

A GENERAL ANALYSIS OF GAS CENTRIFUGATION
WITH EMPHASIS ON THE COUNTERCURRENT
PRODUCTION CENTRIFUGE

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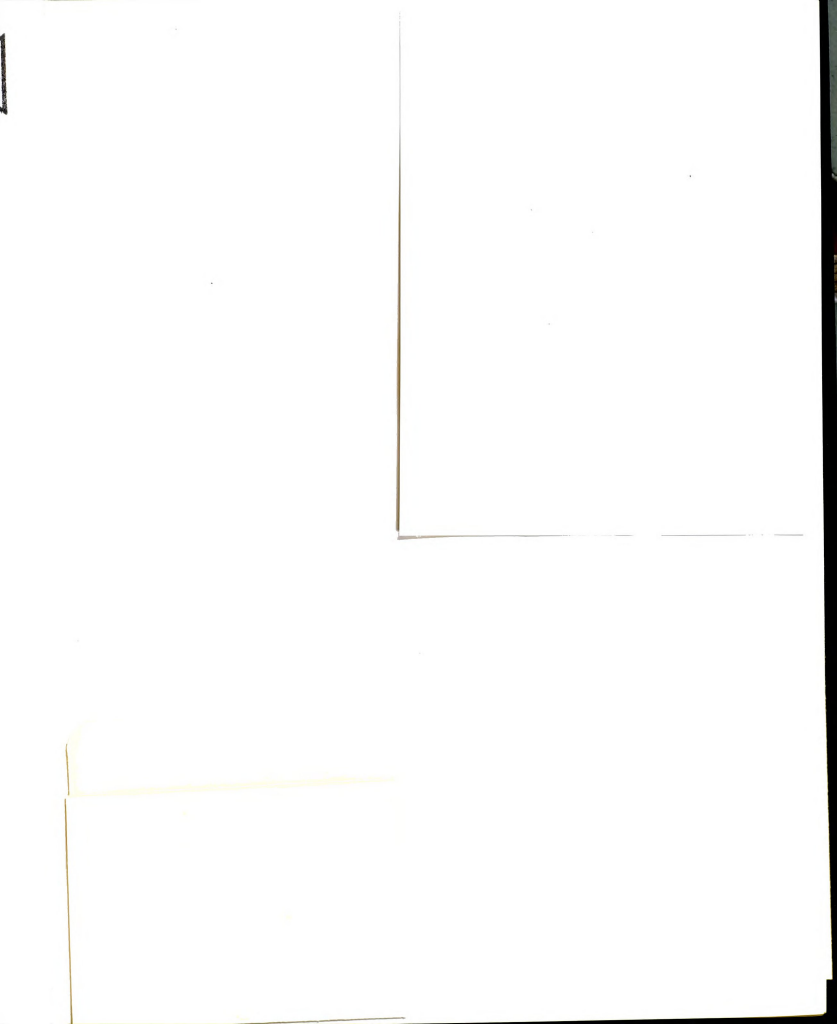
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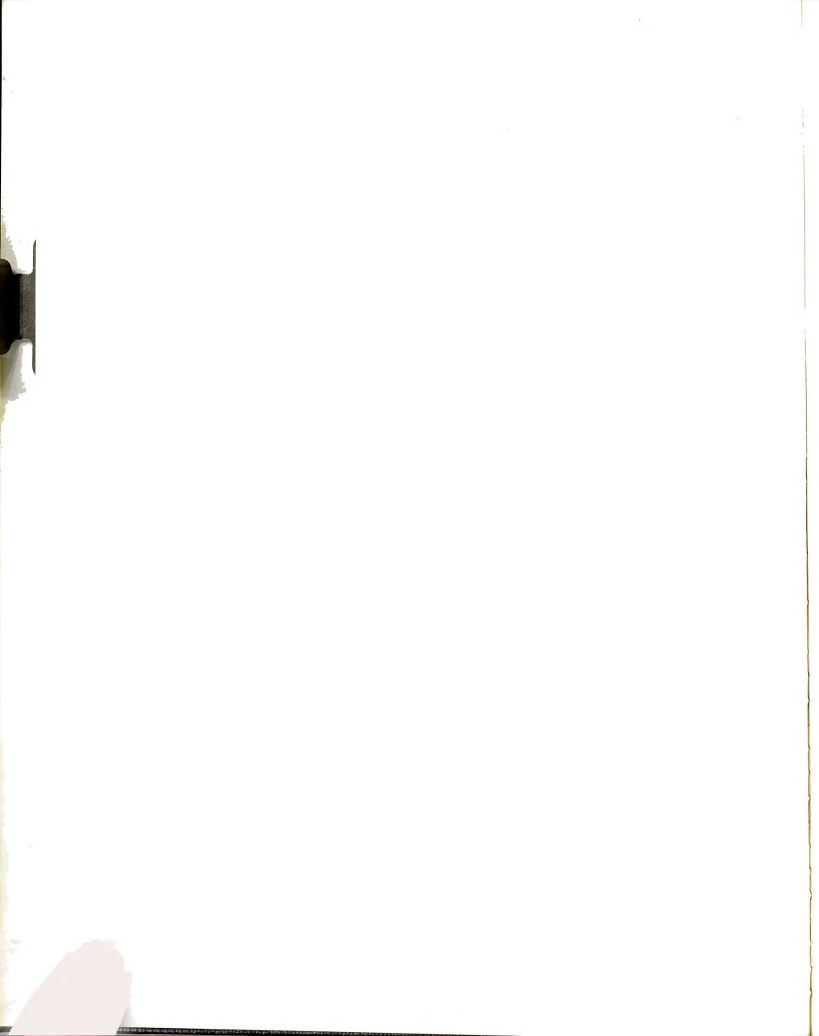
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ABSTRACT

A GENERAL ANALYSIS OF GAS CENTRIFUGATION WITH EMPHASIS ON THE COUNTERCURRENT PRODUCTION CENTRIFUGE

By

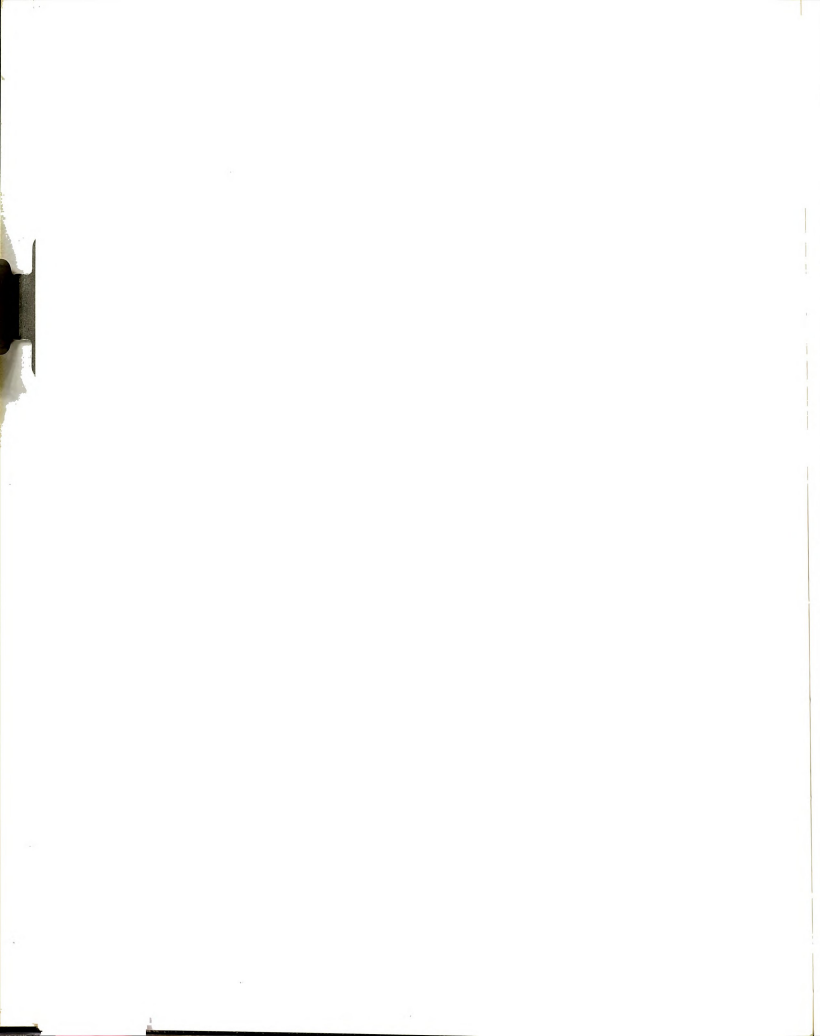
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Contained in this work is a theoretical analysis of gas centrifugation with emphasis on the countercurrent production centrifuge. The in-depth analysis of gas centrifugation presented in this work significantly updates the previously available literature. Results are presented which allow an evaluation to be made regarding the applicability of the gas centrifuge to perform a given separation. Operating variables such as pressure, temperature, rotational speed, centrifuge diameter and length, throughput, molecular weight differences and diffusion coefficients, among others, are discussed in detail for the gas centrifuge separation of a binary gas mixture. Included as Appendices are user instructions, descriptions and listings of computer programs that are based on this work which can be used to model (predict) the performance of either a stripping, rectifying or Zippe type gas centrifuge in a given situation. Results predicted by the programs agree very well to separations presented in the literature for Uranium isotope (as UF_6) separations.

Throughout the work many significant points are illustrated using the gas pairs $\text{SO}_2\text{-N}_2$, $\text{SO}_2\text{-H}_2$ and UF_6 (235 and 238 isotopes). The $\text{SO}_2\text{-N}_2$ gas pair reflects the desire to determine the applicability of gas centrifugation as a viable means for removing SO_2 from power plant stack gas.

Equations were developed describing the equilibrium pressure and composition profiles and the times required for the development of these profiles in a simple centrifuge containing a binary gas mixture. This analysis illustrated that, while an 8-inch diameter simple centrifuge charged at 70°F and 1 atmosphere with an $\text{SO}_2\text{-N}_2$ gas mixture (5000 ppm SO_2) and then rotated at 20000 RPM would give a 39.4% increase in SO_2 concentration going from the axis to the wall, it would take approximately 43 seconds for 50% of this separation to occur. The diffusion coefficient for the gas pair was found to be the only factor controlling the rate of separation. With such slow rates of mass transfer, it was concluded that long residence times would be required to realize the separating potential of the counter-current production centrifuge.

To meet the demands of high rotational speeds and long residence times, the mechanical limitations (size versus rotational speeds) of the centrifuge were investigated. Expressions were developed for the bursting and whirling speeds of a simply supported cylinder, illustrating that Aluminum and Magnesium alloys were best suited for centrifuge design. It was shown for these alloys that a peripheral speed of 700 ft/sec was well below the bursting speed of an 8-inch diameter rotating cylinder with a 1/4-inch wall thickness,



r, at this speed the length to diameter ratio has to be less for safe operation under the first whirling speed.

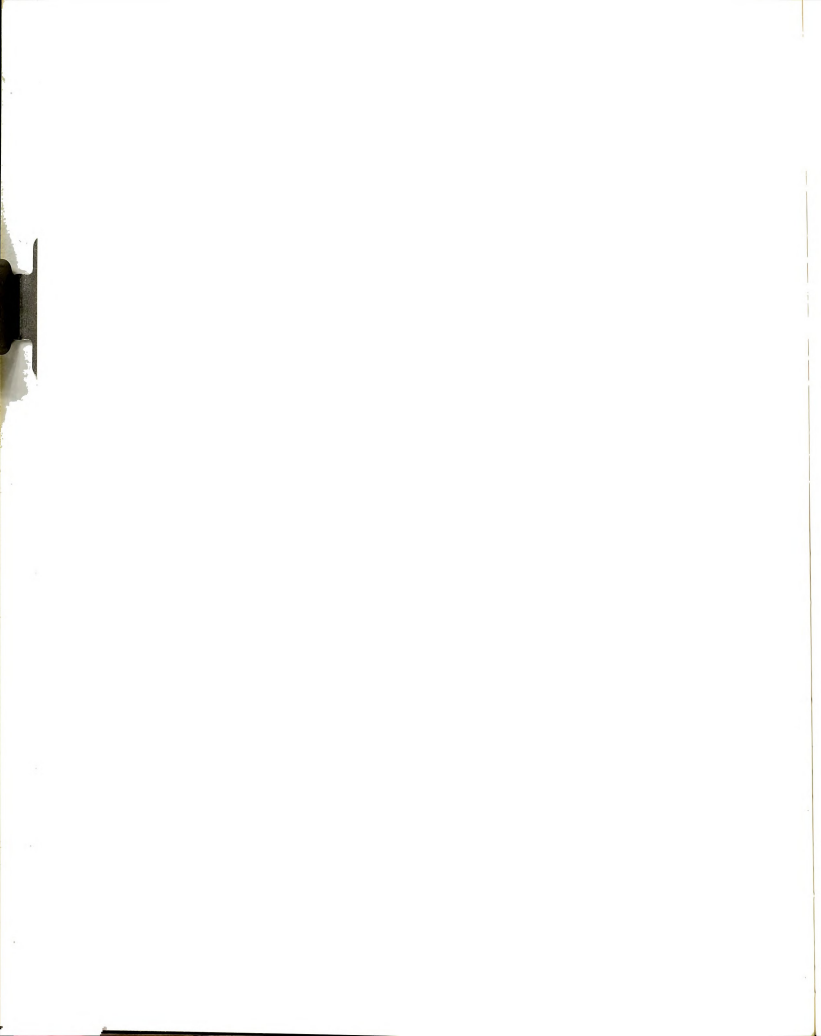
Expressions were developed describing the separations in a concurrent gas centrifuge. It was determined that in the operation of a countercurrent rectifying (concentrates the heavy species) stripping (concentrates the light species) centrifuge that an optimum feed rate (OFR) existed, yielding a maximum in the separation (MSF). For the gas pair $\text{SO}_2\text{-N}_2$ at 70°F and 1 atmosphere axis to radius in an 8-inch diameter by 36-inch long rectifying centrifuge operating at 15000 RPM, the OFR was found to be 0.0169 scfm giving an MSF of 2.337 at total reflux. If a rich product stream equal to 10% of the feed stream is removed the OFR increases to 0.0191 scfm but the MSF (rich to lean stream) to 1.696 or a reduction of 28%.

It was shown that the OFR and the MSF could be quickly and accurately estimated for any gas pair in any size rectifying centrifuge at any operating conditions by using the following equations:

$$\text{OFR} \approx a \cdot (\text{diffusivity times pressure, cm}^2 \cdot \text{atm/sec}) / (\text{diameter, inches}),$$

$$\text{MSF} \approx \text{Exp} [b \cdot (\text{rotational speed, ft/sec})^2 / (\text{molecular weight difference}) (\text{length/diameter}) / (\text{temperature, } ^\circ\text{F})],$$

where $a = .0157$ and $b = 1.013 \times 10^{-5}$ at total reflux, and

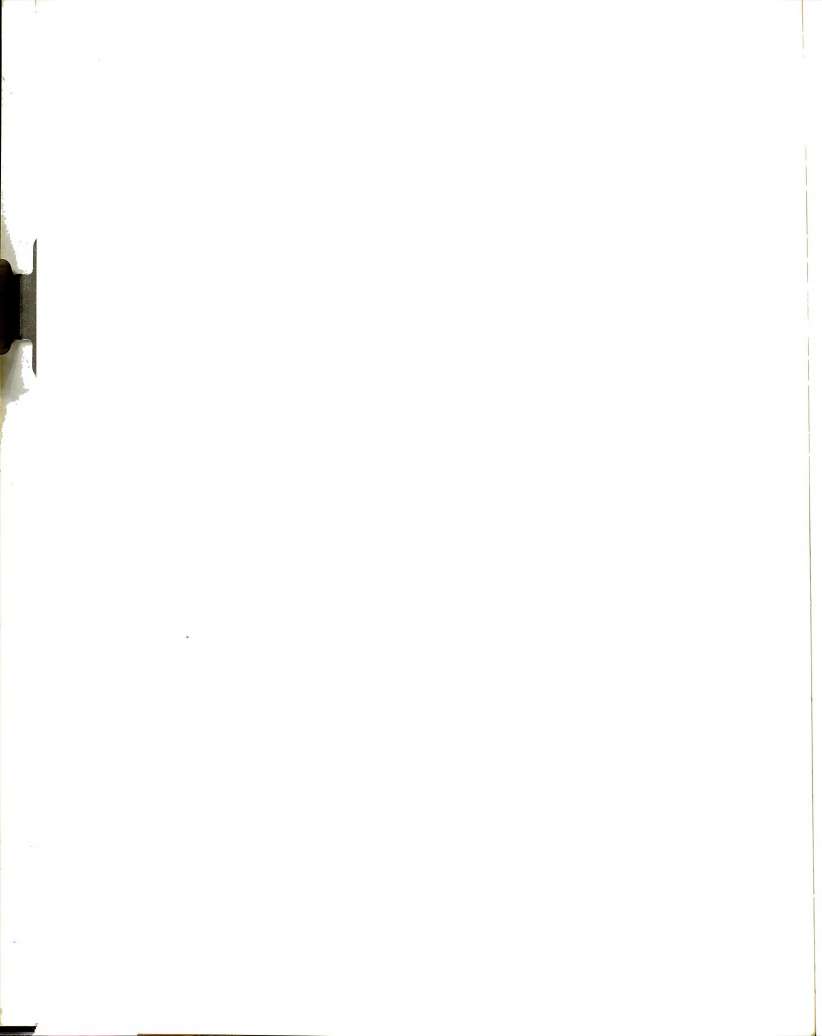


$a = .0178$ and $b = 6.304 \times 10^{-6}$ where the rich stream is 10% of the feed stream.

As is shown in the above estimating equations, increasing the speed but maintaining a constant peripheral speed increases the MSF directly; however, the reduction in the length to diameter ratio initially decreases the MSF. Hence, to sustain a given level of SO_2 removal when scaling up a centrifuge design, the length and diameter must increase by the same percentage. Also, shown in this work is the fact that removal of a product stream rather sharply reduces the MSF regardless of the centrifuge length. This is an equilibrium limitation which was shown to be characteristic of the gas centrifuge.

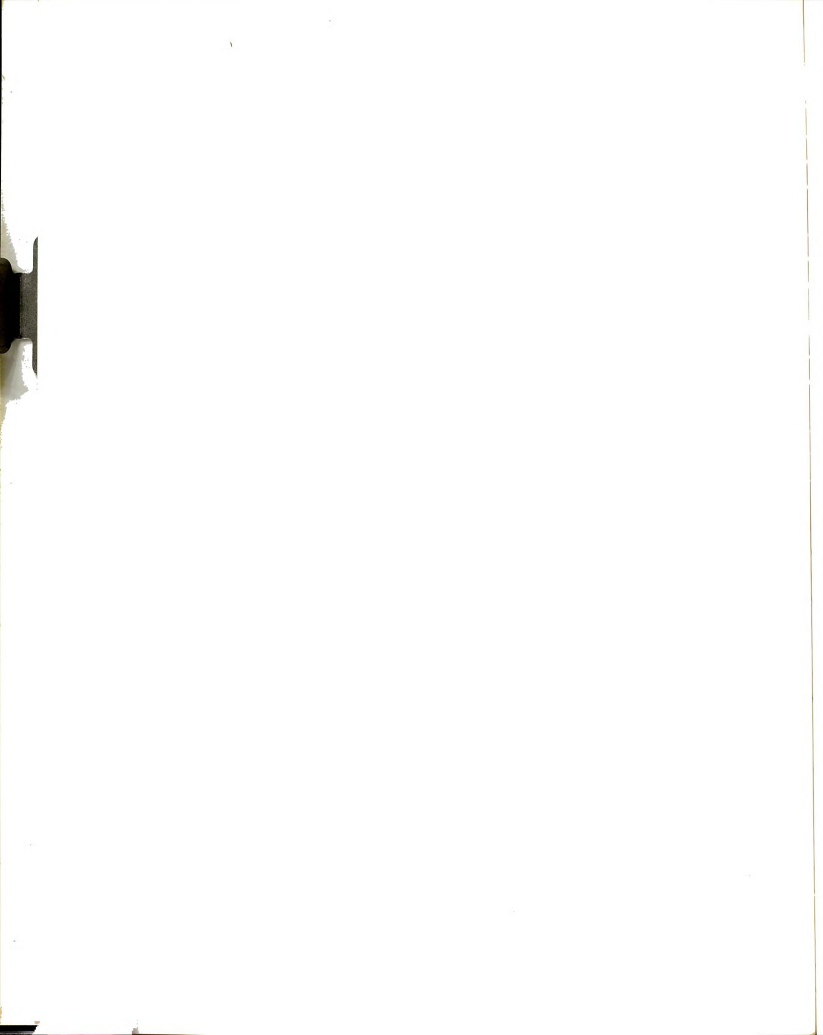
The results of this work clearly indicate that for the gas SO_2 - N_2 in the 8-inch diameter centrifuge operated as described with the OFR of 0.0191 scfm and corresponding MSF of 1.696 with a gas stream removal of 0.0019 scfm (10% of the feed) cannot be significantly altered by any operating parameters. These very small MSFs and low MSFs are incompatible with the tremendous volumes of gas produced by power plants and the high degree (90+%) of SO_2 removal required. Gas centrifugation for this purpose cannot begin to compare with the many conventional SO_2 removal processes proposed for removal of SO_2 from coal fired power plant stack gases.

Included as part of the Appendices is a description and analysis of the experimental program which paralleled this work. The centrifuge used in the experimental program, which was modeled after a design by Zippe (University of Virginia, 1960), had 34 inches available



axial flow, a 7.5-inch diameter, and was rotated at 11000 RPM. Zippe's experiments were with UF₆ (235 and 238) separations with pressures less than 0.1 mm Hg, the above experimental program carried out at atmospheric pressure with SO₂-N₂ gas mixtures. The feed rate (limited by equipment design and sampling methods for analysis) which was used was 0.1 scfm. No measurable separation was observed at this feed rate or at any other higher feed rate. The analyses presented in this work, which predict Zippe's observations accurately, show the separation factor predicted at the above feed rate to be only 1.045. This very low predicted separation factor corresponds to SO₂ concentration differences much too small to be seen in the infrared spectrophotometer used for gas analysis. Furthermore, the uncontrollable and unpredictable increase in internal turbulence promoted by the Zippe type centrifuge operated at atmospheric pressure was expected to have reduced if not destroyed this small, expected, separation factor.

The very small feed rate and predicted separation factor, coupled with the turbulence problems fundamental to the Zippe centrifuge design when operated at pressures near 1 atmosphere, resulted in termination of the experimental program.



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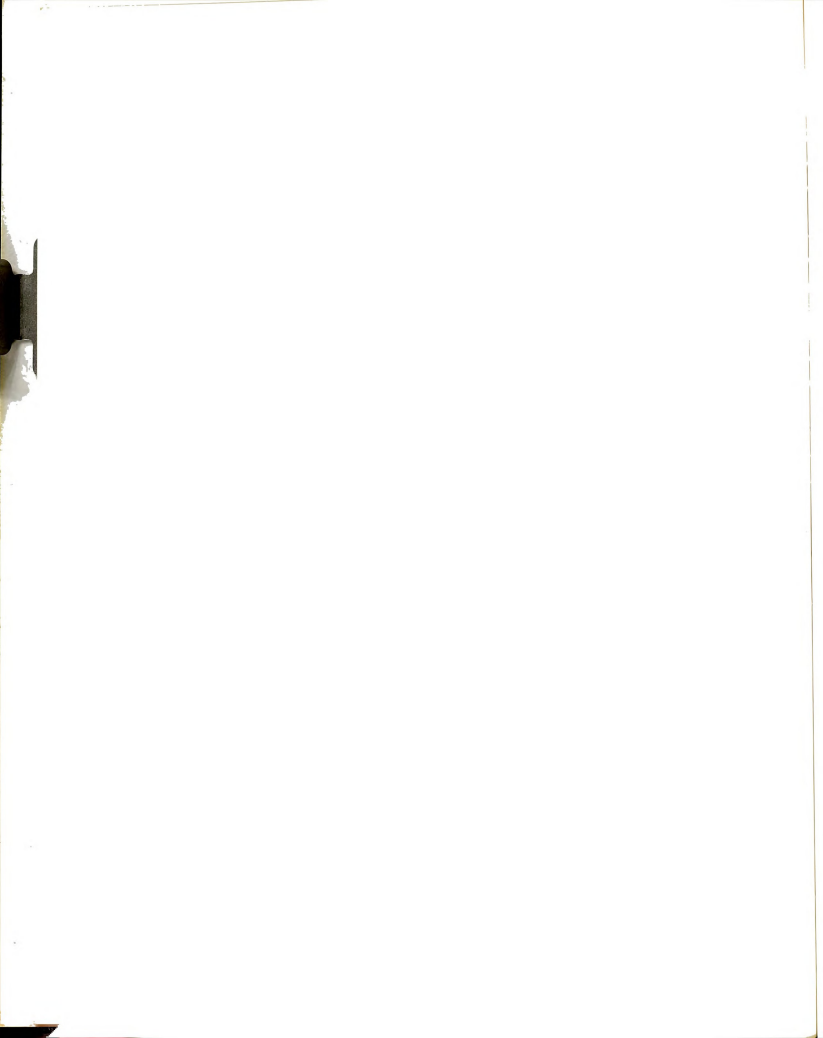
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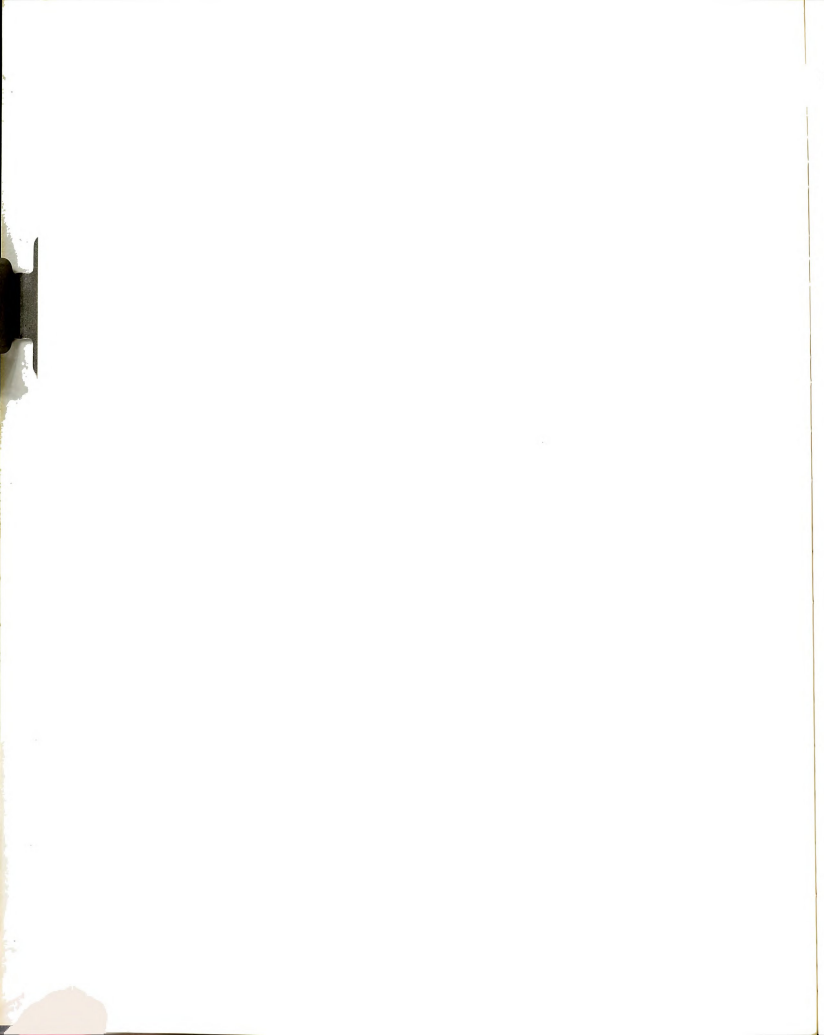
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The understanding and patience of the author's wife, Pam, is greatly appreciated.

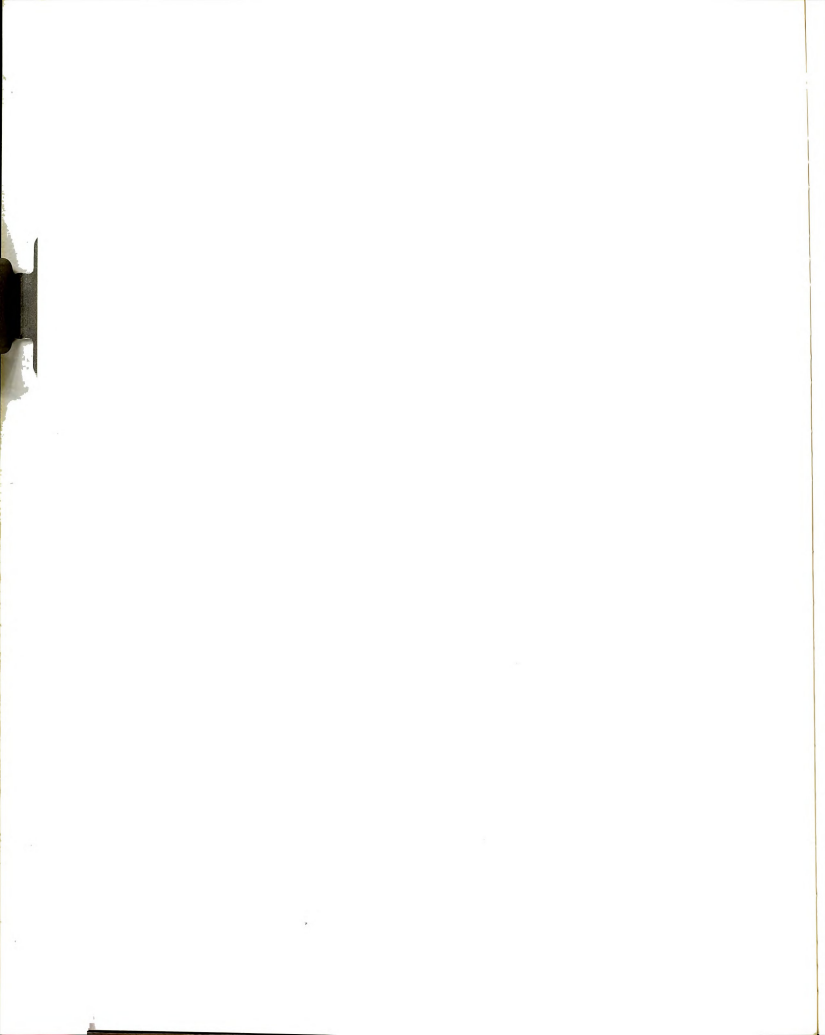


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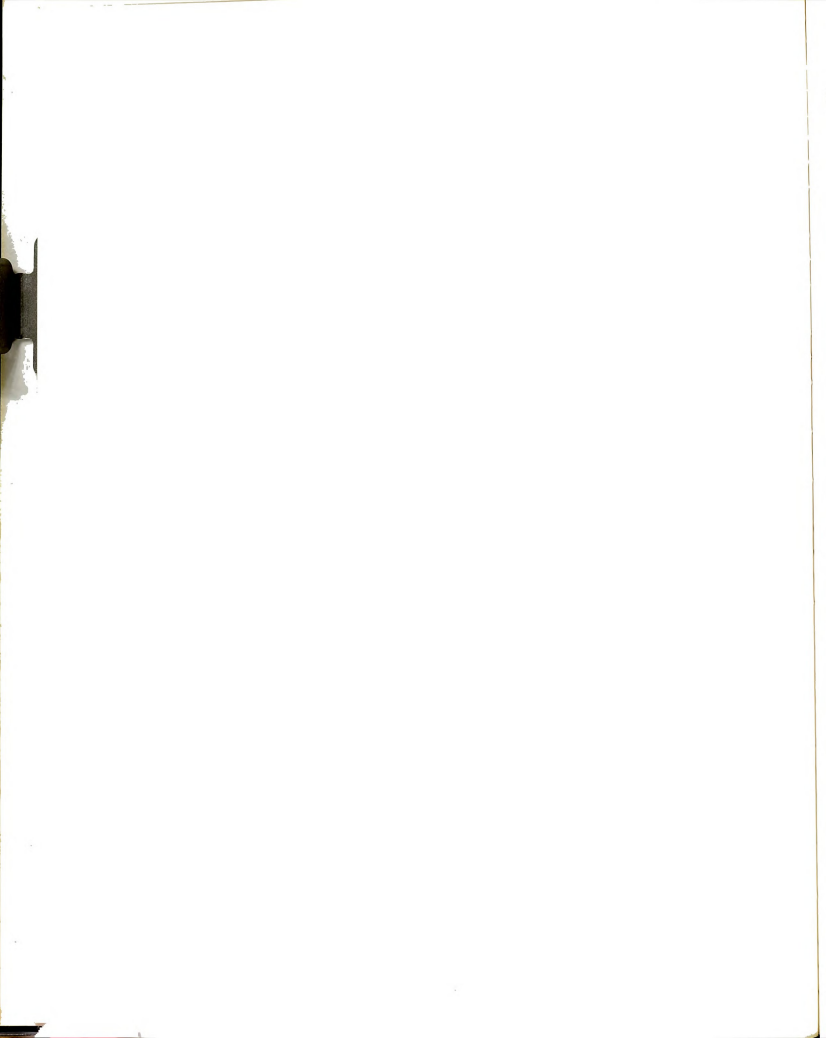


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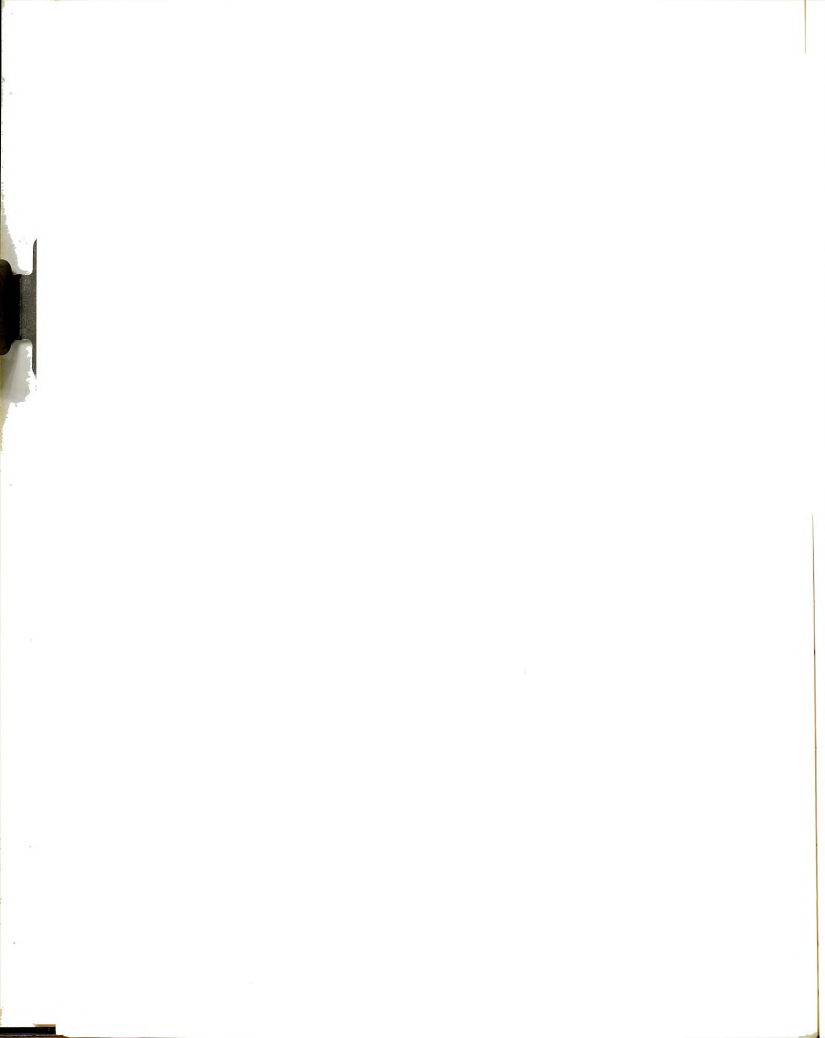


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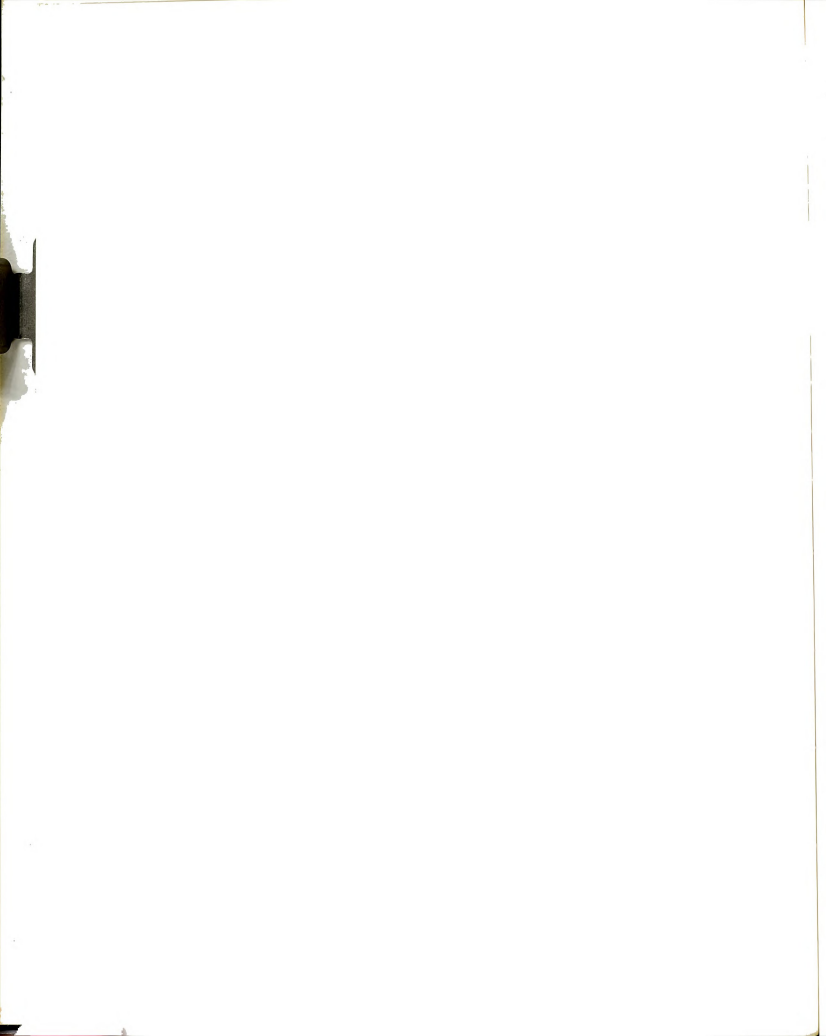
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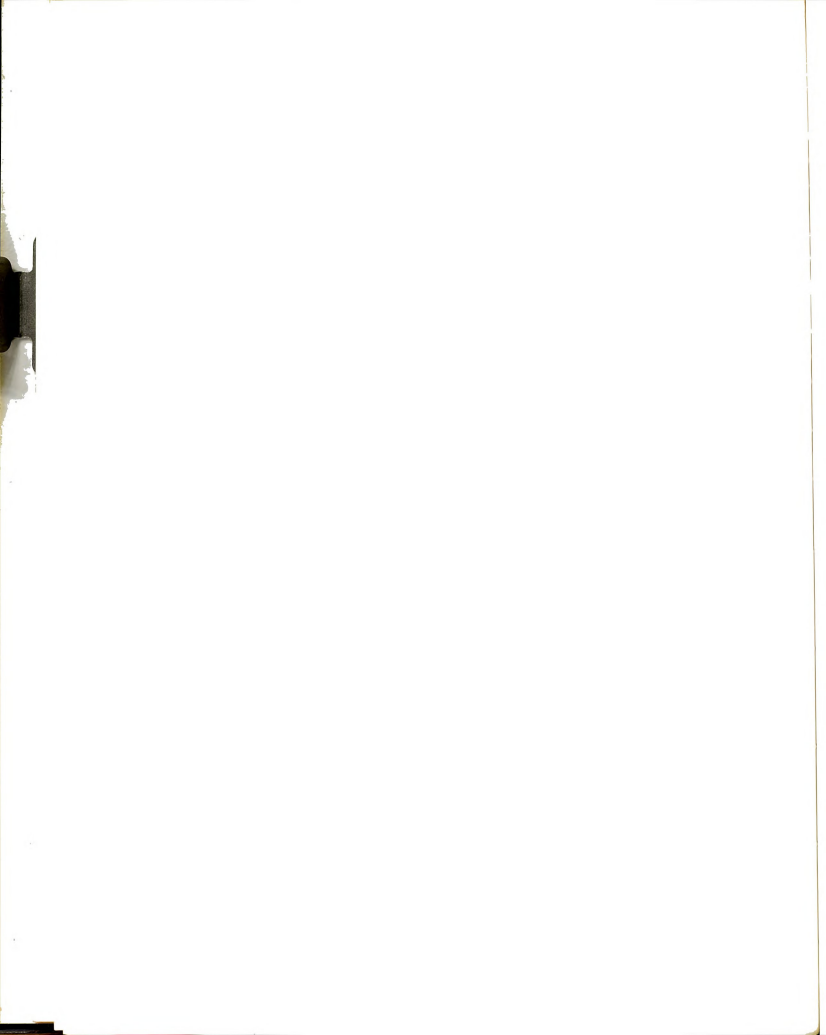
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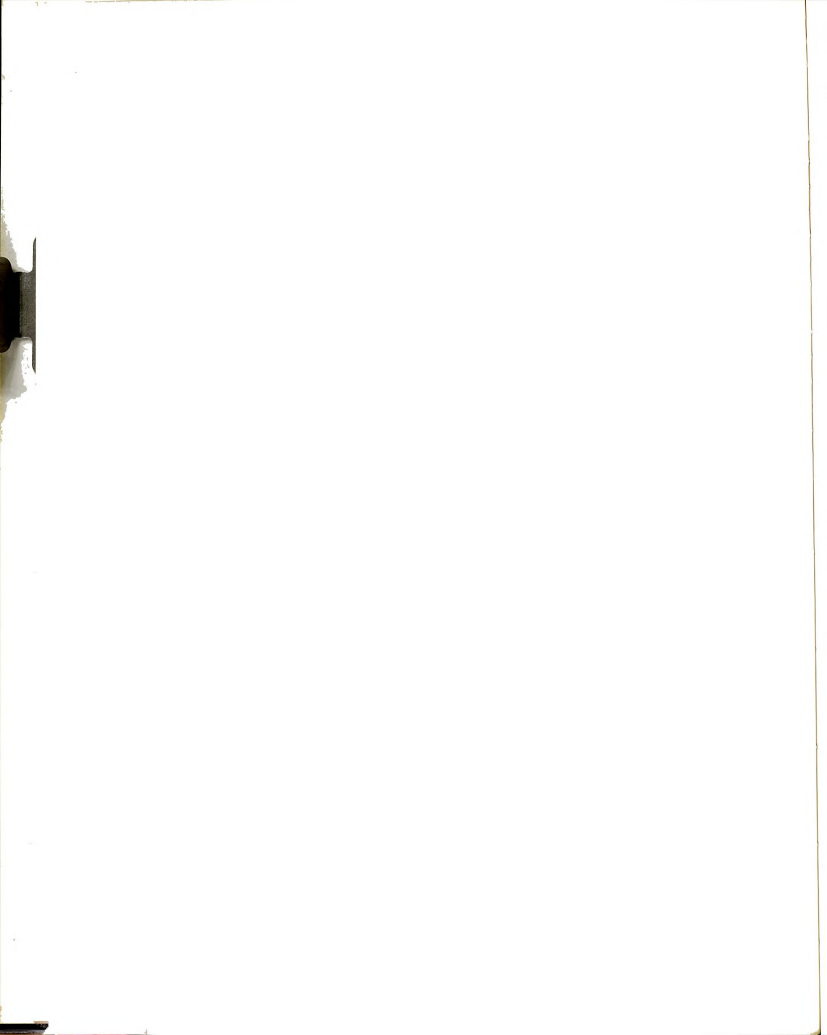


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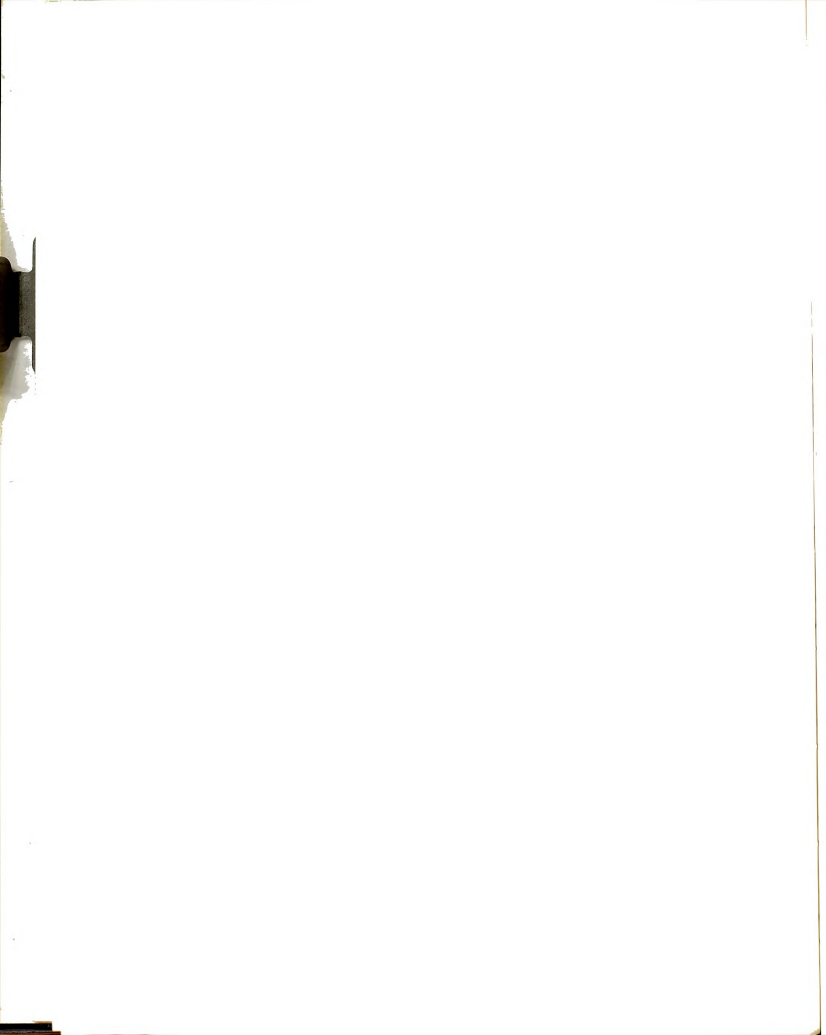


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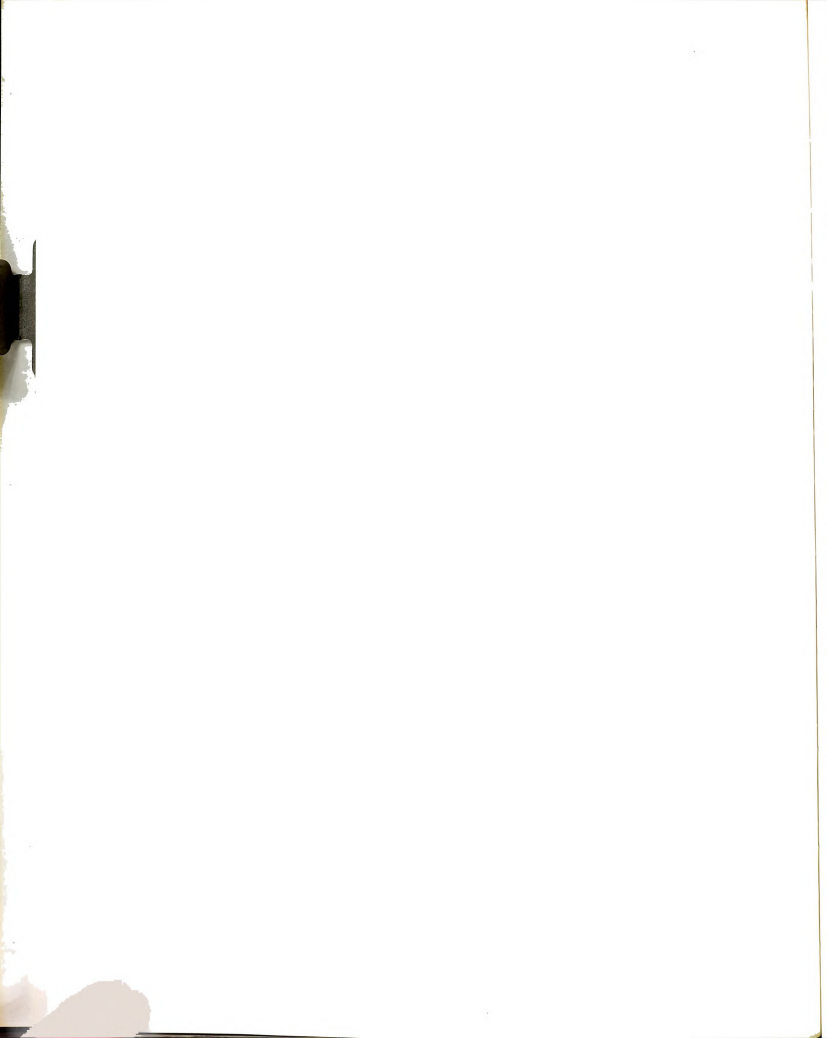
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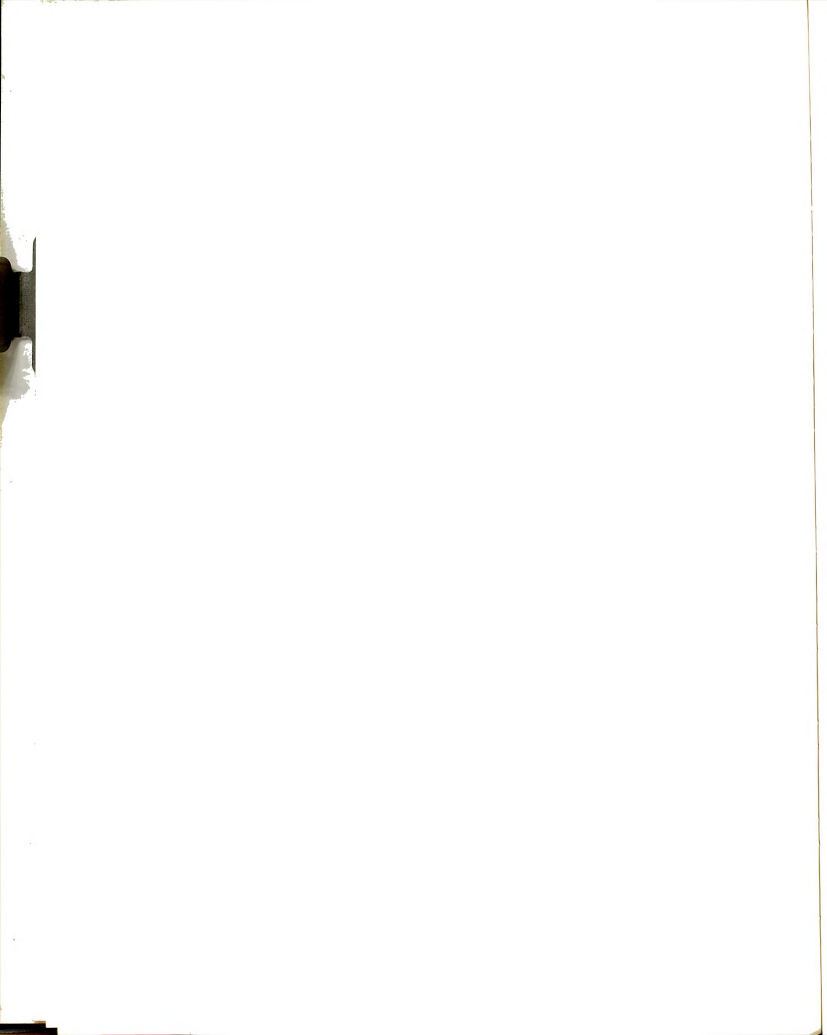


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CHAPTER I

INTRODUCTION

A. Gas Separations in a Gravitational Field

The change in composition of the atmosphere with altitude is a known effect of the Earth's gravitational field. The effect of the acceleration of gravity, g , is to set up a force, g/g_c , per unit mass. Under the influence of this force, a pressure gradient is established for each species according to

$$\frac{\partial P_i}{\partial h} = -\rho_i \frac{g}{g_c},$$

P_i = the partial pressure of species i ,

ρ_i = the concentration of species i , and

h = the height.

