S,XW)
A2=H*F6(X+0.5*A1,Y+0.5*B1,Q,P,S,XW)
B2=H*F7(X+0.5*A1,Y+0.5*B1,Q,P,S,XW)
A3=H*F6(X+0.5*A2,Y+0.5*B2,Q,P,S,XW)
B3=H*F7(X+0.5*A2,Y+0.5*B2,Q,P,S,XW)
A4=H*F6(X+A3,Y+B3,Q,P,S,XW)
B4=H*F7(X+A3,Y+B3,Q,P,S,XW)
T1=X*(A1+A4+2.*(A2+A3))/6.
T2=Y*(B1+B4+2.*(B2+B3))/6.
RETURN
END

```

```

FUNCTION F6(X,Y,Q,P,S,XW)
F6=((Y-X)*(S*(Q*X-P*Y)*(1.-X)-X*(Q*(1.-X)-P*(1.-Y))))/(Y-XW)

```



```

C
C
C
THIS PROGRAM IS FOR HOLLOW FIBER FEED OUTSIDE MODE
OPERATING IN COUNTER CURRENT MODE WHEN FLOW RATE IS VARIED.
PROGRAM FOR HOLLOW FIBRE MEMBRANE.
DIMENSION X(110),Y(110),U(110),V(110),PR(110),RX(110)
EXTERNAL F1,F2,F3,F4,F5,F6,F7,F8,F9,F10
OPEN(1,FILE='FLOW.DAT',STATUS='OLD')
OPEN(2,FILE='FLOW.OUT',STATUS='NEW')
READ(1,*)DO,DI,VIS,R,TEMP,FL,TNF
READ(1,*)Q2,PF,SF,XF,XW
READ(1,*)PRO,N,RXL,FLAST,TOL,FLINC
WRITE(2,*)DO,DI,VIS,R,TEMP,FL,TNF
WRITE(2,*)Q2,PF,SF,XF,XW
WRITE(2,*)PRO,N,RXL,FLAST,TOL,FLINC
DLM=(DO-DI)/ALOG(DO/DI)
A1=256*VIS*R*TEMP*(FL**2)
A2=(3.14**2)*Q2*DLM*(DI**4)*(PF**3)*TNF
B6=A1/A2
AN=N
B=RXL/AN
RXO=0.0
X(1)=XW
PR(1)=PRO
RX(1)=RXO
XI=X(1)
CALL FIND(S,PRO,XI,YI)
Y(1)=YI
DO 10 I=2,N+1
K=I-1
IF(K.NE.1)GO TO 11
AN=X(K)
YK=Y(K)
CALL RKD(SF,PRO,XK,YK,H,XI,YI)
Y(I)=YI
X(I)=XI
RX(I)=RX(1)+H
GO TO 10
AN=X(K)
YK=Y(K)
CALL RKB(SE,PRO,XW,XK,YK,RXK,H,XI,YI,RXI)
X(I)=XI
Y(I)=YI
RX(I)=RXI
CONTINUE
YF=Y(N+1)
WRITE(2,17)
FORMAT(10X,FL,9X,X,9X,Y,9X,U,9X,V,9X,PR,9X,XW,/)
DLM=(DO-DI)/ALOG(DO/DI)
A1=256*VIS*R*TEMP*(FL**2)
A2=(3.14**2)*Q2*DLM*(DI**4)*(PF**3)*TNF
B6=A1/A2
B=RXL/AN
X(1)=XW
XI=X(1)
PR(1)=PRO
CALL FIND(SF,PRO,XI,YW)
Y(1)=YW
A1=(N/10)+1
RXO=0.0
DO 20 J=2,N+1
I=J-1
IF(I.NE.1)GO TO 12
XD=X(L)
YL=Y(L)
CALL RKD(SF,PRO,XL,YL,H,XJ,YJ)
X(J)=XJ

```