Using the ideal gas law and assuming constant temperature and constant g/g_c , this equation may be integrated giving the ratio of the partial pressure of gas species i at any height to that at a reference level, i.e.,

$$\frac{P_i(h)}{P_i(0)} = \exp \left(\frac{-MW_i g h}{RT g_c} \right),$$

MW_i = the molecular weight of species i ,

R = the gas constant, and

T = the absolute temperature.



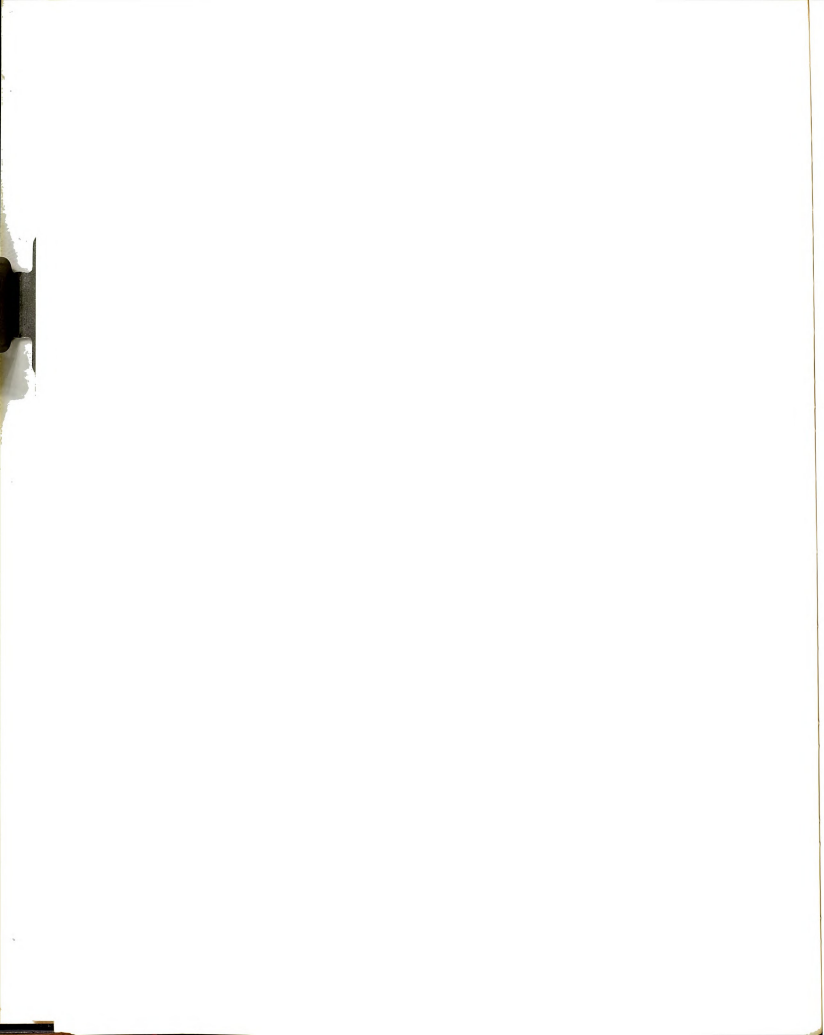
example, at an altitude of 10,000 ft, assuming a constant temperature of 40°F, the ratio of the partial pressure of oxygen to that at ground level is calculated to be 0.661.

Since the ratio of the partial pressures is dependent on the molecular weight of the species, the ratios of the partial pressures of different species will decrease at different rates. This is illustrated by taking the ratio of the partial pressures of species i and j at height, h ,

$$\frac{P_i(h)}{P_j(h)} = \frac{P_i(0)}{P_j(0)} \exp \left[\frac{-(MW_i - MW_j)gh}{RT g_c} \right] .$$

If the ratio of the partial pressure of oxygen to nitrogen is taken as 0.237 at ground level, then at 10,000 ft, assuming a constant temperature of 40°F, the ratio reduces to 0.237.

In 1919, Lindeman and Aston (1) suggested that the gas separations caused by the Earth's gravitational field could be duplicated by using a centrifugal field. That is, for separations in a centrifugal field the gravitation energy term, gh/g_c , could be replaced by the equivalent centrifugal energy term, $(\omega^2 r^2 / 2g_c)$, where ω is the rotational speed, and r is the radius of rotation. Equating the two energy terms it can be shown that for a radius of 10 inches a rotational speed of 22980 RPM is required to create an effect identical to that caused by the Earth's gravitational field at an altitude of 10,000 ft.

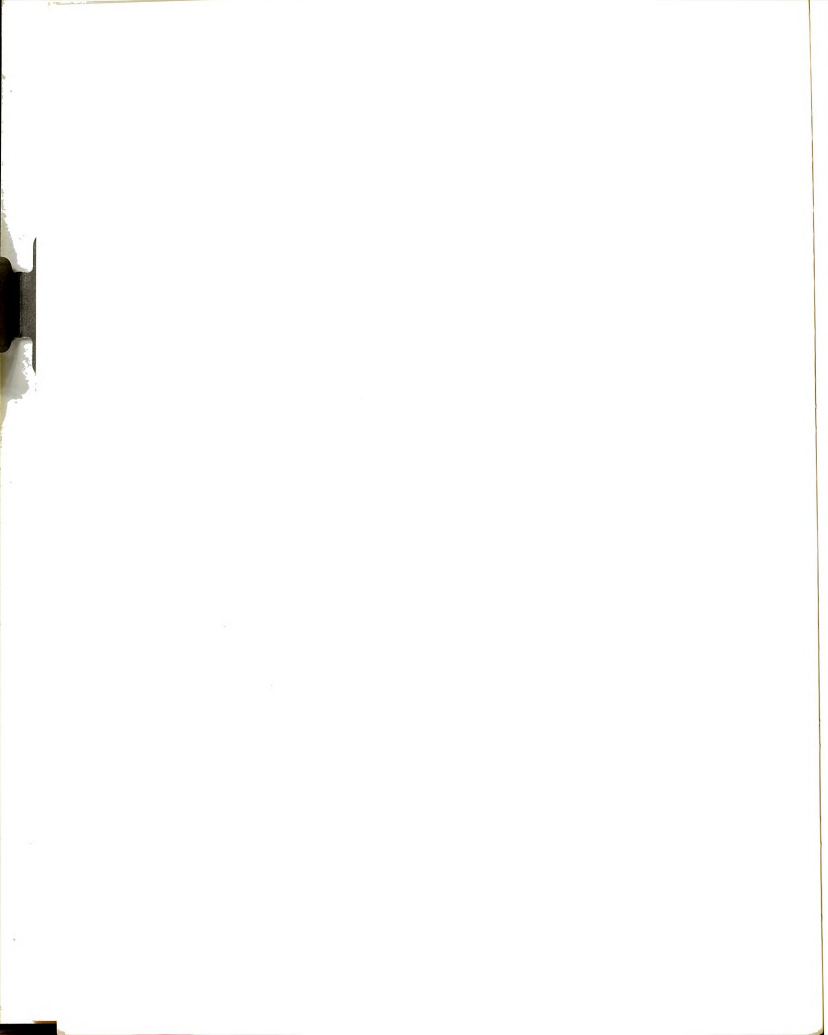


B. Centrifuge Types

One year after the suggestion by Lindeman and Aston, the first publication appeared marking the beginning of research in the area of centrifugation. The first experiments involving centrifugation directed towards realizing the equilibrium separation as predicted by the above equation. However, by 1940, with several researchers having demonstrated that the equilibrium separation could be realized, the basis was turned to gas centrifuge designs which could be operated continuously separating, to some degree, a gas mixture.

The idea of an evaporative centrifuge was introduced by H. S. G. (2) in 1922 as a means of realizing the equilibrium separation. This type of centrifuge is a very short device (length to diameter ratio ~ 0.1) in which a small amount of liquid containing different gaseous species is placed. As the centrifuge is brought up to operating speed, the liquid forms a layer at the periphery. Vapor is removed from the centrifuge very slowly via a hollow shaft at the axis. As long as the vapor is drawn off very slowly, an equilibrium condition is established throughout the vapor in the centrifuge.

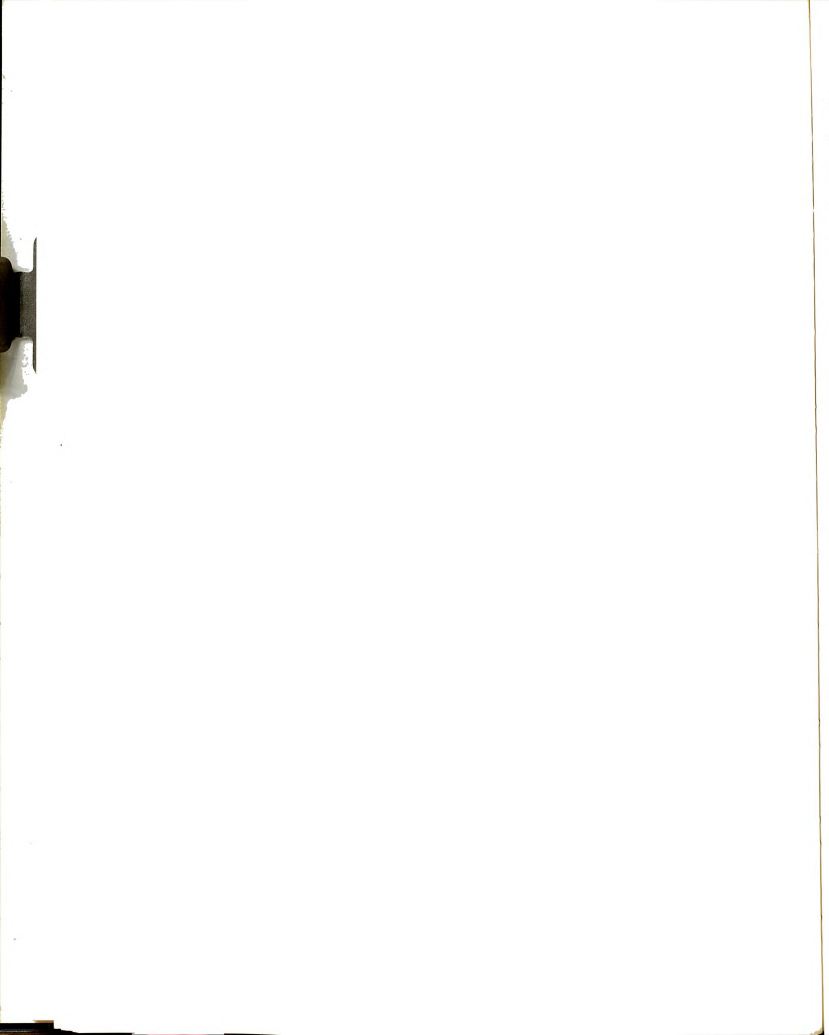
The vapor that is extracted is supplied by the evaporation of the liquid at the periphery which must diffuse along the centrifuge wall against the centrifugal field. The result is that the vapor drawn off the axis is richer in the lighter species and the remaining liquid is richer in the heavier species than the original liquid. Further work along these lines was done by Beams and Skarstrom (3) in



The idea of the cream separator as applied to gas mixture separations resulted in the concept of a flow-through centrifuge. In this type of centrifuge design a gas mixture enters the cylinder at one end via a hollow shaft. As the gas traverses the length of the cylinder (length to diameter ratio ~ 5) the equilibrium composition profile develops. At the other end, two streams are taken off, one from the periphery (rich stream) and one near the axis (lean stream). Work on such devices has been reported by Beams (4), Groth (5), and Kistemaker (6) among others.

The third and final centrifuge type to be mentioned here is the countercurrent centrifuge. In this centrifuge design two concentric gas streams flow in opposite axial directions. As a result the inner stream becomes richer in the lighter species near its exit and the outer stream becomes richer in the heavier species near its exit. Since the opposing flow continually upsets the establishment of an equilibrium composition profile, separations greater than equilibrium can be achieved. Work on the development of the countercurrent centrifuge has been reported by Beams (4), Groth (5), Kistemaker (6), and Zippe (7), among others. The centrifuge used by Beams was the largest reported having a length of $11 \frac{2}{3}$ ft, a radius of 3.75 inches and rotating at 1000 RPM.

While the performance of the evaporative and the flow-through centrifuges have a definite place in the overall understanding of gas separation by centrifugation, only the countercurrent centrifuge has the potential to be used as a production device. That is to say, the "best" that either the evaporative or flow-through centrifuge can ever achieve is an equilibrium separation. On the other hand, the

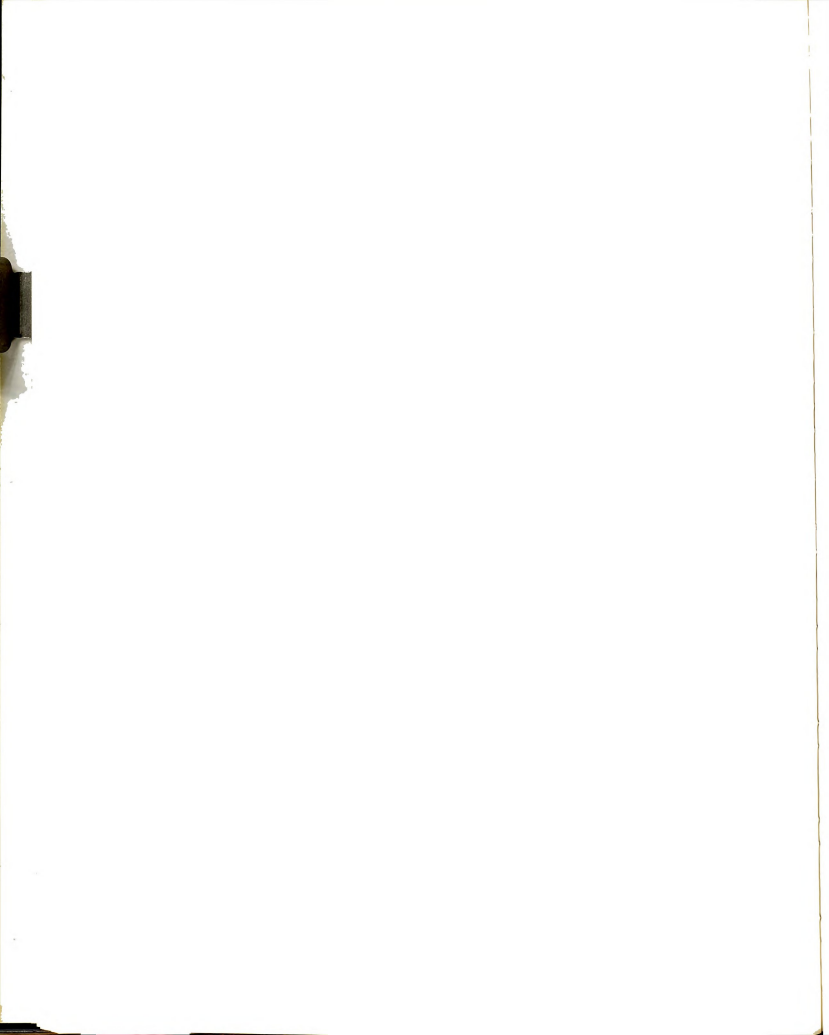


recurrent centrifuge has the capability of yielding separations greater than equilibrium. This conclusion is supported in the literature where a major portion of the work that has been done in centrifuge research has been done using the countercurrent centrifuge separations reported exceeding corresponding equilibrium values.

C. Scope of Past Work

The suggestion by Lindeman and Aston that centrifugation was a simple means of separating gas mixtures reflected their desire to develop a new technique to separate mixtures of isotopes. The simple physical nature and higher expected separations of the gas centrifuge compared to complex diffusion processes made it a definite avenue of investigation for the difficult problem of isotope separation. Consequently, almost all of the research which has been published deals with the separation of isotopes of such elements as Fluorine, Chlorine, Neon, Krypton, Xenon, Selenium and Uranium. The few gas mixtures employed, that were not isotopes, were used merely as test gases and were the basis of the experimental work.

Until 1951, all of the investigations of the gas centrifuge were experimental in nature with the published results consisting of centrifuge design, operating conditions and the separations obtained. Usually the results were compared to those predicted by equilibrium calculations. In 1951, however, the first and only available theoretical analysis of gas centrifugation was presented by (8). The analysis was contained in a collection of theories available for various processes which could be used in the

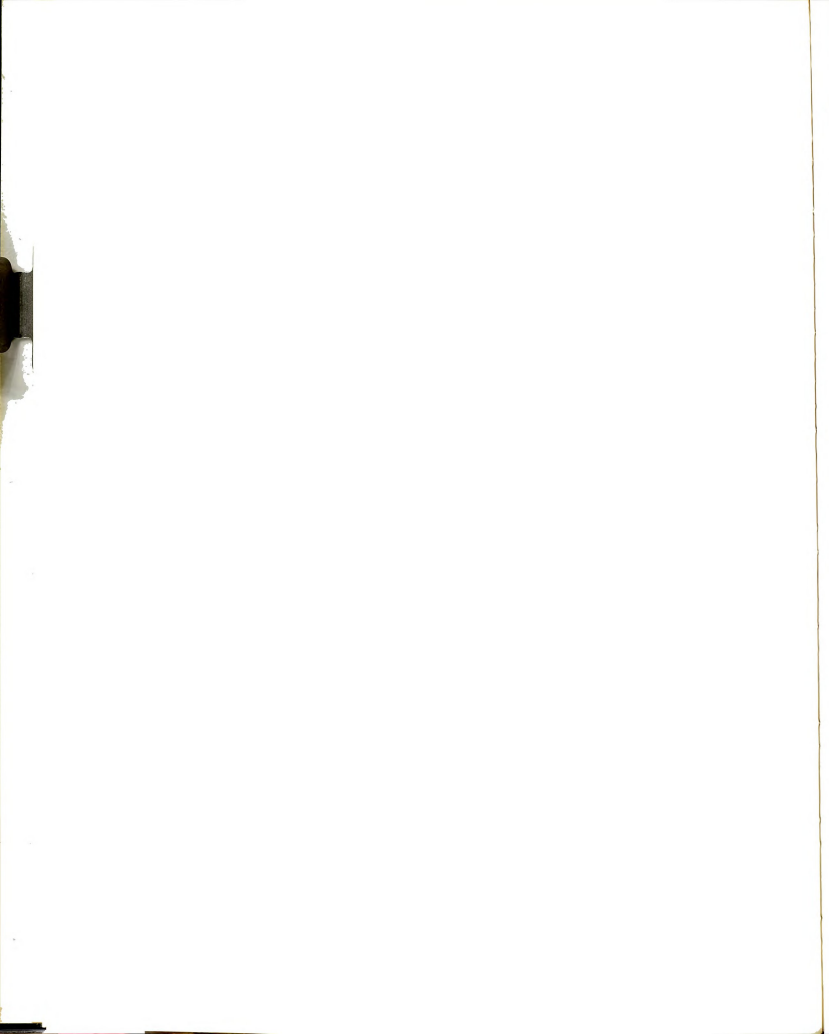


ge-scale separation of uranium isotopes. Equations resulting from Cohen's analysis of the countercurrent centrifuge, although containing several approximations, were used to predict (with reasonable success) experimental results in future published experimental works. A few investigators modified Cohen's equations slightly, while others explained differences between their experimental results and those predicted by assumptions that were incorporated in Cohen's analysis.

At this point in time, 1951, with the demand for fissionable uranium beginning to grow very quickly, investigations involving the centrifuge were being entirely directed toward its applicability as an efficient means of enriching Uranium. In this country, much such work was, and still is, sponsored and funded by the Atomic Energy Commission. The results of this change in emphasis and motivation was a steady decline in the number of publications available for general review, varying from a few publications of demonstration work at the University of Virginia in the late 1950s to the early 1960s, to no publications currently.

D. Scope of This Work

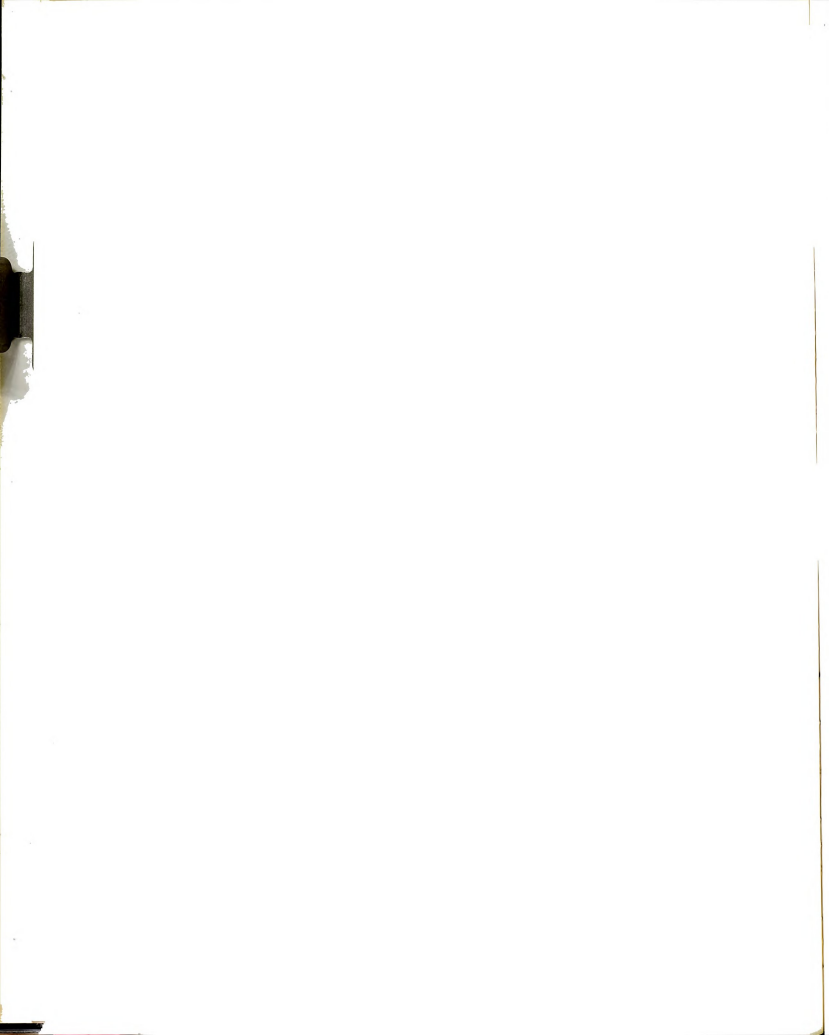
Even though research on the subject began in the 1920s, still missing from the available literature is a general analysis of the centrifuge. An analysis in which a thorough study of the countercurrent gas centrifuge is made, detailing important operating variables, the restrictions, allowable flow rates, and any other fundamental limitations that may exist, is needed. With such an analysis, a question such as, "May the gas centrifuge be considered as a viable



to separate sulfur dioxide from flue gas?" could be answered directly. However, as stated above, information to answer such a question is simply not available in the unclassified literature. Therefore, it was with this goal in mind that the analyses presented in this work were made.

Throughout the body of this work important points are illustrated by using the gas pairs $\text{SO}_2\text{-N}_2$, $\text{SO}_2\text{-H}_2$ and UF_6 (235 and 238 isotopes). The sulfur dioxide-hydrogen combination was chosen to reflect the current interest in removing SO_2 from stack gases. The sulfur dioxide-hydrogen combination was used as a variation to give a mixture with a very low density at standard conditions (at low concentrations), large diffusion coefficient and large molecular weight difference. The gasified Uranium isotopes (as UF_6), on the other hand, represent an opposite extreme having a relatively large density at standard conditions, low self-diffusion coefficient and small molecular weight difference. The use of any additional gas pair for illustration was found unnecessary, since the analysis conducted, and the use of the above three gas pairs concurred, that no special properties exist for particular gas pairs.

Paralleling this work from its beginning was an experimental program which was initiated to demonstrate the performance of a (7) type gas centrifuge, when used to separate the gas pair $\text{SO}_2\text{-H}_2$ at one atmosphere and 70°F . The centrifuge constructed was 24 inches long and 8 inches in diameter, operating at speeds up to 10,000 RPM. The experimental program, however, was terminated after several efforts failed to yield any measurable separations. Faced

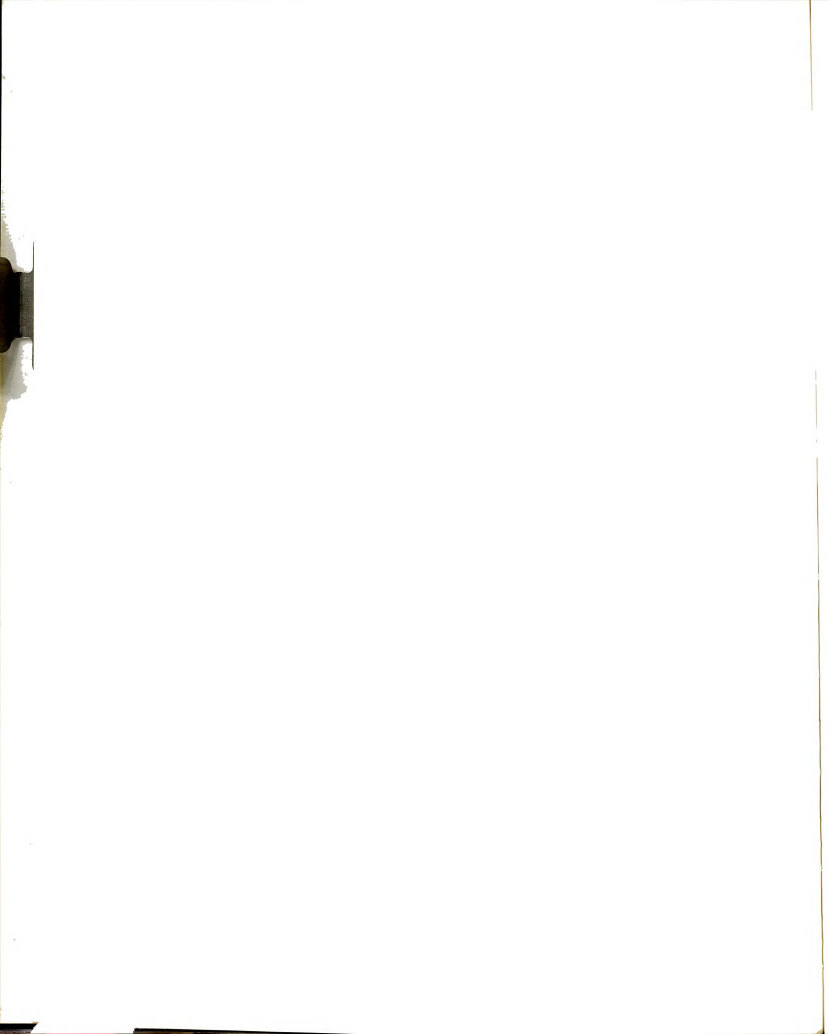


this situation, an even more exhaustive effort was undertaken to understand the gas centrifuge in order to determine whether the design was in fact simply not applicable to the situation and/or whether there existed fundamental reasons for not observing a measurable separation.

It was found that the information and conclusions contained throughout the body of this work, coupled with basic problems associated with the "soundness" of the Zippe gas centrifuge design, indeed provided more than sufficient reasons to expect that no measurable separations would be seen. A complete description and analysis of the experimental program may be found in Appendix F.

E. The Organization of the Information Provided in This Work

The analysis of gas centrifugation put forth in the body of this work is contained in six chapters. The analysis begins in Chapter II with the simple equilibrium centrifuge. Although such a centrifuge is defined to be simply a sealed rotating cylinder containing a mixture, the analysis illustrates the magnitude of pressure gradients and equilibrium separations, setting the ground work necessary for the analysis of production centrifuges. In Chapter III the simple equilibrium centrifuge is analyzed with respect to the times required for the equilibrium composition profiles to develop. With the aid of this section a feel for the expected performance and limitations of the gas centrifuge begin to develop. Furthermore, it was established that while the degree of separation varies with different gas pairs, all gas pairs behave similarly in the gas centrifuge.

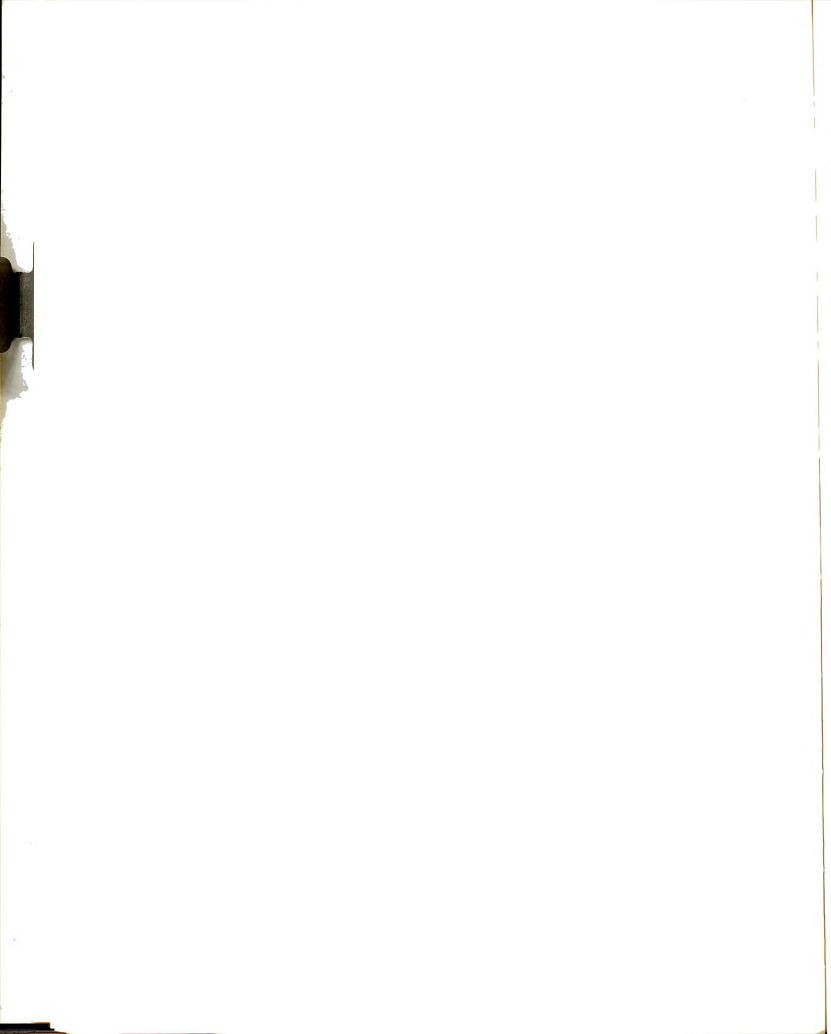


In Chapter IV attention is turned to actual limitations of centrifuge itself. That is, how fast may the centrifuge be rotated without bursting and/or entering into a critical mode of vibration which could destroy it? These analyses gave the necessary perspective on considering production centrifuges which require not only high rotational speeds, but length to diameter ratios greater than four.

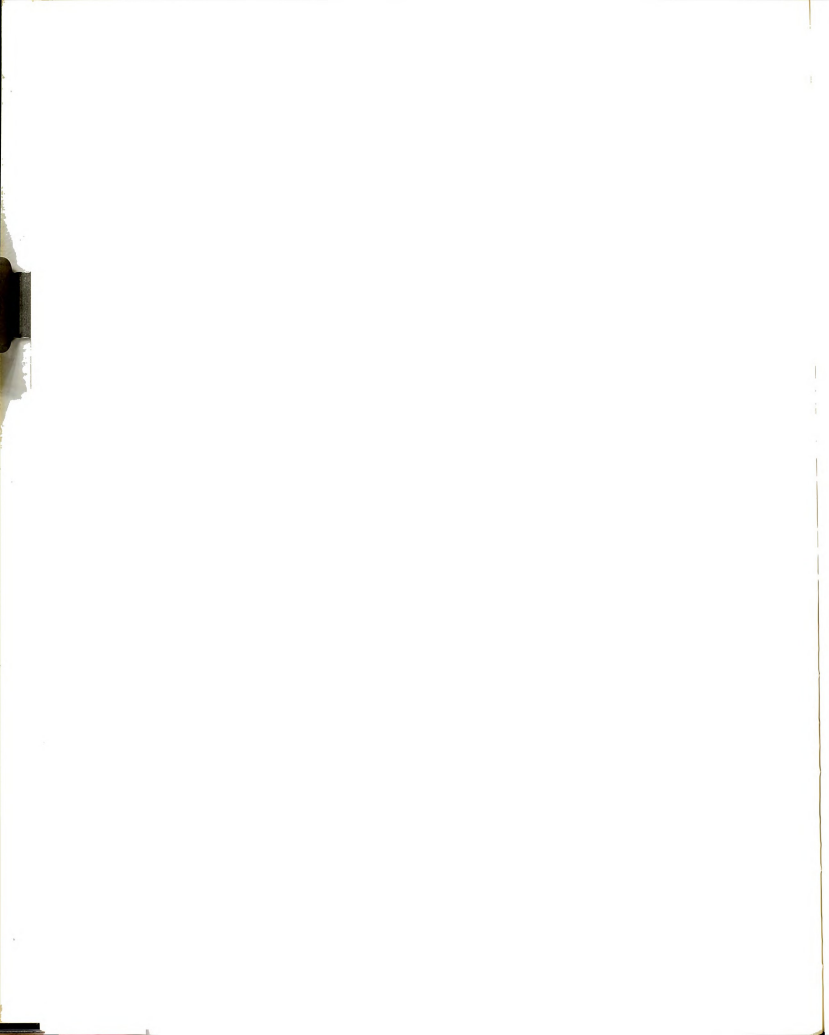
With all the ground work laid in the previous sections, the analysis of the countercurrent production centrifuge is undertaken in Chapter V. The necessary equations are developed and a numerical and approximate analytical solution are developed. Conclusions that may be drawn immediately regarding the solutions are put forth and maintained.

Having developed the necessary equations and drawn several preliminary conclusions, the countercurrent rectifying centrifuge (produces a product stream richer in the heavy species) is analyzed in great detail in Section VI. Changes in performance with various changes in operating conditions are illustrated and explained.

Chapter VII concludes this work by illustrating perhaps the most significant aspects limiting the use of a gas centrifuge. Several example calculations are used to illustrate the magnitude of the limitations. Also included in this section is a list of the results contained in this work. However, this list is not meant to be complete, since the entire text contains numerous pertinent points and examples which lose their significance when taken out of context and simplified to enter into a table or list.



Appendices following the text contain such things as calculated
used to construct figures in the text and complete descriptions
heral computer programs that may be used to analyze, with great
, the expected performance of the gas centrifuge. Also included
appendix is a description of the experimental program which
eled this work, as referenced above.



CHAPTER II

STEADY STATE SIMPLE GAS CENTRIFUGE THEORY

A. Pressure Gradients, Pure Gases

A simple gas centrifuge shall be defined as a closed rotating cylinder containing an isothermal pure gas or gas mixture. The gas rotates uniformly at the same speed as the cylinder, i.e., ω rad/sec, with no radial or axial motions. To prevent radial flow a pressure gradient is established in the radial direction balancing the centrifugal force per unit mass ($\omega^2 r / g_c$) created by the rotation of the gas.

$$\frac{1}{\rho} \frac{\partial P}{\partial r} = \frac{\omega^2 r}{g_c},$$

ρ = mass density (lb_m/ft^3),

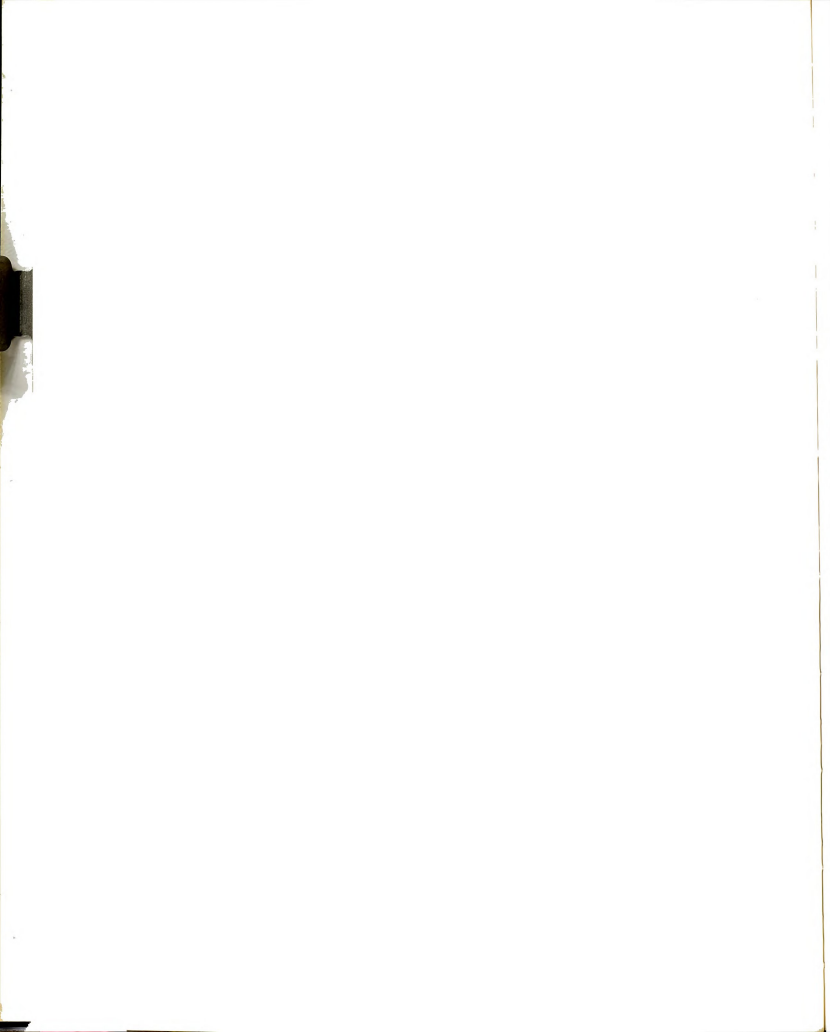
P = pressure (lb_f/ft^2), and

g_c = gravitational constant, $32.174 \text{ lb}_m/\text{lb}_f \text{ ft/sec}^2$.

Using the ideal gas law and assuming a pure gas with molecular weight MW , the pressure gradient equation can be written as

$$\frac{1}{P} \frac{\partial P}{\partial r} = \frac{MW \omega^2 r}{RT g_c},$$

upon integration gives



$$\frac{P(r)}{P(0)} = \exp \left(\frac{MW \omega^2 r^2}{2RT g_c} \right),$$

where $P(0)$ is the pressure at the axis, $r = 0$.

At the cylinder wall ($r = R_w$) the quantity ωR_w represents the inner peripheral speed of the cylinder, s (ft/sec), i.e.,

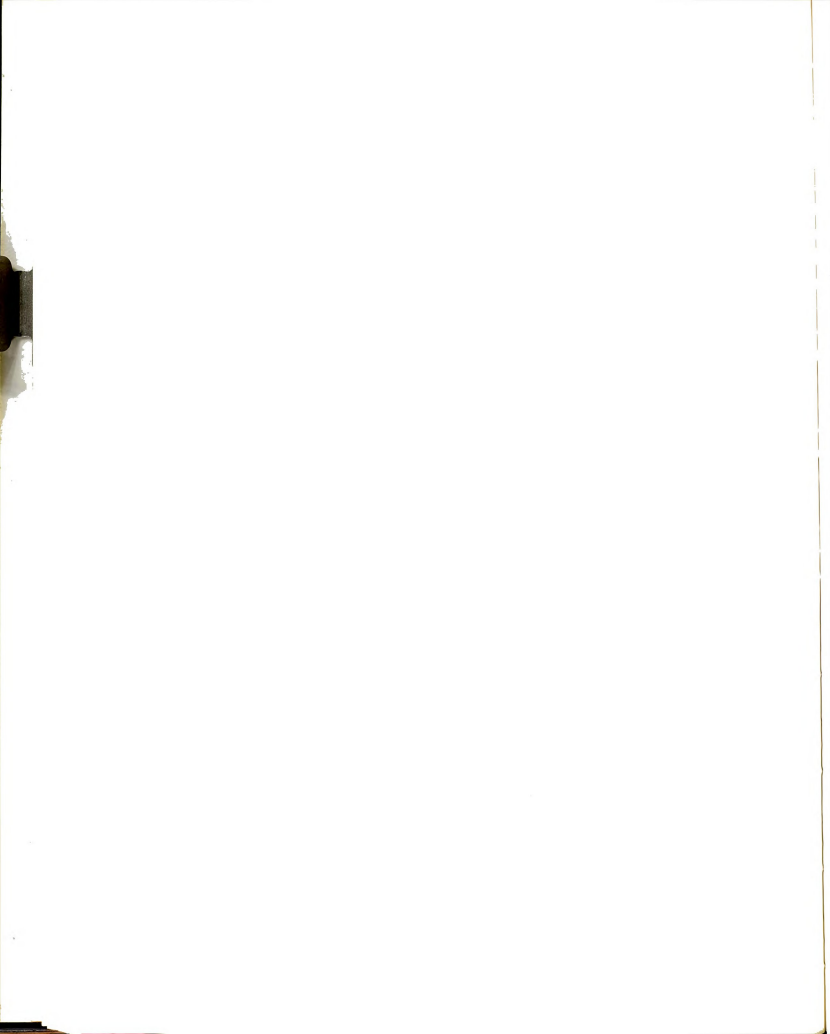
$$P(\text{wall})/P(\text{axis}) = \exp \left(\frac{MW s^2}{2RT g_c} \right).$$

Figures 1 and 2 illustrate values of the ratio, $P(\text{wall})/P(\text{axis})$, obtainable in a simple gas centrifuge operating at different peripheral speeds and containing pure gases of different molecular weights at 70°F.

Data used to construct the Figures are found in Appendix A. As can be seen from the equation for $P(\text{wall})/P(\text{axis})$, the limiting value of the ratio, as s and/or MW go to zero, is one. Hence, in order to distinguish small changes from one, Figure 1 contains a plot of $P(\text{wall})/P(\text{axis}) - 1$, due to the small molecular weights (2-100), whereas Figure 2 contains a plot of simply $P(\text{wall})/P(\text{axis})$ with molecular weights between 100 and 400.