```

12
Y(J)=YJ
GO TO 20
PR(2)=PR(1)
PRL=PR(L)
XL=X(L)
YL=Y(L)
CALL RKC(SF,XW,XF,YF,BE,XL,YL,FRL,H,XJ,YJ,FRL)
X(3)=XJ
Y(3)=YJ
PR(3)=PRJ
U(J)=(Y(J)-X(1))/(Y(J)-X(J))
V(J)=(X(J)-X(1))/(Y(J)-X(J))
CONTINUE
WRITE(*,16)FL,X(N+1),Y(N+1),U(N+1),V(N+1),PR(N+1),XW
YF=Y(N+1)
IF (ABS(XF-X(N+1)) .LE. TOL)GO TO 40
XW=XW-.0001
GO TO 25
WRITE(*,16)FL,X(N+1),Y(N+1),U(N+1),V(N+1),PR(N+1),XW
WRITE(2,16)FL,X(N+1),Y(N+1),U(N+1),V(N+1),PR(N+1),XW
FORMAT(4X,E9,3,2X,6(2X,F8,4)/)
IF(ABS(FL-FLAST).LE.0.00000001)GO TO 13
FL=FL+FLINC
GO TO 25
STOP
END

```

```

C
C
SUBROUTINE TO FIND Y0
SUBROUTINE FIND(S,P,X,Y)
A=P*(S-I.)
B=1.+(S-I.)*(P+X)
C=X+S
Y=1B-SORT(B**2-4.*A*C)/(2.*A)
RETURN
END

```

```

C
C
SUBROUTINE RKB(S,P,XW,X,Y,RX,H,T1,T2,T3)
A1=B+F1(X,Y,S,P,XW)
B1=B+F2(X,Y,S,P,XW)
A2=B+F1(X+0.5*A1,Y+0.5*B1,S,P,XW)
B2=B+F2(X+0.5*A1,Y+0.5*B1,S,P,XW)
A3=B+F1(X+0.5*A2,Y+0.5*B2,S,P,XW)
B3=B+F2(X+0.5*A2,Y+0.5*B2,S,P,XW)
A4=B+F1(X+A3,Y+B3,S,P,XW)
B4=B+F2(X+A3,Y+B3,S,P,XW)
T1=X+(A1+A4+2.*(A2+A3))/6.
T2=Y+(B1+B4+2.*(B2+B3))/6.
T3=RX+H
RETURN
END

```

```

FUNCTION F1(X,Y,S,P,XW)
F1=((Y-X)*(S*(1.-X)*(X-P+Y)-X*(1.-X)-P*(1.-Y)))/(Y-XW)
RETURN
END
FUNCTION F2(X,Y,S,P,XW)
F2=((Y-X)*(S*(1.-Y)*(X-P+Y)-Y*(1.-X)-P*(1.-Y)))/(X-XW)
RETURN
END

```

```

C
C
C
SUBROUTINE RKC(S,XW,XF,YF,BE,XL,YL,FRL,H,XJ,YJ,T2,T3)

```

```

A1=H*F6(X,Y,P,S,XW)
B1=H*F7(X,Y,P,S,XW)
C1=H*F8(X,Y,P,S,XW,XF,YF,BE)
A2=H*F6(X+0.5*A1,Y+0.5*B1,P+0.5*C1,S,XW)
B2=H*F7(X+0.5*A1,Y+0.5*B1,P+0.5*C1,S,XW)
C2=H*F8(X+0.5*A1,Y+0.5*B1,P+0.5*C1,S,XW,XF,YF,BE)
A3=H*F6(X+0.5*A2,Y+0.5*B2,P+0.5*C2,S,XW)
B3=H*F7(X+0.5*A2,Y+0.5*B2,P+0.5*C2,S,XW)
C3=H*F8(X+0.5*A2,Y+0.5*B2,P+0.5*C2,S,XW,XF,YF,BE)
A4=H*F6(X+A3,Y+B3,P+C3,S,XW)
B4=H*F7(X+A3,Y+B3,P+C3,S,XW)
C4=H*F8(X+A3,Y+B3,P+C3,S,XW,XF,YF,BE)
T1=X*(A1+A4+2.*(A2+A3))/6.
T2=Y*(B1+B4+2.*(B2+B3))/6.
T3=P*(C1+C4+2.*(C2+C3))/6.
RETURN
END

FUNCTION F6(X,Y,P,S,XW)
F6=((Y-X)*(S*(1.-X)*(X-P*Y)-X*((1.-X)-P*(1.-Y))))/(Y-XW)
RETURN
END

FUNCTION F7(X,Y,P,S,XW)
F7=((Y-X)*(S*(1.-Y)*(X-P*Y)-Y*((1.-X)-P*(1.-Y))))/(X-XW)
RETURN
END

FUNCTION F8(X,Y,P,S,XW,XF,YF,BE)
F8=(-BE*(X-XW)*((XF-YF)**2))/(2*P*(Y-X)*((XW-YF)**2))
RETURN
END

SUBROUTINE RKD(S,P,X,Y,H,T1,T2)
A1=H*F9(X,Y,S,P)
R1=H*F10(X,Y,S,P)
A2=H*F9(X+0.5*A1,Y+0.5*B1,S,P)
R2=H*F10(X+0.5*A1,Y+0.5*B1,S,P)
A3=H*F9(X+0.5*A2,Y+0.5*B2,S,P)
R3=H*F10(X+0.5*A2,Y+0.5*B2,S,P)
A4=H*F9(X+A3,Y+B3,S,P)
R4=H*F10(X+A3,Y+B3,S,P)
T1=X*(A1+A4+2.*(A2+A3))/6.
T2=Y*(B1+B4+2.*(B2+B3))/6.
RETURN
END

FUNCTION F9(X,Y,S,P)
F9=S*(1.-X)*(X-P*Y)-X*(1.-X)-P*(1.-Y)
RETURN
END

FUNCTION F10(X,Y,S,P)
F10=((Y-X)*(S-(S-1.)*Y)*(S*(1.-X)*(X-P*Y)-X*((1.-X)-P*(1.-Y))))/
1*(S*(1.-X)*(X-P*Y)-X*((1.-X)-P*(1.-Y)))-(Y-X)*((S-1.
2*(2.-P*Y-X-P)-1.))
RETURN
END

```

```

C THIS PROGRAM IS FOR HOLLOW FIBER COUNTER CURRENT MODE
C WHEN TEMPERATURE IS VARIED.
C PROGRAM FOR HOLLOW FIBRE MEMBRANE.
DIMENSION X(110),Y(110),U(110),V(110),PR(110),RX(110)
EXTERNAL F1,F2,F3,F4,F5,F6,F7,F8,F9,F10
OPEN(1,FILE='TEMP.DAT',STATUS='OLD')
OPEN(2,FILE='TEMP.OUT',STATUS='NEW')
READ(1,*)DO,DI,VIS1,R,TEMP1,TEMP2,FL,INF
READ(1,*)Q1T,Q2T,EQ1,EQ2,FF,SE,XF,XW,FW
READ(1,*)PRO,N,RXL,TLAST,TOL,TINC
WRITE(2,*)DO,DI,VIS1,R,T1,T2,FL,INF
WRITE(2,*)Q1T,Q2T,EQ1,EQ2,FF,SE,XF,XW,FW
WRITE(2,*)PRO,N,RXL,TLAST,TOL,TINC
AT=(TEMP2-TEMP1)/(TEMP2+TEMP1)
Q1=Q1T*EXP(EQ1*AT/R)
Q2=Q2T*EXP(EQ2*AT/R)
SF=Q1/Q2
VIS=VIS1*((TEMP2/TEMP1)**PW)
DUM=(DO-DI)/ALOG(DO/DI)
A1=256*VIS*R*TEMP2*(FL**2)
A2=(3.14**2)*Q2*DLM*(DI**4)*(FF**3)*INF
SE=AI/A2
AN=N
H=RXL/AN
RXO=0.0
X(1)=XW
PR(1)=PRO
RX(1)=RXO
X1=X(1)
CALL FIND(SF,PRO,X1,Y1)
Y(1)=Y1
DO 10 I=2,N+1
K=I-1
IF(K.NE.1)GO TO 11
XK=X(K)
YK=Y(K)
CALL RMD(SF,PRO,XK,YK,B,XI,YI)
Y(I)=YI
X(I)=XI
RX(I)=RX(1)+H
GO TO 10
XK=X(K)
YK=Y(K)
RXK=RX(K)
CALL RKB(SF,PRO,XW,XK,YK,RXK,B,XI,YI,RXI)
X(I)=XI
Y(I)=YI
RX(I)=RXI
CONTINUE
WRITE(2,17)
FORMAT(9X,'TEMP',9X,'X',9X,'Y',9X,'U',9X,'V',9X,'PR',9X,'RX','XW'//)
DUM=(DO-DI)/ALOG(DO/DI)
AT=(TEMP2-TEMP1)/(TEMP2+TEMP1)
Q1=Q1T*EXP(EQ1*AT/R)
Q2=Q2T*EXP(EQ2*AT/R)
SF=Q1/Q2
VIS=VIS1*((TEMP2/TEMP1)**PW)
A1=256*VIS*R*TEMP2*(FL**2)
A2=(3.14**2)*Q2*DLM*(DI**4)*(FF**3)*INF
SE=AI/A2
H=RXL/AN
X(1)=XW
X1=X(1)
PR(1)=PRO
CALL FIND(SF,PRO,X1,YM)

```