To illustrate the use of Figures 1 and 2, consider Sulfur dioxide ($MW = 64$) in a simple gas centrifuge operating at 70°F with a peripheral speed of 500 ft/sec. From Figure 1, $P(\text{wall})/P(\text{axis}) - 1$ is equal to .36 (actual value = .3547).

Since the ratio MW/T appears in the pressure equation, a correction to the true molecular weight can be used to determine pressure ratios, $P(\text{wall})/P(\text{axis})$, at temperatures other than those at 70°F shown in Figures 1 and 2. That is,



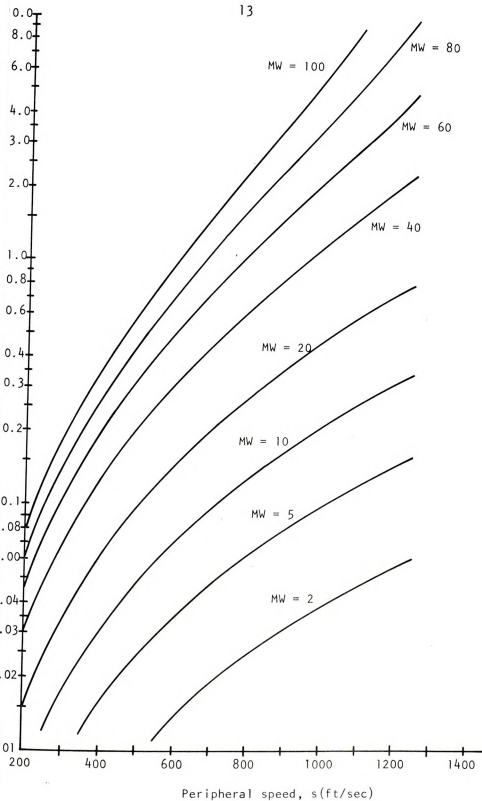
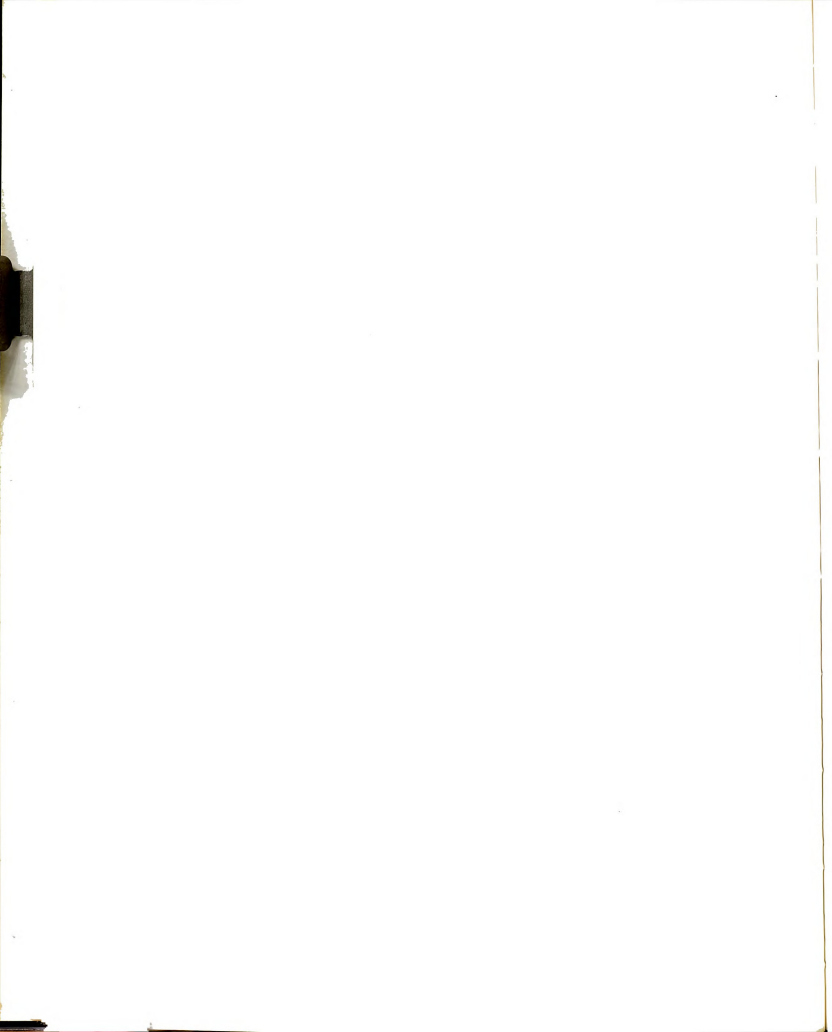


Figure 1.--Wall to Axis Pressure Ratios Minus 1 Versus Peripheral
for Various Molecular Weights Between 2 and 100.



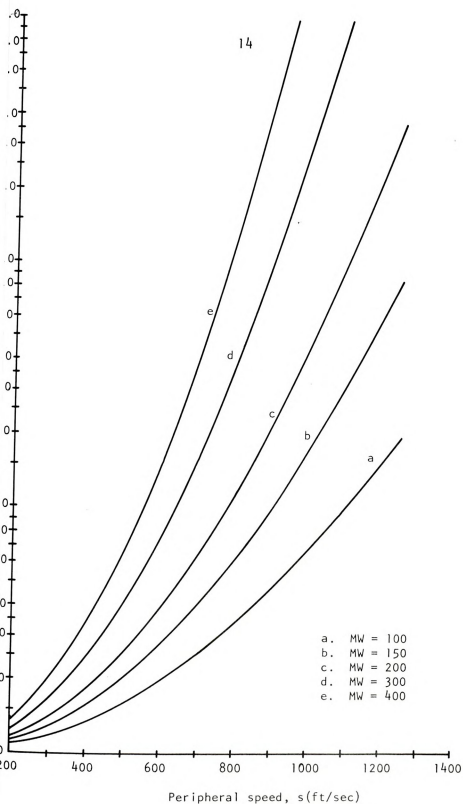
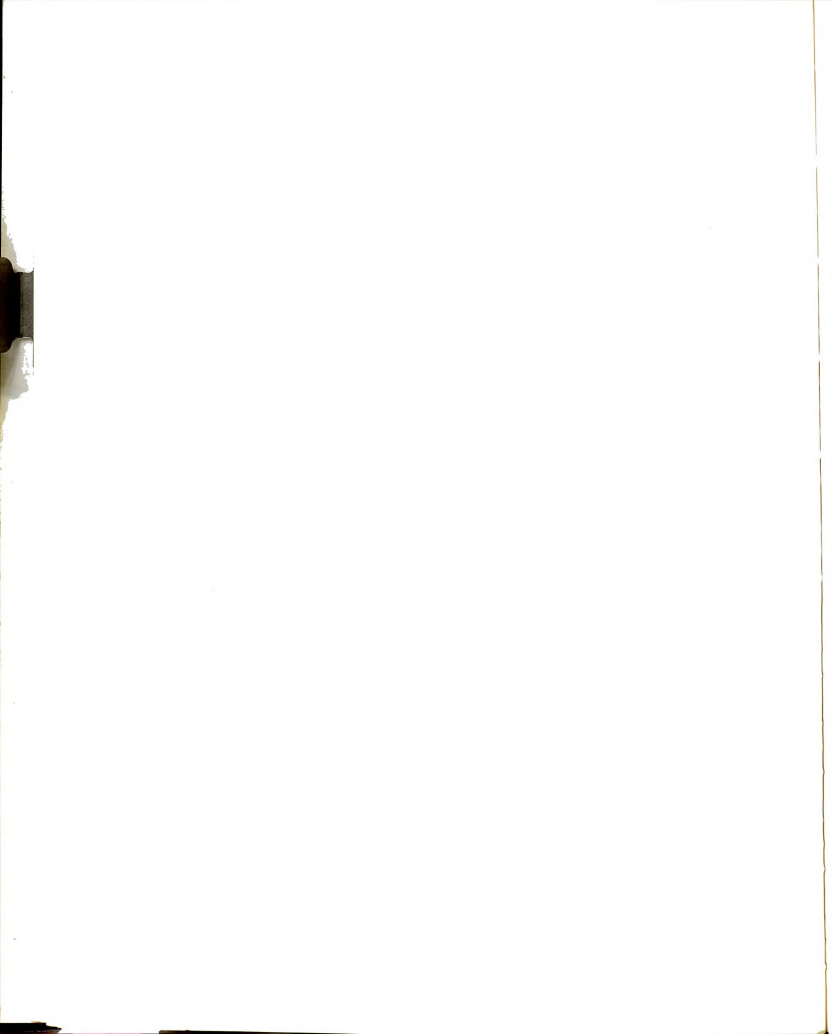


Figure 2.--Wall to Axis Pressure Ratios Versus Peripheral Speed
Various Molecular Weights Between 100 and 400.



$$MW_e = MW_{\text{true}} [530/(460 + ^\circ\text{F})],$$

where MW_e is the effective molecular weight to be used in place of true molecular weight. Figure 3 contains a plot of the corrected molecular weight versus the true molecular weight with temperature as a parameter. Data used to construct the Figure are found in Appendix A. For example, had the above illustration been worked at $^\circ\text{F}$, a $MW_e = 44.6$ is read from Figure 3 and from Figure 1, $P(\text{wall})/P(\text{axis}) - 1 = .24$ (actual value = .2358). The fact that increasing temperature can be thought of as decreasing the effective magnitude of the molecular weight of a gas species will serve as a useful concept in the analysis of gas centrifugation.

B. Pressure Gradients, Gas Mixtures

If a perfect mixture of gas species is placed in a simple centrifuge a pressure gradient will be established for each species according to the equation developed in Section A. For example, for species i we have

$$\frac{1}{P_i} \frac{\partial P_i}{\partial r} = \frac{MW_i \omega^2 r}{RT g_c},$$

integrating as before gives

$$\frac{P_i(r)}{P_i(0)} = \exp \left(\frac{MW_i \omega^2 r^2}{2RT g_c} \right)$$

total pressure at any point r is then defined by

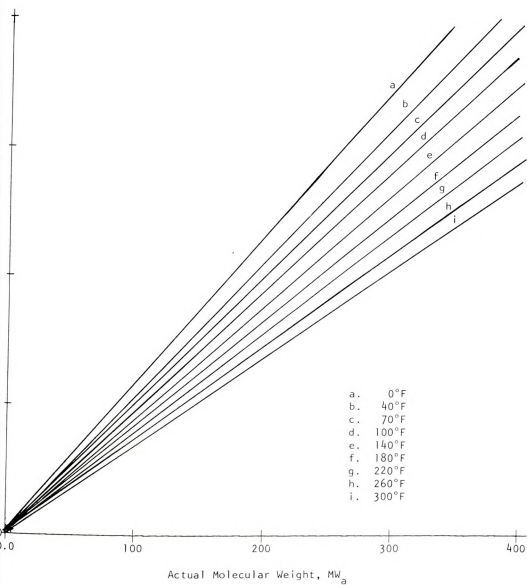
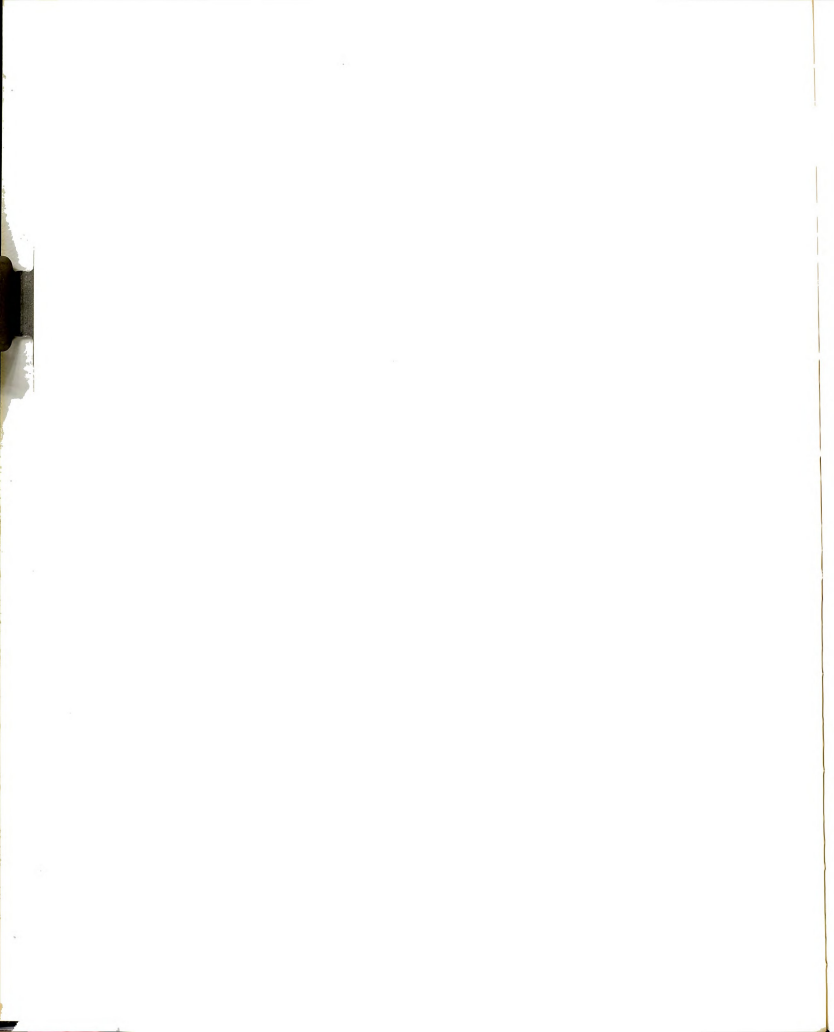


Figure 3.--Effective Molecular Weights Versus Actual Molecular Weights at Temperatures Between 0 and 300°F.



$$P(r) = \sum_{i=1}^n P_i(0) \exp \left(\frac{MW_i \omega^2 r^2}{2RT g_c} \right),$$

where n = number of species.

Due to the different molecular weights of each species, the individual partial pressures increase at different rates proceeding from the axis to the wall. Thus, the ratio of species i and j at the axis will differ from their ratios at any other position. This fact is illustrated by taking the ratios of the partial pressures of species i and j , i.e.,

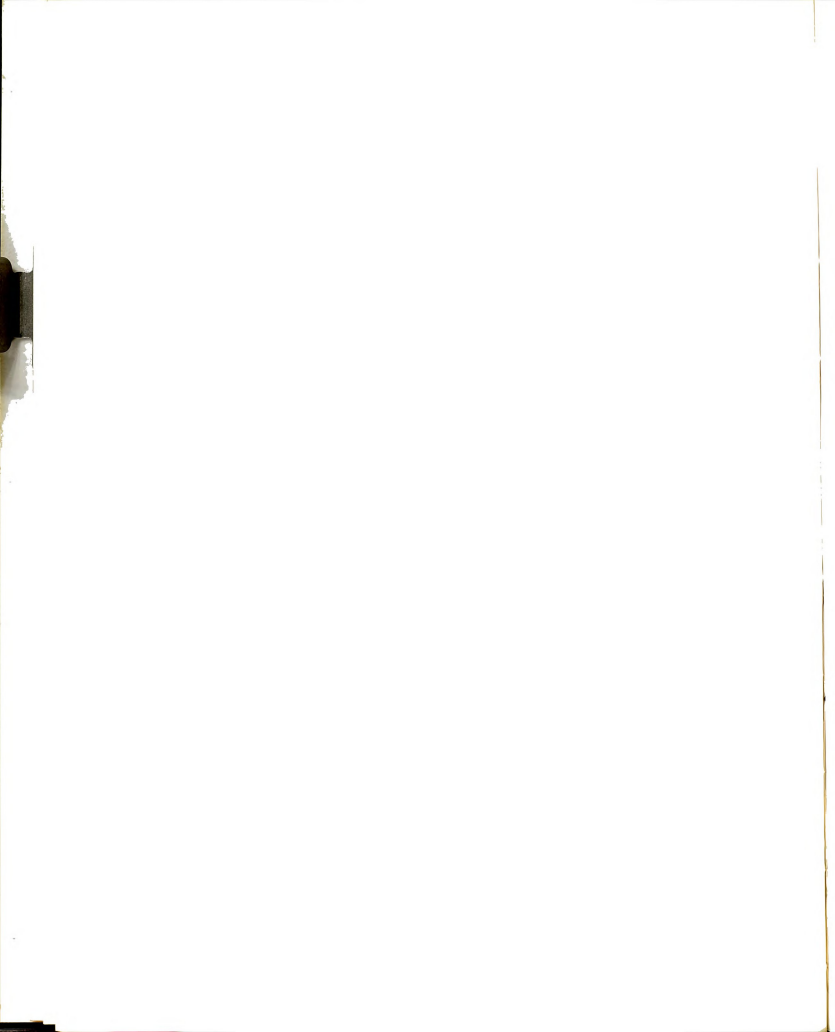
$$\frac{P_i(r)}{P_j(r)} = \frac{P_i(0)}{P_j(0)} \exp \left[\frac{(MW_i - MW_j) \omega^2 r^2}{2RT g_c} \right].$$

Thus, if MW_i is greater than MW_j , the gas mixture near the wall will be more concentrated in the heavier (i^{th}) species.

With this observation in mind, all further analyses embodied in this work will be restricted to binary gas mixtures. This is not to indicate that the concepts developed are restricted to only binary mixtures, but was done simply to simplify the equations and simplify the methods by which they may be analyzed.

C. Mole Fraction Distributions and Simple Separation Factors

In a binary gas mixture (species 1 and 2) the mole fraction (y) of the heavy species (taken as species 1) in a simple gas centrifuge can be written in terms of the partial pressures of the species, i.e.,



$$y(r) = \frac{P_1(0) \exp\left(-\frac{MW_1 \omega^2 r^2}{2RT g_c}\right)}{P_1(0) \exp\left(-\frac{MW_1 \omega^2 r^2}{2RT g_c}\right) + P_2(0) \exp\left(-\frac{MW_2 \omega^2 r^2}{2RT g_c}\right)},$$

$$y(r) = \frac{1}{1 + \frac{P_2(0)}{P_1(0)} \exp\left[-\frac{(MW_2 - MW_1) \omega^2 r^2}{2RT g_c}\right]}.$$

$y(0)$ is the mole fraction at the axis, then

$$P_2(0) = [1 - y(0)] P(0), \text{ and}$$

$$P_1(0) = y(0) P(0).$$

Substitution of this information into the mole fraction equation and rearranging gives

$$y(r) = \frac{y(0) \exp\left(\frac{Ar^2}{2}\right)}{y(0) \left[\exp\left(\frac{Ar^2}{2}\right) - 1\right] + 1},$$

where

$$A = \frac{(MW_1 - MW_2) \omega^2}{RT g_c} = \frac{\Delta MW \omega^2}{RT g_c}.$$

This expression allows one to compute the mole fraction profile in a gas centrifuge given A and $y(0)$.

A separation factor for the simple gas centrifuge may be defined as the ratio of species 1 to 2 at the wall to the ratio of species 1 to 2 at the axis, i.e.,

$$\alpha = \frac{y(R_w)}{1-y(R_w)} \cdot \frac{1-y(0)}{y(0)} .$$

in terms of the mole fraction distribution given above,

$$\alpha = \frac{1-y(0)}{y(0)} \cdot \frac{y(0) \exp\left(\frac{AR_w^2}{2}\right)}{y(0) \left[\exp\left(\frac{AR_w^2}{2}\right) - 1\right] + 1 - y(0) \exp\left(\frac{AR_w^2}{2}\right)} ,$$

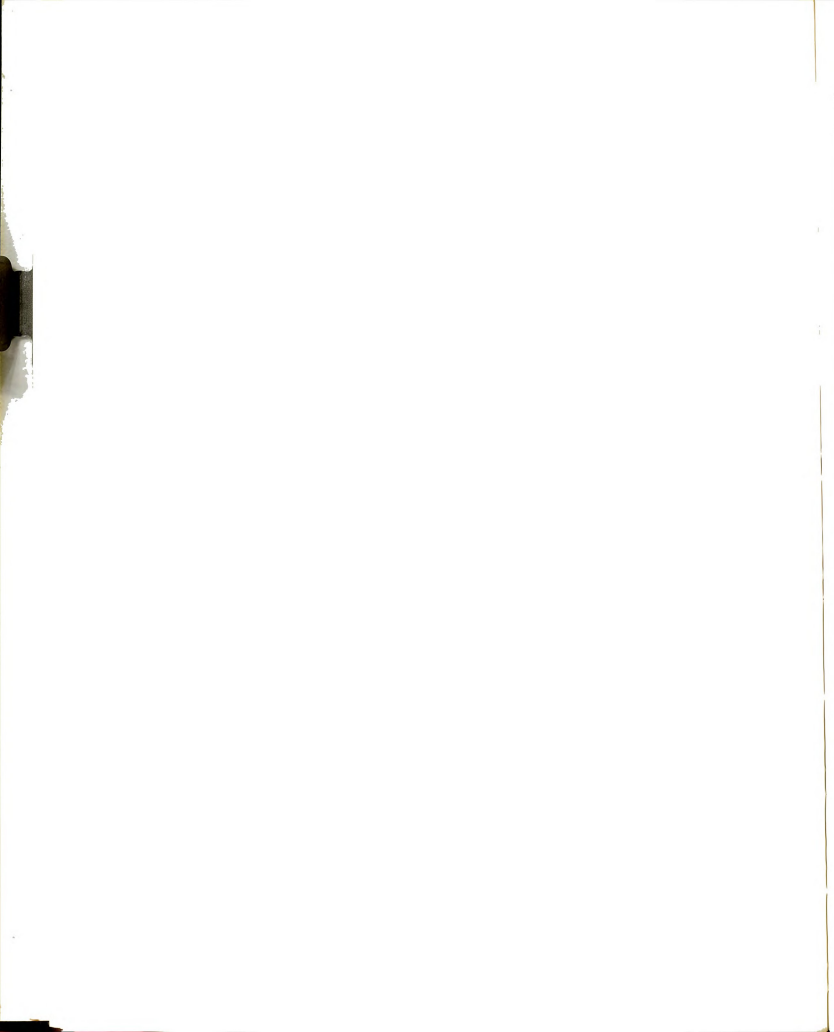
which simplifies to

$$\alpha = \exp\left(\frac{AR_w^2}{2}\right) .$$

The expression for $y(R_w)$ can now be written in terms of α , i.e.,

$$y(R_w) = \frac{\alpha y(0)}{y(0) (\alpha - 1) + 1} .$$

Since the expression for α is identical to that developed for the ratio $P(\text{wall})/P(\text{axis})$ for a pure gas, except that molecular weight difference appears in the exponential instead of an actual molecular weight, Figures 1 and 2 can be used to estimate values of α by just substituting molecular weight difference. For example, consider a mixture of Hydrogen (MW=2) and Sulfur Dioxide (MW=64) at 70°F in a simple centrifuge with a peripheral speed of 500 ft/sec. From Figure 1



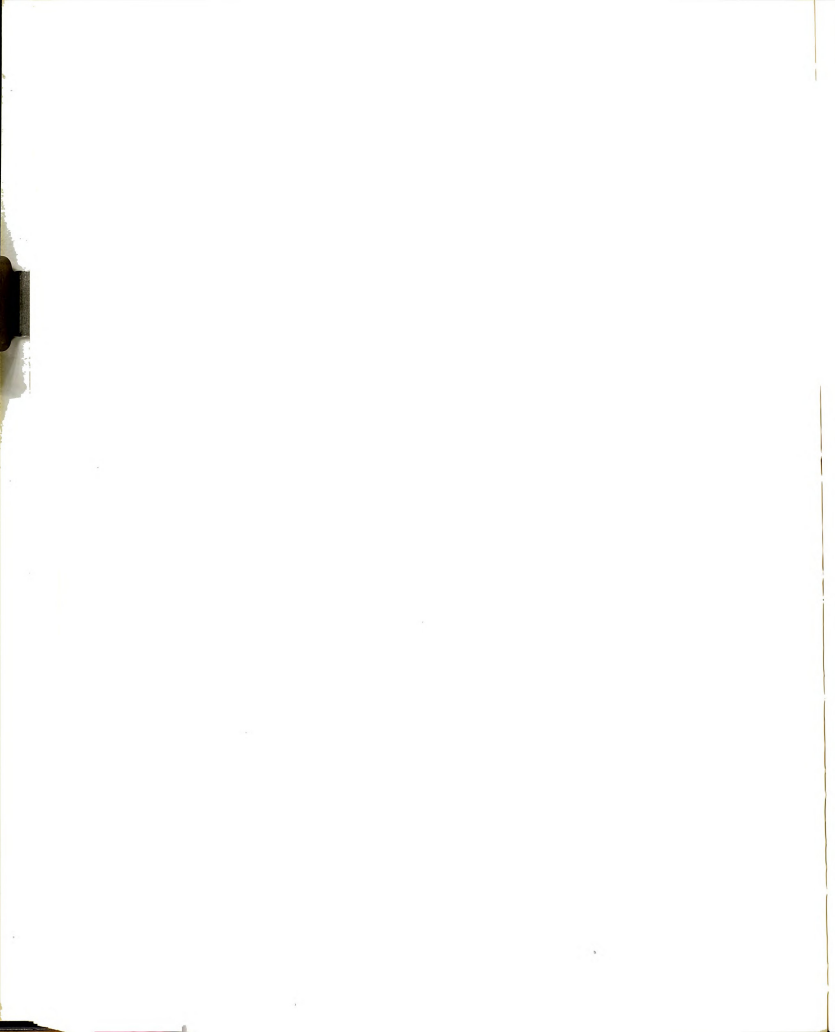
with $MW=62$, $\alpha - 1$ is found to be .34 (actual value = .3419). The value of $\alpha - 1$ at a different temperature, say 300°F , can be found by first using Figure 3 which gives an effective $\Delta MW=43.2$ and then using Figure 1 giving $\alpha - 1 = .22$ (actual value = .2198).

An important aspect to be noted in the expression for α is that it is a function of molecular weight difference, not the ratio of the molecular weights or the molecular weight difference divided by the sum of molecular weights as in diffusion processes. This gives the gas centrifuge an important advantage for separating heavy gases, hence the interest in the field of gas centrifugation for the separation of Uranium isotopes (5, 6, 7, and 8) ($\Delta MW=3$) when gasified as Uranium Hexafluoride ($MW=352$).

Although α is a fundamental quantity depicting the separating potential of a gas pair, a more tangible quantity is the increase of $y(R_w)$ over the value of $y(0)$ as a function of α , i.e.,

$$\frac{y(R_w) - y(0)}{y(0)} = \frac{\alpha}{y(0)(\alpha - 1) + 1} - 1.$$

Figure 4 contains a plot of $[y(R_w) - y(0)]/y(0)$ versus $y(0)$ for various values of α . Data used to construct Figure 4 are found in Appendix A. As can be seen in Figure 4, the greatest increase in the value of $y(R_w)$ over the value of $y(0)$ occurs at low concentrations [$y(0) \leq 0.3$] regardless of the value of α . The curve in Figure 4 for a very large value of α corresponds to $y(R_w) \approx 1$ for all values of $y(0)$.



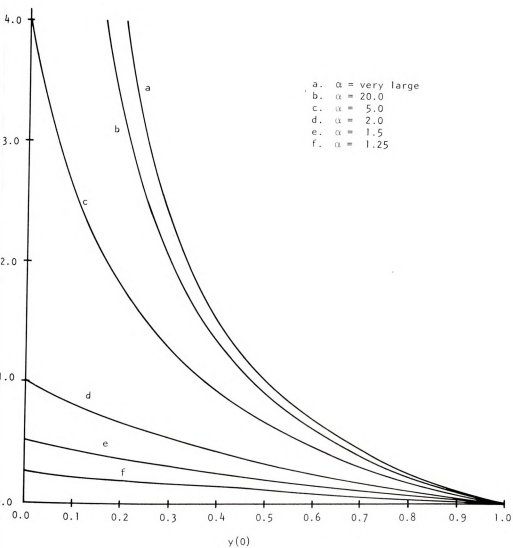
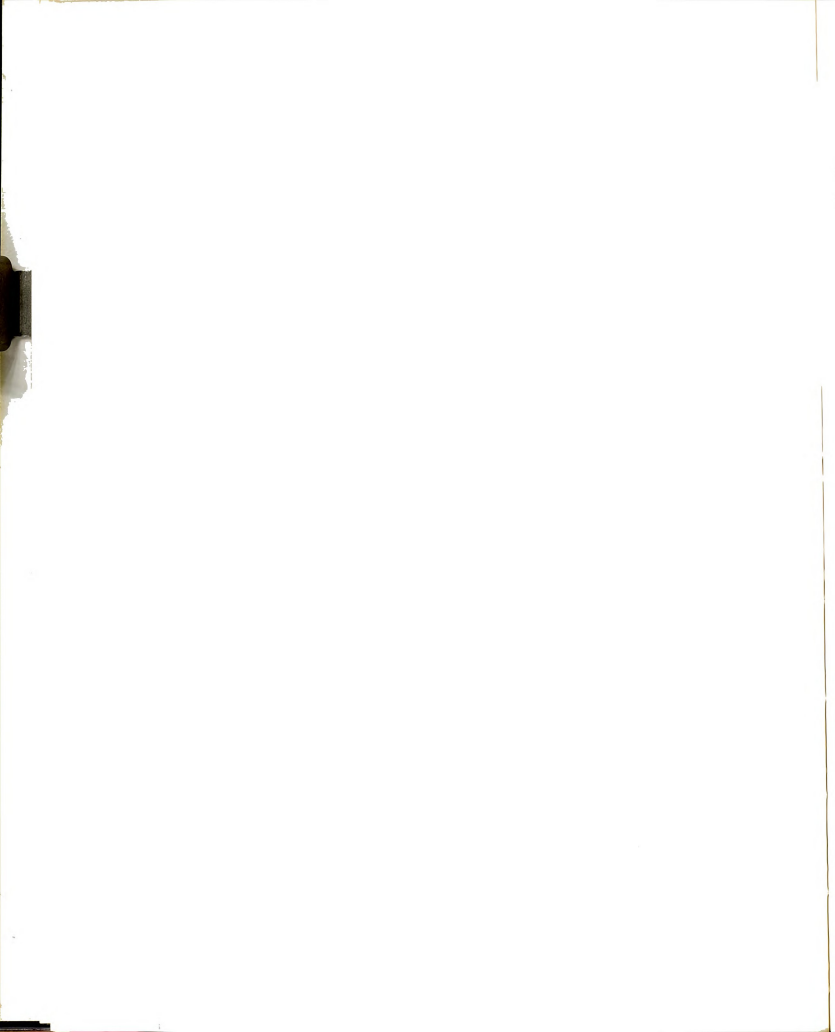


Figure 4.-- $[y(R_w) - y(0)]/y(0)$ Versus $y(0)$ for Values of α .



D. Axis Composition in a Simple Centrifuge

In Section C a relationship was given between $y(R_w)$ and $y(0)$ as a function of α , a quantity which only depends on the molecular weight difference of the gas pair, temperature, and the peripheral speed. This expression, however, lacks usability when applied to a real situation. For example, if a simple gas centrifuge is charged with a gas of known composition, y_f , and then rotated until the steady state mole fraction distribution has developed, the mole fraction profile cannot be computed. Knowing the value of $y(0)$, however, would allow the calculation of the mole fraction profile [giving $y(R_w)$]. It should be pointed out that if $y(R_w)$ was known instead of $y(0)$ the profile could also be computed; however, analytically computing $y(0)$ is an easier task.

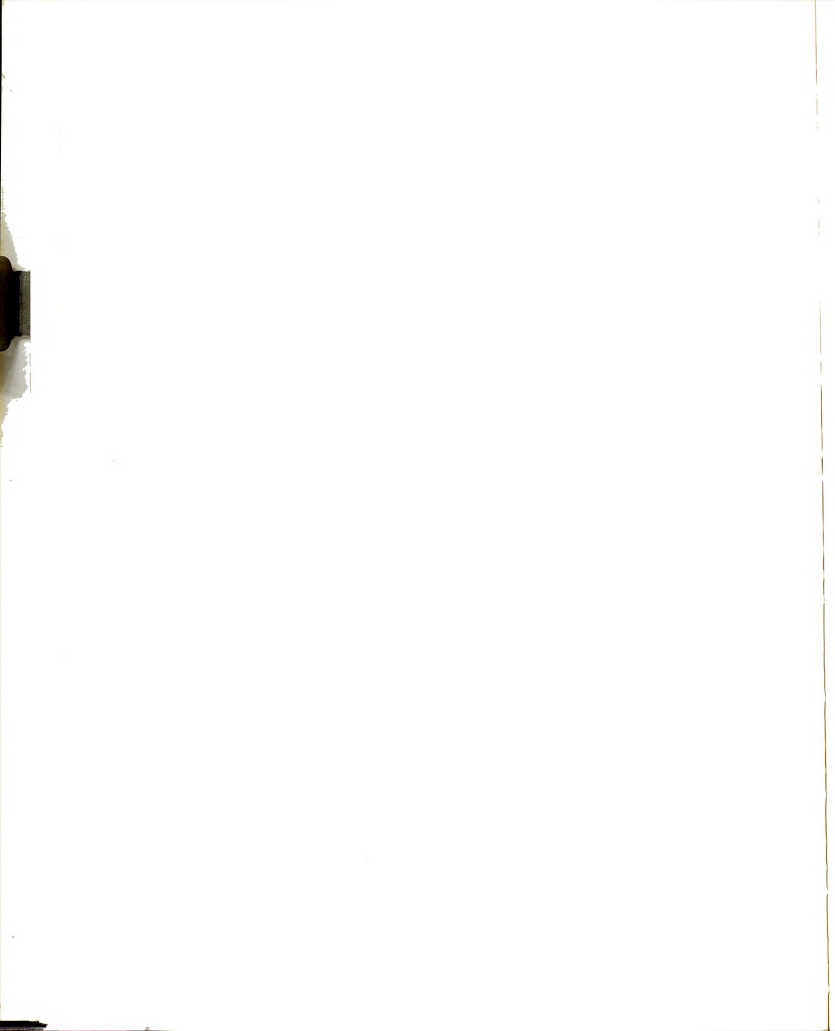
If B moles of gas had been used to charge the simple gas centrifuge, then the following relationship representing conservation of mass must be satisfied:

$$B = 2\pi L \int_0^{R_w} \rho_1 r dr + 2\pi L \int_0^{R_w} \rho_2 r dr ,$$

where ρ_1 and ρ_2 are the molar densities of species 1 and 2 respectively, in the mixture.

Or, using the ideal gas law and the pressure ratio equations developed previously,

$$B = \frac{2\pi L P_1(0)}{RT} \int_0^{R_w} \exp\left(-\frac{Q_1 r^2}{2}\right) r dr + \frac{2\pi L P_2(0)}{RT} \int_0^{R_w} \exp\left(-\frac{Q_2 r^2}{2}\right) r dr ,$$



where

$$Q_1 = \frac{MW_1 \omega^2}{RT g_c}, \quad Q_2 = \frac{MW_2 \omega^2}{RT g_c}, \quad \text{and}$$

L = length of the simple centrifuge.

Also, the conservation of species 1 must be maintained, thus

$$y_f B = \frac{2\pi L P_1(0)}{RT} \int_0^{R_w} \exp\left(\frac{Q_1 r^2}{2}\right) r dr.$$

Integrating and solving for y_f gives

$$y_f = \frac{P_1(0) [\exp(Q_1 R_w^2) - 1] / Q_1}{P_1(0) [\exp(Q_1 R_w^2 / 2) - 1] / Q_1 + P_2(0) [\exp(Q_2 R_w^2 / 2) - 1] / Q_2}.$$

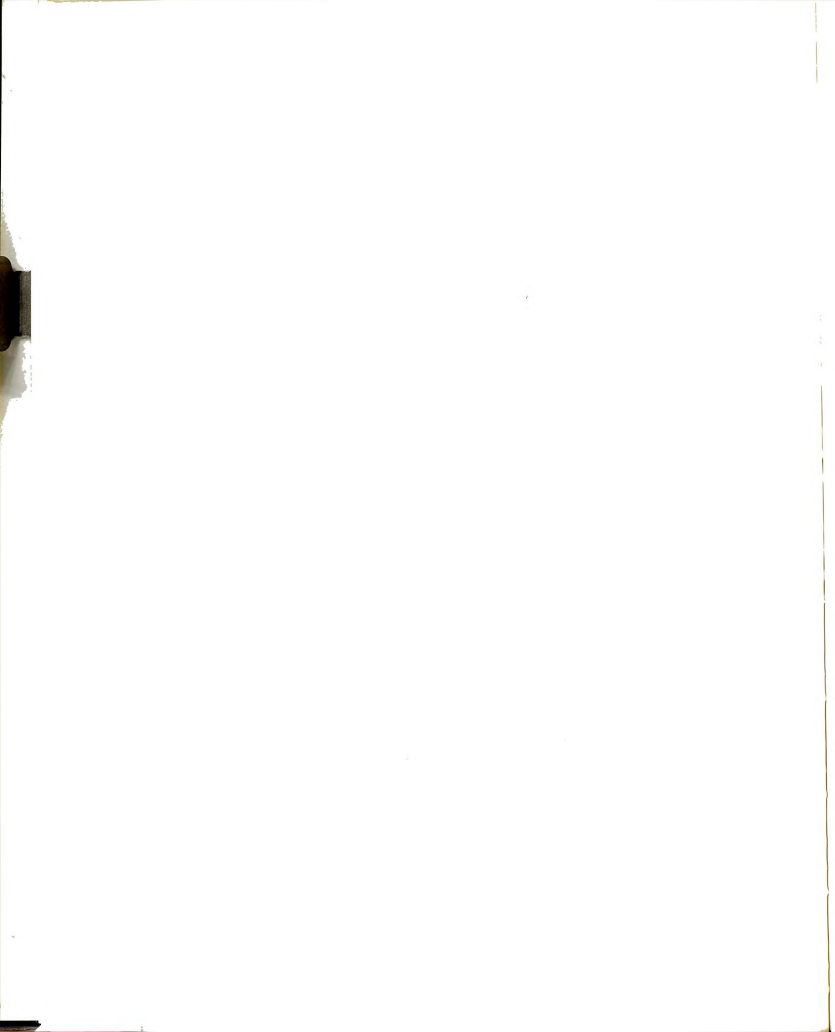
Substituting for $P_1(0)$ and $P_2(0)$ in terms of $P(0)$ and $y(0)$ gives the following expression for $y(0)$:

$$y(0) = \frac{y_f \frac{Q_1}{Q_2} C}{1 + y_f \left(\frac{Q_1}{Q_2} C - 1\right)},$$

where

$$C = \frac{\exp(Q_2 R_w^2 / 2) - 1}{\exp(Q_1 R_w^2 / 2) - 1}.$$

Using this expression, Figure 5 was constructed showing the mole fraction profiles developed in a simple centrifuge for the following



- a. Charge composition, $y_f = 0.002$
- b. $\text{SO}_2\text{-H}_2$, $y = \text{mole fraction } \text{SO}_2$
- c. $\text{SO}_2\text{-N}_2$, $y = \text{mole fraction } \text{SO}_2$
- d. UF_6 (235, 238 isotopes), $y = \text{mole fraction } \text{U}_{235}$

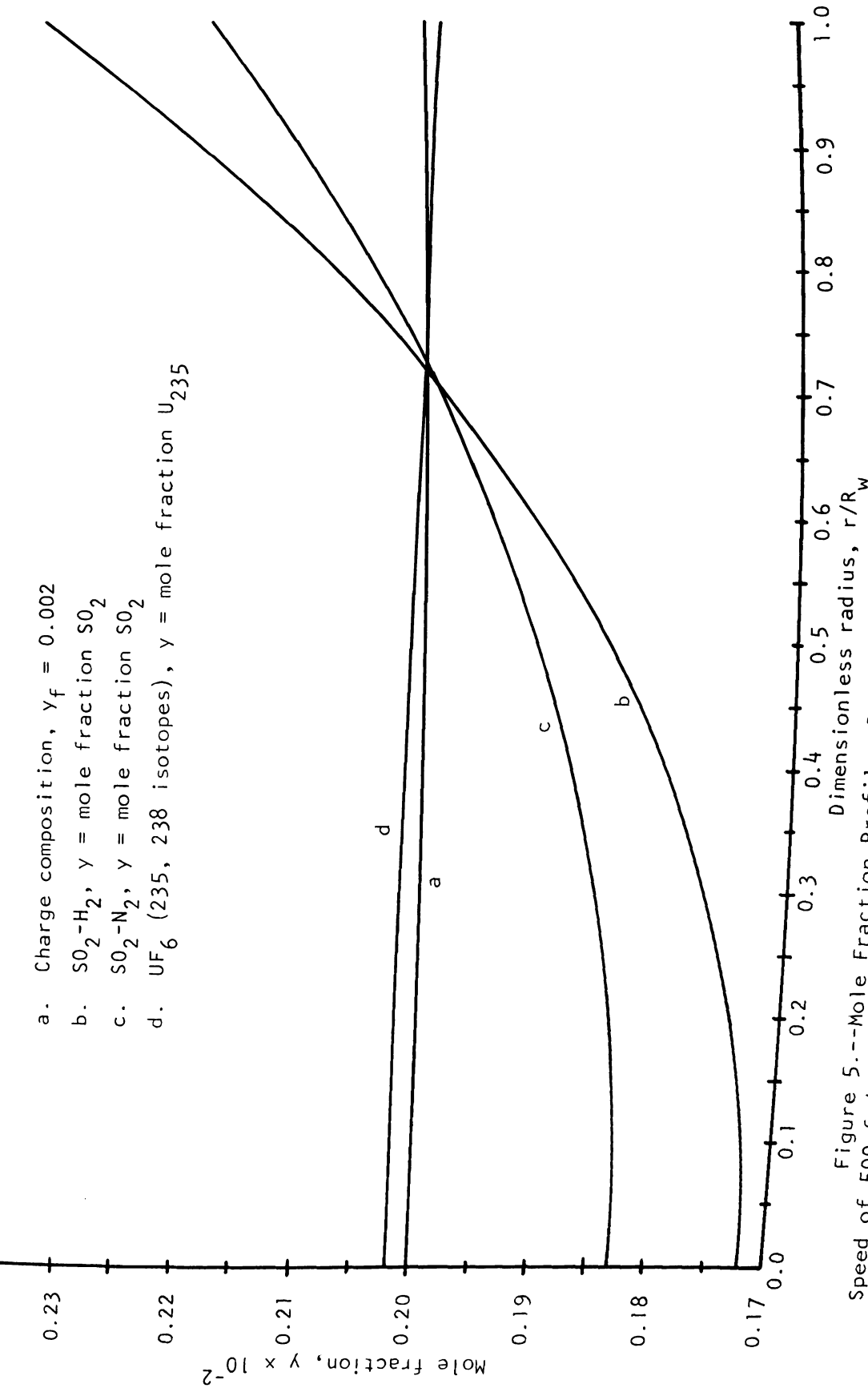
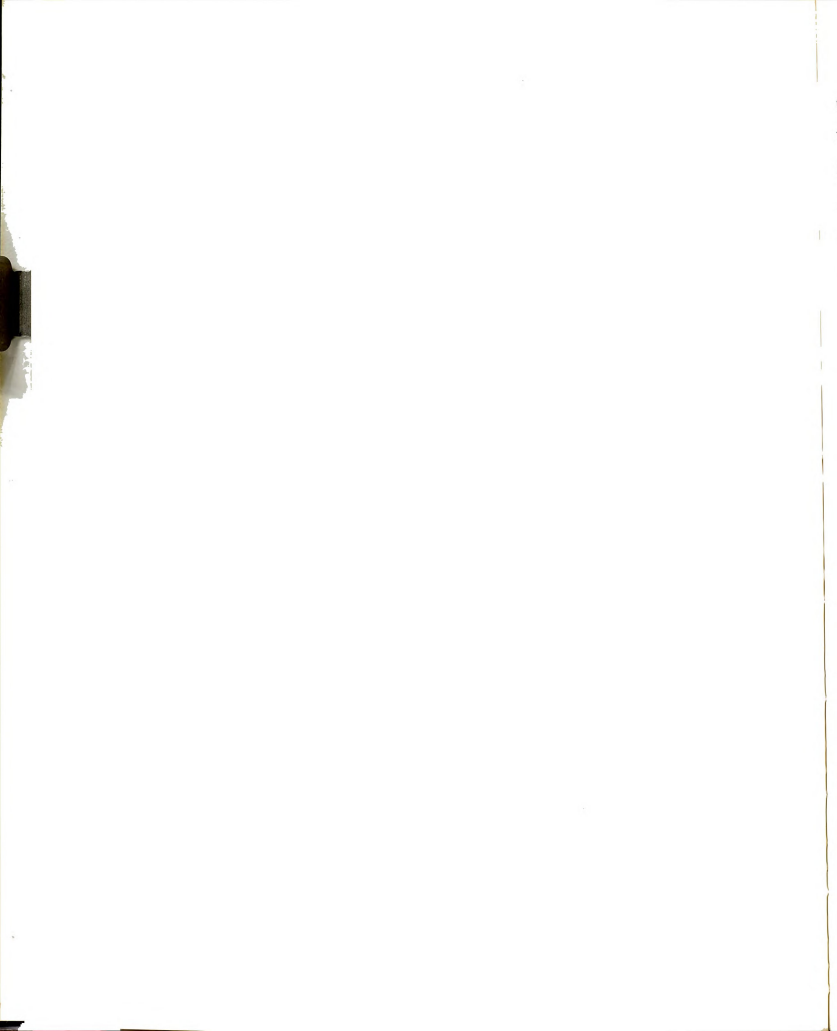


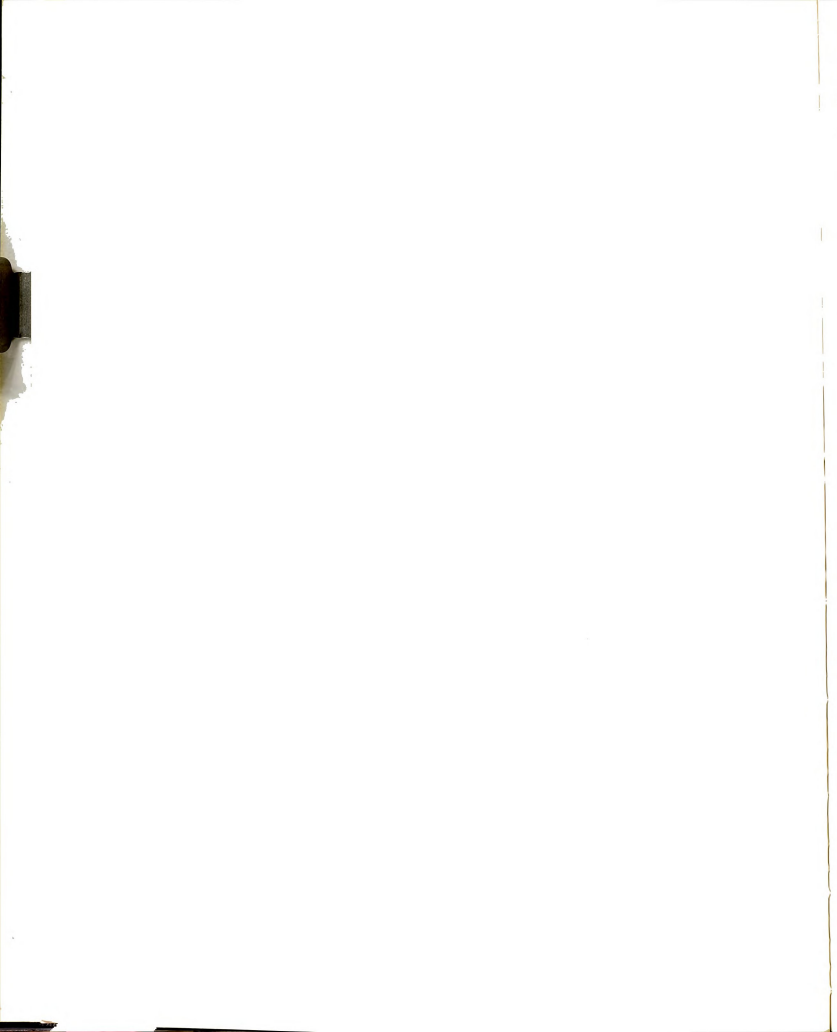
Figure 5.--Mole Fraction Profiles Developed in a Simple Centrifuge With a Peripheral Speed of 500 ft/sec for the Gas Pairs: $\text{SO}_2\text{-H}_2$, $\text{SO}_2\text{-N}_2$ and UF_6 (235, 238 isotopes) at 70°F .



three gas pairs: $\text{SO}_2\text{-H}_2$, $\text{SO}_2\text{-N}_2$ and UF_6 (235, 238 isotopes) at 70°F . The composition of the charge (y_f) in the $\text{SO}_2\text{-H}_2$ and $\text{SO}_2\text{-N}_2$ pairs is 0.002 mole fraction SO_2 (a typical flue gas composition), whereas y_f is 0.002 for the UF_6 (235 isotope). Data used to construct this figure are found in Appendix A. The centrifuge operating speed is 500 ft/sec. Table 1 contains a list of some observations taken from Figure 5 for comparison. As expected (due to the large ΔMW) the $\text{SO}_2\text{-H}_2$ mixture separates best as indicated by the separation factors. Also, due to the radial pressure gradient, the point at which the mole fraction profile crosses the value of y_f does not occur at the equal area position ($s = 353.5$ ft/sec). Instead, the crossing point is 358 ft/sec for $\text{SO}_2\text{-H}_2$, 360 ft/sec for $\text{SO}_2\text{-N}_2$, and 398 ft/sec for UF_6 (235, 238 isotopes). The large molecular weight of the UF_6 (larger pressure gradient) pushes the crossing point closest to the periphery. Also worth noting is that the values of $y(0)$ and $y(R_w)$ are not equal distances on either side of y_f , and the mole fraction profile becomes flat as

TABLE 1.--Simple Centrifuge Separations of the Gas Pairs: $\text{SO}_2\text{-H}_2$, $\text{SO}_2\text{-N}_2$, UF_6 (235, 238 isotopes) at 70°F . Centrifuge Peripheral Speed = 500 ft/sec.