```

Y(1)=YW
KI=(N/10)+1
RXO=0.0
DO 20 J=2,N+1
L=J-1
IF(L.NE.1)GO TO 12
XL=X(L)
YL=Y(L)
CALL RKB(SF,PRO,XL,YL,B,XJ,YJ)
X(J)=XJ
Y(J)=YJ
GO TO 20
PR(2)=PR(1)
PRL=PR(L)
XL=X(L)
YL=Y(L)
CALL RKB(SF,XW,XF,YF,SE,XL,YL,FRL,B,XJ,YJ,PRJ)
X(J)=XJ
Y(J)=YJ
PR(J)=PRJ
U(J)=(Y(J)-X(1))/(Y(J)-X(J))
V(J)=(X(J)-X(1))/(Y(J)-X(J))
CONTINUE
WRITE(*,18)TEMP2,X(N+1),Y(N+1),U(N+1),V(N+1),PR(N+1),XW
YF=Y(N+1)
IF (ABS(XF-X(N+1)).LE.TOL)GO TO 40
XW=XW-.0001
GO TO 25
WRITE(*,18)TEMP2,X(N+1),Y(N+1),U(N+1),V(N+1),PR(N+1),XW
FORMAT(4X,F8.3,2X,6(2X,F8.4))//)
18 IF(ABS(TEMP2-TLAST).LE.0.0001)GO TO 13
TEMP2=TEMP2+TINC
GO TO 25
13 STOP
END
C
SUBROUTINE TO FIND,YO
SUBROUTINE FIND(S,F,X,Y)
A=P*(S-1.)
B=1.+(S-1.)*(P+X)
C=X*S
Y=(B-SQRT(B**2-4.*A*C))/(2.*A)
RETURN
END
C
SUBROUTINE RKB(S,F,XW,X,Y,RX,H,T1,T2,T3)
A1=H*F1(X,Y,S,F,XW)
A2=H*F2(X,Y,S,F,XW)
A3=H*F3(X+0.5*A1,Y+0.5*B1,S,F,XW)
A4=H*F4(X+0.5*A1,Y+0.5*B1,S,F,XW)
A5=H*F5(X+0.5*A2,Y+0.5*B2,S,F,XW)
A6=H*F6(X+0.5*A2,Y+0.5*B2,S,F,XW)
A7=H*F7(X+A3,Y+B3,S,F,XW)
A8=H*F8(X+A3,Y+B3,S,F,XW)
T1=X+(A1+A4+2.*(A2+A3))/6.
T2=Y+(B1+B4+2.*(B2+B3))/6.
T3=RX+8
RETURN
END
FUNCTION F1(X,Y,S,F,XW)
F1=((Y-X)*(S+(1.-X)*(X-P*Y))-X*(1.-X))-P*(1.-X)
RETURN
END

```

2\*(2.\*P\*Y-X-P)-1.))  
 RETURN  
 END

FUNCTION F2(X,Y,S,P,XW)  
 F2=((Y-X)\*(S\*(1.-Y)\*(X-P\*Y)-Y\*((1.-X)-P\*(1.-Y))))/(X-XW)  
 RETURN  
 END

C  
 C  
 C

SUBROUTINE RKC(S,XN,XF,YF,BE,X,Y,P,H,T1,T2,T3)  
 A1=H\*F6(X,Y,P,S,XW)  
 B1=H\*F7(X,Y,P,S,XW)  
 C1=H\*F8(X,Y,P,S,XW,XF,YF,BE)  
 A2=H\*F6(X+0.5\*A1,Y+0.5\*B1,P+0.5\*C1,S,XW)  
 B2=H\*F7(X+0.5\*A1,Y+0.5\*B1,P+0.5\*C1,S,XW)  
 C2=H\*F8(X+0.5\*A1,Y+0.5\*B1,P+0.5\*C1,S,XW,XF,YF,BE)  
 A3=H\*F6(X+0.5\*A2,Y+0.5\*B2,P+0.5\*C2,S,XW)  
 B3=H\*F7(X+0.5\*A2,Y+0.5\*B2,P+0.5\*C2,S,XW)  
 C3=H\*F8(X+0.5\*A2,Y+0.5\*B2,P+0.5\*C2,S,XW,XF,YF,BE)  
 A4=H\*F6(X+A3,Y+B3,P+C3,S,XW)  
 B4=H\*F7(X+A3,Y+B3,P+C3,S,XW)  
 C4=H\*F8(X+A3,Y+B3,P+C3,S,XW,XF,YF,BE)  
 T1=X\*(A1+A4+2.\*(A2+A3))/6.  
 T2=Y\*(B1+B4+2.\*(B2+B3))/6.  
 T3=P\*(C1+C4+2.\*(C2+C3))/6.  
 RETURN  
 END

FUNCTION F6(X,Y,P,S,XW)  
 F6=((Y-X)\*(S\*(1.-X)\*(X-P\*Y)-X\*((1.-X)-P\*(1.-Y))))/(Y-XW)  
 RETURN  
 END

FUNCTION F7(X,Y,P,S,XW)  
 F7=((Y-X)\*(S\*(1.-Y)\*(X-P\*Y)-Y\*((1.-X)-P\*(1.-Y))))/(X-XW)  
 RETURN  
 END

FUNCTION F8(X,Y,P,S,XW,XF,YF,BE)  
 F8=(-BE\*(X-XW)\*((XF-YF)\*\*2))/((2\*P\*(Y-X)\*((XW-YF)\*\*2))  
 RETURN  
 END

SUBROUTINE RKD(S,P,X,Y,H,T1,T2)  
 A1=H\*F9(X,Y,S,P)  
 B1=H\*F10(X,Y,S,P)  
 A2=H\*F9(X+0.5\*A1,Y+0.5\*B1,S,P)  
 B2=H\*F10(X+0.5\*A1,Y+0.5\*B1,S,P)  
 A3=H\*F9(X+0.5\*A2,Y+0.5\*B2,S,P)  
 B3=H\*F10(X+0.5\*A2,Y+0.5\*B2,S,P)  
 A4=H\*F9(X+A3,Y+B3,S,P)  
 B4=H\*F10(X+A3,Y+B3,S,P)  
 T1=X\*(A1+A4+2.\*(A2+A3))/6.  
 T2=Y\*(B1+B4+2.\*(B2+B3))/6.  
 RETURN  
 END

FUNCTION F9(X,Y,S,P)  
 F9=S\*(1.-X)\*(X-P\*Y)-X\*((1.-X)-P\*(1.-Y))  
 RETURN  
 END

FUNCTION F10(X,Y,S,P)  
 F10=((Y-X)\*(S\*(1.-Y)\*(X-P\*Y)-Y\*((1.-X)-P\*(1.-Y))))/(S-1.)  
 RETURN  
 END

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