Gas Pair	y_f	$y(0)$	$y(R_w)$	$\frac{y_f - y(0)}{y_f}$	$\frac{y(R_w) - y_f}{y_f}$	α
$\text{SO}_2\text{-H}_2$	0.002	.00172	.00231	.140	.155	1.3419
$\text{SO}_2\text{-N}_2$	0.002	.00183	.00217	.085	.085	1.1862
UF_6 (235, 238)	0.002	.002018	.001989	-.0090	-.0053	.9859



the axis approached. This situation exists since as the axis is approached the centrifugal force diminishes and the concentration decreases simply to make up for what has moved to the wall. On the other hand, near the periphery where the difference in the centrifugal forces acting on the heavy and light species is growing farther apart, the mole fraction profile increases quite rapidly.

E. A Simple Centrifuge Containing a Stationary Pipe Centered Along the Axis

Before leaving this chapter it is worth mentioning that the experimental gas centrifuge enrichment of the Uranium isotopes has been accomplished by using centrifuges containing no internals and to a lesser extent by using centrifuges containing a stationary pipe centered along the axis. Such work had been done by Zippe (7) and Groth (5). The question then at this point is what effect does the stationary center pipe have on the pressure ratios and separation factors found for the simple centrifuge containing no center pipe?

To answer this question the following assumptions must be made:

1. The centrifuge is sufficiently long so that end effects may be neglected.
2. The radial pressure changes are small enough so that viscosity changes can be neglected. This is a good assumption at pressures around 1 atmosphere and lower.
3. The flow between the cylinders is laminar.

Of the assumptions, number 3 requires the closest analysis. Since, if the tangential flow is not laminar, the mixing associated with turbulent flow would destroy the desired concentration profiles.

Intuitively, because of the centrifugal forces involved, one may conclude that laminar flow is favored. That is, the gas near the wall will not tend to move inward because the centrifugal forces are greater near the wall than near the axis. Likewise, gas near the axis will not tend to move outward because of the higher centrifugal forces on the particles it would have to replace. Hence, shear rates higher than those encountered in normal gas flows in a pipe are expected to be possible.

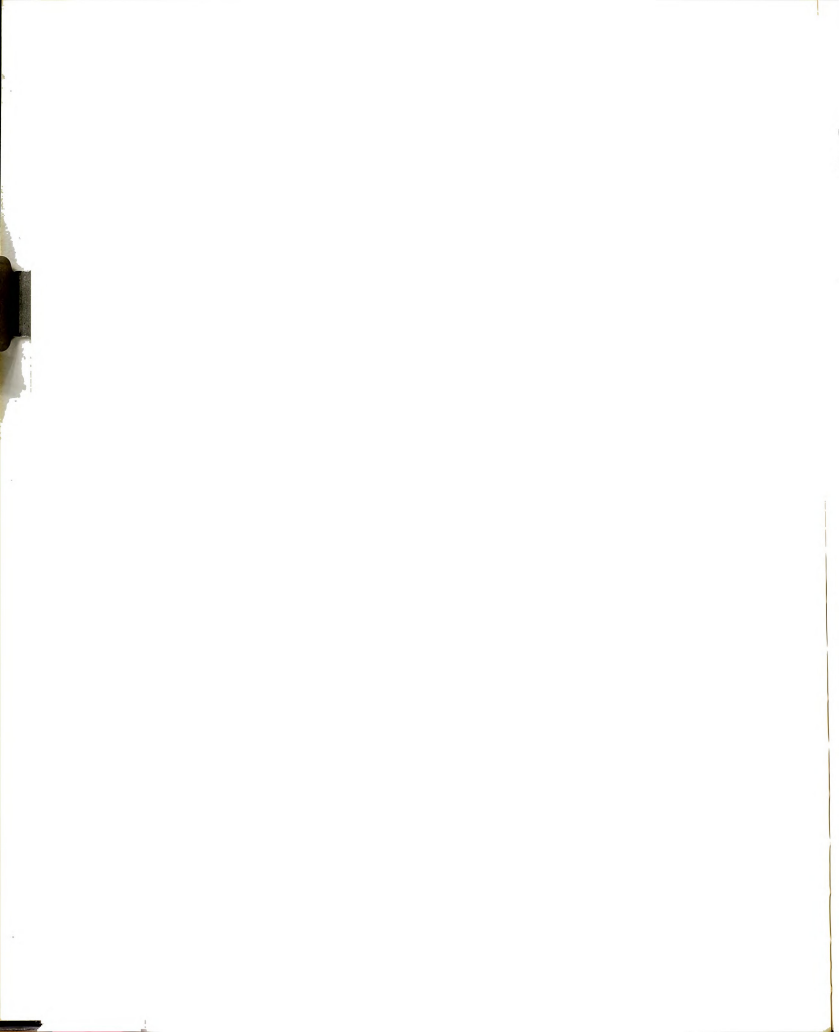
H. Schlichting (9) determined the transition (changing from laminar to turbulent flow) Reynold's number, $\omega_o R_w^2 \rho / \mu$, giving the transition RPM, for tangential flow between a stationary inner cylinder (pipe) and a rotating outer cylinder. From the results of his work, it was determined that for a ratio of pipe to centrifuge diameter of 1/16, the transition Reynold's number is 20×10^4 , while for a ratio of 1/2 the transition Reynold's number is 16×10^4 . Table 2 contains all the parameters and their values required to compute the transition RPMs of an 8-inch diameter centrifuge containing either $\text{SO}_2\text{-N}_2$ or $\text{SO}_2\text{-H}_2$ gas mixtures. Since in practice one would expect the center pipe to be small in diameter as compared to the centrifuge, a center pipe diameter of 1/2 inch is used in Table 2.

As can be seen from Table 2, the transition RPMs at 70°F and 1 atmosphere are rather small (~2790 and ~2080) for the gas pair $\text{SO}_2\text{-N}_2$ with SO_2 mole fractions of 0.002 and 0.2. The reduction in the transition RPM going from an SO_2 mole fraction of 0.002 to 0.2 reflects the change in density of the gas (viscosity only changes by 6.3% whereas the density changes 25.5%). This is especially true for

TABLE 2.--Predicted Transition RPMs for the Gas Pairs $\text{SO}_2\text{-N}_2$ and $\text{SO}_2\text{-H}_2$ in a Simple Centrifuge Containing a Stationary Center Pipe.

Parameter	Value			
	$\text{SO}_2\text{-N}_2$		$\text{SO}_2\text{-H}_2$	
R_{cp} (center pipe), inches	1/4		1/4	
R_w , inches	4		4	
$(\frac{\omega_o R_w^2 \rho}{\mu})$ trans	20×10^4		20×10^4	
T , $^{\circ}\text{R}$	530		530	
P (average), psia	14.696		14.696	
Mole fraction SO_2	0.002	0.2	0.002	0.2
ρ , lb_m/ft^3	0.0725	0.091	0.0055	0.0372
μ , cp	0.0175	0.0164	0.0090	0.0096
ω_o (trans), RPM	2788	2082	18900	2980

the gas pair $\text{SO}_2\text{-H}_2$ where the transition Reynold's numbers are ~18900 and 2980 for SO_2 mole fractions of 0.002 and 0.2, respectively (density change of 576%). The transition RPMs, however, could be increased by either increasing the temperature or decreasing the pressure. The latter is the case for Uranium isotope separation where low pressures (approximately 1/10 atmosphere or less) are necessary to keep the UF_6 vaporized for feed stock and at the centrifuge wall. At normal pressures (near 1 atm) and the high rotational speeds necessary in gas centrifugation, however, the operation of a centrifuge with a center pipe does not seem very promising due to the problem of turbulence.



Nevertheless, with assumptions 1, 2 and 3 the equation of motion for the tangential flow of the gas in the annular space can be written as

$$\frac{d}{dr} \left[\frac{1}{r} \frac{d}{dr} (r^2 \omega) \right] = 0$$

where $\omega = 0$ at $r = R_{cp}$ (center pipe), and $\omega = \omega_o$ at $r = R_w$. This equation can be integrated, giving

$$\omega = C \left(\frac{k R_w^2}{r^2} - \frac{1}{k R_w} \right),$$

where $C = \frac{\omega_o R_w}{(k-1/k)}$, and $k = R_{cp}/R_w$.

Substituting this expression for ω in the pressure equation derived in Chapter II-A gives (for a pure gas)

$$\frac{1}{P_c} \frac{dP_c}{dr} = \frac{MW}{RT} \frac{C^2}{g_c} \left(\frac{k^2 R_w^2}{r^4} - \frac{2}{r^2} + \frac{1}{k^2 R_w^2} \right) r,$$

where $P_c = P_c(R_{cp})$ at $r = k R_w$.

Integrating gives the following expression for the ratio of the pressure at the wall to that at the center pipe, i.e.,

$$\ln P_c(R_w)/P_c(R_{cp}) = \frac{A R_w^2}{2} \frac{(1/k^2 - k^2 + 4 \ln k)}{(1/k^2 + k^2 - 2)},$$

where $A = MW \omega_o^2 / RT g_c$ as before.

Remembering that without a center pipe

$$\ln P(R_w)/P(0) = \frac{AR_w^2}{2},$$

allows the following comparative expression to be written:

$$\ln P_c(R_w)/P_c(R_{cp}) = \theta \ln P(R_w)/P(0),$$

or

$$\frac{P_c(R_w)}{P_c(R_{cp})} = \left[\frac{P(R_w)}{P(0)} \right]^\theta,$$

where

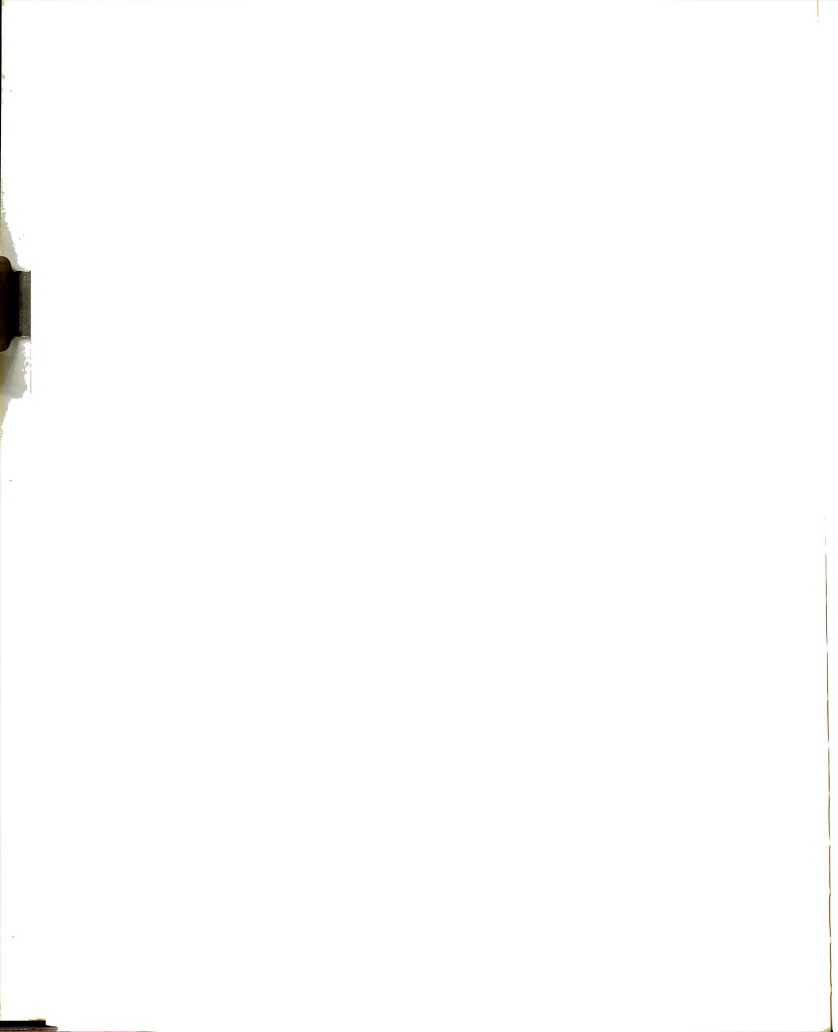
$$\theta = \frac{(1/k^2 - k^2 + 4 \ln k)}{(k^2 + 1/k^2 - 2)}.$$

The limit of θ can easily be seen to be 1 and 0 as k approaches its limits of 0 and 1.

Since the above expression is valid for either species in a binary gas mixture, a relation can also be written for the separation factors, i.e.,

$$\alpha_c = \alpha^\theta.$$

Figure 6 contains a plot of θ versus k . The calculated data used to construct the figure can be found in Appendix A. For a given simple centrifuge containing a center pipe (given k), the value of θ



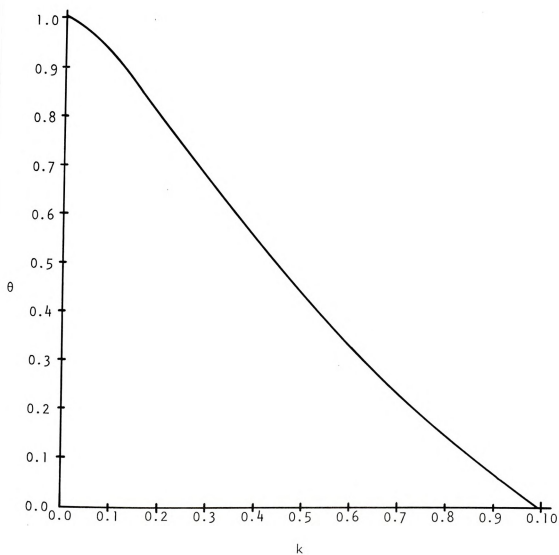


Figure 6.-- θ Versus k for a Simple Centrifuge Containing a Stationary Center Pipe.

can be taken from Figure 6. This value of θ can then be used to compute the pressure ratios and/or the simple separation factors by raising the corresponding value taken from Figure 1 or 2 for a simple centrifuge without a center pipe to the θ power.

CHAPTER III

UNSTEADY STATE SIMPLE GAS CENTRIFUGE THEORY

A. Concentration and Pressure Diffusion Fluxes

In Chapter II the steady state mole fraction profiles for a binary, perfect gas mixture were derived and analyzed from a pressure gradient approach. This approach made use of the fact that the centrifugal force, which is tending to pile all the gas up at the periphery, acts to a greater degree on the heavier species giving rise to the mole fraction profile.

From a molecular point of view, however, what the steady state operation implies is a no net flux condition. That is, at any radial position r , the flux of say, species 1, by diffusion is equal and opposite to the flux of species 1 caused by the centrifugal field tending to pile it up at the wall. In terms of transport properties, the sum of the terms describing ordinary concentration diffusion and pressure diffusion is zero.

From Bird, Stewart, and Lightfoot, Transport Phenomena (10), for a perfect gas mixture the one dimensional molar flux of species 1 for concentration is given by

$$F_{1y} = - \frac{2\pi P}{RT} D_{12} r \frac{\partial y}{\partial r},$$

and the one dimensional molar flux of species 1 for pressure diffusion is given by

$$F_{1p} = - \frac{2\pi P}{RT} \frac{MW_1 y}{RT} D_{12} \left(\frac{\bar{V}_1}{MW_1} - \frac{1}{\rho} \right) r \frac{\partial p}{\partial r},$$

where F_{1y} and F_{1p} are expressed in lb-mole/ft²-sec,

$D_{12} = D_{21}$ is the diffusion coefficient, ft²/sec, and

$\bar{V}_1$ is the partial molar volume of species 1, ft³/lb-mole.

Using the following relations:

$$\frac{\bar{V}_1}{MW_1} = \frac{RT}{MW_1 P} = \frac{1}{\rho_1} \text{ for a perfect gas mixture,}$$

where ρ_1 = the mass density of species 1, and

$$\frac{\partial P}{\partial r} = \frac{\rho \omega^2 r}{g_c} \text{ in the simple centrifuge,}$$

where ρ = the mass density of the mixture,

allows F_{1p} to be written as

$$F_{1p} = - \frac{2\pi P}{RT} \frac{MW_1 y}{RT} D_{12} \frac{\omega^2 r^2}{g_c} \left(\frac{\rho}{\rho_1} - 1 \right).$$

Since $\rho = \frac{P}{RT} [y MW_1 + (1-y) MW_2]$ and $\rho_1 = \frac{P MW_1}{RT}$, F_{1p} may be further reduced to

$$F_{1p} = \frac{2\pi P}{RT} D_{12} A r^2 y(1-y),$$

where $A = \frac{(MW_1 - MW_2)\omega^2}{RT g_c}.$

In the steady state operation of the simple gas centrifuge, where the two diffusional fluxes are equal and opposite in sign, the following expression results:

$$\frac{\partial y}{\partial r} = Ar y(1-y).$$

Integrating and using the fact that at $r = 0$, $y = y(0)$, gives

$$y(r) = \frac{y(0) \exp (Ar^2/2)}{y(0) [\exp (Ar^2/2)-1] + 1}$$

which is identical to the expression derived in Chapter II-C.

B. The Partial Differential Equation for the Unsteady State Operation of the Simple Centrifuge

The analysis of the unsteady state operation of the simple centrifuge will provide insight as to how fast the equilibrium mole fraction profile develops, hence yielding information about the ability of the centrifugal forces to perform a separation. This simpler analysis, which is being carried out before the analysis of gas centrifuges with axial flows, will give a very good indication of the magnitude of the flows that may be expected and the centrifuge lengths required to perform a separation.

Consider a simple centrifuge that has been filled with a perfect binary gas mixture (total pressure = P_0) with composition y_f (heavy species) and then quickly brought up to rotational speed. Certainly from a practical point of view, it would be impossible to bring the machine instantly up to speed nor would it be possible to

overcome the inertia of the gas (without perhaps the aid of radial baffles, etc.) so that angular velocity gradients did not develop. Nevertheless, the above hypothetical situation is proposed for the purpose of this analysis. The first thing to occur will be a rapid bulk radial flow of gas to the wall. When this flow essentially stops, diffusional flow will establish the equilibrium mole fraction profile. Starting from this point in time (when the gas is still of uniform composition, y_f) the unsteady state problem will be solved.

By using the diffusional flux equations developed in Chapter III-A, the equation of continuity for the heavy species in the rotating cylinder is given by

$$\frac{\partial}{\partial t} \left(\frac{P y}{RT} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{P}{RT} D_{12} [Ar^2 y(1-y) - r \frac{\partial y}{\partial r}] \right) = 0.$$

At this point it is worthwhile to note that the product PD_{12} can be taken as a constant. That is, in expressions for the diffusivity (binary mixture), resulting from kinetic theory and corresponding states arguments, at low pressures, the diffusivity was found to vary inversely with pressure to the first power. Such expressions are given by, among others, Hirschfelder, Bird and Spotz (11).

Taking the necessary partial derivatives and simplifying, the equation of continuity becomes

$$P \frac{\partial y}{\partial t} + y \frac{\partial P}{\partial t} + D_{12} P \left(2 Ay(1-y) + [(Ar(1-2y) - \frac{1}{r}] \frac{\partial y}{\partial r} - \frac{\partial^2 y}{\partial r^2} \right) = 0.$$

The boundary conditions are that there is no flux at the axis or the wall as expressed by the following equations:

$$\text{at } r = 0, \frac{\partial y}{\partial r} = 0, \text{ and}$$

$$\text{at } r = R_w, \frac{\partial y}{\partial r} = Ar Y(1 - y).$$

The initial condition is that the mole fraction is uniform at the value y_f .

As the equilibrium mole fraction profile develops, the pressure profile also changes due to changing centrifugal forces coupled with the fact that conservation of mass must be maintained. This gives rise to the partial derivative of pressure with respect to time.

The pressure distribution can be computed from the pressure gradient equation developed in Chapter II-A with the mass density of the gas mixture used in place of a pure gas density. That is,

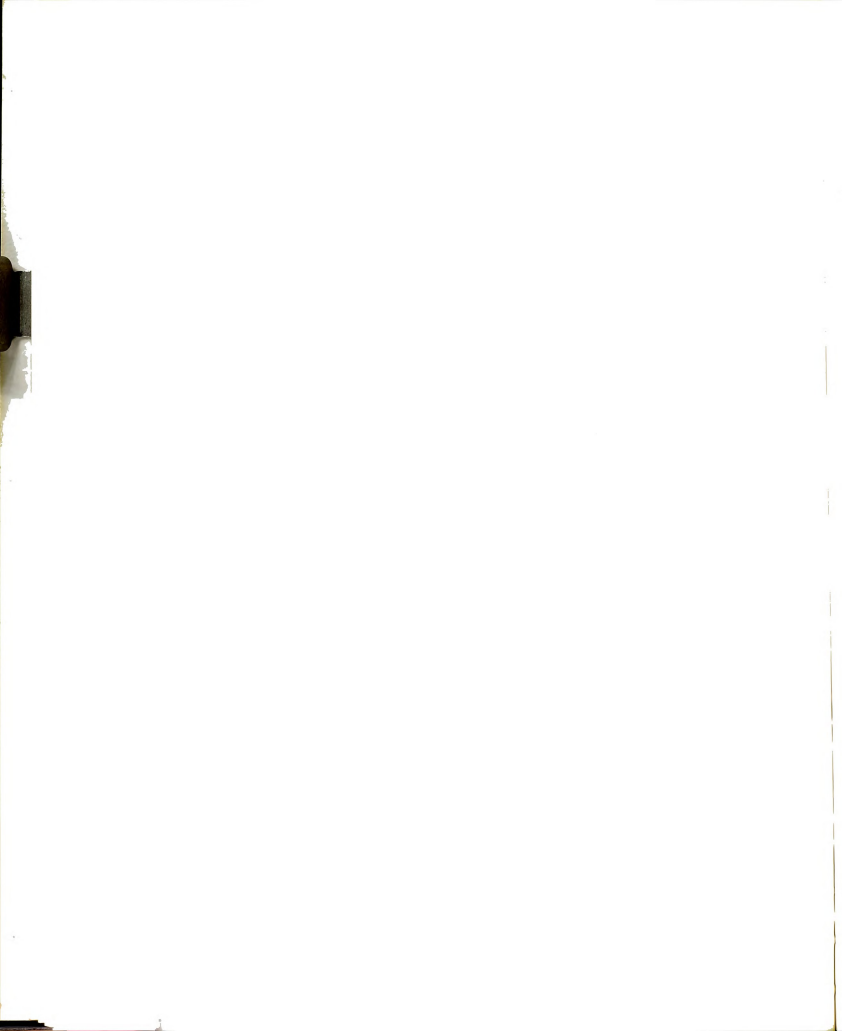
$$\frac{\partial P}{\partial r} = \frac{P \omega^2}{RT g_c} (\Delta MW y + MW_2) r,$$

$$\text{and at } r = 0, P = P(0).$$

The pressure at the axis, $P(0)$, may be computed by using the fact that the centrifuge contains a fixed amount of mass. Thus, the expression for $P(0)$ can be written as

$$P(0) = \frac{B/L}{\frac{2\pi}{RT} \int_0^{R_w} P r dr},$$

where B/L are the moles per foot in the centrifuge, i.e., $B/L = 2\pi P_0 / RT$.



C. The Method of Solution Used to Solve the Partial
Differential Equation for the Unsteady State
Operation of the Simple Centrifuge

Due to the coupling of P and y and hence nonlinearity of the partial differential equations which had to be solved, a numerical solution was sought. The numerical approach chosen was to solve the partial differential equations implicitly. That is, all partial derivatives were approximated with fourth order finite difference formulas at the next increment in time, resulting in a set of simultaneous equations.

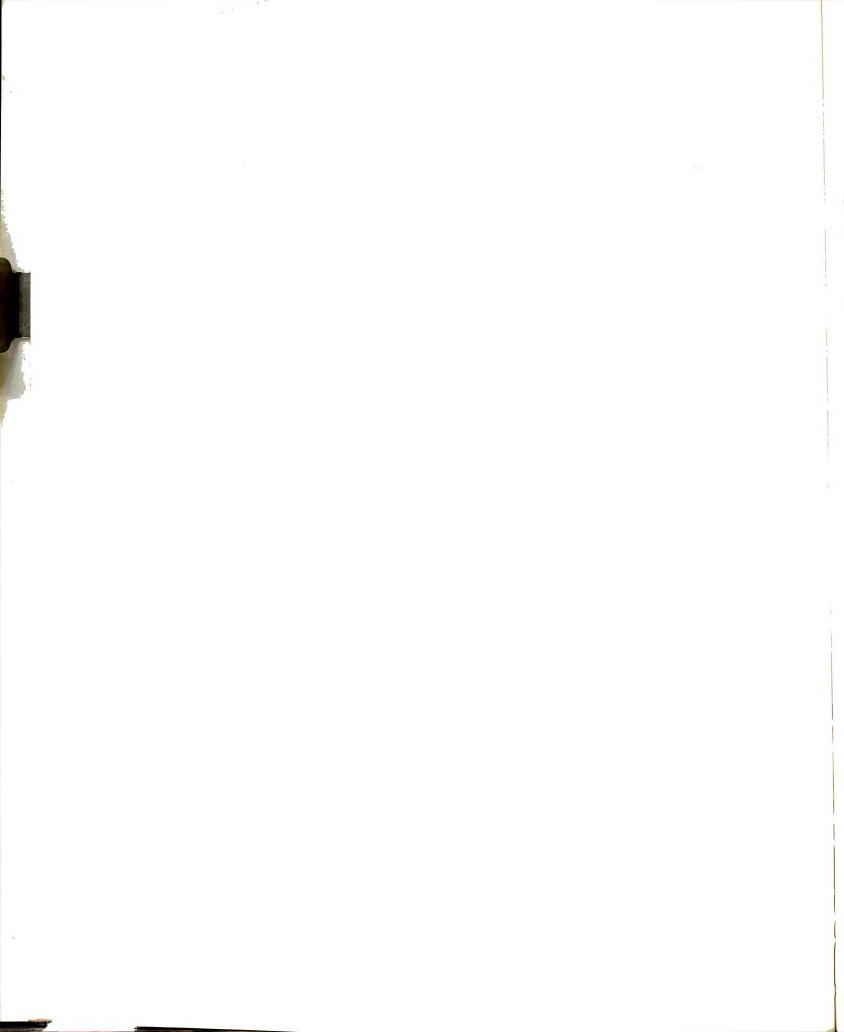
To obtain the numerical solution a general FORTRAN program, UNSTEADY, aided by the scientific subroutine ONEDIAG to solve the simultaneous equations, was written. The program was constructed so that it could be used to analyze any gas pair in any size centrifuge operating at any rotational speed.

A complete listing of the finite difference formulas used to approximate the various partial derivatives and a complete listing of the FORTRAN program and subprogram can be found in Appendix C. The following is a brief outline of the calculational steps used in the program:

1. Input operating conditions.
2. Divide the radius ($R_w = 4$ inches) into 21 equally spaced grid points. The time increments were chosen so the $PD_{12}\Delta T \approx 0.5 \text{ lb}_f$. Using more radial and/or time increments gave essentially no improvement in the solutions.
3. Compute the initial pressure profile using the uniform composition y_f . The axis pressure is such that the known moles per foot are maintained.

4. Compute the equilibrium mole fraction profile so that a comparison can be made to the actual mole fraction profile as a function of time.
5. Based on past information, estimate the values of P and y at the next position in time. This must be done because of the nonlinearity of the equations.
6. Compute the partials, $\partial P / \partial t$, at each grid point.
7. Using finite difference approximations for the partials of y , an equation is written for each grid point at the next position in time. This results in 21 simultaneous equations which are solved for the new values of y .
8. Using the new values of y , the finite difference approximations are written for the pressure equation at each grid point resulting in 21 simultaneous equations. The equations are solved with the axis pressure arbitrarily taken at 1.0.
9. Using the new values of P , the integration for the total moles present is performed which gives the axis pressure. The correct pressure profile can be obtained by multiplying all the values of P by the axis pressure.
10. Due to the nonlinear nature of the equations, which requires the estimation of P and y at a new position in time (step 5), statements 6 through 9 are executed twice during each incremental move ahead in time. More iterations did not significantly affect the results.
11. Output results and increment time. If the time interval over which the calculations were desired is exceeded, calculations are complete. Otherwise, return to step 5.

The program was executed on a Control Data Corporation 6500 digital computer and required approximately 15 seconds of central processor time to march 100 time increments.



D. The Mole Fraction Profiles Developed in the
Unsteady State Operation of the Simple Gas
Centrifuge for the Three Gas Pairs: $\text{SO}_2\text{-N}_2$,
 $\text{SO}_2\text{-H}_2$, and UF_6 (235, 238 isotopes)

With the aid of the above equations the separation of the two gas pairs, $\text{SO}_2\text{-N}_2$ and $\text{SO}_2\text{-H}_2$, was analyzed in the unsteady state simple centrifuge at temperatures of 70° and 300°F with centrifuge RPMs of 10000 and 20000. Also, a mixture of Uranium isotopes (as UF_6) was analyzed at a temperature of 80°F and a centrifuge RPM of 20000.

Table 3 contains a complete tabulation of the operating conditions and diffusivities used. Values of the diffusivities were either calculated or found in the literature. All information regarding the diffusivities may be found in Appendix B.

TABLE 3. Operating Conditions and Diffusivities Used in the Unsteady State Analysis of the Gas Pairs $\text{SO}_2\text{-N}_2$, $\text{SO}_2\text{-H}_2$ and UF_6 (235, 238 isotopes).

Parameter	Gas Pairs		
	$\text{SO}_2\text{-N}_2$	$\text{SO}_2\text{-H}_2$	UF_6 (235, 238 isotopes)
Charge pressure, psia	14.696	14.696	2.1
Charge composition, y	0.002(SO_2)	0.002 (SO_2)	0.002(U_{235})
Temperatures, °F	70, 300	70, 300	80
Centrifuge radius, inches	4.0	4.0	4.0
Centrifuge RPM	10000, 20000	10000, 20000	20000
Molecular weights	64, 28	64, 2	349, 352
Diffusivities, cm^2/sec			
@ 70°F and 14.696 psia	0.1346	0.5282	---
@ 80°F and 2.1 psia	---	---	0.1136
@ 300°F and 14.696 psia	0.2590	0.9869	---

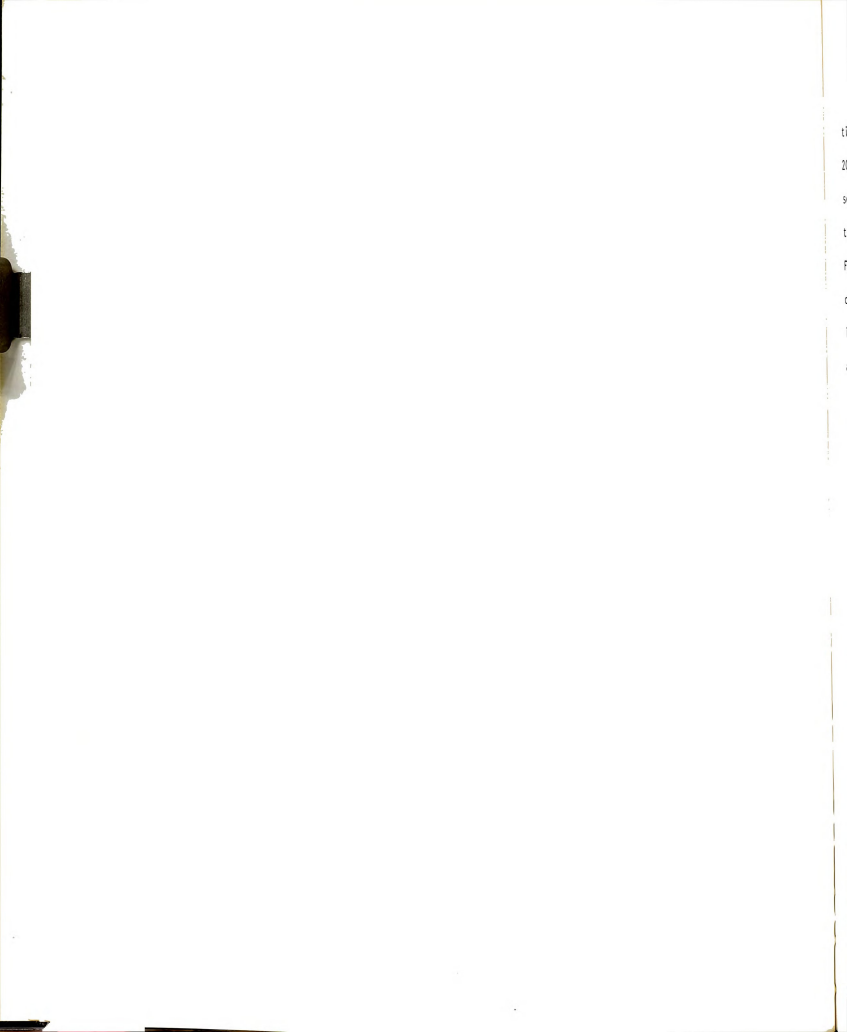
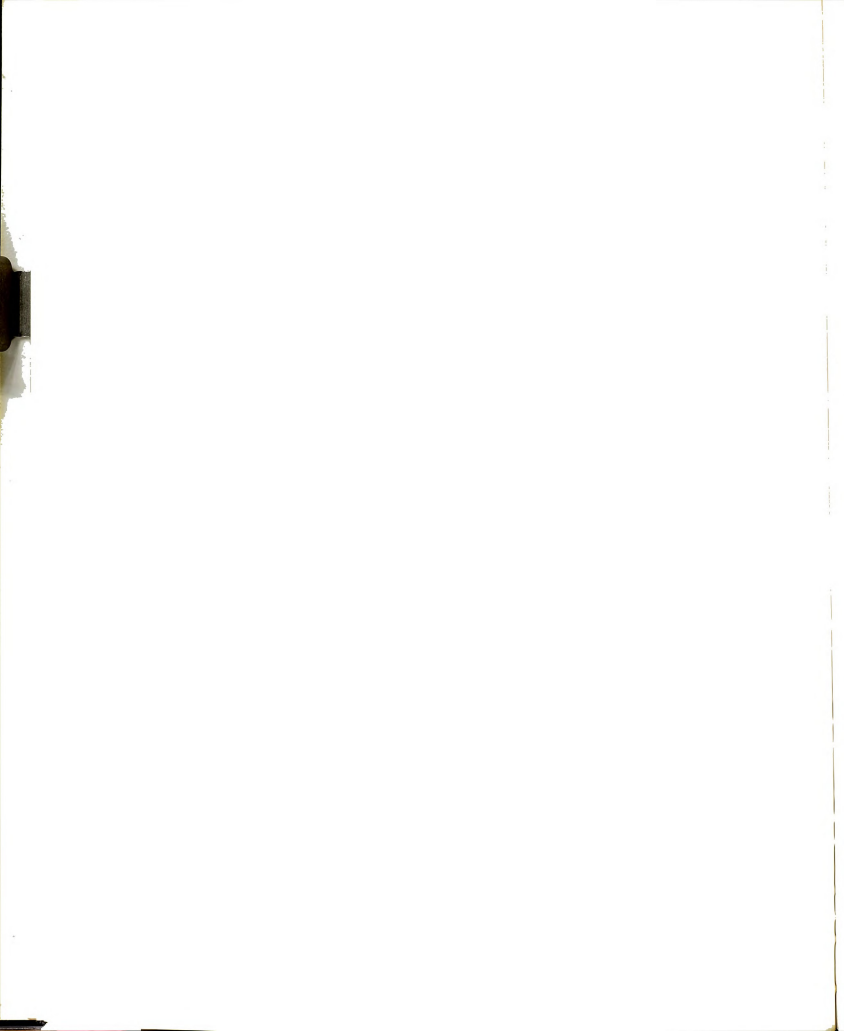


Figure 7 illustrates the changing mole fraction profiles with time for the gas pair $\text{SO}_2\text{-H}_2$ at 70°F and a centrifuge rotation of 20000 RPM. The profiles given are for times of 0, 3.6, 7.2 and 14.4 seconds. Also included is the equilibrium mole fraction profile, i.e., the profile established after a long time period. The curves in Figure 7 illustrate the expected fact that the profile develops much quicker near the wall than near the axis. This fact is further illustrated by Tables 4, 5 and 6 which contain values of $(y-y_f)/(y_e-y_f)$ at the axis and the wall for each of the pairs and all the operating

TABLE 4.--Values of $(y-y_f)/y_e-y_f \times 100$ Versus Time at the Axis and the Wall for the Gas Pair $\text{SO}_2\text{-N}_2$ in the Unsteady State Simple Centrifuge, Radius = 4 inches.

Time (sec)	70°F and 10000 RPM		70°F and 20000 RPM		300°F and 10000 RPM		300°F and 20000 RPM	
	axis	wall	axis	wall	axis	wall	axis	wall
9	8.7	39.9	9.7	39.2	16.6	52.5	17.8	52.0
18	18.4	54.2	20.3	53.7	34.7	68.8	36.6	68.7
27	27.9	63.5	30.5	63.2	51.2	78.5	53.2	78.5
36	37.2	70.3	40.1	70.2	64.4	84.9	66.4	85.0
45	45.9	75.5	49.0	75.5	74.5	89.2	76.1	89.4
54	53.8	79.7	56.9	79.9	81.8	92.3	83.2	92.5
63	60.8	83.1	63.8	83.3	--	--	--	--
72	66.9	85.9	69.7	86.2	--	--	--	--
81	72.2	88.2	74.8	88.5	--	--	--	--
90	76.7	90.1	79.0	90.4	--	--	--	--
99	80.5	91.7	82.6	92.0	--	--	--	--



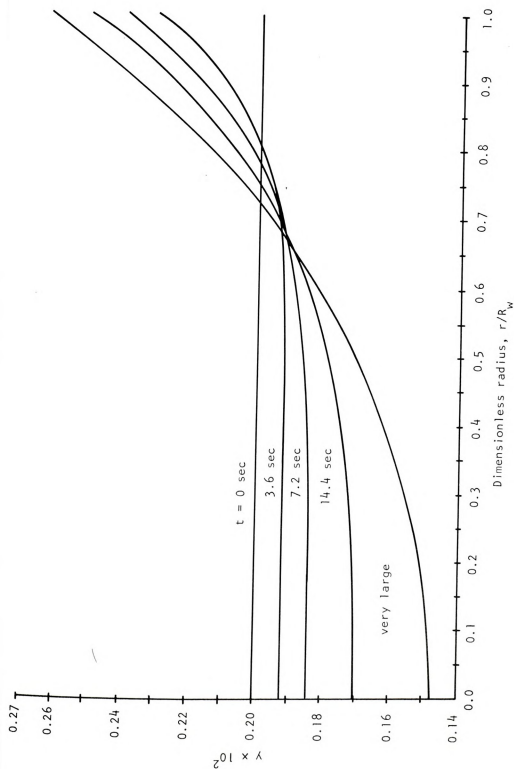


Figure 7.--Mole Fraction Profiles for SO_2 , Y , versus Dimensionless Radius, r/R_w ($R_w = 4$ inches), at Various Times in the Unsteady State Operation of a Simple Centrifuge Containing $\text{SO}_2\text{-H}_2$ at 70°F . RPM = 20000.

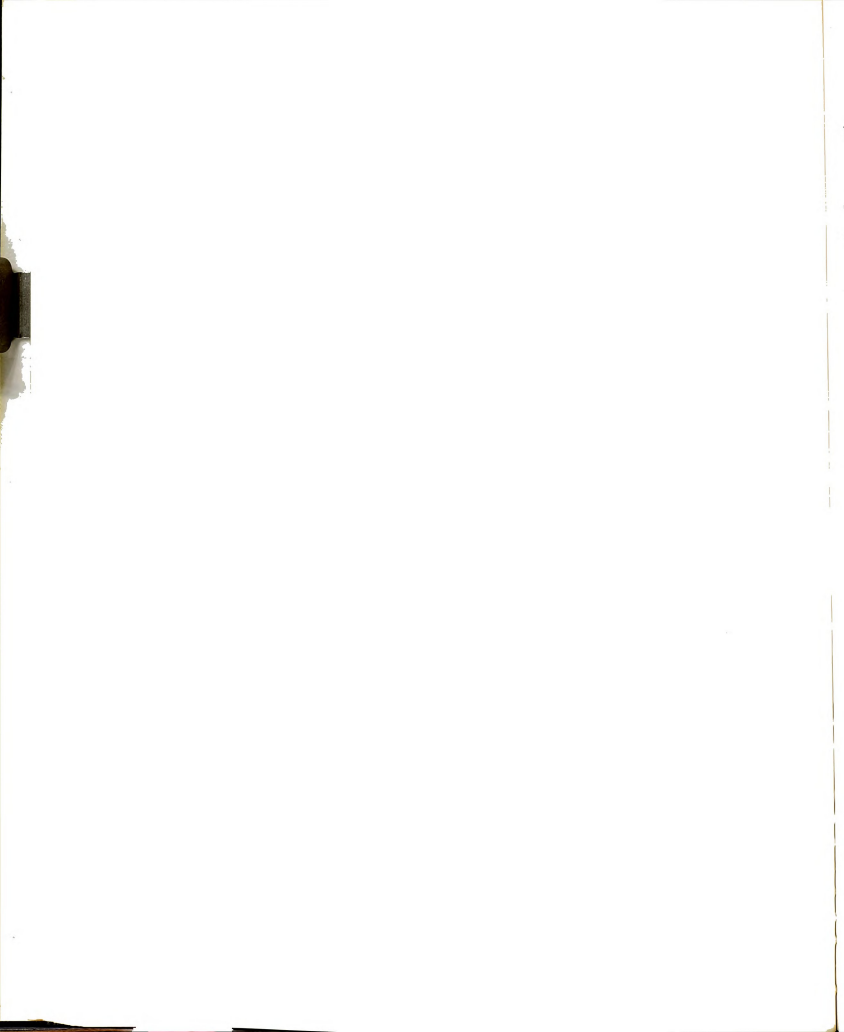


TABLE 5.--Values of $(y-y_f)/(y_e-y_f) \times 100$ Versus Time at the Axis and the Wall for the Gas Pair $\text{SO}_2\text{-H}_2$ in the Unsteady State Simple Centrifuge, Radius = 4 inches.

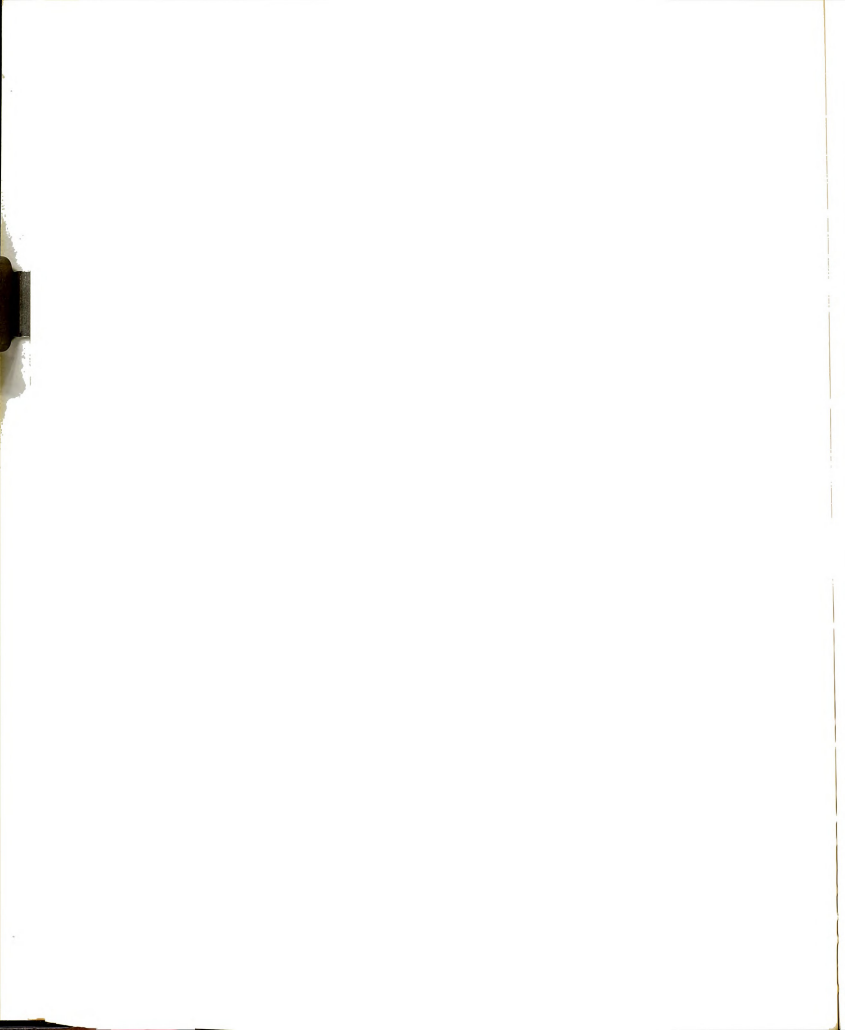
Time (sec)	70°F and 10000 RPM		70°F and 20000 RPM		300°F and 10000 RPM		300°F and 20000 RPM	
	axis	wall	axis	wall	axis	wall	axis	wall
.9	--	--	--	--	6.3	34.9	6.7	34.0
1.8	6.8	35.8	7.4	34.6	13.3	47.8	14.0	47.0
2.7	--	--	--	--	20.3	56.5	21.2	55.7
3.6	14.3	49.0	15.5	47.9	27.2	63.1	28.3	62.4
4.5	--	--	--	--	34.0	68.3	35.2	67.7
5.4	21.8	57.9	23.3	56.9	40.5	72.6	41.8	72.0
6.3	--	--	--	--	46.7	76.1	48.0	75.7
7.2	29.2	64.5	31.0	63.6	52.5	79.2	53.7	78.8
8.1	--	--	--	--	57.8	81.8	58.9	81.5
9.0	36.4	69.8	38.3	69.0	62.6	84.0	63.7	83.8
9.9	--	--	--	--	67.0	86.0	68.0	85.8
10.8	43.3	74.0	45.2	73.4	70.8	87.7	71.8	87.5
11.7	--	--	--	--	74.3	89.2	75.2	89.0
12.6	49.8	77.6	51.6	77.1	77.4	90.5	78.2	90.3
13.5	--	--	--	--	80.1	91.6	80.8	91.5
14.4	55.7	80.6	57.4	80.2	--	--	--	--
16.2	61.0	83.2	62.7	82.8	--	--	--	--
18.0	65.8	85.4	67.4	85.1	--	--	--	--
19.8	70.1	87.3	71.5	87.1	--	--	--	--
21.6	73.9	88.9	75.2	88.7	--	--	--	--
23.4	77.2	90.3	78.4	90.2	--	--	--	--
25.2	80.2	91.6	81.2	91.5	--	--	--	--

E 6.--Values of $(y-y_f)/(y_e-y_f) \times 100$ Versus Time at the Axis and the Wall for the Gas UF_6 (235 and 238 isotopes) in the Unsteady State Simple Centrifuge. Radius = 4 inches and Charge Pressure = 2.1 psia.

Time (sec)	80°F and 20000 RPM	
	Axis	Wall
7.2	36.6	30.9
14.4	52.2	44.2
21.6	64.2	53.7
28.8	73.7	60.7
36.0	81.1	66.1
43.2	86.8	70.2
50.4	91.3	73.4
57.6	94.8	75.8

itions investigated. For a better comparison of the gas pairs, re 8 contains plots of $(y-y_f)/(y_e-y_f)$ at the axis versus time at of the temperatures investigated. The curves for SO_2-N_2 and SO_2-H_2 are at a centrifuge rotation of 10000 RPM, whereas the e for the UF_6 is at 20000 RPM.

The results presented here are only for a centrifuge having a eter of 8 inches. As shown in Chapter II, varying the radius, maintaining the same peripheral speed, does not affect the magni- of the equilibrium separation. However, in the case of the eady state operation of the simple centrifuge, maintaining the peripheral speed implies the same flux due to pressure diffusion given dimensionless radius, r/R_w . Hence, since increasing the



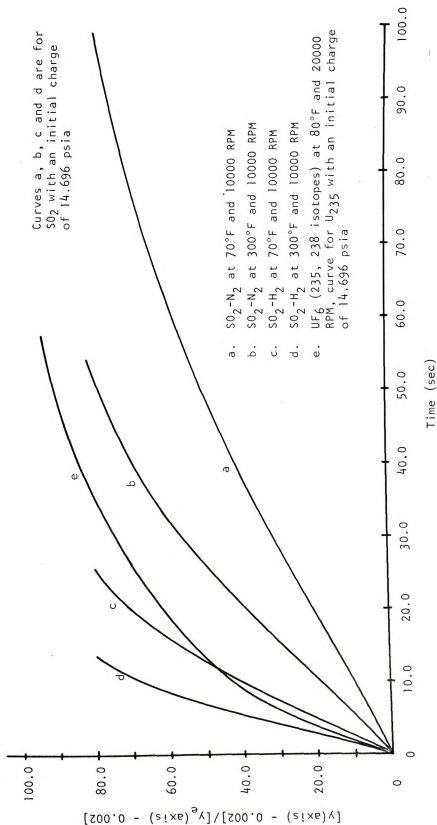
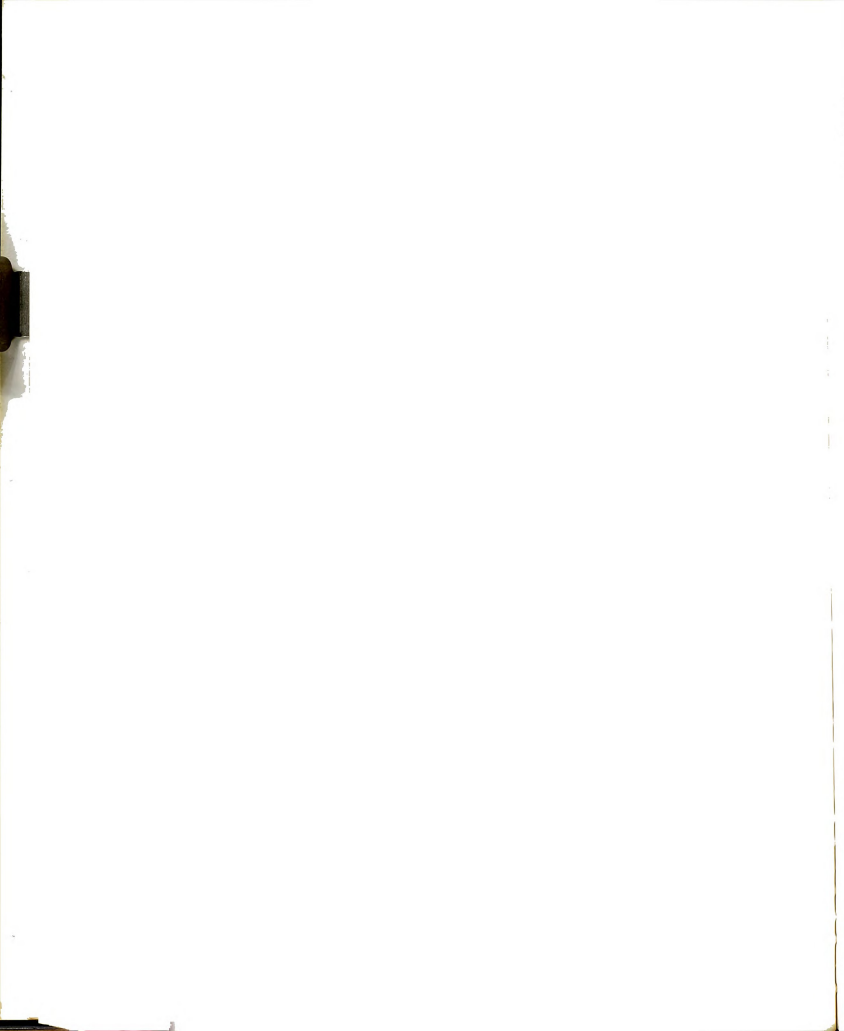


Figure 8.-- $[y(\text{axis}) - 0.002] / [y_e(\text{axis}) - 0.002]$ Versus Time in the Unsteady State Simple Centrifuge With a Radius of 4 Inches.



radius allows more mass to be contained in the centrifuge (all other operating conditions being equal), the time for the separation to occur must necessarily increase. Nevertheless, it was felt that sticking to just one size served the present purpose of establishing and putting into perspective key operating parameters and their effect on the radial fluxes.

From the above information, three observations may be made regarding operating parameters which control the rate of separation in the simple gas centrifuge:

1. As illustrated with the gas pairs $\text{SO}_2\text{-N}_2$ and $\text{SO}_2\text{-H}_2$ in Tables 4 and 5, increasing the rotational speed from 10000 to 20000 RPM had very little effect on the time required for the mole fraction profiles to develop. This is expected since increasing the rotational speed increases the flux due to pressure diffusion (depends on the rotational speed squared) which correspondingly increases the magnitude of the separation as established in Chapter II-C. The fact that increasing the rotational speed moves the gas contained in the centrifuge nearer the wall (steeper pressure profile), leaves less gas near the axis. Hence, as can be seen in Tables 4 and 5, at 20000 RPM as compared to 10000 RPM, the composition approaches equilibrium slightly faster at the axis.

In lieu of the effect of rotational speed, the effect of using charge composition (y_f) of 0.002 mole fraction on the times for the separations to occur as presented in Tables 4, 5 and 6 may be evaluated. If a function ϕ is defined such that $y = \phi y_f$ at every radial position and every point in time, the partial differential

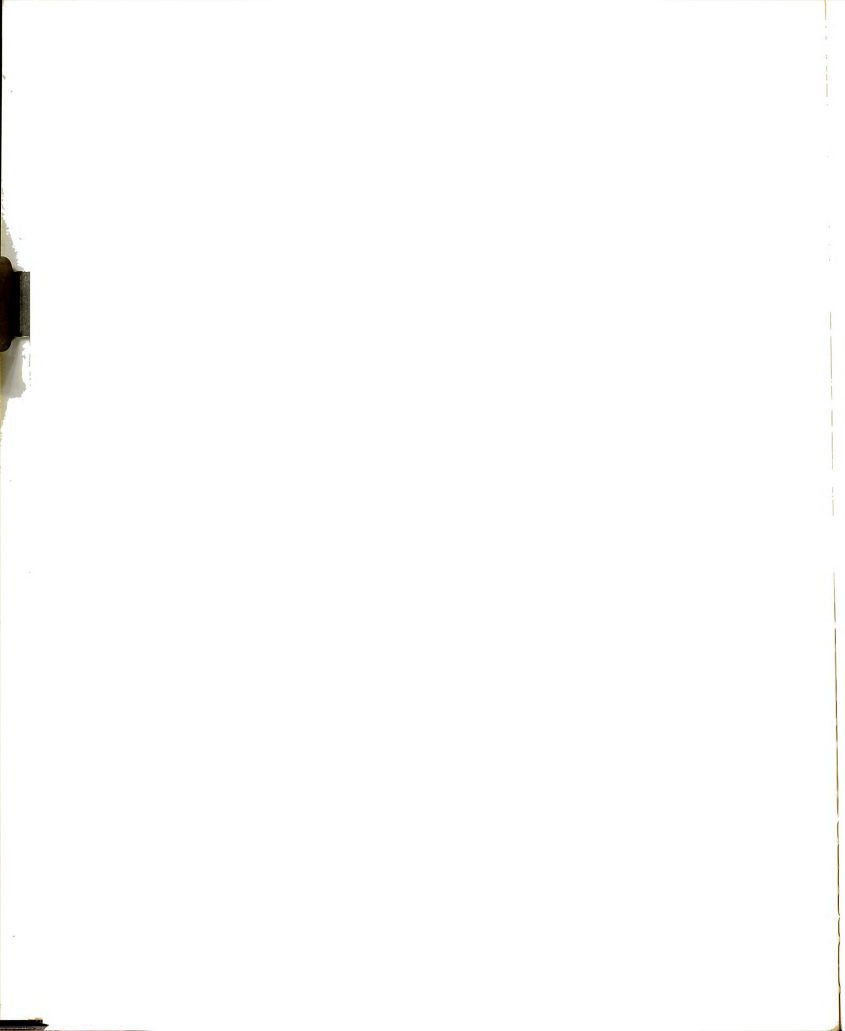
tion for the continuity of Species 1 in the unsteady state simple centrifuge may be rewritten as

$$\frac{\partial}{\partial t} \left(\frac{P\phi}{RT} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{PD_{12}}{RT} [r^2 A(1-\phi y_f) \phi - r \frac{\partial \phi}{\partial r}] \right) = 0 ,$$

At time = 0, $\phi = 1$ for all r . The only remaining dependence on the value of y_f is in the pressure, P , and the term $A(1-\phi y_f)$, which are the same terms which were affected by changing the rotational speed.

Changing the values of y_f changes the average molecular weight of the gas in the centrifuge which changes the steepness of the pressure profile (the greater the molecular weight, the steeper the profile). But, as shown above, for a given charge pressure (fixed amount of gas) the steepness of the pressure profile had very little effect on the time required for the equilibrium separation to occur.

At early times (t close to 0) when ϕ is very nearly equal to 1 at all radial positions, the magnitude of $A(1-\phi y_f) \sim A(1-y_f)$ is mainly determined by the value of y_f . But, as pointed out above, changing the magnitude of $A(1-y_f)$ changes the flux due to pressure diffusion which correspondingly changes the magnitude of the equilibrium separation. Hence, no effect on the time for the separation to occur is expected. After some time has passed, however, the quantity $A(1-\phi y_f)$ is not only changing with radial position but also with time. The maximum radial change that may take place in the term $1-\phi y_f$ is at equilibrium. As illustrated in Chapter 11-C, the composition at the wall, $y(R_w)$, based on the axis composition, $y(0)$, at equilibrium is given by



$$y(R_w) = \frac{y(0)\alpha}{y(0)(\alpha-1) + 1},$$

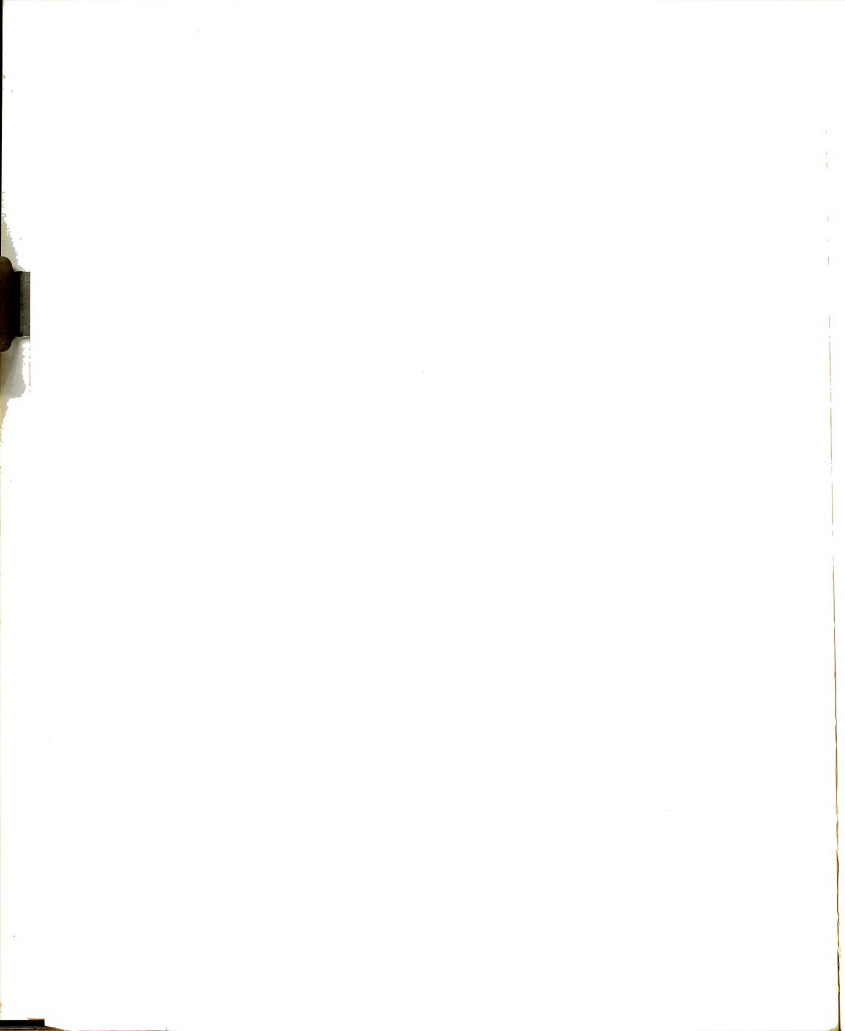
where α is the simple separation factor, $\exp(AR_w^2/2)$. Rearranging the above equation, the following ratio may be obtained:

$$\frac{1-y(R_w)}{1-y(0)} = \frac{1}{y(0)(\alpha-1) + 1}.$$

For small values of $y(0)$, regardless of the value of α , the ratio is near 1. On the other hand, for values of $y(0)$ near 1, the ratio approaches $1/\alpha$. The values of $1/\alpha$ for the gas pairs SO_2-N_2 and O_2-H_2 at $70^\circ F$ and 20000 RPM ($R_w = 4$ inches) are 0.717 and 0.564, respectively. At $80^\circ F$ the value of $1/\alpha$ for UF_6 (235 and 238 isotopes) is 0.973. Hence, even for large mole fractions the radial change in ϕy_f at equilibrium is not very significant and the term $A(1-\phi y_f)$ may be replaced by $A(1-y_f)$ for all times.

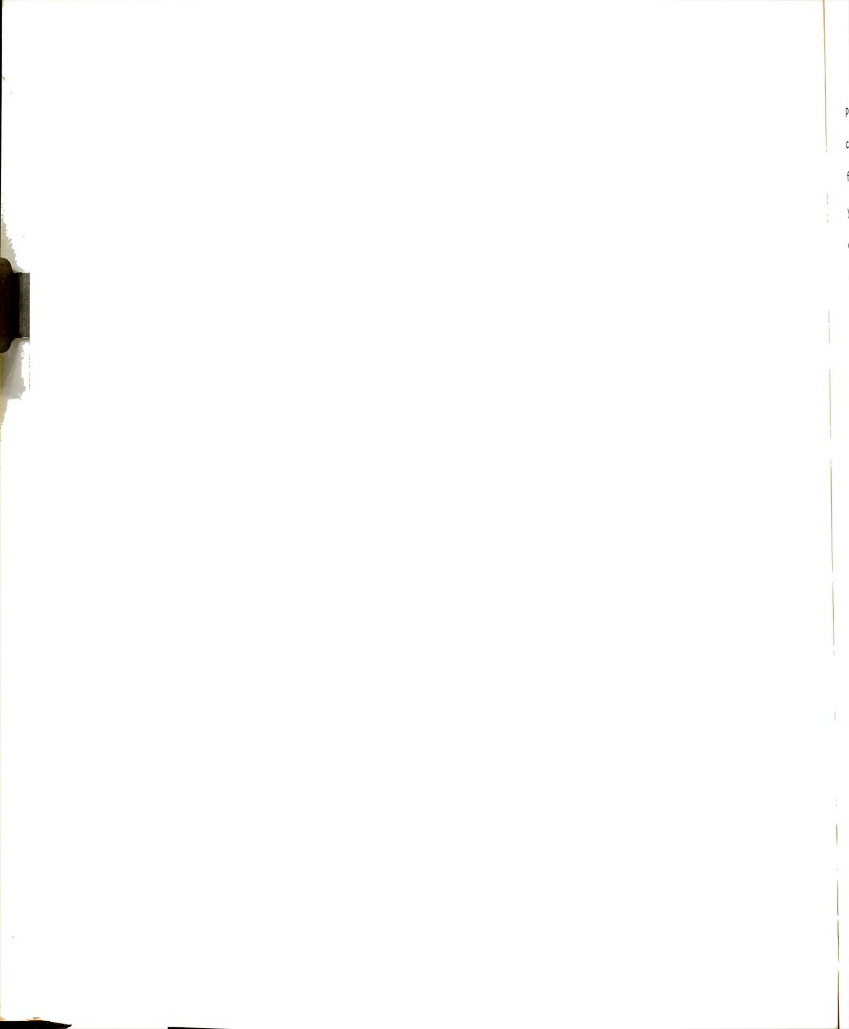
Thus, it would be expected that using the charge composition of 0.002 mole fraction had very little effect on the times for the equilibrium separation to take place and did not bias the times given in Tables 4, 5 and 6. To substantiate this conclusion, consider the gas pair SO_2-N_2 at $70^\circ F$ and 20000 RPM ($R_w = 4$ inches) in the unsteady state operation of the simple centrifuge. For charge mole fractions of SO_2 of 0.002, 0.2, 0.5, 0.75 and 0.9, the values of the quantity $(y-y_f)/(y_e-y_f) \times 100$ at the axis after 81 seconds are 74.8, 75.1, 76.1, 76.8 and 77.1, respectively.

2. As illustrated in Tables 4 and 5, temperature has a substantial effect on the time required for the mole fraction profiles to



develop. The effect of changing the temperature is of an indirect nature, since increasing the temperature from 70°F to 300°F almost doubles the diffusivity (~1.9 times), which in turn almost halves the time for mass transfer to take place. It should be remembered, however, as illustrated in Chapter II-A, that increasing the temperature reduces the effective value of ΔMW (decreases flux due to pressure diffusion), hence decreasing the magnitude of the separation. Along these same lines it should be noted that the ratio of the diffusivities times pressure for SO_2-N_2 at 70°F to the corresponding value for UF_6 at 80°F is 8.3 (Appendix B). This would appear to indicate that if it required 49 seconds in the case of SO_2-N_2 for the dimensionless axis composition $[(y-y_f)/(y_e-y_f)]$ to move within 50% of its equilibrium value, it would require 407 seconds for the corresponding situation to occur for UF_6 due to the much lower radial diffusion flux in the case of UF_6 . However, the actual time calculated for UF_6 is only 13 seconds. The key to this apparent inconsistency is that not only was the charge pressure in the case of the UF_6 1/7 that of the SO_2-N_2 (less total mass present) but at 20000 RPM the much greater molecular weight of UF_6 further reduces the ratio of the pressures at the axis to 0.024. Correcting for such a reduction in the mass present at the axis reduces the expected time from 407 seconds to approximately 10 seconds.

3. Perhaps the most important is the fact that the times required for mass transfer to take place in the gas centrifuge are relatively large when compared to times for mass transfer to take place in conventional gas separation. For example, consider the gas

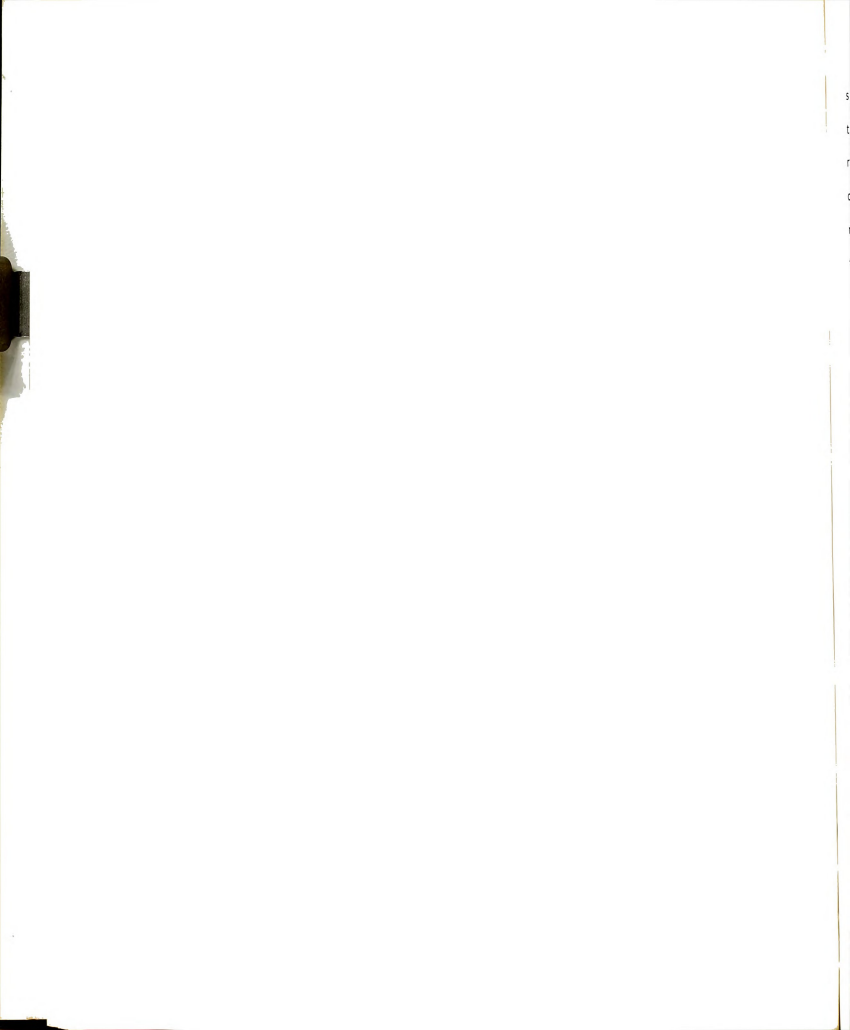


$\text{SO}_2\text{-N}_2$ at 70°F , 10000 RPM and $t = 0$ in the unsteady state simple centrifuge, the flux due to concentration diffusion is zero and the flux due to pressure diffusion is 4.11×10^{-10} lb moles/sec/ft² with $\Delta p = 0.002$ and $r = 2.9$ inches. At future times the net flux, of course, becomes smaller as the flux due to the concentration gradient decreases. In a gas centrifuge with axial flow, the effect of the small net fluxes is to require long residence times.

With these three points the following conclusions can be drawn regarding the production gas centrifuge with a feed and product stream:

1. To make the best use of the small fluxes the device should have an axial countercurrent flow. That is, the device should have an axial flow in one direction and an annular outer flow in the opposite direction. Their combined effect would be to continually retard the establishment of an equilibrium profile, allowing the fullest utilization of the flux by pressure diffusion. Also, separations faster than those in the simple centrifuge could be realized.

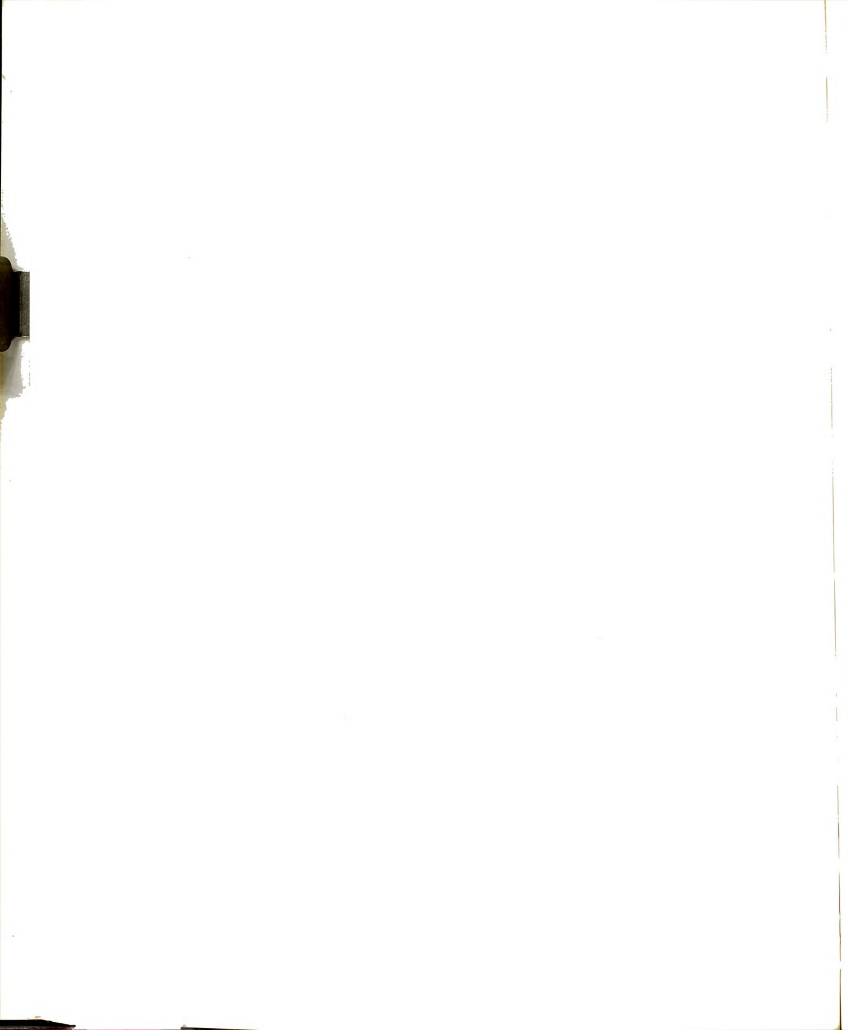
2. As observed in 2 above, the magnitude of the fluxes due to pressure diffusion are very small. In the production centrifuge this means very large residence times will be required for a separation to take place. The significance of this aspect is that the throughput rates will correspondingly have to be very small. This is certainly not in line with the use of the gas centrifuge to process flue gas where the tremendous volumes of gas to be processed necessarily dictate high throughput rates. Although increasing the



size of the centrifuge (increasing the length and/or diameter) rather than decreasing the throughput rate is also a means of increasing the residence time, certain mechanical limitations on the size of the centrifuge as presented in Chapter IV prohibit this from being a reasonable approach. It was shown above that increasing the temperature and hence, increasing the diffusivity, correspondingly increases the radial flux rate, and to a certain degree, provides a means of decreasing the required residence time.

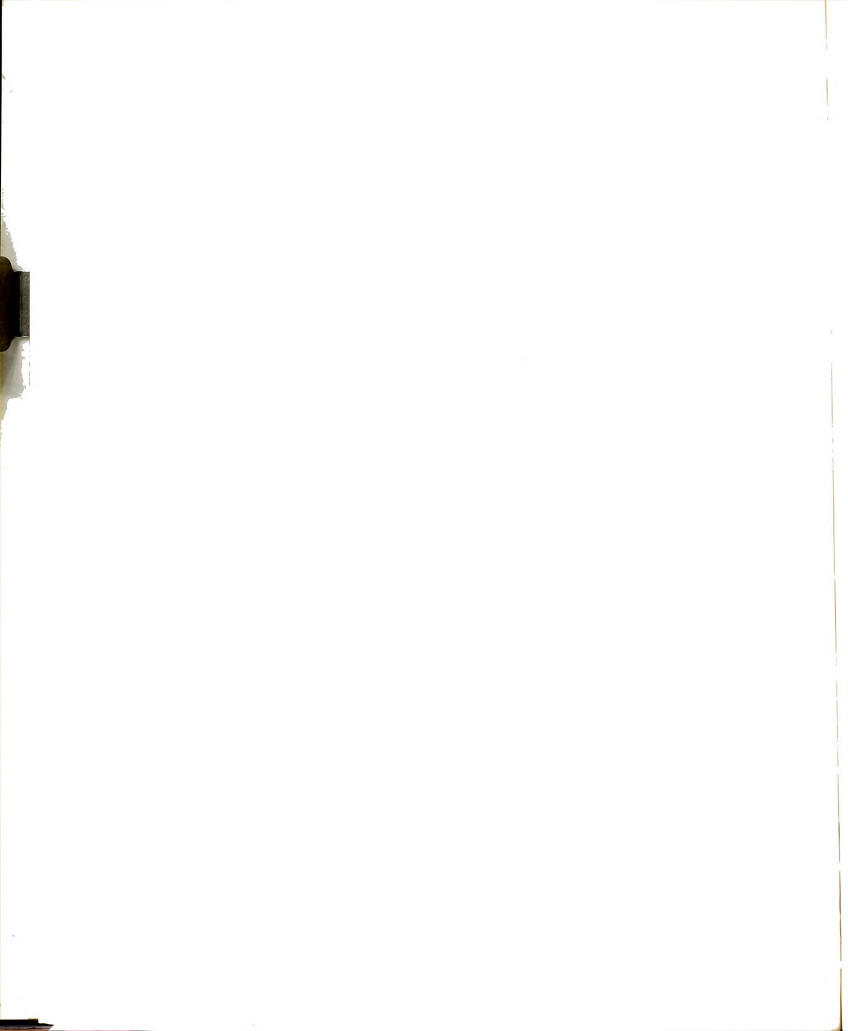
3. The magnitude of the centrifuge's rotation and the charge composition had very little effect on the time required to establish the mole fraction profiles as shown above. Thus, these two parameters can be expected to have very little effect on the residence time required in the production centrifuge, but, of course, have a substantial effect on the magnitude of the separation.

One final point to be mentioned in this chapter is that regarding the magnitude of the pressure changes as the mole fraction profile developed in the unsteady state simple centrifuge. This observation will give insight regarding the importance of including derivatives of pressure with respect to distance in the axial direction when analyzing the production centrifuge. Table 7 contains the total pressure profile at $t = 0$ and at equilibrium for the gas pair $\text{SO}_2\text{-N}_2$ at 70°F and 10000 RPM. Table 7 illustrates that the change in the pressure profile is very small for charge compositions of 0.002, and 0.2 mole fraction of SO_2 . For two heavy gases like UF_6 (U_{235} , U_{238}) with a small molecular weight difference the change in the pressure profile is essentially, for practical purposes, nonexistent.



LE 7.--Total Pressure Profiles in the Unsteady State Simple Centrifuge for the Gas Pair $\text{SO}_2\text{-N}_2$ at 70°F and 10000 RPM. Radius = 4 inches.

r/R_w	Total Pressures (psia)			
	$y_f = 0.002$		$y_f = 0.2$	
	$t = 0$	$t = \infty$	$t = 0$	$t = \infty$
0.0	14.224	14.224	14.106	14.108
0.1	14.233	14.233	14.117	14.119
0.2	14.287	14.287	14.152	14.154
0.3	14.307	14.307	14.210	14.212
0.4	14.372	14.372	14.291	14.293
0.5	14.457	14.457	14.396	14.397
0.6	14.560	14.560	14.525	14.525
0.7	14.684	14.684	14.680	14.680
0.8	14.827	14.827	14.860	14.861
0.9	14.992	14.992	15.067	15.068
1.0	15.178	15.178	15.302	15.303



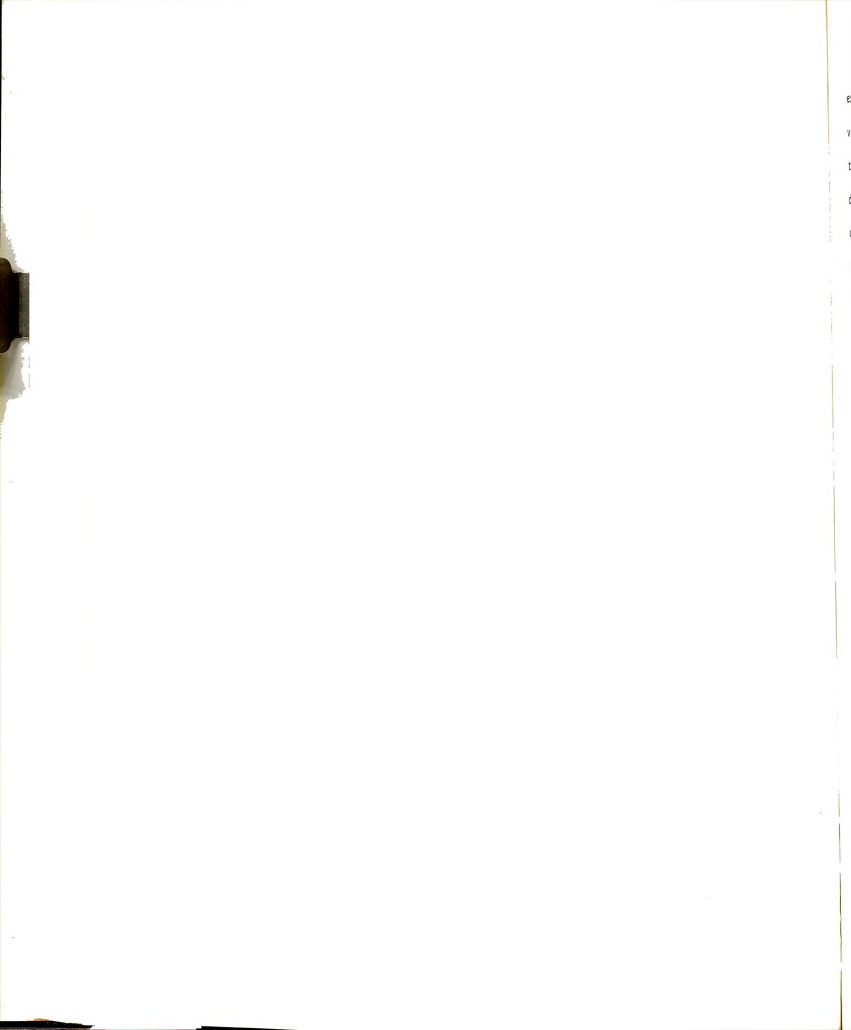
CHAPTER IV

THE ESTIMATION OF THE BURSTING AND WHIRLING SPEEDS OF A GAS CENTRIFUGE

As determined in the previous chapter, large rotational speeds and long residence times are necessary for significant separations to occur in a gas centrifuge. It was also pointed out that for a production centrifuge (feed and product streams) the residence time could be controlled by the size of the centrifuge and/or the feed rate. However, as will be shown in this section, the choice of the rotational speeds and the ratios of length to diameter of a centrifuge are not arbitrary, but must lie in a certain range dictated by the material of which the centrifuge is constructed.

As the rotational speed of a given centrifuge is increased, a point will be reached where either the centrifuge will burst or enter a critical vibrational mode which will destroy it if it is left to operate at this speed. It is possible for both the bursting and whirling speeds to be identical.

The bursting speed can be simply thought of as a speed at which the centrifugal forces acting on the wall of the centrifuge exceed the ultimate (ultimate) strength of the metal (alloy) of which it is composed. The whirling speed, however, is a slightly more complex phenomenon. It is, as the centrifuge is rotating its centerline will not



tly coincide with the geometric centerline due to eccentricities, vibrations and other causes. Hence, due to the inertia of the cylinder, centrifugal forces will produce a bending moment tending to deflect the centerline of rotation even farther from the geometric centerline. These centrifugal forces which are proportional to the rotational speed squared and to the deflection are countered only by the elastic forces of the cylinder. Thus, as the rotational speed is increased a value will be reached where the elastic forces cannot counter the centrifugal forces, and if the centrifuge is left to operate at this speed, it will destroy itself.

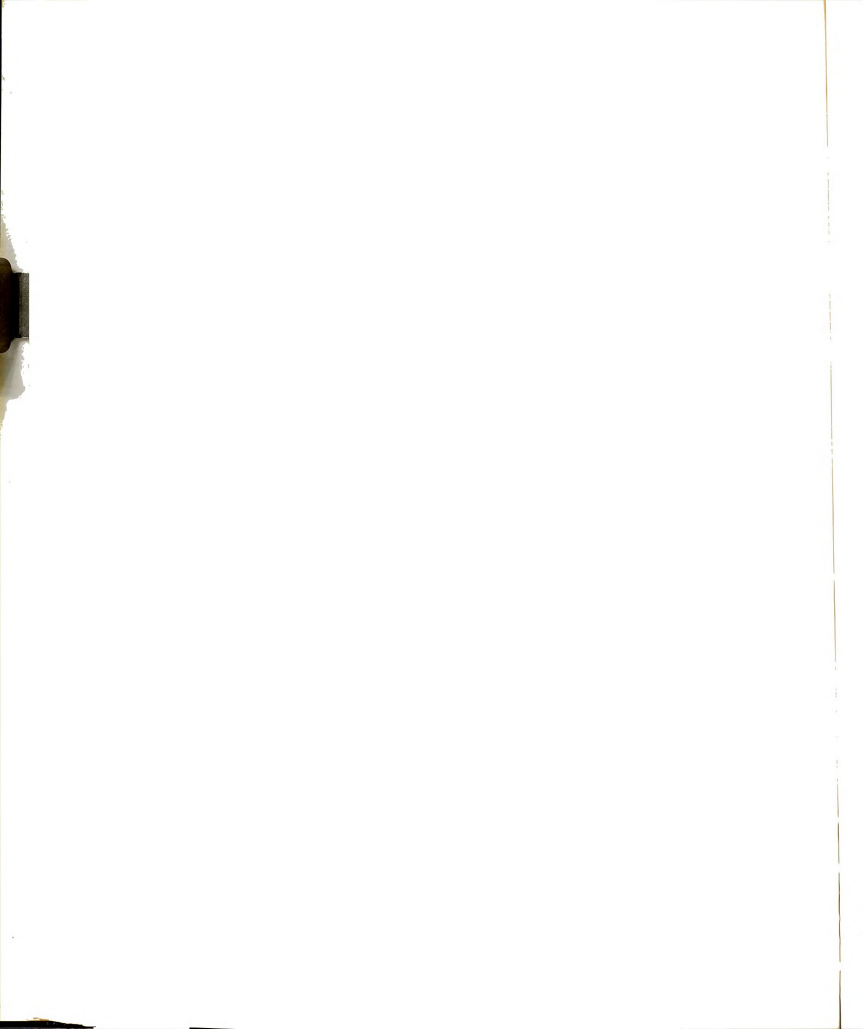
A. Bursting Speed Analysis¹

To determine the intensities of the stresses in a cylinder rotating about its axis a few simple assumptions are made:

1. The material of which it is composed is isotropic.
2. The length of the cylinder is greater than the radius [length to diameter (L/D_0) greater than 1].
3. The principal stresses are in the radial, circumferential, and axial directions.
4. The plane sections perpendicular to the axis remain so after straining due to the rotation of the cylinder. For a long cylinder this is very nearly correct everywhere except near the ends.

Figure 9 illustrates a disk formed by the cutting of a cylinder by two parallel planes Δz apart and perpendicular to the axis of the cylinder. Also shown is a small element of the disk subtended by the

¹This section is composed (in part) of an overview of a detailed analysis dealing with the stresses developed in a rotating cylinder by Morley (12).



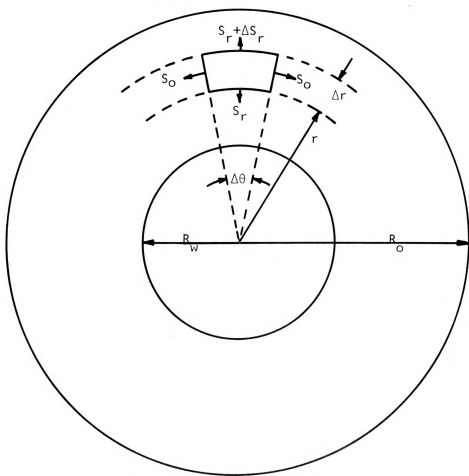
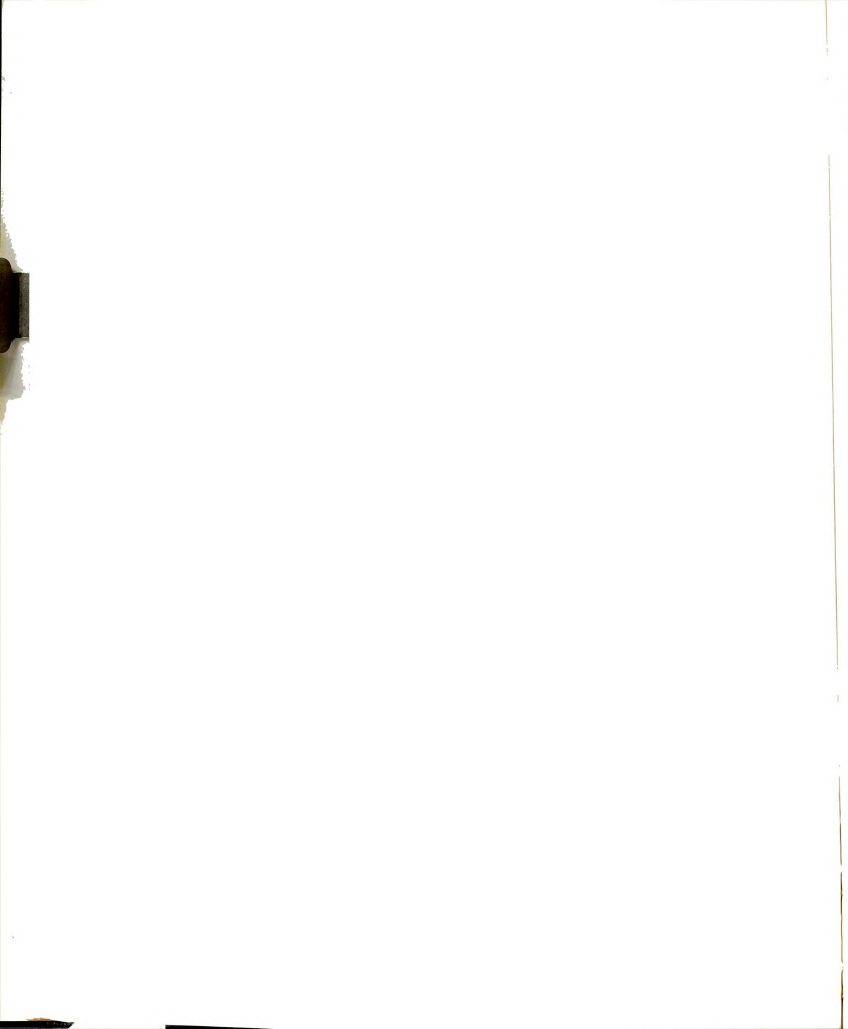


Figure 9.--The Cross Section of a Rotating Cylinder Illustrating Radial and Circumferential Stresses, S_r and S_θ , Acting on a Small Element.



angle $\Delta\theta$, with width Δr and thickness Δz . The volume of the mass contained in the element is given by

$$v = r \Delta r \Delta\theta \Delta z,$$

and the centrifugal force acting on this element is given by

$$F_c = \frac{\rho}{g_c} \omega^2 r^2 \Delta r \Delta\theta \Delta z$$

after neglecting second order quantities. The quantity ρ is the density of the material.

The centrifugal force acting on the element is countered by the equal and opposite forces due to the radial and circumferential stresses S_r and S_θ . The force due to these stresses is given by

$$F_s = \Delta z \left[2 S_\theta \sin \frac{\Delta\theta}{2} \Delta r + 2 S_r r \sin \frac{\Delta\theta}{2} - 2(S_r + \Delta S_r) \cdot (r + \Delta r) \sin \frac{\Delta\theta}{2} \right].$$

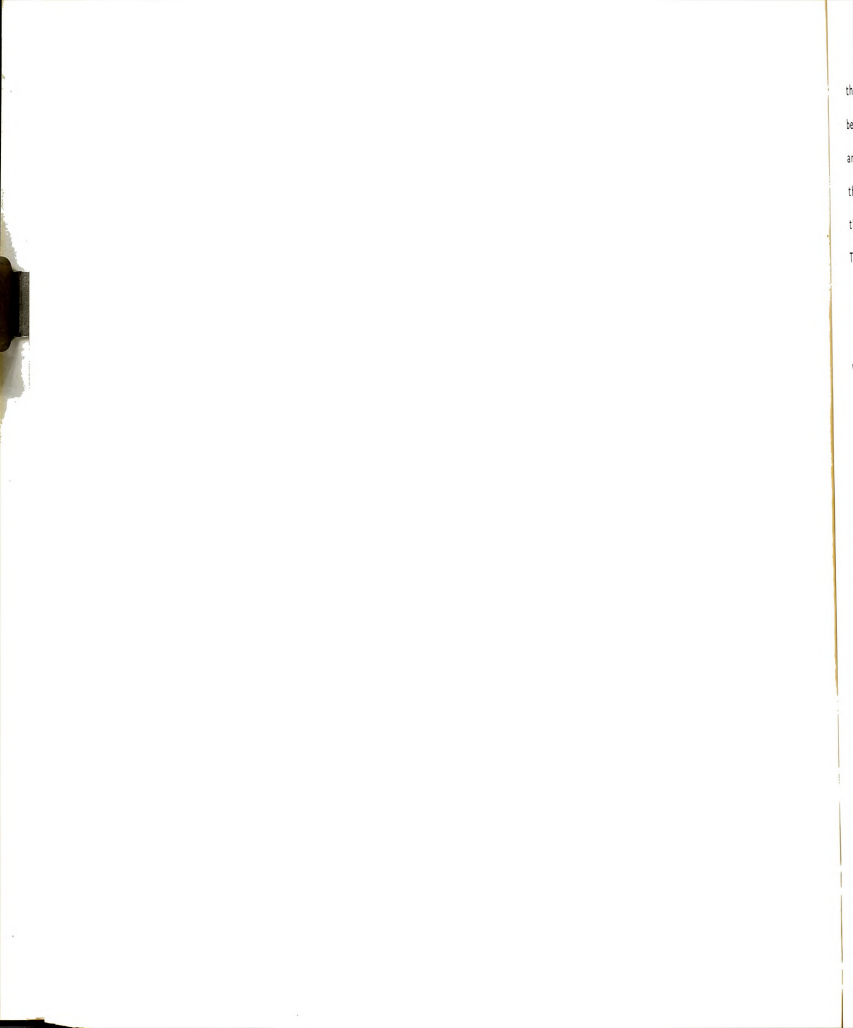
For small angles, $\sin \frac{\Delta\theta}{2}$ is approximately $\frac{\Delta\theta}{2}$ and the above expression reduces to

$$F_s = \Delta z \Delta\theta (S_\theta \Delta r - S_r \Delta r - r \Delta S_r).$$

Equating F_c and F_s and taking the limit as Δr , $\Delta\theta$, and Δz go to zero gives

$$F = \frac{\rho \omega^2 r^2}{g_c} + S_r + \frac{r dS_r}{dr}.$$

The circumferential stress, or hoop tension as it is sometimes called, is the quantity of interest, since as S_θ approaches the yield point of



the material, bursting will occur. To determine S_θ , however, use must be made of the strains taking place as the stresses, S_r , S_θ , and S_z , are applied. The strain in the θ direction is given by the ratio of the stress in that direction to Young's modulus of elasticity (E) minus the contraction that takes place due to the r and z direction stresses. That is,

$$e_\theta = [S_\theta - p(S_r + S_z)]/E,$$

where p is Poisson's ratio which varies from .25 for steel to .33 for aluminum. Likewise the strains in the r and z directions are given by

$$e_r = [S_r - p(S_\theta + S_z)]/E, \text{ and}$$

$$e_z = [S_z - p(S_r + S_\theta)]/E.$$

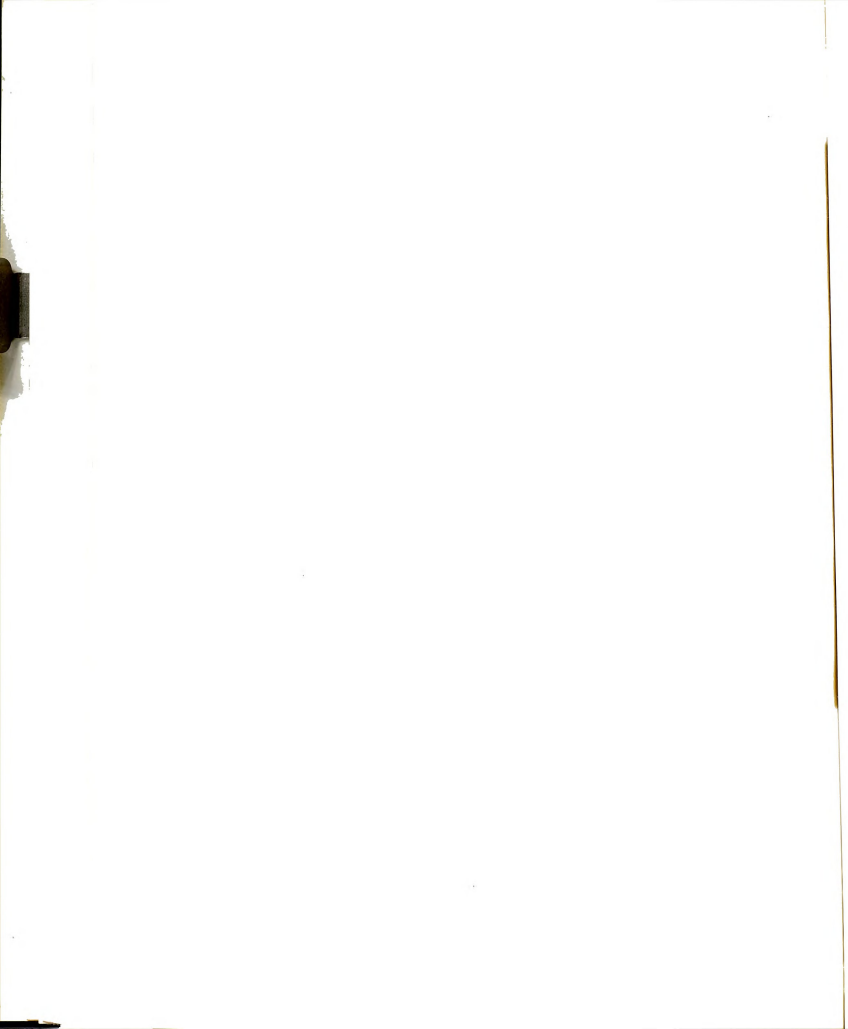
If as assumed, the displacement of points in the disk are purely radial then the points at a position r move to a position r + q and the circumferential strain can also be written as

$$e_\theta = \frac{2\pi(r+q) - 2\pi r}{2\pi r} = \frac{q}{r},$$

and the radial strain is given by

$$e_r = \frac{dq}{dr}.$$

Substituting these expressions in the strain equations and solving for S_r and S_θ gives



$$S_r = \frac{Ep}{(1-2p)(1+p)} \left[\frac{(1-p)}{p} \frac{dq}{dr} + \frac{q}{r} + e_z \right] \quad \text{and}$$

$$S_\theta = \frac{Ep}{(1-2p)(1+p)} \left[\frac{(1-p)}{p} \frac{q}{r} + \frac{dq}{dr} + e_z \right] .$$

using assumption 4 (plane sections remain perpendicular after strain) e_z must be constant with respect to r . Thus, the above expressions for S_r and S_θ may be substituted into the force balance equation giving

$$\frac{r}{dr} \frac{d^2 q}{dr^2} + \frac{dq}{dr} - \frac{q}{r} + \frac{\rho \omega^2}{g_c} \frac{(1+p)(1-2p)}{E(1-p)} r^2 = 0 .$$

One additional equation must be used to determine e_z . This equation can be written by symmetry considerations, since, midway between the ends of the cylinder there can be no net forces in the axial direction. Thus, the following equation can be written

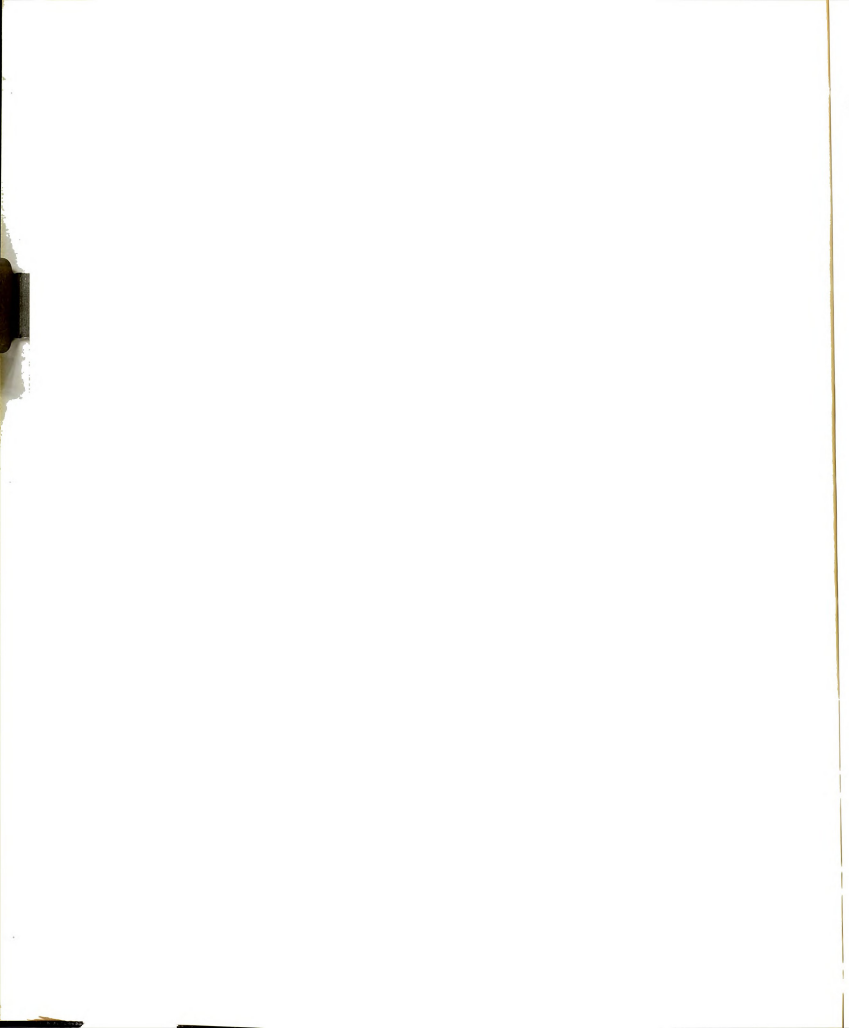
$$2\pi \int_{R_w}^{R_o} S_z \, r dr = 0 .$$

Integrating the second order ordinary differential equation for q and using the boundary conditions plus the above equation gives

$$= \frac{\rho \omega^2}{g_c 8E} \left[\frac{(3-5p)}{(1-p)} (R_w^2 + R_o^2) + \frac{(1+p)(3-2p)}{(1-p)} \frac{R_o^2 R_w^2}{r^2} - \frac{(1+p)(1-2p)}{(1-p)} r^2 \right] .$$

The circumferential stress is then given by

$$S_\theta = \frac{\rho \omega^2}{8g_c} \left[\frac{(3-2p)}{(1-p)} (R_o^2 + R_w^2) + \frac{R_o^2 R_w^2}{r^2} - \frac{(1+2p)}{(1-p)} r^2 \right] ,$$



and has its maximum value at R_w , given by

$$S_{\theta(\max)} = \frac{\rho \omega^2}{4g_c} \left[\frac{(3-2p)}{(1-p)} R_o^2 + \frac{(1-2p)}{(1-p)} R_w^2 \right] .$$

The above expression can be rewritten in a more general form as

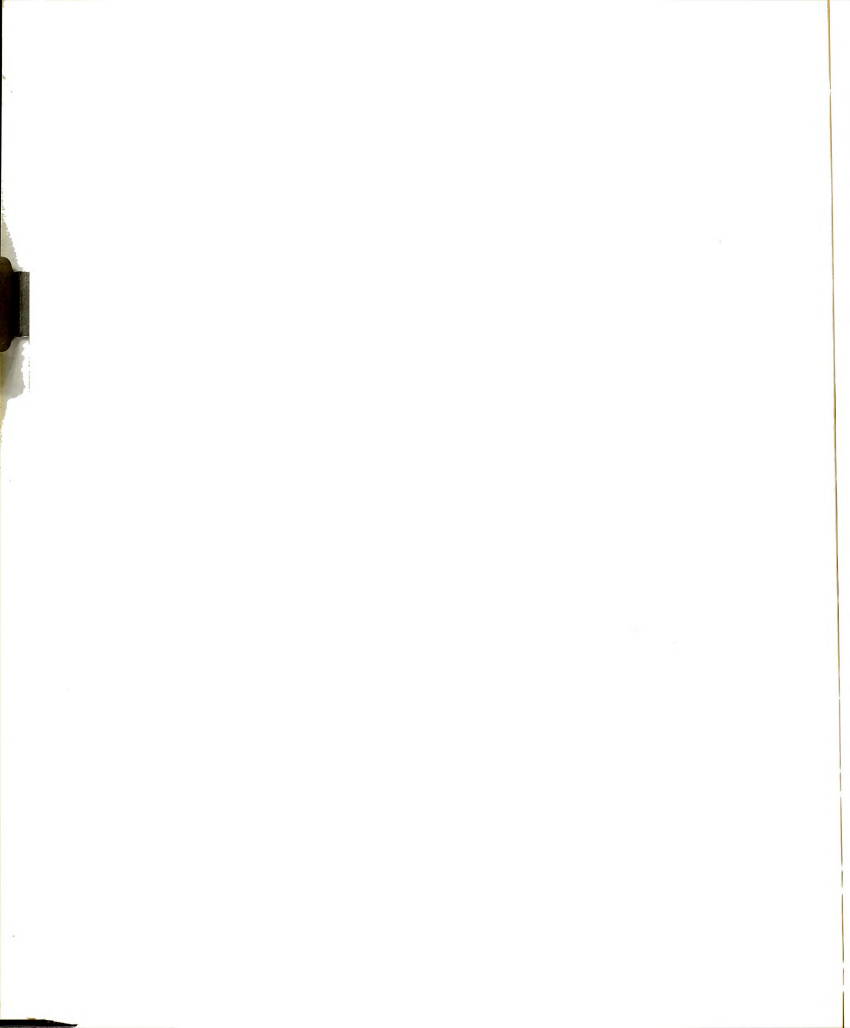
$$\frac{S_{\theta(\max)}}{\rho/g_c} = \frac{s_o^2}{4} \left[\frac{(3-2p)}{(1-p)} + \frac{(1-2p)}{(1-p)} k^2 \right] ,$$

where s_o = the outer peripheral speed, ωR_o , and $k = R_w/R_o$.

Using a value of .33 for Poisson's ratio for common materials of the construction of a centrifuge (Aluminum alloys, and Magnesium alloys) is on the side of safety and simplifies the above equation, giving

$$\frac{S_{\theta(\max)}}{\rho/g_c} = \frac{s_o^2}{8} (3 + 5k^2) .$$

Figure 10 contains a plot of $S_{\theta(\max)}/(\rho/g_c)$ versus s_o for k values of 0.9, 0.95, and 1.0. Data used to construct Figure 10 can be found in Appendix A. At each outer peripheral speed, s_o , the value $S_{\theta(\max)}/(\rho/g_c)$ must lie below (within a certain safety factor) the value $Y/(\rho/g_c)$ corresponding to the metal or alloy of which the cylinder in question is composed. The quantity Y is the yield (ultimate) strength of the metal or alloy. Table 8 contains some values of the ratio of the yield (ultimate) strength to density for some common metals and their alloys, computed from data taken from Perry's Chemical Engineers' Handbook (13). As can be seen by comparing Figure 10 with alloys in Table 8,



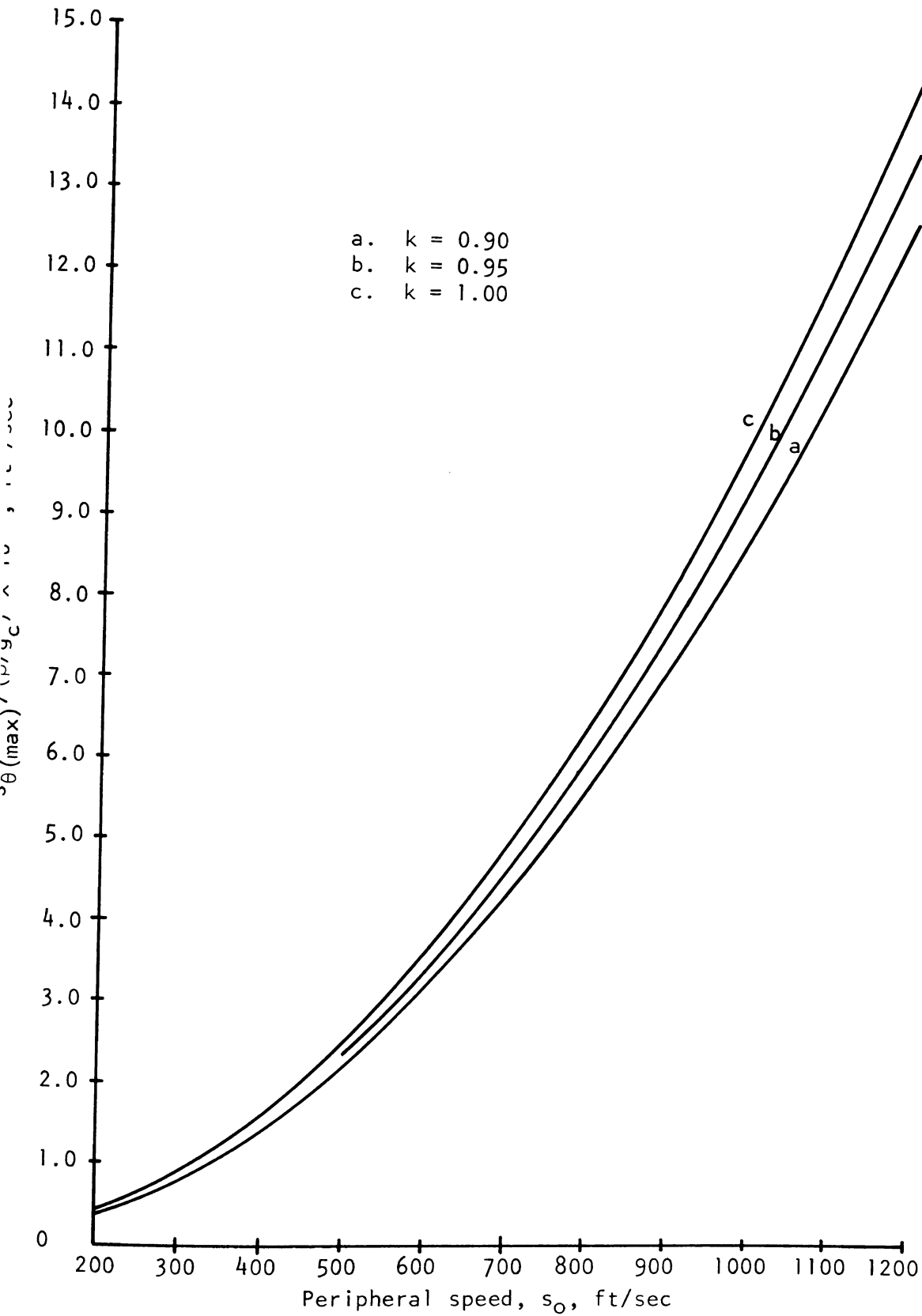


Figure 10.-- $\omega_{\theta(\max)} / (\rho/g_c)$ Versus Peripheral Speed, s_o , for values of 0.90, 0.95, and 1.00.

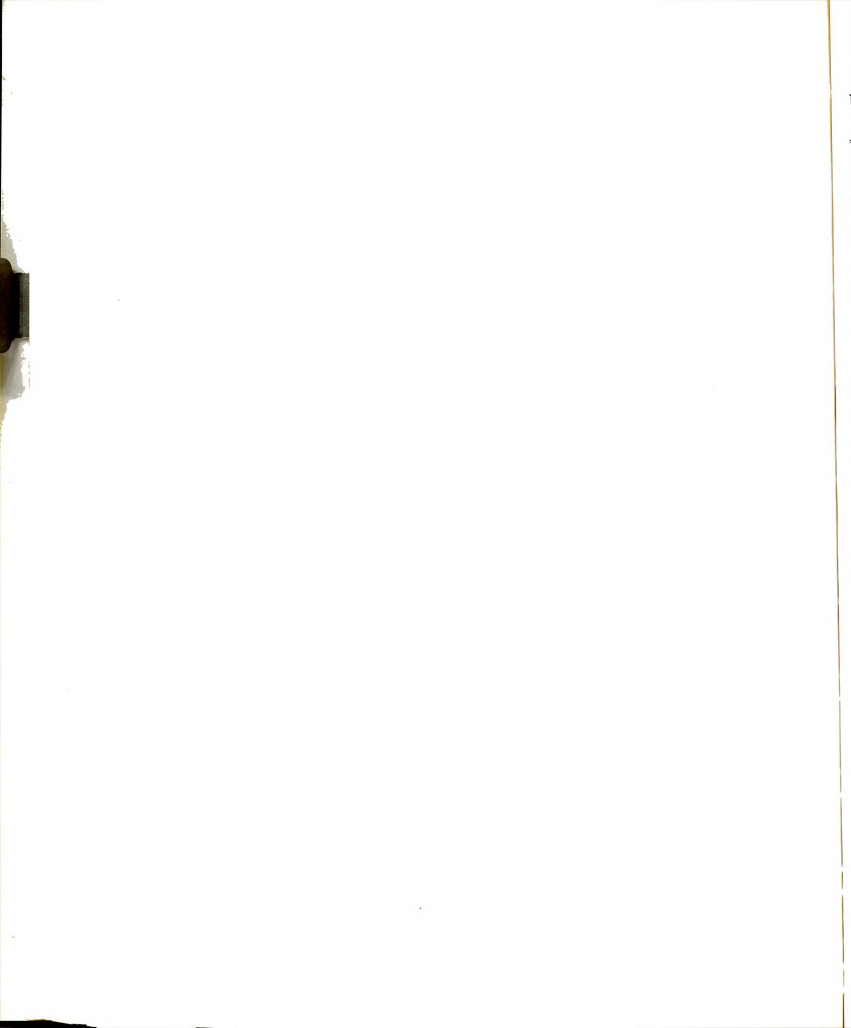


TABLE 8.--Ratios of Yield (Ultimate) Strength to Density for Some Common Metals and Their Alloys.

Alloy	Condition	$Y/(\rho/g_c) \times 10^{-5},$ ft^2/sec^2
Aluminum		
alloy 1100	99+% cold-rolled-H14	4.65
alloy 2017	Heat treated T4	10.62
alloy 7075	Heat treated T6	19.38
Red Brass (wrought)	Cold drawn	1.74
Cartridge Brass	Cold rolled	5.48
Magnesium		
alloy AZ80A	Extruded	14.85
Carbon Steel	Hot rolled	3.97
Wrought Iron (pipe)	Hot rolled	2.89

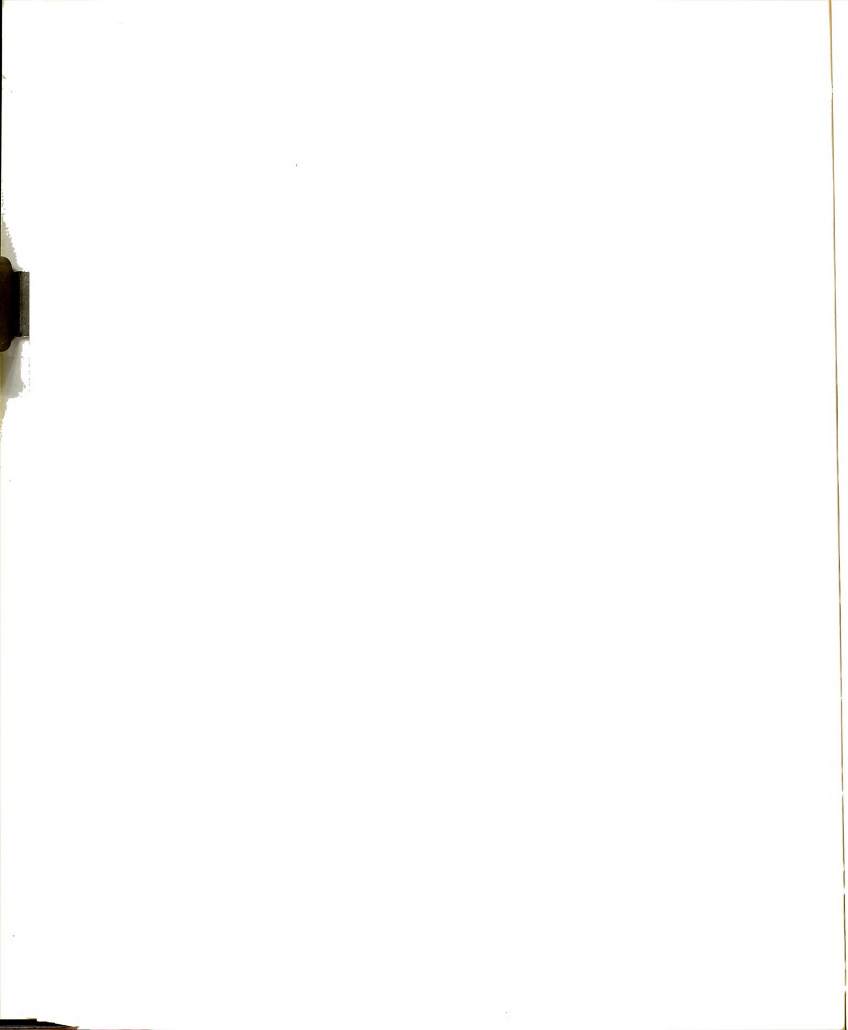
the alloys of Aluminum and Magnesium are the only materials that can safely be used to construct a centrifuge where a typical peripheral velocity might be 700 ft/sec ($R_o = 4$ inches, $\omega = 20000$ RPM).

B. Whirling Speed Analysis²

To determine the whirling speeds of a centrifuge the following assumptions are made:

1. The material of which the centrifuge is composed is isotropic.
2. The centrifuge can be thought of as a uniform shaft simply supported at both ends; i.e., neither end can be displaced nor support a bending moment.

²Contained in this section is information taken (in part) from the analyses of buckling shafts by J. P. DenHartog (14).



3. The only thrust felt by the centrifuge will be due to the weight of the top end cap. This is assumed even though the material at the base of the centrifuge must support the weight of the centrifuge above it plus the end cap. Whereas, the material at the top of the centrifuge need only support the end cap. The validity of this assumption will be evaluated later.

Let y be the deflection of the shaft from the geometric centerline at a distance z from one end. The centrifugal force acting on the shaft at this point is given by

$$F_c = m\omega^2 y / g_c ,$$

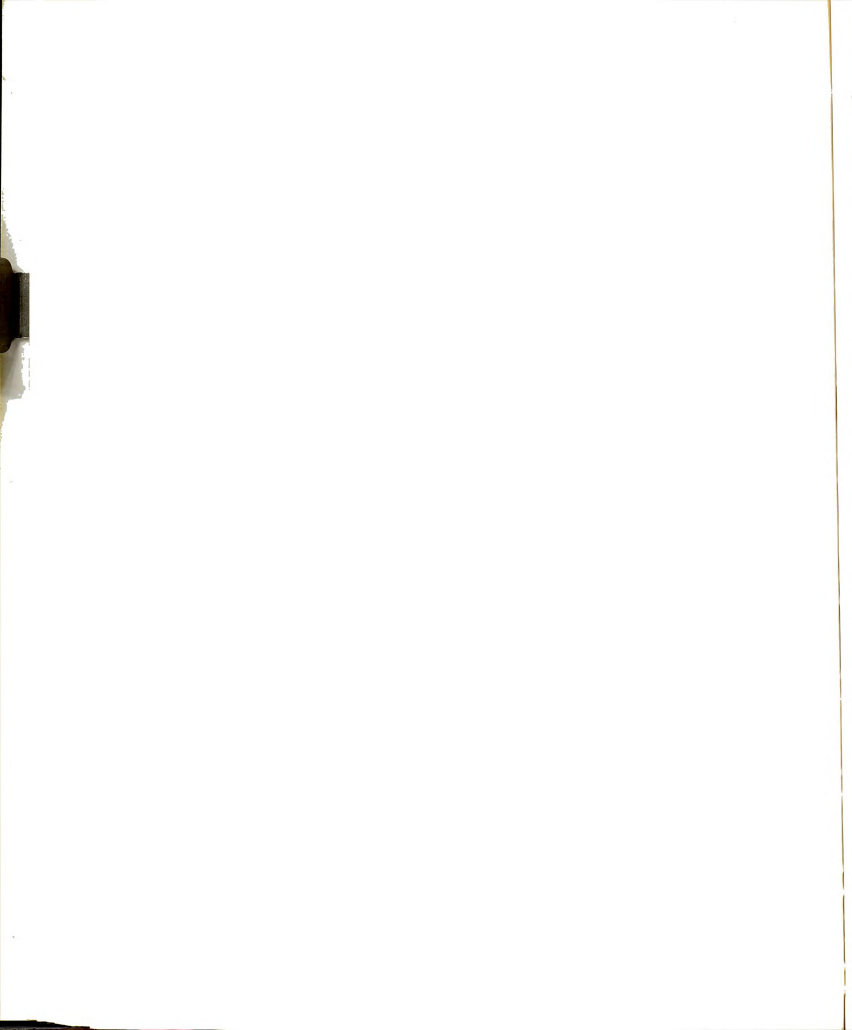
where m = the mass per unit length $= \pi(R_o^2 - R_w^2)\rho$.

Since the shaft will be concave to its unstrained position, the sign convention is to consider the bending moment due to the end cap weight as negative, i.e.,

$$F_w = -Wy ,$$

where W = the weight of the end cap. The total bending moment is then the sum of that due to the centrifugal force and the end cap weight and must be countered by the stiffness of the shaft. This fact may be expressed as follows:

$$EI \frac{d^4 y}{dz^4} + W \frac{d^2 y}{dz^2} - m \frac{\omega^2 y}{g_c} = 0 ,$$



where E = modulus of elasticity, and

I = the moment of inertia of the cross-sectional area about a diameter, $\pi(R_O^4 - R_W^4)/4$.

The boundary conditions as stated in assumption 2 can be written as

$$y = \frac{d^2 y}{dz^2} = 0 \quad \text{at } z = 0, \text{ and}$$

$$y = \frac{d^2 y}{dz^2} = 0 \quad \text{at } z = L.$$

The fourth order ordinary differential equation for the deflections has the complete solution

$$y = A \cos c_1 z + B \sin c_1 z + C \cosh c_2 z + D \sinh c_2 z$$

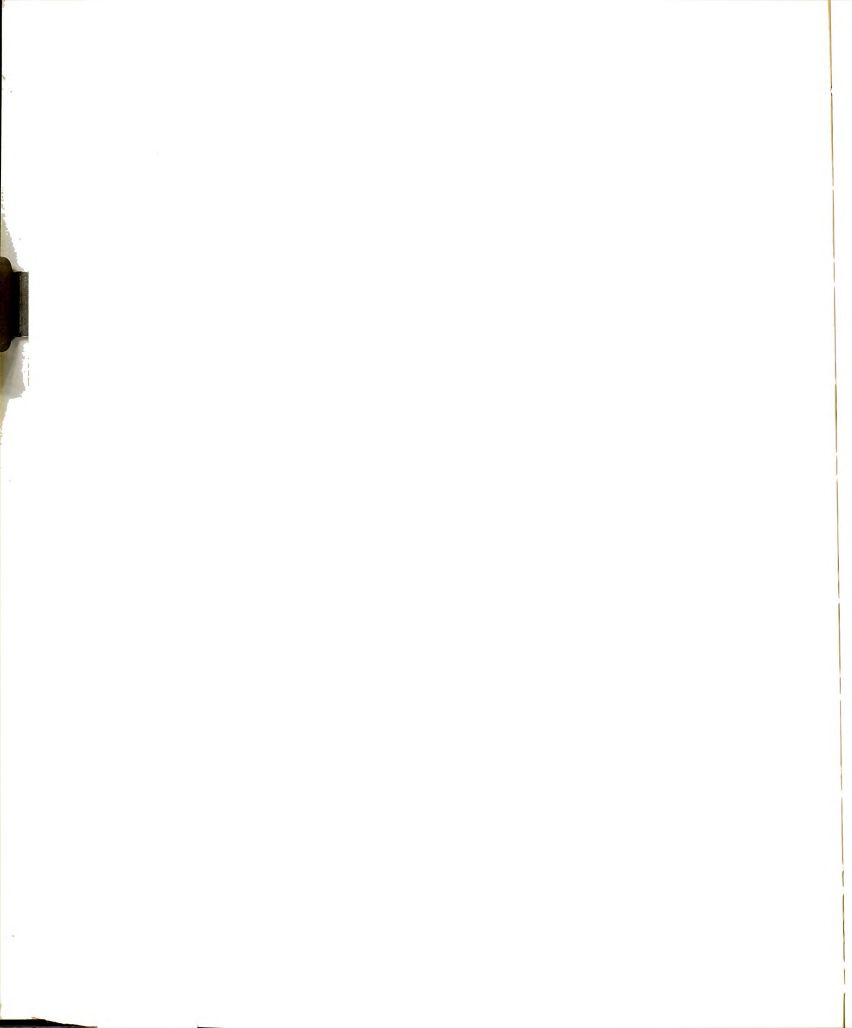
where

$$c_1^2 = \left[\frac{W^2}{4(EI)^2} + \frac{m\omega^2}{9_c EI} \right]^{1/2} + \frac{W}{2EI},$$

$$c_2^2 = \left[\frac{W^2}{4(EI)^2} + \frac{m\omega^2}{9_c EI} \right]^{1/2} - \frac{W}{2EI},$$

and A , B , C , and D are constants.

Using the boundary conditions that y and $d^2 y/dz^2$ are zero at $z = 0$, it may be concluded that $A = 0$ and $C = 0$. Applying the boundary conditions at $z = L$ gives the two equations



$$B \sin c_1 L + D \sinh c_2 L = 0 \quad \text{and}$$

$$-B c_1^2 \sin c_1 L + D c_2^2 \sinh c_2 L = 0 ,$$

which may be solved, giving

$$(c_1^2 + c_2^2) D \sinh c_2 L = 0 \quad \text{and}$$

$$(c_1^2 + c_2^2) B \sin c_1 L = 0 .$$

Since the quantity $(c_1^2 + c_2^2)$ cannot be zero and $\sinh$ is only zero when its argument is zero, $D = 0$. If B was also zero, the solution would be the trivial solution, $y = 0$. To avoid this situation the values of $c_1 L$ must be multiples of π so that $\sin c_1 L = 0$, i.e., $c_1 L = \pi, 2\pi, 3\pi$, etc. Thus, there exists characteristic values of ω such that $c_1 L$ is exact multiples of π and the deflection, y , is undefined. These values of ω are the so-called "whirling speeds" of the shaft.

In the remainder of this analysis only the lowest whirling speed, corresponding to $c_1 L = \pi$, will be considered, i.e.,

$$\left[\frac{W^2}{4(EI)^2} + \frac{m\omega^2}{g_c EI} \right]^{1/2} + \frac{W}{2EI} = \frac{\pi^2}{L^2} .$$

Squaring and rearranging the terms in the above equation gives the following:

$$\omega^2 = \frac{\pi^4}{L^4} \left(\frac{g_c EI}{m} \right) - \frac{\pi^2 g_c W}{m L^2} .$$

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At this point the validity of assumption 3 can be tested by using $\bar{\omega}$ as the whirling speed obtained had only the centrifugal force been taken into account, i.e.,

$$\bar{\omega}^2 = \frac{\pi^4}{L^4} \frac{g_c EI}{m} ,$$

W has been replaced by zero. Taking the ratio of the two critical speeds gives

$$\frac{\omega}{\bar{\omega}} = \left(1 - \frac{L^2 W}{\pi^2 EI}\right)^{1/2} .$$

From this expression, an upper limit can be found for W, such that $\omega/\bar{\omega}$ is no smaller than 0.99. The upper bound placed on W by this restriction may be written as

$$W \leq 0.0199 \pi^2 EI / L^2 .$$

To evaluate the actual magnitudes of W, consider centrifuges 18 inches long and constructed from one of the alloys of Aluminum which typically have moduli of elasticities around 10.2×10^6 lb/in² and densities around 0.1 lb_m/in³. By assuming radii of 2, 3, 4 inches and different wall thickness, several corresponding values of the upper bound of W can be computed. These values are presented in Table 9. The results in Table 9 indicate how very large end cap weights must be to affect the critical speeds by 1%. Furthermore, when the large values of W are compared to the various weights of the

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9.--Upper Bounds for W for an Aluminum Alloy Centrifuge 40 Inches Long.

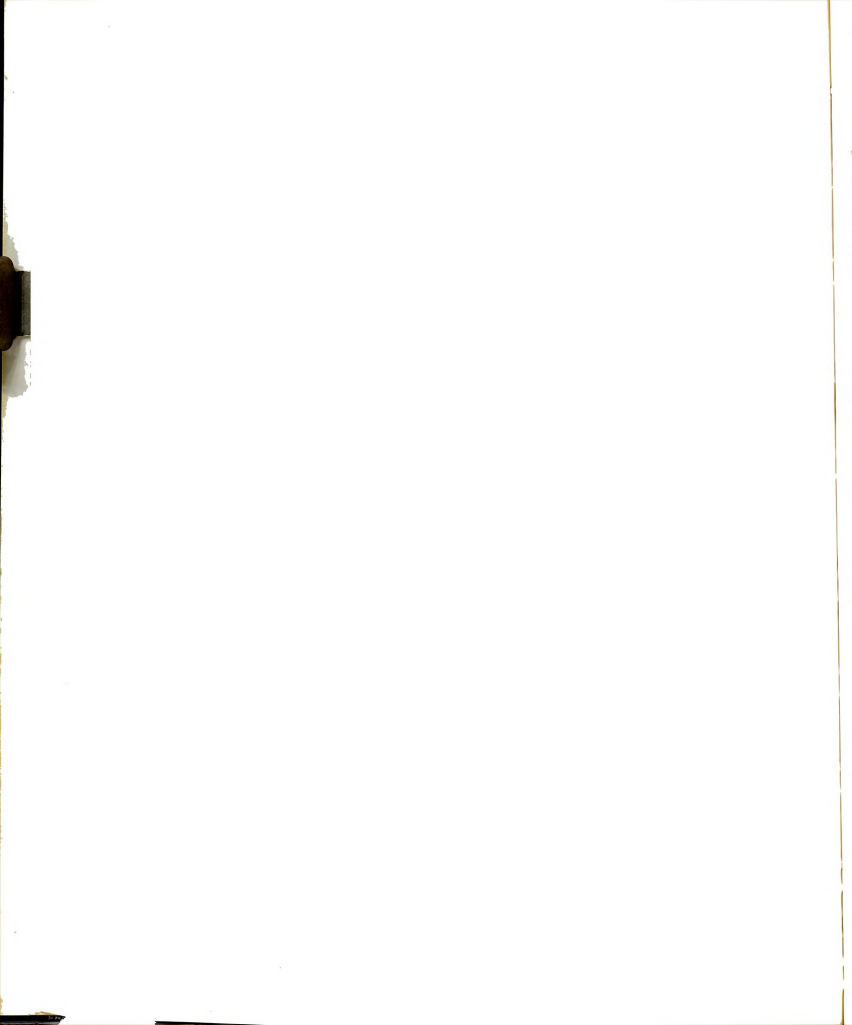
$E = 10.2 \times 10^6 \text{ lb}_f/\text{in}^2, \rho = 0.1 \text{ lb}_m/\text{in}^3$			
Radius (inches)	Wall Thickness (inches)	Centrifuge Weight (lb _f)	W (lb _f)
2	1/4	11.8	6511
	1/8	6.1	3580
	1/16	3.1	1876
	1/32	1.6	961
3	1/4	18.1	23410
	1/8	9.2	12470
	1/16	4.7	6433
	1/32	2.3	3267
4	1/4	24.3	57280
	1/8	12.4	30020
	1/16	6.2	15370
	1/32	3.1	7775

ifuges the assumption made to neglect the effect of the weight
e centrifuge itself is valid.

Dropping the special symbols used to differentiate between
two critical speeds and hence dropping the term involving W, the
wing general expression may be written:

$$\omega^2 = \frac{\pi}{L} \frac{g_c E R_o^2}{4\rho} (1+k^2),$$

$\pi(R_o^4 - R_w^4)/4$ and $\pi\rho(R_o^2 - R_w^2)$ have been substituted for I and m
ctively. k is the ratio of inner to outer radii as previously
ed. The above expression may be further generalized as follows:



$$E/(\rho/g_c) = \frac{64}{(1+k^2)\pi^4} \left(\frac{L}{D_o}\right)^4 s_o^2 ,$$

D_o = the outside diameter, and s_o = outer peripheral speed.

Figure 11 contains a plot of $E/(\rho/g_c)$ versus s_o for L/D_o values of

3, 5, and 6. To construct Figure 11, a value of 0.95 was chosen

for k . Data used to construct Figure 11 can be found in Appendix A.

To operate below the whirling speed a given centrifuge design

rotational speed must be adjusted so that the value of

$E/(\rho/g_c)$ read from Figure 11 is less than the value of $E/(\rho/g_c)$ for

material of construction (within certain safety limits). Table 10

gives the ratio of the elastic modulus to the density for some

metals and their alloys. These values are computed from data

from Perry's Chemical Engineers' Handbook (13).

As can be seen from Table 10, all the metal and alloys,

except for Brass, have essentially the same value of $E/(\rho/g_c)$.

From the conclusion derived from the bursting analysis, that only

Aluminum and Magnesium alloys (of those investigated) were acceptable,

no restrictions have to be modified. However, what the whirling analysis

provides are restrictions on the length to diameter ratio of the

centrifuge. For example, an Aluminum alloy centrifuge with an

outside diameter, 1/4-inch wall, and rotating at 20000 RPM, must be

12 inches or less in length to maintain a safety factor of 15% below

the first critical value of L/D_o .

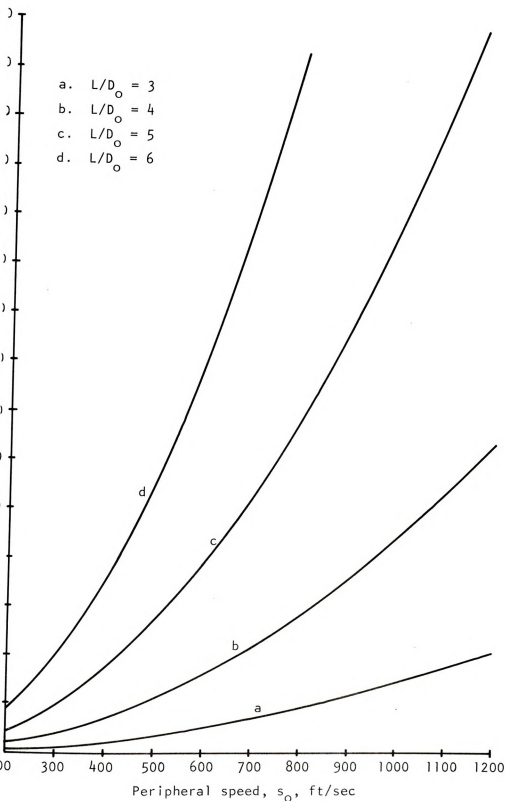


Figure 11.--Critical Elastic Modulus Over Density, $E/(\rho/g_c)$ versus Peripheral Speed, s_o , for Length to Diameter Ratios, L/D_o of 3, 4, 5, and 6.

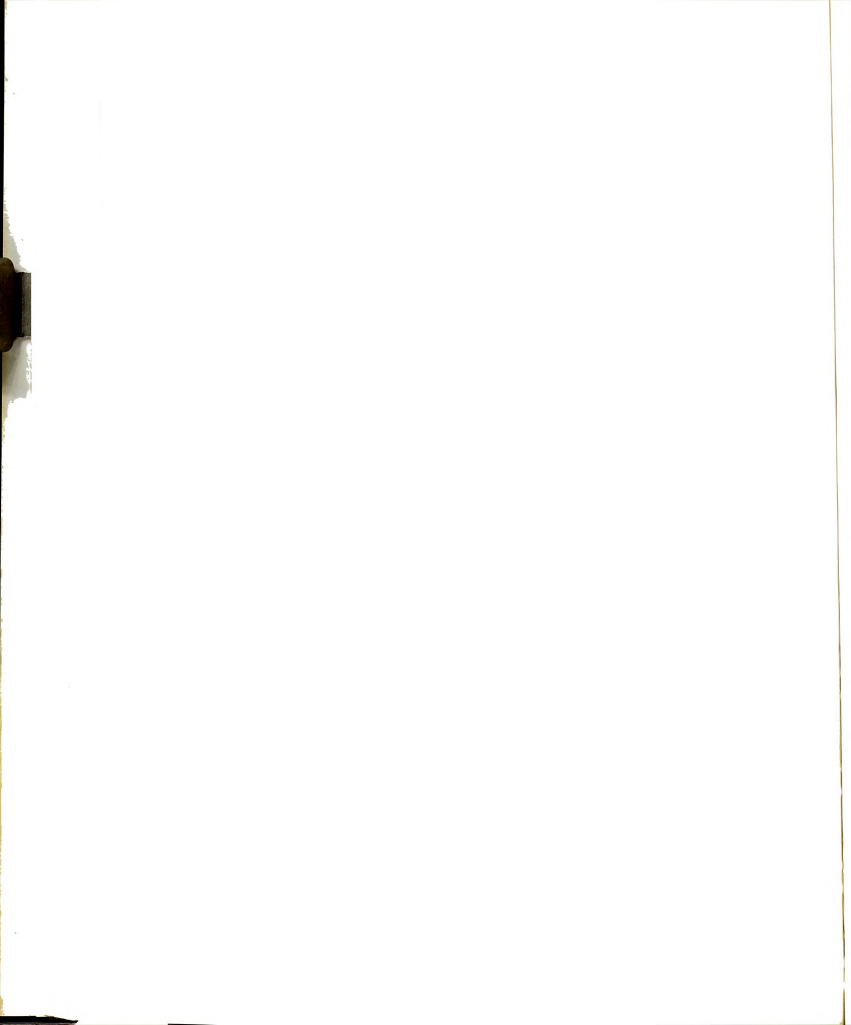
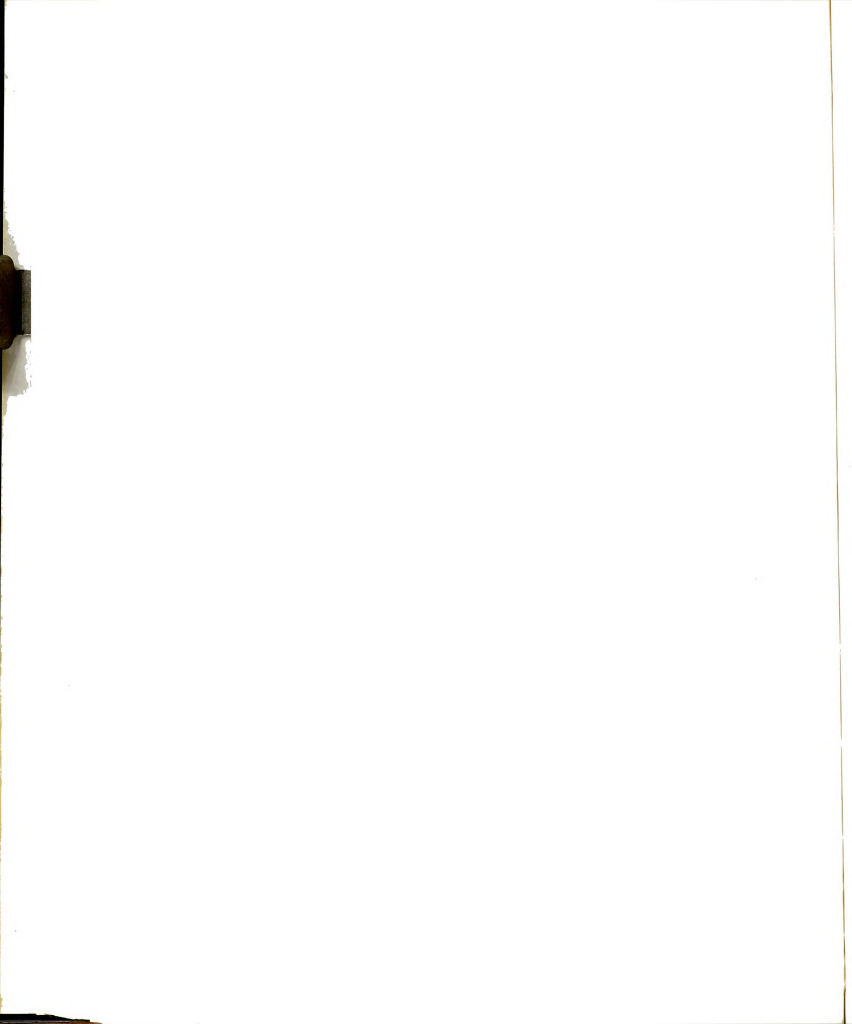


TABLE 10.--Ratios of the Elastic Modulus to Density for Some Common Metals and Their Alloys.

Alloy	Condition	$E/(\rho/g_c) \times 10^{-6}$, ft ² /sec ²
Aluminum		
Alloy 1100	99+ % cold-rolled-H14	273.6
Alloy 2017	Heat treated T4	278.7
Alloy 7075	Heat treated T6	276.1
Brass (wrought)	Cold drawn	144.2
Cartridge Brass	Cold rolled	139.3
Titanium		
Alloy AZ80A	Extruded	268.1
Carbon Steel	Hot rolled	283.2
Cast Iron (pipe)	Hot rolled	279.7

To keep the sizes and rotational speeds realistic, the analyses undertaken in the remaining chapters of this work will have incorporated them the restrictions on the rotational speed and on the length to diameter ratio established in the above two sections (A and B). To facilitate this, it will further be assumed that the material of construction of all centrifuge designs is either an Aluminum or titanium alloy.



CHAPTER V

THE COUNTERCURRENT PRODUCTION CENTRIFUGE

Figure 12 illustrates a countercurrent rectifying (enriches heavy species) centrifuge. The feed gas stream enters at the top of the centrifuge and proceeds downward in an annular stream, near the periphery. As the outer annular stream passes down the centrifuge, it is enriched in the heavy species by the radial flux of the light species from the inner stream. After the outer stream leaves the centrifuge, a portion of it is directed off as the rich product stream and the remainder recycled to the centrifuge. The recycle stream enters the bottom of the centrifuge flowing upward in the inner stream. The inner stream leaving the top of the centrifuge is the lean product stream.

Not illustrated is a countercurrent stripping centrifuge. In this type of centrifuge the feed would enter the bottom of the centrifuge flowing upward in the inner stream. A portion of the inner stream leaving the top of the centrifuge is directed off as the lean product stream with the remainder recycled to the centrifuge. The recycle stream entering the top of the centrifuge would proceed downward in the annular outer stream. The outer stream leaving the bottom of the centrifuge would be the rich product stream.

- a. Feed stream
- b. Rich product stream
- c. Light product stream
- d. Recycle Stream

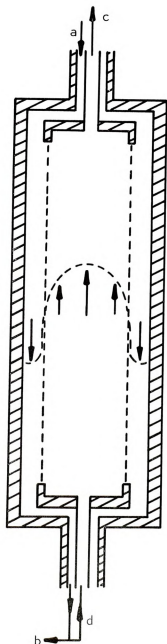
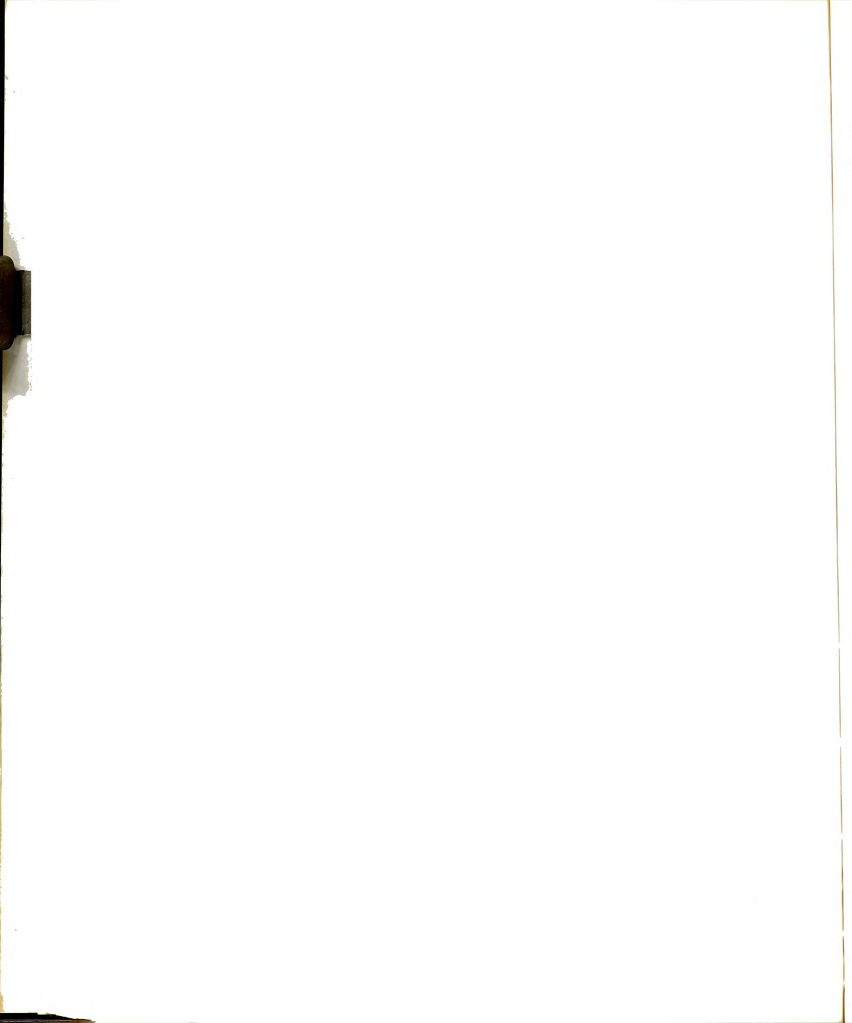


Figure 12.--Countercurrent Rectifying Centrifuge Illustrating Outer Axial Flows and Feed and Product Streams.



It is worth mentioning at this point that a rectifying centrifuge produces a richer heavy product stream than does a stripping centrifuge. The opposite is true if a lean stream containing the maximum amount of the heavy species is desired. This result has analogies with the distillation of a binary mixture in a rectifying or stripping column where in centrifugation the heavy species may be transferred to the more volatile component in distillation.

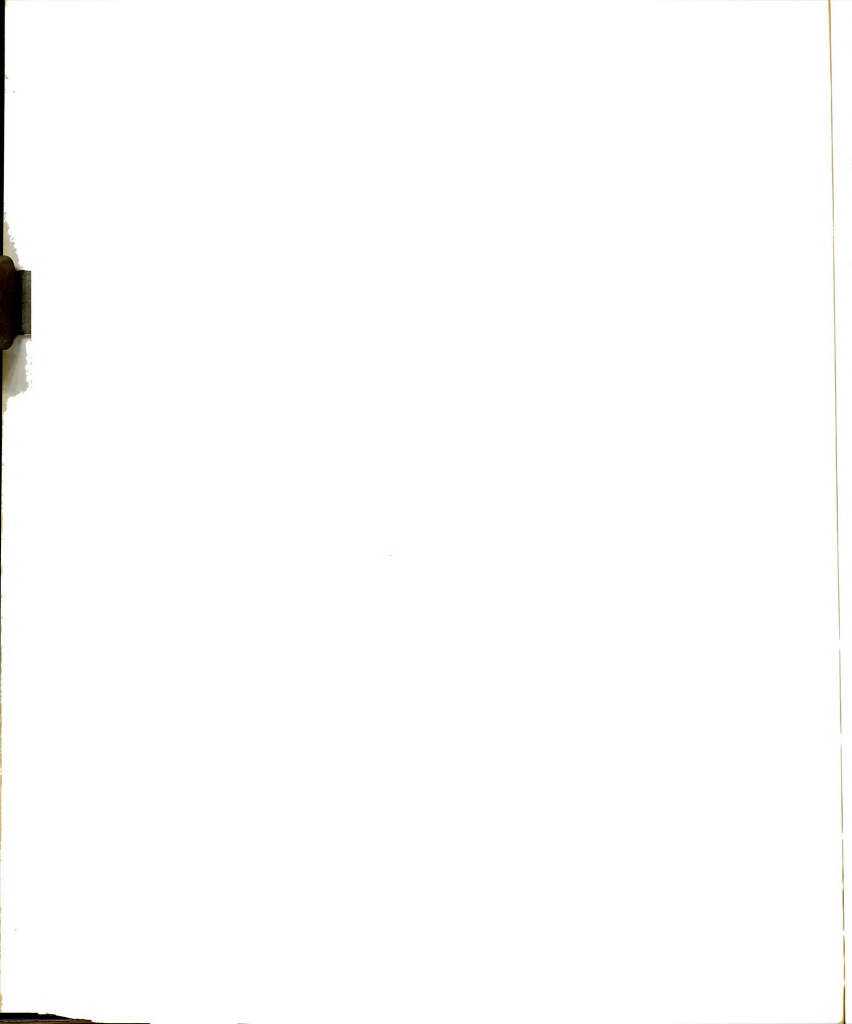
A. Partial Differential Equation for the Countercurrent Centrifuge

When the differential equations for the simple centrifuge were derived, it was assumed that the gas in the centrifuge was isothermal and rotated uniformly at the speed of the centrifuge. These assumptions are necessary for the development of the equations describing the countercurrent centrifuge, in addition to the following assumptions:

1. All bulk flows are in the axial direction and are not turbulent. The axial flows are further assumed to only be a function of radial position.
2. All derivatives of pressure with respect to axial position may be ignored.

Further assumed in assumption 1 is that the axial flow may be between "plug or rod" type flow and laminar flow. The importance of the actual shape of the velocity profile and the radial position of the intersection of the inner and outer flows will be evaluated in a subsequent section.

Differential equations representing the concentration and pressure diffusion in the radial direction in a gas centrifuge were developed in Section III-A. They are rewritten here for convenience, where



$$F_{ly} = - \frac{2\pi P}{RT} D_{12} r \frac{\partial y}{\partial r}$$

the radial flux due to a concentration gradient, and

$$F_{lp} = \frac{2\pi P}{RT} D_{12} A r^2 y(1-y) ,$$

$$A = \frac{(MW_1 - MW_2) \omega^2}{RT g_c}$$

the radial flux due to a pressure gradient.

In the countercurrent centrifuge an expression is also needed

flux in the axial direction. This flux is made up of the flux

the bulk flow of the gas minus the flux due to diffusion in the

direction. The axial flux may thus be written as

$$F_{lz} = 2\pi \left[\frac{Pv(r)ry}{RT} - \frac{PD_{12}}{RT} r \frac{\partial y}{\partial z} \right] ,$$

) is the axial velocity profile assumed to be a function of position only.

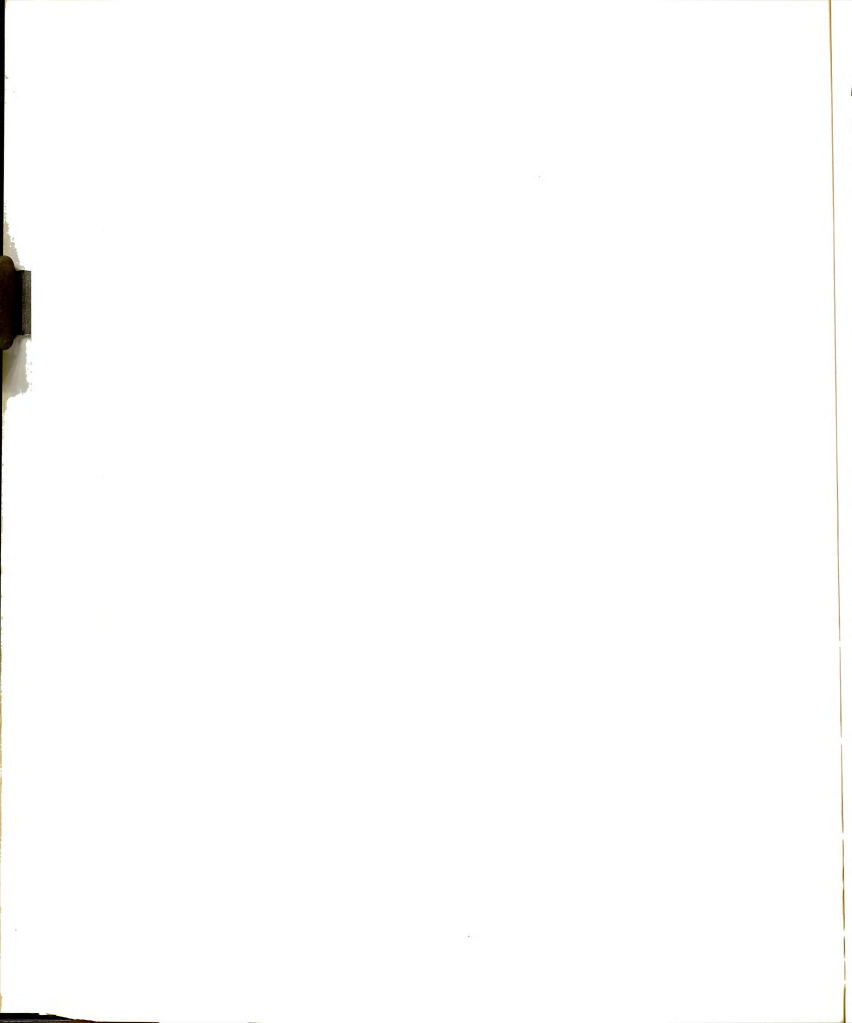
With expressions for the fluxes in the radial and axial direc-

the partial differential equation for the continuity of species 1

steady state operation of the countercurrent centrifuge may be

as

$$\frac{1}{r} \frac{\partial}{\partial r} [A r^2 y(1-y) - r \frac{\partial y}{\partial r}] + \frac{Pv(r)}{D_{12}P} \frac{\partial y}{\partial z} - \frac{\partial^2 y}{\partial z^2} = 0 .$$



case with the unsteady state simple centrifuge, the radial boundary conditions for the countercurrent centrifuge are that there is no flow through the axis or the wall. These boundary conditions as previously are

$$\frac{\partial y}{\partial r} = 0 \text{ at } r = 0, \text{ and}$$

$$\frac{\partial y}{\partial r} = A y (1-y) \text{ at } r = R_w.$$

The axial boundary conditions depend on the type of centrifuge considered: rectifying or stripping. Letting R_m be the radial distance at which the inner and outer flows intersect, the axial boundary conditions may be stated as follows:

Rectifying Centrifuge

At the top of the centrifuge where the feed enters becoming the outer stream, the boundary condition is that $y = y_f$ for the interval $R_m \leq r \leq R_w$. At the bottom the average composition of the outer stream leaving the centrifuge is given by

$$y_r = \frac{\frac{2\pi}{RT} \int_{R_m}^{R_o} P[v(r)y - D_{12} \frac{\partial y}{\partial z}] r dr}{\frac{2\pi}{RT} \int_{R_m}^{R_o} P v(r) r dr}.$$

This equation is simply the moles of species 1 leaving the centrifuge in the outer stream divided by the total moles leaving the centrifuge in the outer stream. After a portion of the outer stream

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ected off as the rich product stream, the remaining gas of
 ition y_r is recycled becoming the inner stream. Thus, the
 ry condition at the bottom is that

$$y = y_r \text{ for all } r \text{ in the interval } 0 \leq r \leq R_m.$$

Stripping Centrifuge

At the bottom of the centrifuge where the feed enters becoming
 her stream, the boundary condition is that

$$y = y_f \text{ for all } r \text{ in the interval } 0 \leq r \leq R_m.$$

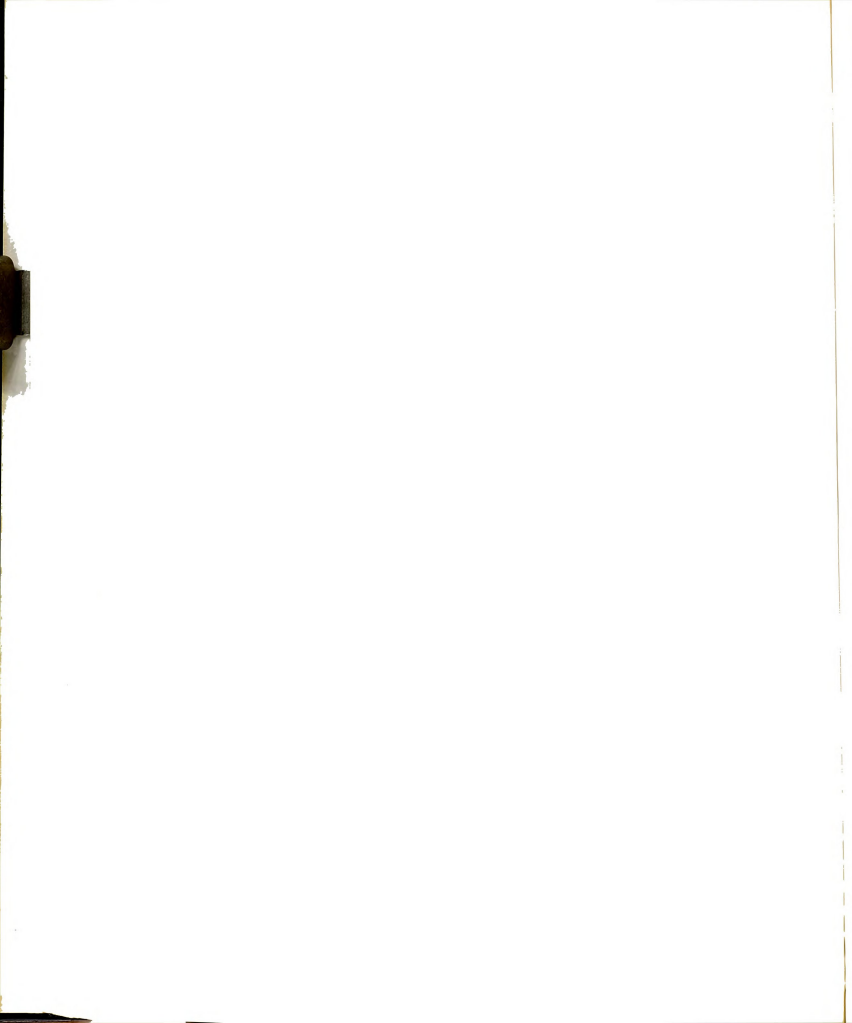
top of the centrifuge the average composition of the inner
 leaving the centrifuge is given by

$$y_1 = \frac{\frac{2\pi}{RT} \int_0^{R_m} P[v(r)y - D_{12} \frac{\partial y}{\partial z}] r dr}{\frac{2\pi}{RT} \int_0^{R_m} P v(r) r dr}.$$

a portion of the inner stream is directed off as the lean product
 , the remaining gas of composition y_1 is recycled making up the
 r outer stream. Thus, the boundary condition at the top is that

$$y = y_1 \text{ for all } r \text{ in the interval } R_m \leq r \leq R_w.$$

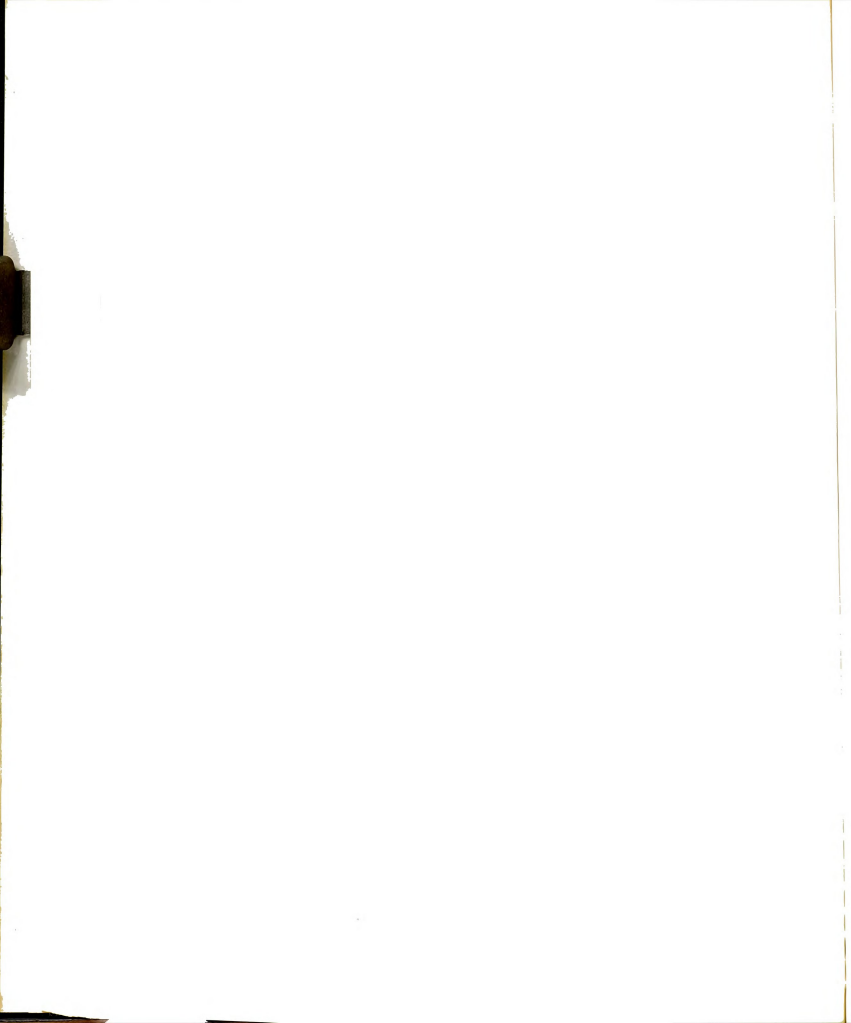
With some reflection on the radial fluxes taking place and
 magnitudes (Chapter III), two extremes in the operation of the
 r current centrifuge can be visualized. In one case, the rate of
 nput is made very small in hopes of allowing the radial fluxes to



antly move the heavy species from the inner to the outer stream. However, with the very small axial bulk flows, axial diffusion is the large axial gradient hoped for. In the other extreme, the rate of throughput is made quite large, to eliminate the total effect of axial diffusion, the very small radial fluxes would be able to move the heavy species from the inner to the outer stream before the end of the centrifuge is reached. Thus, in both of these two extremes very little separation would be seen. It is suggested by this reasoning is that a rate of throughput be chosen such that the separation achieved in a countercurrent centrifuge be maximized.

B. Velocity Profiles

This work does not deal with the analysis and computation of the exact shape of the velocity profiles and hence, the exact position of the flow intersection, R_m , of the inner and outer stream in the countercurrent centrifuge. Instead, two different velocity profiles are assumed: "plug or rod" type flow and laminar flow. This approach is considered more in line with the fundamental problem of determining the range of separations that may be expected along with the magnitude of the allowable flows in the countercurrent centrifuge. Also, by assuming two quite different velocity profiles and different flow intersection points, R_m , the importance of knowing the exact shape of the velocity profiles and the flow intersection position could be evaluated. To compute the actual magnitude of an assumed velocity profile, the density profile is needed. By knowing the pressure



and the shape of the velocity profile in a stream, the magnitude of the velocity profile is determined by equating the integral of velocity times velocity, over the area of flow, to the known flow rate in the stream.

To compute the pressure profile, a molecular weight equal to the feed gas was used. The pressure profile is then given by the equation derived in Chapter 11-A. That is,

$$P(r) = P(0) \exp \left(-\frac{A r^2}{2} \right),$$

$$A = \frac{MW_{avg} \omega^2}{RT g_c}, \quad MW_{avg} = MW_1 y_f + MW_2 (1 - y_f), \quad \text{and}$$

$P(0)$ is the axis pressure.

The axis pressure, $P(0)$, in the countercurrent centrifuge is determined under the desired operating conditions. This is unlike the analysis of the unsteady state simple centrifuge where a special equation was used to compute it.

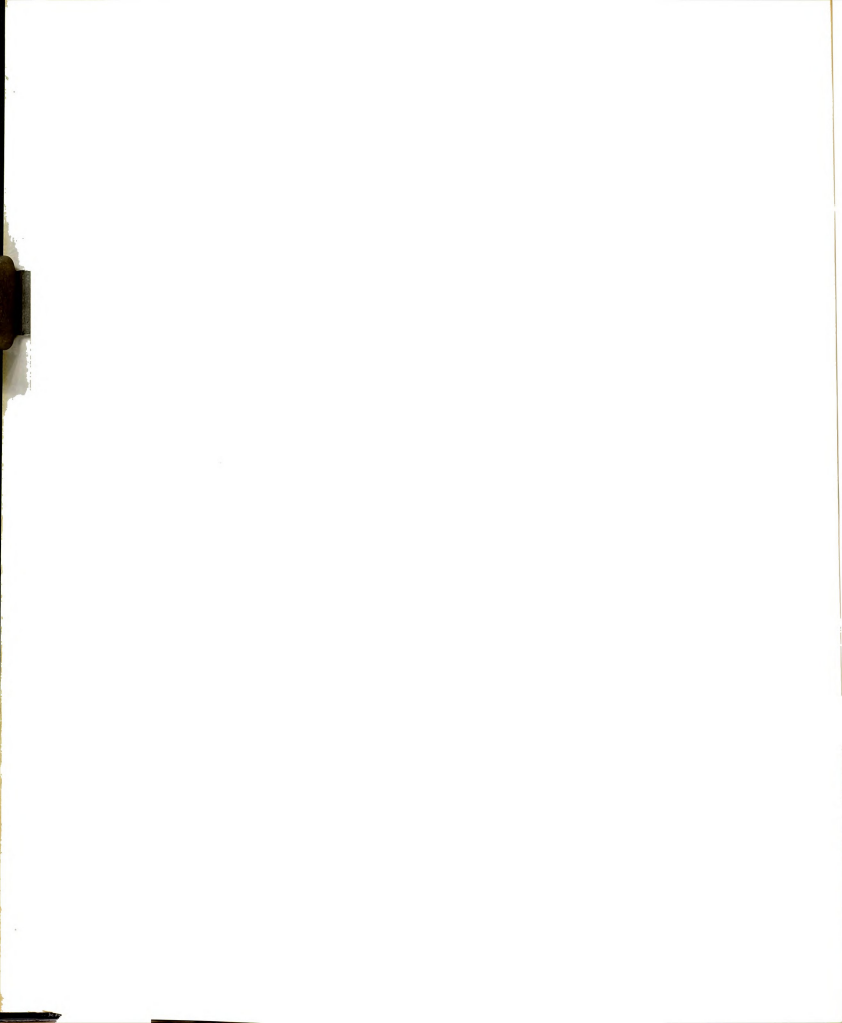
With the aid of the above pressure equation the velocity profile may be computed by evaluating the integral

$$\text{Flow} = \frac{2\pi}{RT} \int_{r_1}^{r_2} P v(r) r dr,$$

Flow = the flow rate of the stream,

$v(r)$ = the velocity profile, and

and r_2 is the region in which the flow takes place.



ug (Rod) Type Flow

By definition, the velocity profiles for both the inner and outer streams are constant with radial position. This result may be expressed as

$$v_i = \text{constant for all } r \text{ in the interval } 0 \leq r \leq R_m, \text{ and}$$

$$v_o = \text{constant for all } r \text{ in the interval } R_m \leq r \leq R_w,$$

$$v_i = v_o = 0 \text{ at } r = R_m \text{ and } v_o = 0 \text{ at } r = R_w.$$

The integral for the inner flow may be written as

$$\text{Flow}_i = \frac{2\pi P(0) v_i}{RT} \int_0^{R_m} \exp(-Ar^2/2) r dr,$$

after integrating gives the following expression for v_i :

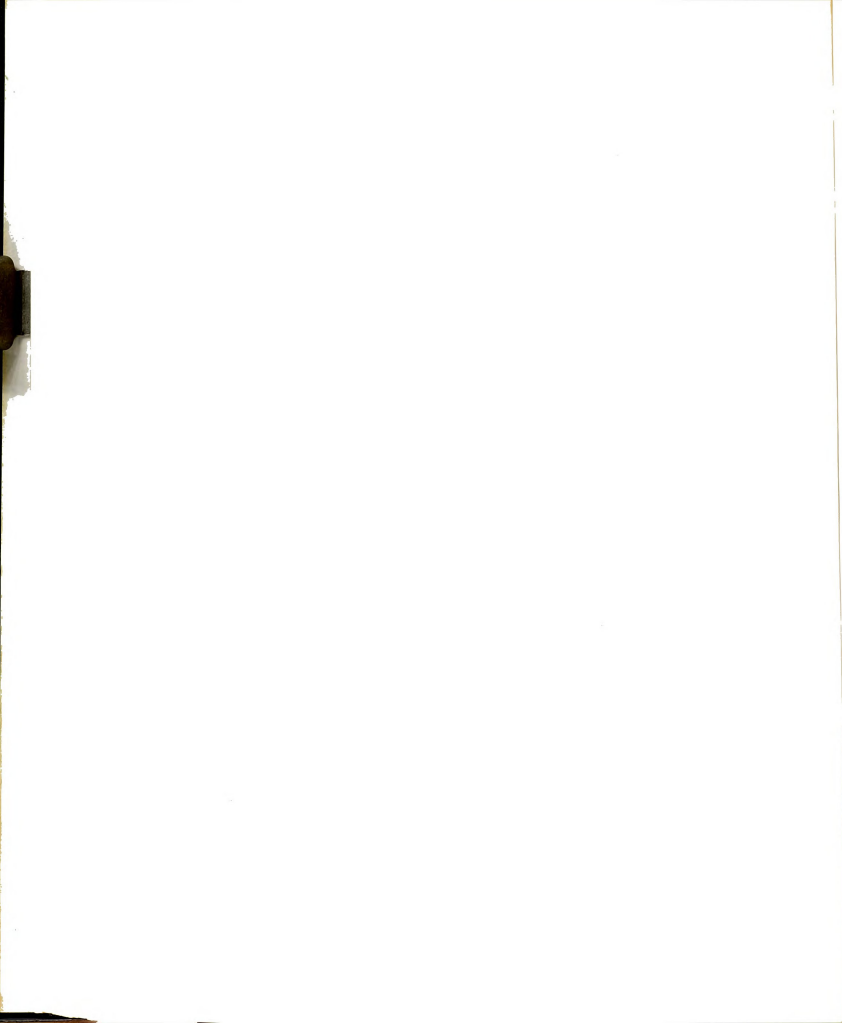
$$v_i = \frac{\text{Flow}_i RT A}{2\pi P(0) (e^a - 1)},$$

$$a = A R_m^2/2.$$

By a similar approach, an expression may be found for v_o , i.e.,

$$v_o = \frac{\text{Flow}_o RT A}{2\pi P(0) (e^b - e^a)},$$

$$b = A R_w^2/2.$$



Laminar Flow

The shape of the inner stream velocity profile will be assumed that for laminar flow in a circular pipe, given by

$$v_i(r) = v_{i(\max)} [1 - (r/R_m)^2] .$$

this expression in the integral for the inner flow gives

$$\text{Flow}_i = \frac{2\pi P(0) v_{i(\max)}}{RT} \int_0^{R_m} [1 - (r/R_m)^2] \exp(A r^2/2) r dr ,$$

after integrating gives the following expression for $v_{i(\max)}$:

$$v_{i(\max)} = \frac{\text{Flow}_i RT A}{2\pi P(0) [(e^a - 1)/a - 1]} ,$$

a is defined as above.

The shape of the outer stream velocity profile will be assumed that for laminar flow through an annulus given by

$$v_o(r) = \frac{v_{o(\max)}}{C} [1 - (r/R_w)^2 + d \ln(r/R_w)] ,$$

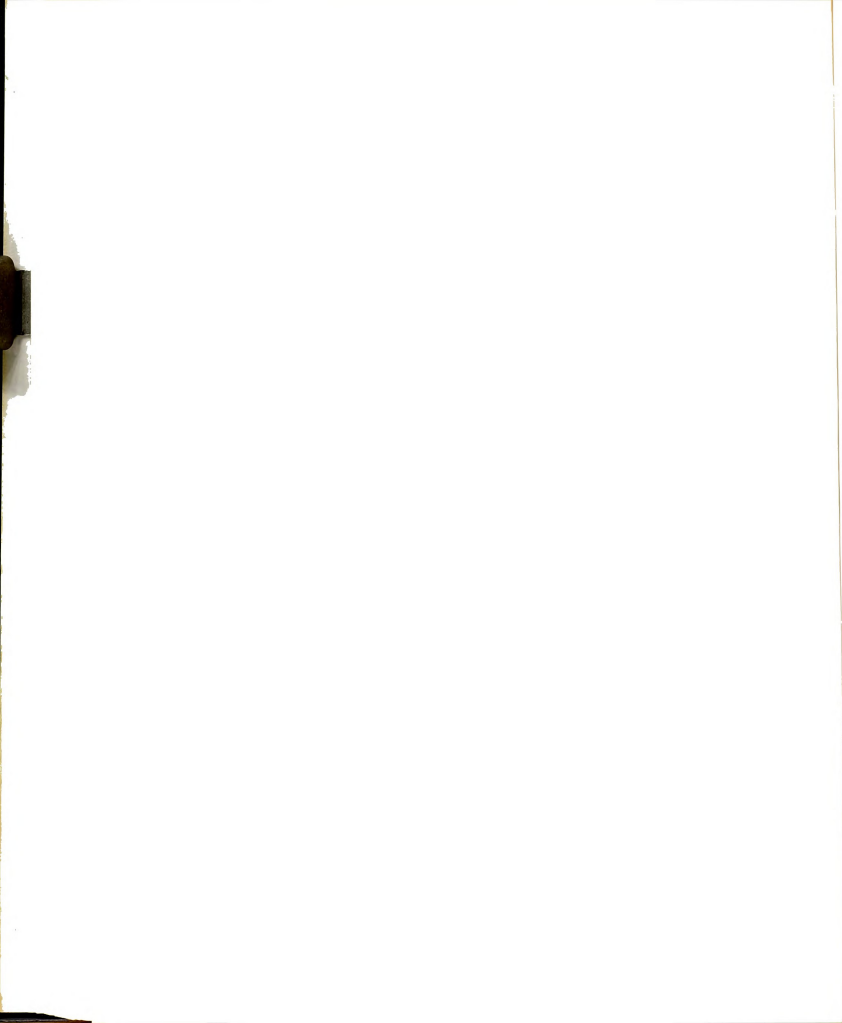
$$d = (1 - k^2) / \ln(1/k) ,$$

$$C = 1 - d[1 - \ln(d/2)]/2 , \text{ and}$$

$$k = R_m/R_w .$$

this expression in the integral for the outer flow gives

$$= \frac{2\pi P(0)}{CRT} v_{o(\max)} \int_{R_m}^{R_w} [1 - (r/R_w)^2 + d \ln(r/R_w)] \exp(A r^2/2) r dr$$



her complicated integral may be integrated analytically, after manipulation, giving the following expression for $v_o(\max)$:

$$v_o(\max) = \frac{\text{Flow}_o \text{ CRT } A}{2\pi P(0) f},$$

$$= (e^b - e^a)/b - e^a(1 - k^2) + d \ln(1/k)(e^a - 1) - \frac{d}{2} \sum_{n=1}^{\infty} \frac{b^n - a^n}{n \cdot n!}$$

and b are as defined above.

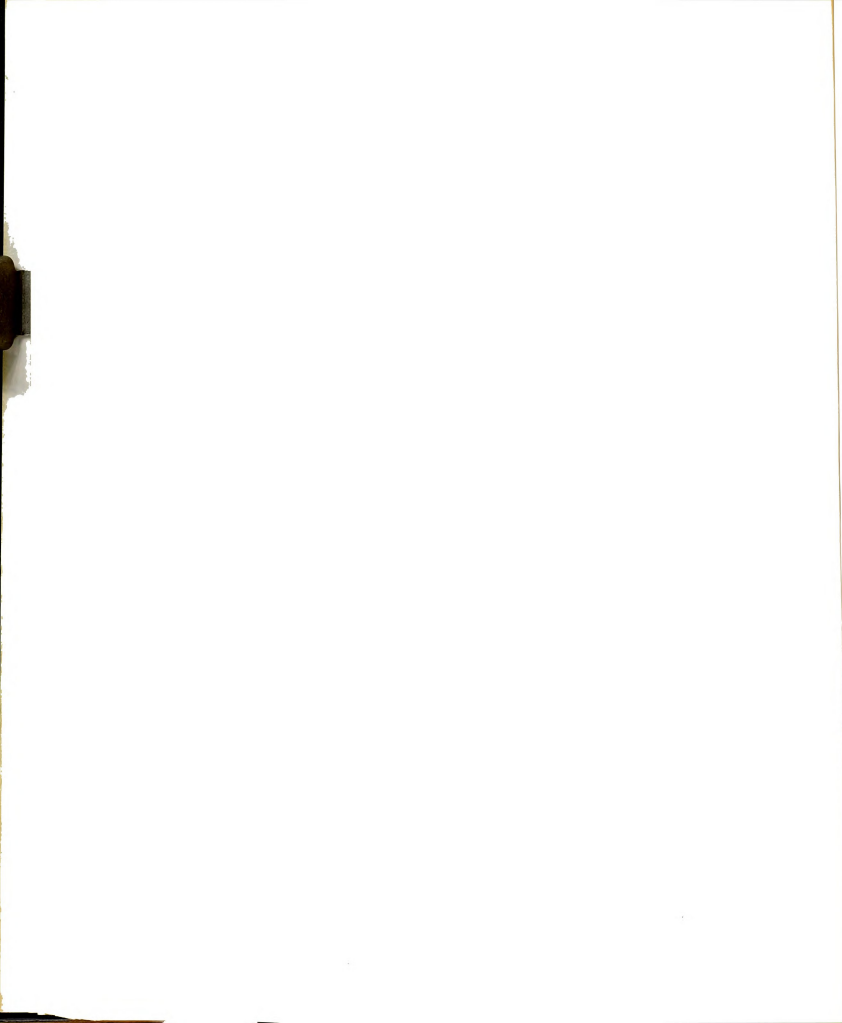
Since the inner and outer flows oppose one another, regardless of the shape of the profile, a sign convention was adopted to further define the velocity profiles. The top of the centrifuge was considered as the zero position in the axial direction ($z = 0$), thus fixing the sign of the velocity. Downward flowing outer stream as positive and the upward flowing inner stream as negative.

C. The Solution of the Partial Differential Equation for the Countercurrent Centrifuge

The partial differential equation for the conservation of the mass of a species in a countercurrent centrifuge was given above in equation V-A as

$$\frac{1}{r} \frac{\partial}{\partial r} [Ar^2 y(1-y) - r \frac{\partial y}{\partial r}] + \frac{P}{D_{12}} \frac{v(r)}{r} \frac{\partial y}{\partial z} - \frac{\partial^2 y}{\partial z^2} = 0.$$

This equation coupled with its associated boundary conditions may be solved directly by using a numerical approach. However, to find an analytical (approximate) solution the equation must be simplified by making certain assumptions. An analytical (approximate) solution



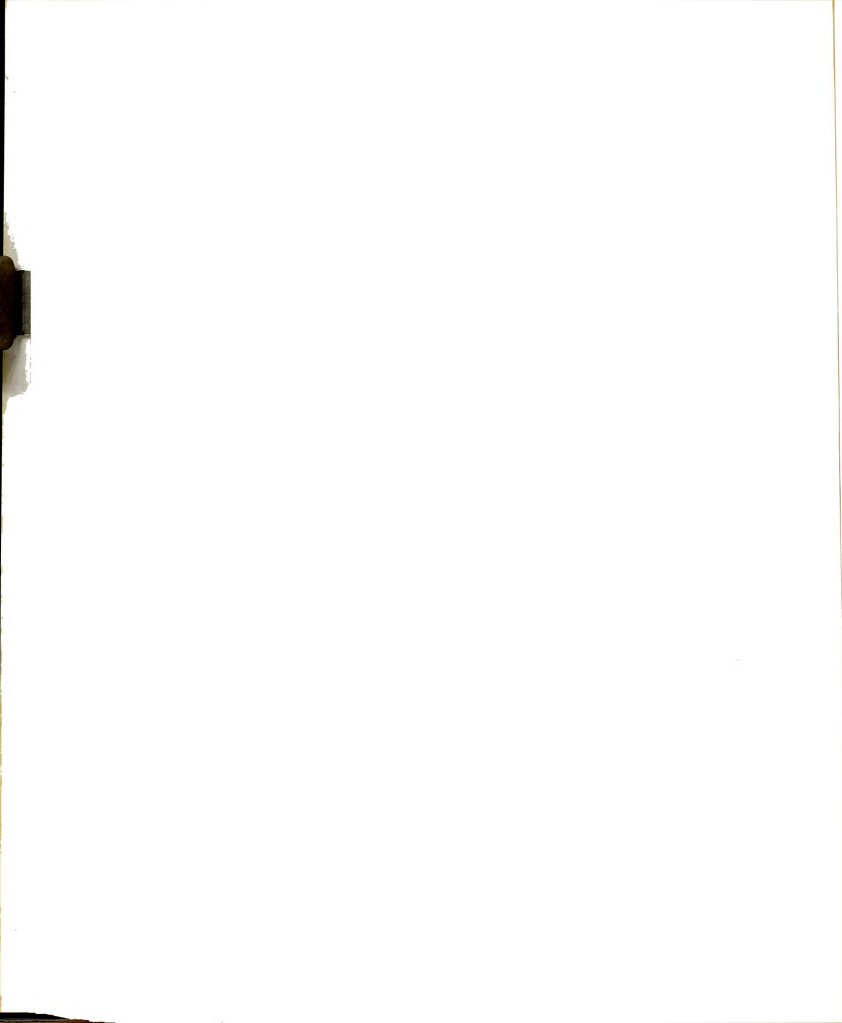
certainly desirable, since finding a numerical solution is itself a rather complex problem.

Numerical Solution

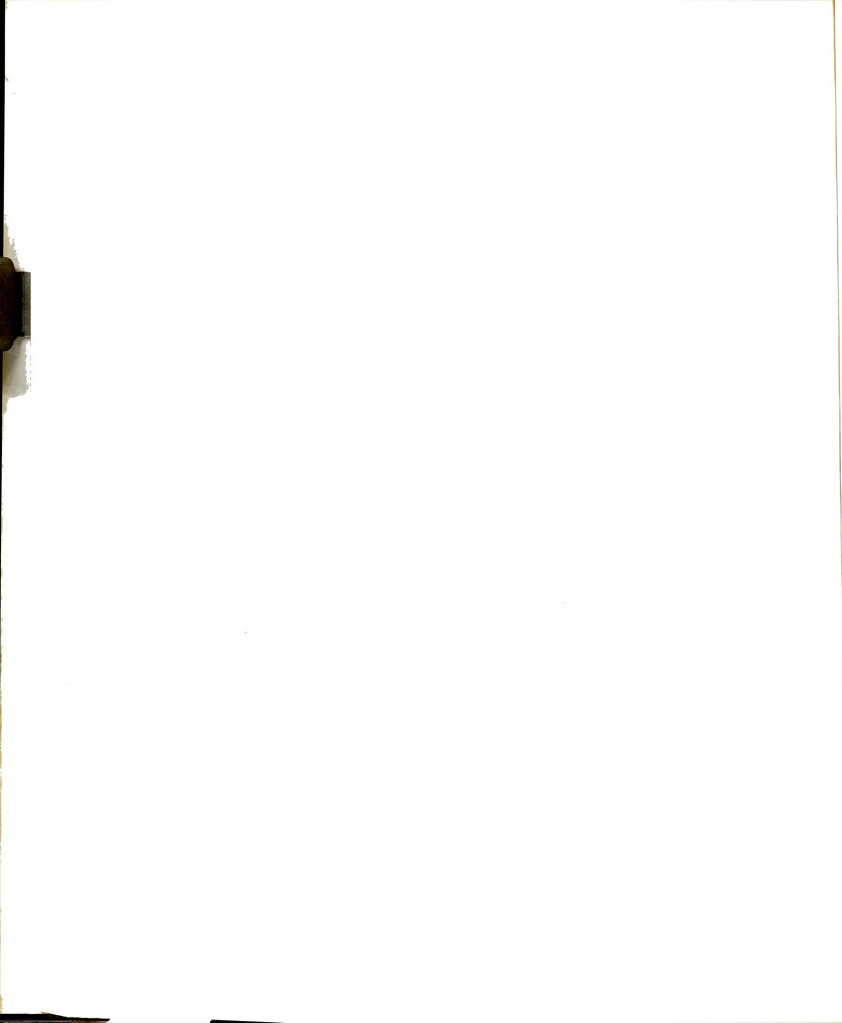
A general FORTRAN program, NCENTRI, was written to solve the governing equation numerically for the steady state mole fraction profiles in a countercurrent rectifying centrifuge. (It was found that having a numerical solution to just the rectifying centrifuge was sufficient to evaluate the analytical [approximate] solution.) The program is written in the sense that it can be used to analyze the separations obtainable in a countercurrent rectifying centrifuge of any size, for any gas pair, and any operating conditions. Also, by giving the user a choice of option, either the plug type or laminar velocity profile can be used in obtaining a numerical solution.

A complete description and listing of the FORTRAN program NCENTRI and its ten associated FORTRAN subprograms may be found in Appendix D. Also included in Appendix D is a sample output from program NCENTRI. The numerical approach used by the program to find the mole fraction profile is best illustrated by the following steps which, in a general sense, outline the flow of calculations:

1. Input the gas properties, operating conditions, centrifuge dimensions, and the number of increments into which the radius and the axial distance is to be divided. The program is written so that regardless of the position of the flow intersection, R_m , the radial distances from the intersection to R_m and from R_m to the wall, R_w , are divided into the same number of increments.



2. Compute the pressure and velocity profiles.
3. Output all the input information along with the pressure and velocity profiles.
4. Compute special fourth order finite difference equations to be used to approximate the first and second partials of y with respect to radius at one grid point before, one grid point after and at the grid point corresponding to the flow intersection. These special equations are needed due to the changing increment size at the flow intersection.
5. Due to the nonlinear nature of the partial differential equation, the entire mole fraction grid is initialized with values computed from a simplified version of the analytical (approximate) solution.
6. By using fourth order finite difference approximations for the partial derivatives appearing in the partial differential equation and the boundary conditions, an equation is written for each grid point. Thus, for example, if the grid consisted of 15 radial grid points and 21 axial grid points, a set of 315 simultaneous equations can be written for the 315 unknown mole fractions at each grid point.
7. Solve simultaneously the set of equations.
8. If the proper option is given, the newly computed mole fractions are used as a better approximation to the true values and steps 6 and 7 are repeated a specified number of times. It was found in all cases investigated that repeating steps 6 and 7 once was sufficient to account for the nonlinearity.
9. Compute the average mole fraction of the lean stream leaving the centrifuge and output it along with the entire mole fraction profile.



2. Approximate Analytical Solution

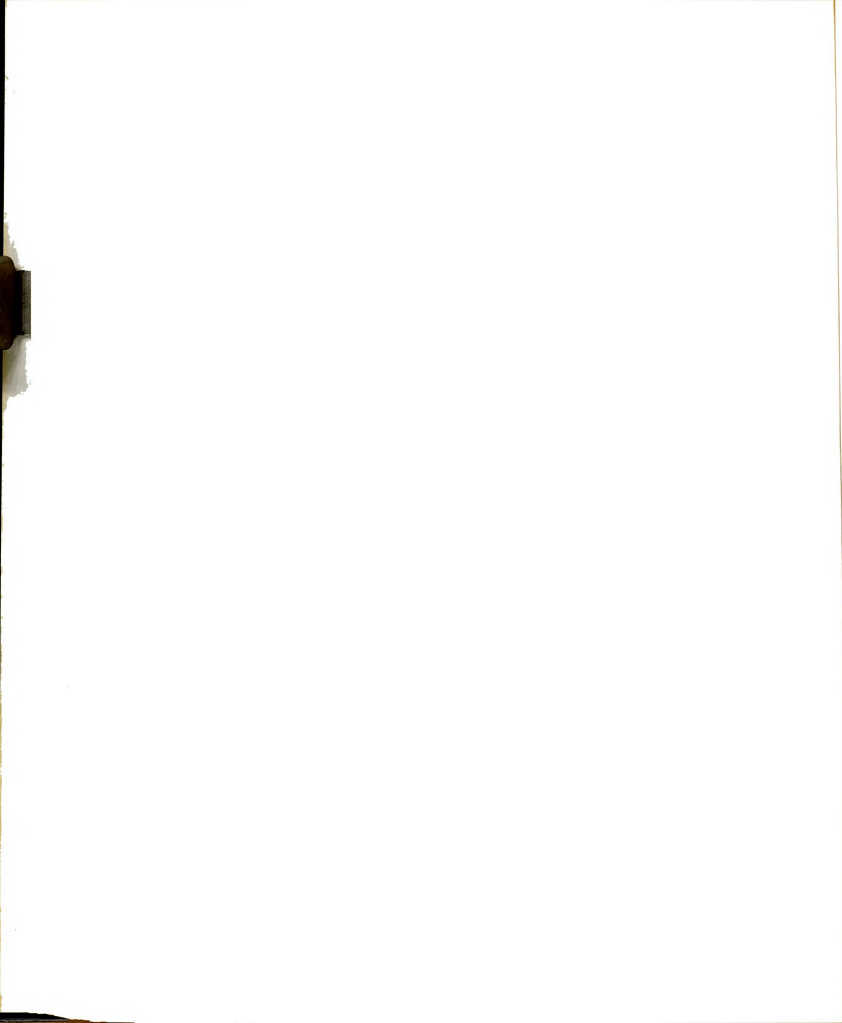
The analytical (approximate) solution of the partial differential equation for the countercurrent centrifuge was obtained by following an approach similar to that used by Furry, Jones, and Onsager (15) for the thermal-diffusion column. This approach was also used by Benedict and Pigford (16) and Cohen (8) in their analysis of Uranium isotope separation by gas centrifugation.

The method used depends on the fact that the term $\partial y / \partial r$ is of the order of the term $Ar y(1-y)$ (Chapter III), which is a small quantity. Thus, the change in y in the radial direction as compared to the variation of r , P , or $P v(r)$ is small and may be neglected. This assumption, for instance, is certainly more reasonable under total reflux operating conditions (no products) than when a rich product stream is taken from a rectifying centrifuge. In the total reflux case the composition of the leaving inner stream must equal to feed composition. However, when a rich product stream is taken, the leaving inner stream by necessity of mass balance must be less concentrated than the feed. Consequently, a significant change in y must take place in the radial direction.

Nevertheless, by using the above assumption, the partial differential equation may be integrated with respect to r , giving

$$Ar^2 y(1-y) - r \frac{\partial y}{\partial r} + \frac{\partial y}{\partial z} \int_0^r \frac{P v(r)}{P D_{12}} r dr + \text{Constant} = 0,$$

where the second order term $\partial^2 y / \partial z^2$ has been neglected. Using the boundary condition that



$\partial y / \partial r = 0$ at $r = 0$, gives: Constant = 0 .

The second integration with respect to r requires the following relationship to get a form that may be integrated:

$$2\pi \int_0^R \left[\frac{P_v(r)}{RT} - \frac{PD_{12}}{RT} \frac{\partial y}{\partial z} \right] r dr = y_p Q ,$$

where Q is the flow rate of the product stream given by

$$2\pi \int_0^R \frac{P_v(r) r dr}{RT} ,$$

and y_p is the mole fraction of the product stream. The above equation is simply a statement of the mass balance for the heavy species at any axial position with respect to the product stream. The first term on the left-hand side of the above integral may be integrated by parts, giving

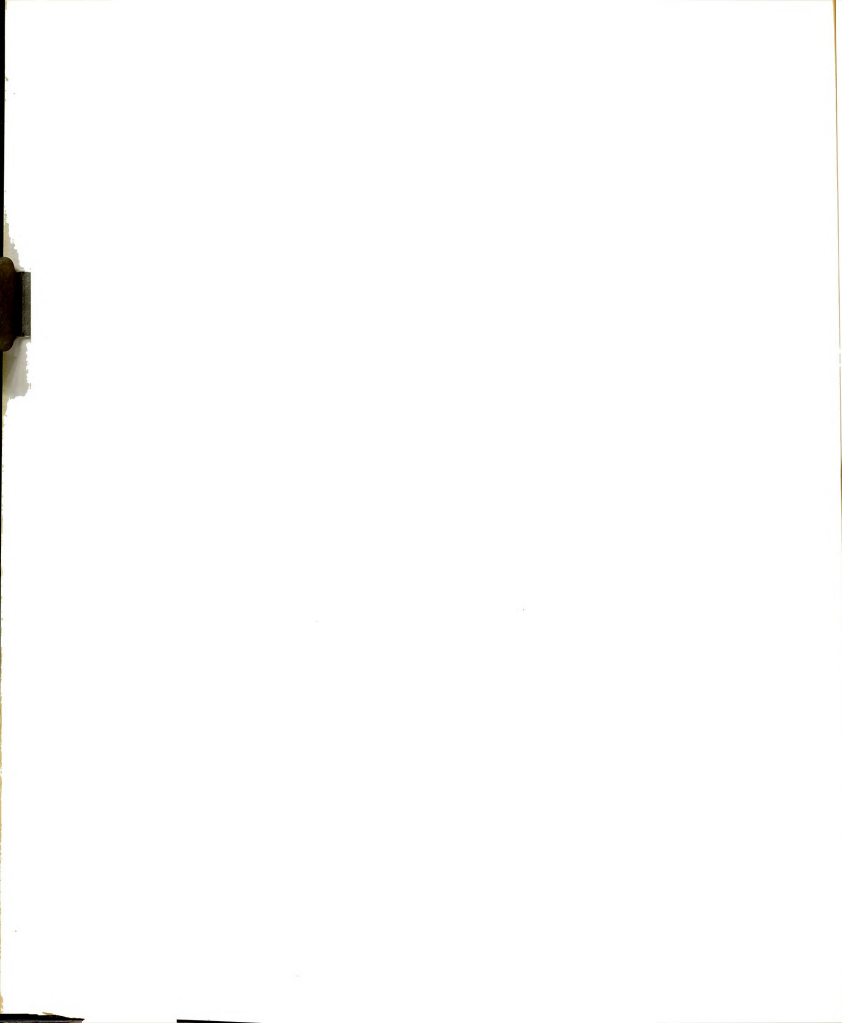
$$\begin{aligned} 2\pi \int_0^R \frac{P_v(r) y}{RT} r dr &= \frac{2\pi y}{RT} \int_0^R P_v(r) r dr \\ &- \frac{2\pi}{RT} \int_0^R \frac{\partial y}{\partial r} dr \int_0^r P_v(r) r dr . \end{aligned}$$

After substituting for $\partial y / \partial r$, the above equation may be rewritten as

$$\frac{2\pi}{RT} \int_0^R P_v(r) y r dr = yQ - C_1 y(1-y) - C_3 \frac{\partial y}{\partial z} ,$$

where

$$C_1 = \frac{2\pi A}{RT} \int_0^R r dr \int_0^r P_v(r) r dr , \text{ and}$$



$$C_3 = \frac{2\pi}{RT} \frac{1}{PD_{12}} \int_0^R w \frac{dr}{r} \left[\int_0^r P_v(r) r dr \right]^2 .$$

The integral for the mass balance may now be written as

$$-C_5 \frac{\partial y}{\partial z} + [yQ - C_1 y(1-y)] = y_p Q ,$$

where $C_5 = C_2 + C_3$, and

$$C_2 = \frac{2\pi}{RT} \frac{PD_{12} R_w^2}{2} .$$

With all the radial dependence having been integrated, the parameters C_1 , C_2 , and C_3 are constants. The resulting differential equation may then be solved by separating variables,

$$\int_0^L dz = \int_{y_f}^{y_p} \frac{C_5 dy}{C_1 y^2 + (P - C_1)y - Q y_p} .$$

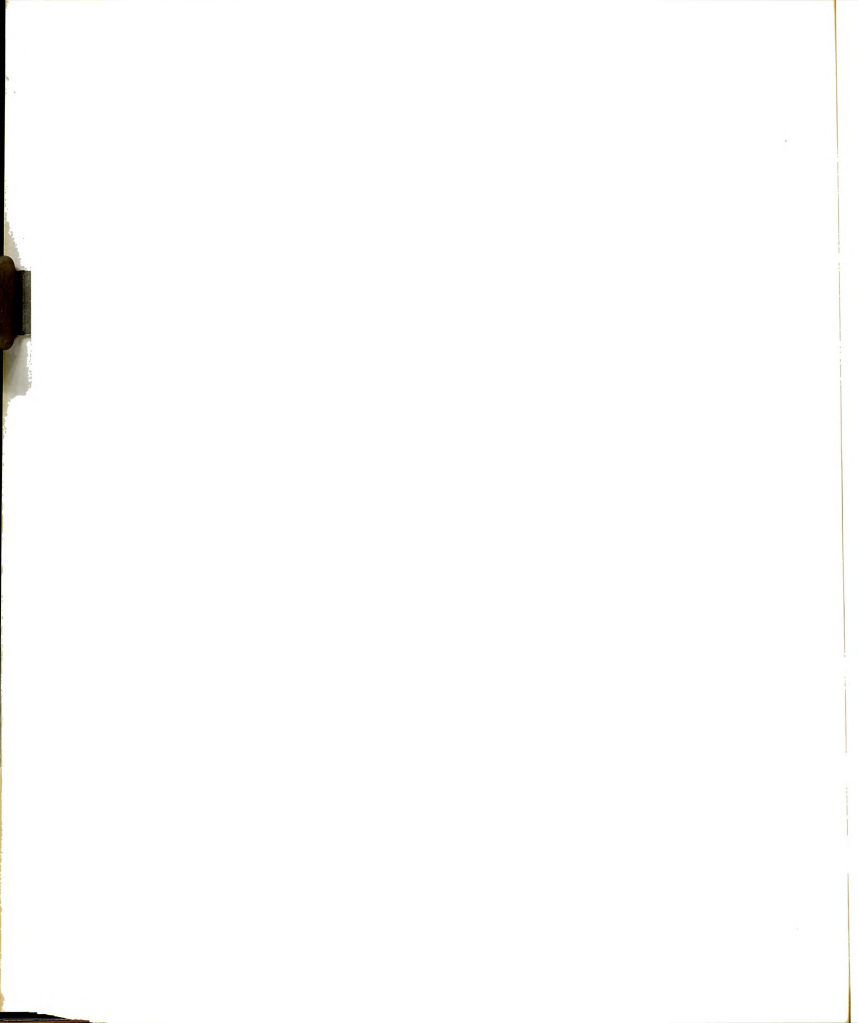
Integrating gives

$$\tanh(uwL) = \frac{(y_p - y_f)w}{y_p - 2y_p y_f + y_f + (y_p - y_f)q} ,$$

where $q = Q/C_1$,

$$w = [1 - 2q(1 - 2y_p) + q^2]^{1/2} , \text{ and}$$

$$u = C_1/C_5^{1/2} .$$



D. Analysis of the Analytical
(Approximate) Solution

For the time being it will be assumed that the following operating parameters are held constant: the shape of the velocity profiles for the inner and outer streams, the flow intersection position, R_m , the ratio of the inner to outer flow rates, F_i/F_o , the pressure, and the temperature. Under these conditions, regardless of the actual magnitude of the inner and outer streams, q is a constant. That is, if the flow rates F_i and F_o are doubled, $F_i - F_o$, which equals Q , is doubled as are the maximum velocities of the inner and outer streams. Thus, since Q is doubled and C_1 is doubled due to the doubling of the maximum velocities, q remains unchanged.

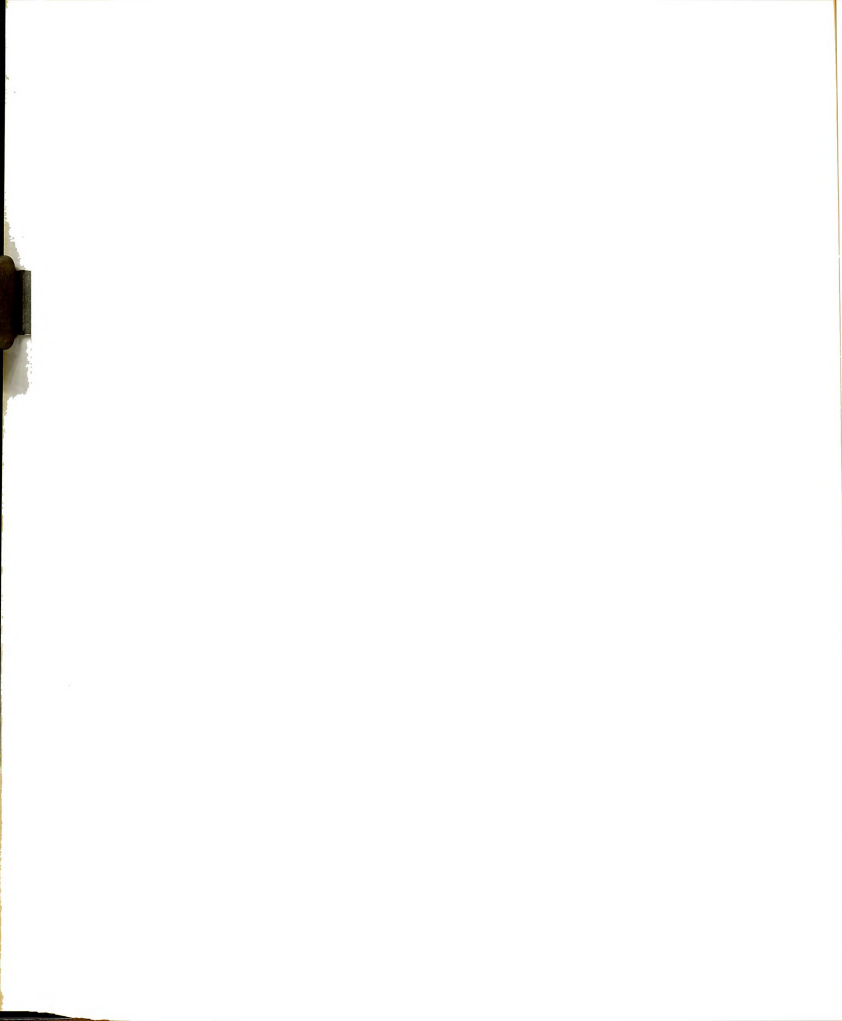
The quantity u , however, is very dependent on the magnitude of the flow rates. From above, u may be written as

$$u_s = \frac{C_{1s}}{2(C_2 + C_{3s})},$$

where the additional subscripts on C_1 and C_3 indicate they were computed for some flow rate, s . Since C_1 is directly related to the flow rates and C_3 is related to the square of the flow rates, u for any other flow rate can be expressed as

$$u = \frac{fC_{1s}}{2(C_2 + f^2C_{3s})}$$

where f is the ratio of the new flow rate to the old flow rate. By taking the derivative of u with respect to f and setting it equal to zero, the value of f which maximized u can be found, i.e.,



$$\frac{du}{df} = 0 = \frac{(c_2 + f^2 c_{3s}) c_{1s} - 2f^2 c_{1s} c_{3s}}{2(c_2 + f^2 c_{3s})^2}$$

giving

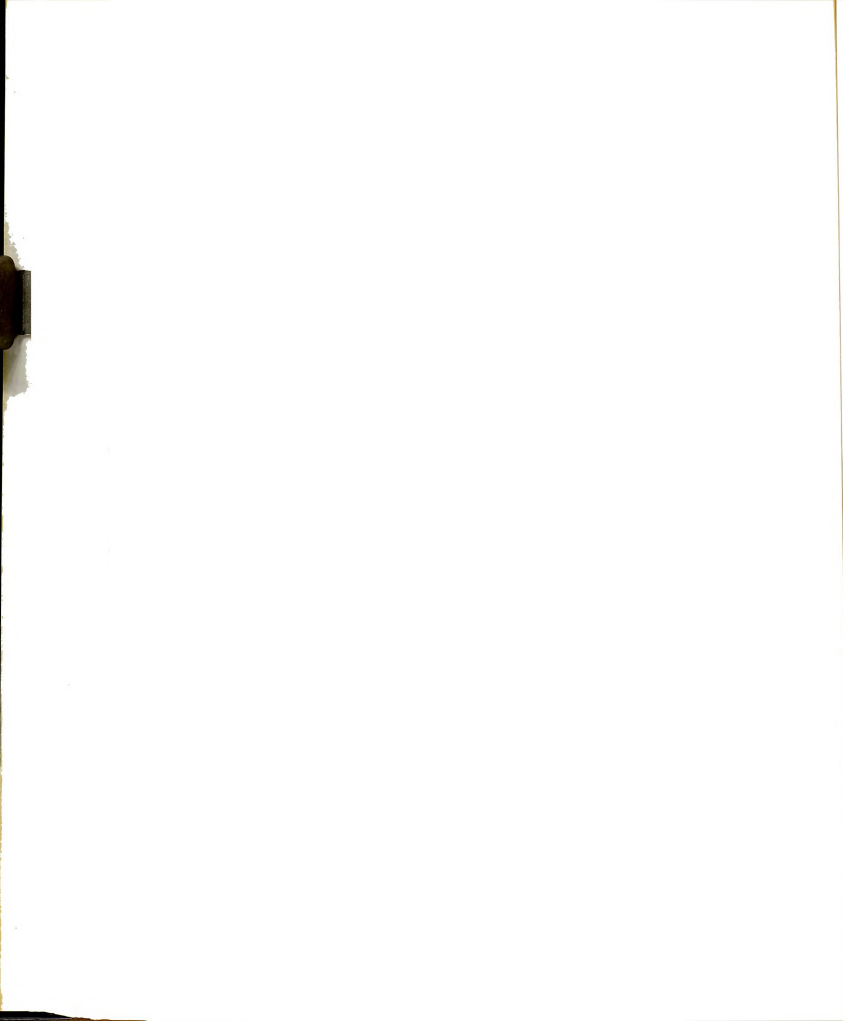
$$f = \left(\frac{c_{2s}}{c_{3s}}\right)^{1/2}.$$

Since u has a maximum value, so does $\tanh(uwL)$ for a fixed L .

Thus, there exists in the analytical (approximate) solution, as expected intuitively, a flow rate such that the separation is maximized.

1. The Effect of Feed Mole Fraction on the Optimum Flow Rate

The effect of the feed mole fraction on the optimum flow rate will be very slight. This is due to the small variation of c_1 and c_3 with a change in the shape of the pressure profile. Feed containing little of the heavy species will give a pressure profile essentially equal to that of the light species and essentially equal to that of the heavy species for feed mole fractions near 1. In either case the magnitude of the velocity profile, having been adjusted to give the proper flow rates, nearly compensates for any changes in the pressure profile, hence little effect on c_1 and c_3 . This agrees with the fact that the charge composition had very little effect on the time required for the equilibrium separation to take place in the unsteady state simple centrifuge (Chapter III-D).



2. The Effect of Rotation Speed on the Optimum Flow Rate

The effect of increasing the rotational speed on the optimum flow rate will also be very slight, although its effect on the actual separation at this flow rate will be great. The change in separation is due to the dependence of C_1 , and likewise u , on the rotational speed squared. Otherwise, changing the rotational speed, as does changing the feed mole fraction, simply changes the shape of the pressure profile. This change, as described above, will very nearly be compensated for by a change in the magnitude of the velocity profile to maintain the proper flow rates. Hence, the effect on the values of C_1 and C_3 caused by the changing pressure profile will be minimal.

3. The Effect of Operating Pressure on the Optimum Flow Rate

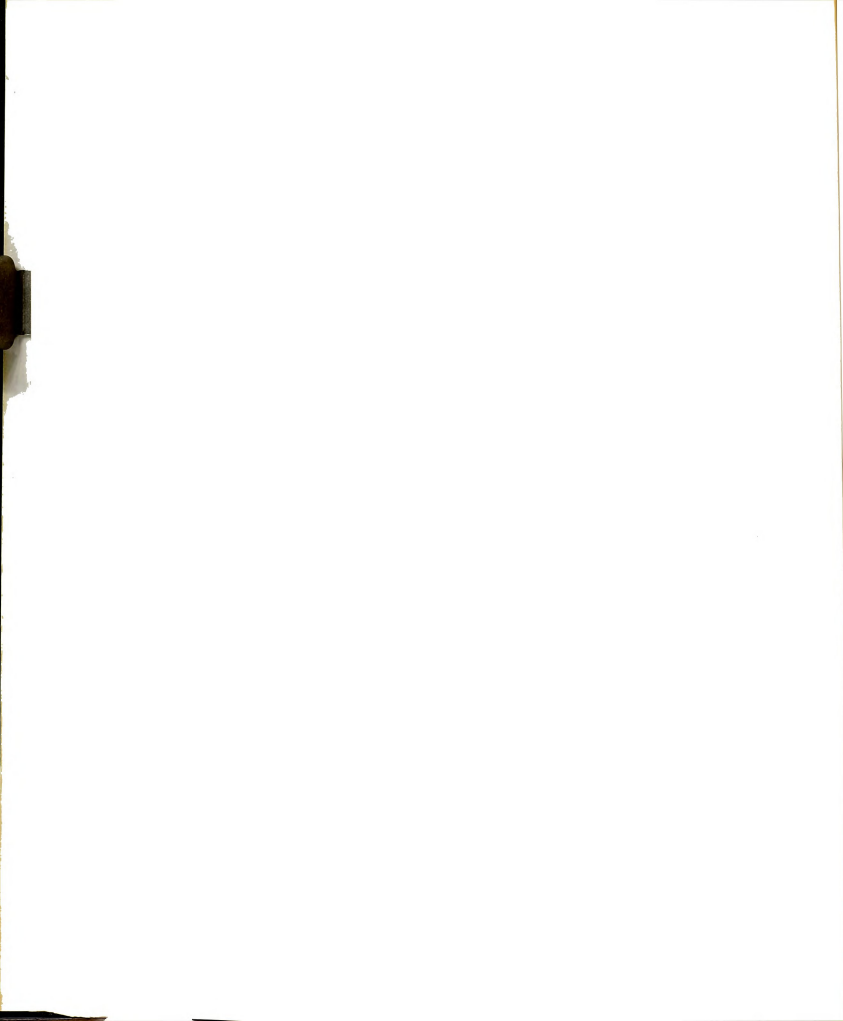
Operating at optimum flow rate conditions, a doubling of the axis pressure would be compensated for by a halving of the magnitude of the velocity profile. Thus, there would be no effect on the values of C_1 and C_3 and hence, on the optimum flow rate.

4. The Effect of Diffusivity Times Pressure on the Optimum Flow Rate

As shown above, the ratio of the optimum flow rate to some other flow rate, f , is given by

$$f = \left(\frac{C_{2s}}{C_{3s}} \right)^{1/2} .$$

Since C_{2s} is directly related to D_{12}^P and C_{3s} is inversely related to D_{12}^P , f is then directly related to D_{12}^P .



This result is of fundamental importance since it and it alone places a definite restriction on the throughput in the operation of the gas centrifuge. That is, for any gas pair, the optimum flow rate is directly related to the quantity $D_{12}P$. Thus, knowing the optimum flow rate for one gas pair, f_1 , the optimum flow for any other gas pair, f_2 , at the same operating conditions is very nearly equal to the known optimum times the ratio of the diffusivities, i.e.,

$$f_2 = f_1 \frac{(D_{12}P)_2}{(D_{12}P)_1}.$$

The small difference expected between the optimum flow rate given above and the actual optimum is due to the different molecular weights of the new gas pair which would affect the pressure profile.

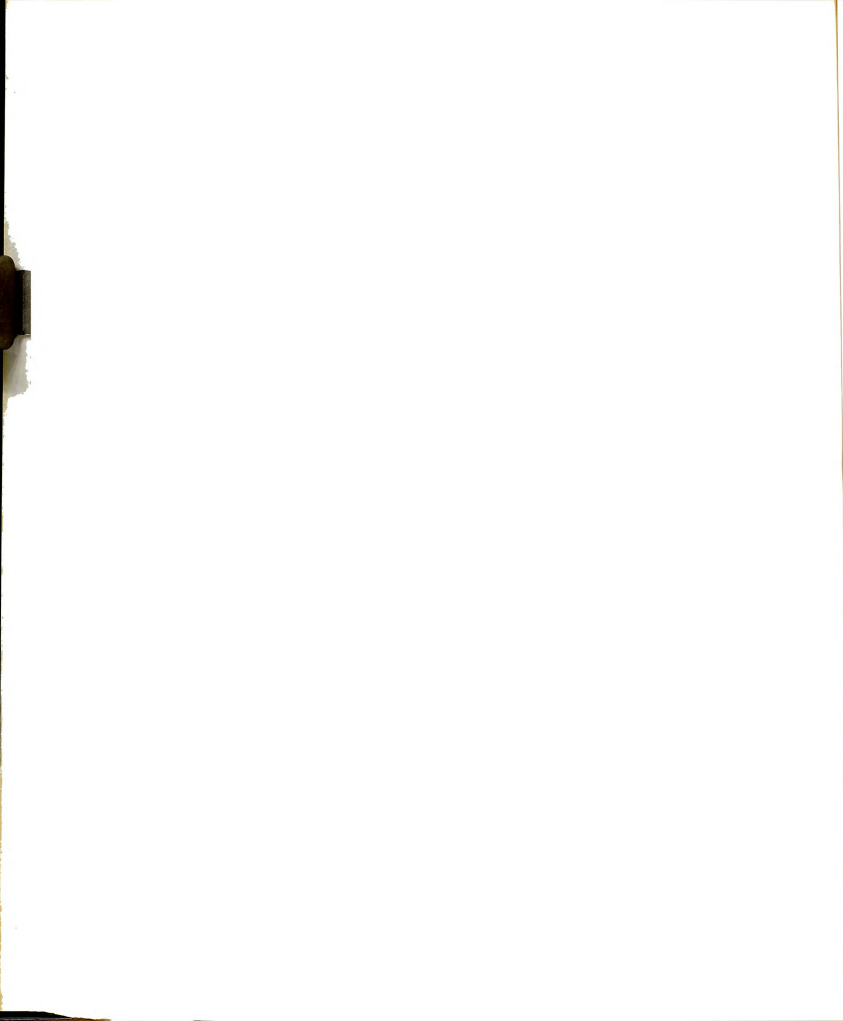
5. The Effect of Temperature on the Optimum Flow Rate

Assuming for the moment that $D_{12}P$ is related directly to the absolute temperature raised to the 3/2 power (see Appendix B), C_2 which is given by

$$C_2 = \frac{2\pi}{RT} \frac{D_{12}P R_w^2}{2},$$

is related directly to $T^{1/2}$. C_3 , which is given by

$$C_3 = \frac{RT}{2\pi} \frac{1}{D_{12}P} \int_0^{R_w} \frac{dr}{r} [2\pi \int_0^r \frac{P}{RT} v(r) r dr]^2,$$



is related inversely to $T^{1/2}$, noting that the effect of temperature in the integral is compensated for by the magnitude of the velocity profile. Thus, the ratio of the optimum flow, f_n , at a new temperature T_n is very nearly given by

$$f_n = \left(\frac{T_n}{T_o}\right)^{1/2} \left(\frac{C_{2o}}{C_{3o}}\right)^{1/2},$$

where the subscript "o" refers to the old temperature.

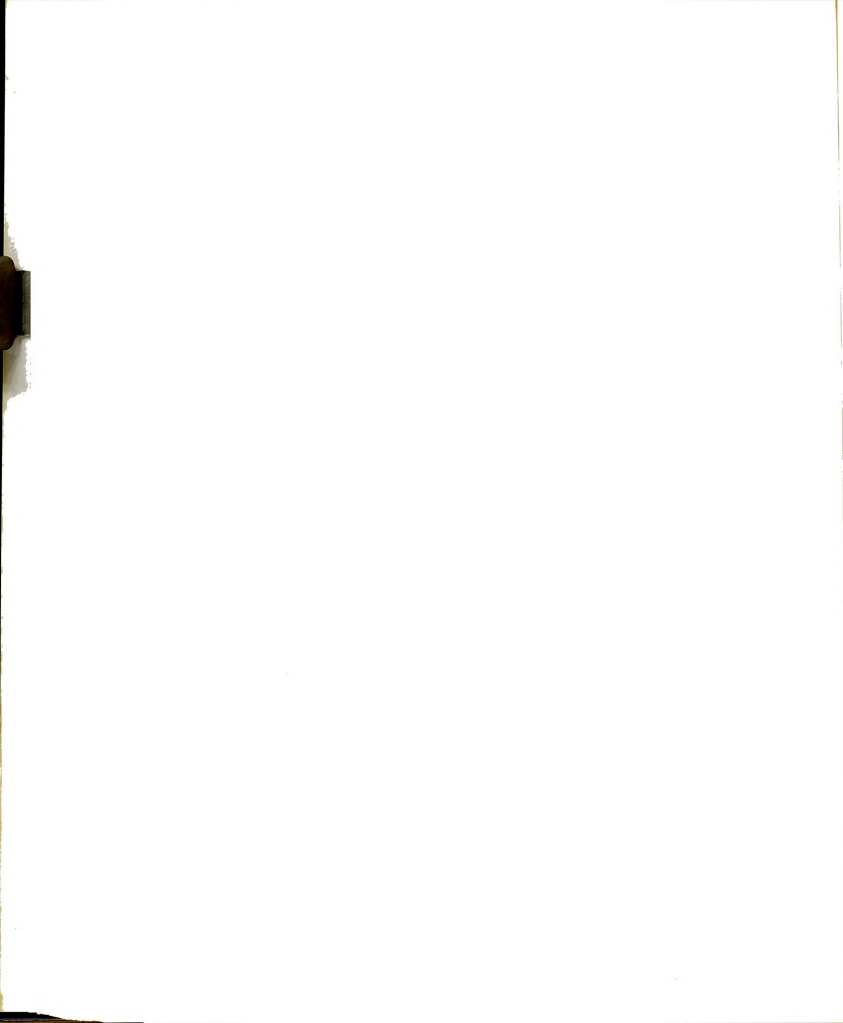
However, recalling that C_1 is given by

$$C_1 = \frac{(MW_1 - MW_2)\omega^2}{RTg_c} \int_0^{R_w} r dr \left[2\pi \int_0^r \frac{P}{RT} v(r) r dr \right]$$

shows that while increasing the temperature increases the optimum flow, it has the adverse effect of decreasing C_1 (effectively decreasing the molecular weight difference, see Chapter 11-A). Since decreasing C_1 decreases u , the optimum separation gets worse.

As the analytical (approximate) solutions for the counter-current centrifuge indicates (as does intuition), the longer the centrifuge, the greater the separation.

The effect of the shape of the velocity profile and the radial position of the intersection of the inner and outer stream on the optimum flow and on the separation will be dealt with in the next chapter. Also covered will be the effect of increasing the centrifuge diameter.



E. Computing the Analytical (Approximate) Solution

A general FORTRAN program, CENTRI, was written to compute the constants and solve the equation resulting from the approximate analytical solution. A detailed description, sample output, and complete listing can be found in Appendix E.

The program was written to be used as a working model for the analysis of any gas in a countercurrent centrifuge. Furthermore, the centrifuge may be operated as a rectifying, stripping or combination rectifying-stripping centrifuge. The numerous capabilities of the general program are listed in Table 11.

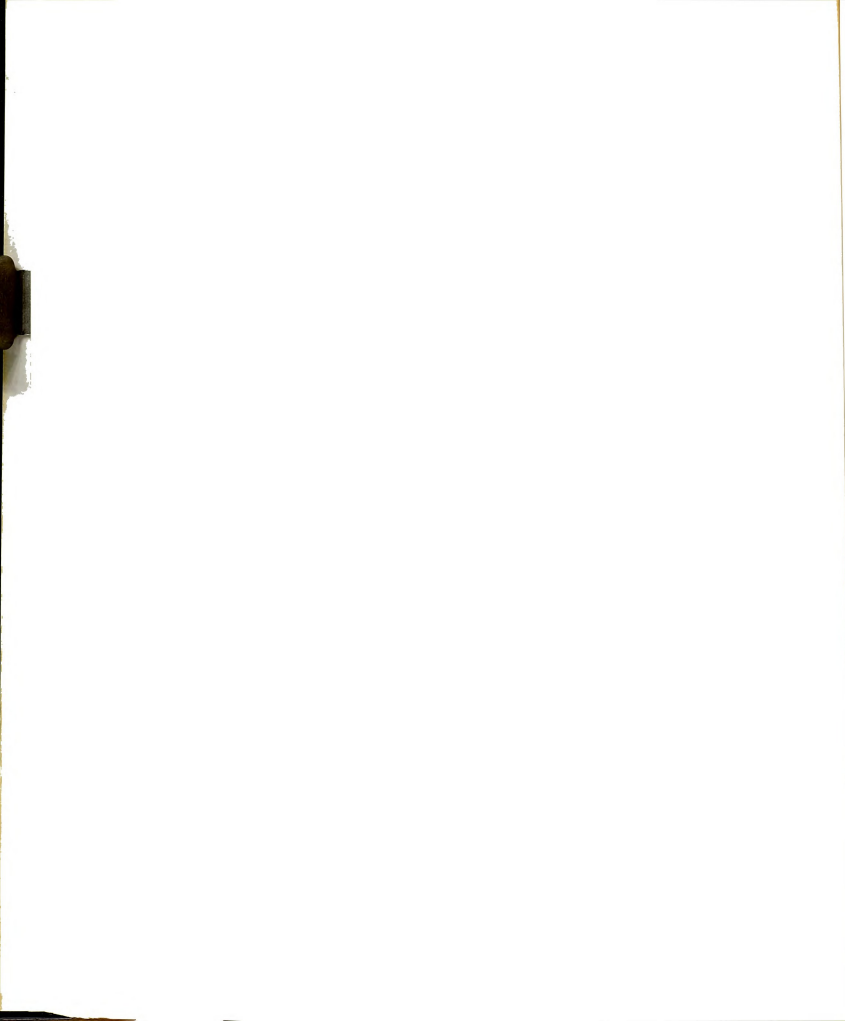
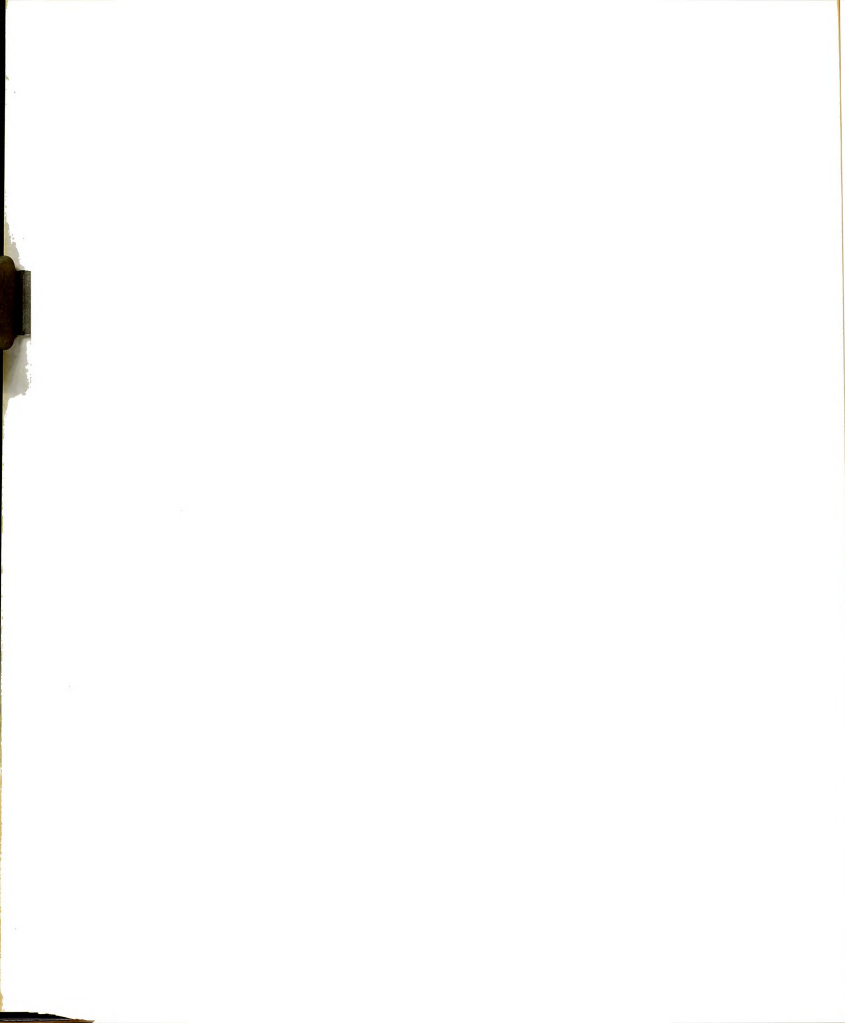


TABLE 11.--The Analysis Capabilities of the FORTRAN Program CENTRI.

Aspect	Needed Parameter	Description and/or Comments
Centrifuge types	An option	Solutions can be found for countercurrent rectifying, or combination rectifying-stripping centrifuges.
Centrifuge size	Radius, length, and rotational speed	If a combination rectifying-stripping centrifuge is used, the lengths for each section are needed.
Centrifuge internals	Radius of center pipe	If the centrifuge contains a center pipe a laminar angular velocity distribution will be used between the stationary center pipe and the wall.
Gas pair	MW_1 , MW_2 , T , $P(\text{axis})$, D_{12} and viscosity	Any gas pair may be analyzed.
Internal flows	Option for type of flow	Any flow profile ranging between plug and laminar may be specified.
	Flow intersection	The flow intersection may be specified or for laminar flow (with an option given) it will be adjusted so that the shear rate of the inner and outer streams at the intersection are equal.
Optimum flows	An option	Using the ratio of the inner to outer stream flow rates given the optimum flow rates will be computed.



CHAPTER VI

ANALYSIS OF THE RESULTS OF THE COUNTERCURRENT CENTRIFUGE

A. A Comparison of the Numerical and Analytical (Approximate) Solutions

The comparison of the numerical and analytical (approximate) solutions was made using the gas pair $\text{SO}_2\text{-N}_2$ in a rectifying counter-current centrifuge. In addition, the following operating conditions were fixed:

Temperature, T , 530°R

Pressure (axis), $P(0)$, 14.7 psia

$y_f = 0.005$

Centrifuge radius, R_w , 4 inches

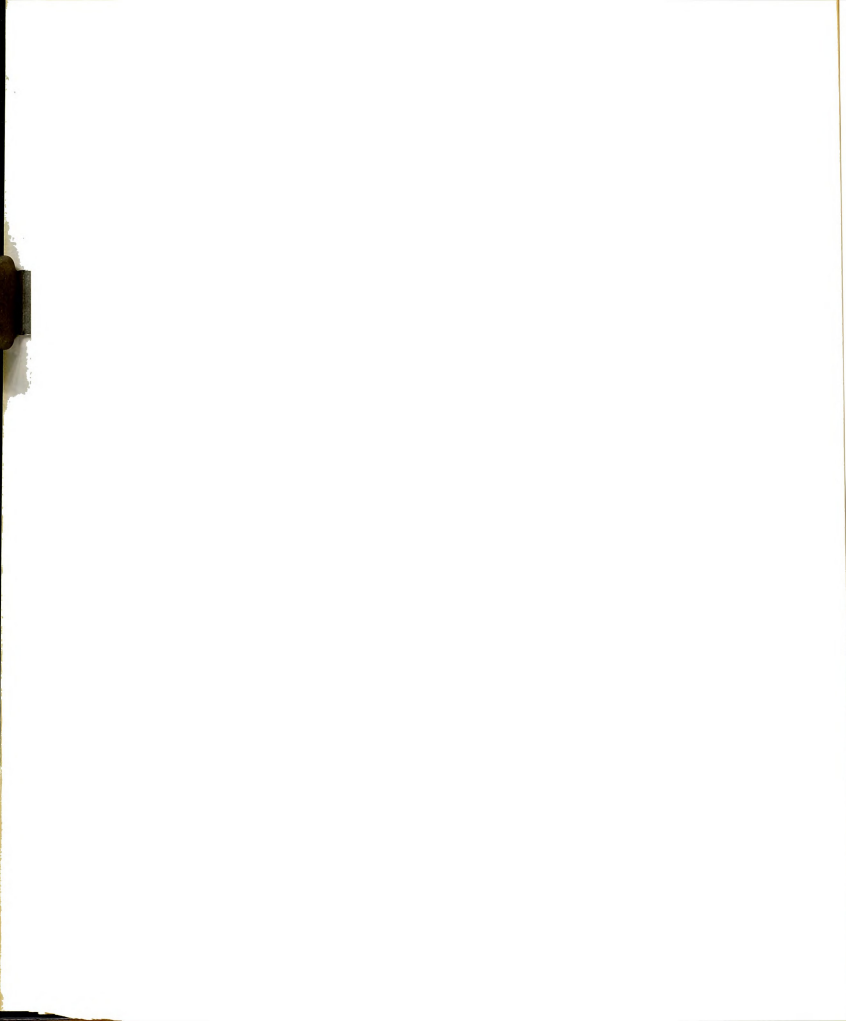
Flow intersection, R_m , 2.25 inches ($R_m/R_w = .5625$)

All numerical calculations were done using 15 radial grid points and 21 axial grid points. In the cases investigated, increasing the number of grid points in either direction, or both, did not significantly affect the results.

Separation factors used are defined as follows:

$$\alpha = \frac{y_r}{(1 - y_r)} \cdot \frac{(1 - y_f)}{y_f},$$

where y_r is the composition at the rich end of the centrifuge.



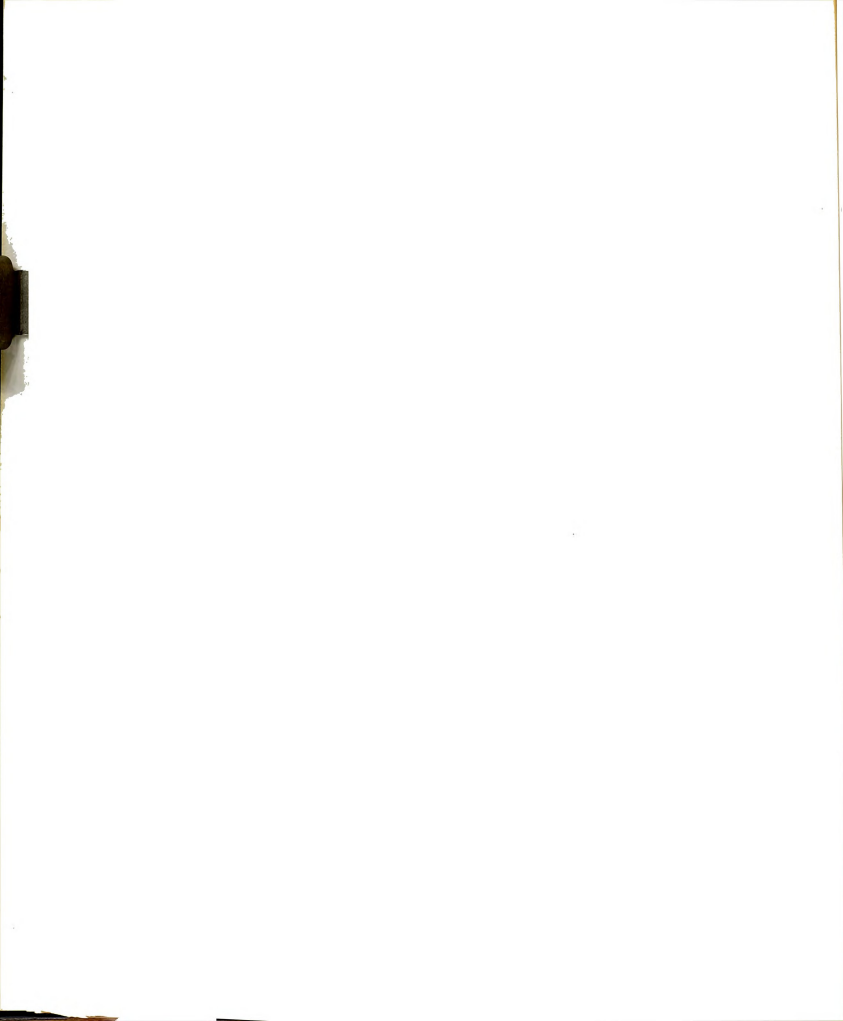
1. Comparison No. 1: $\omega = 10000$ RPM,
Length = 18 and 36 Inches and
Total Reflux

Figure 13 contains plots of the separation factor, α , versus feed rate in standard cubic feet per minute (scfm) computed using the numerical and analytical (approximate) solutions for laminar velocity profiles. Figure 14 contains plots of the separation factor, α , versus feed rate (scfm) computed using the numerical and analytical (approximate) solutions for plug type flow. Data used to construct the figures can be found in Appendix A.

2. Comparison No. 2: $\omega = 20000$ RPM,
Length = 18 inches and Total Reflux

Figure 15 contains plots of the separation factor, α , versus feed rate (scfm) computed using the numerical and analytical (approximate) solutions for laminar velocity profiles. Figure 16 contains plots of the separation factor, α , versus feed rate (scfm) computed using the numerical and analytical (approximate) solutions for plug type flow. Data used to construct the figures can be found in Appendix A.

Total reflux (no products) was used in the comparisons since by mass balance the average composition of the inner stream must equal the average composition of the outer stream at any axial position. This, it was hoped, would be a better approximation of the assumptions made in the process of obtaining an analytical (approximate) solution. That is, that radial changes in y and $\partial y / \partial z$ were small and could be neglected at any axial position. Also, total reflux represents the



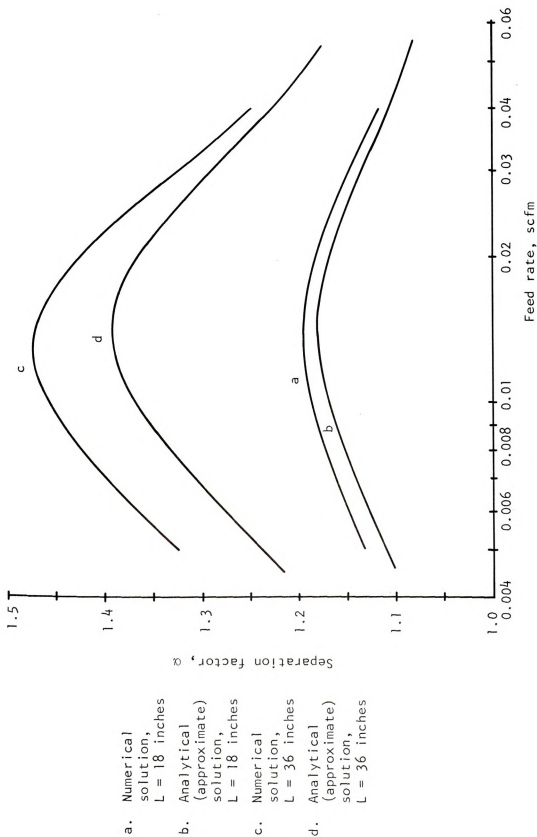
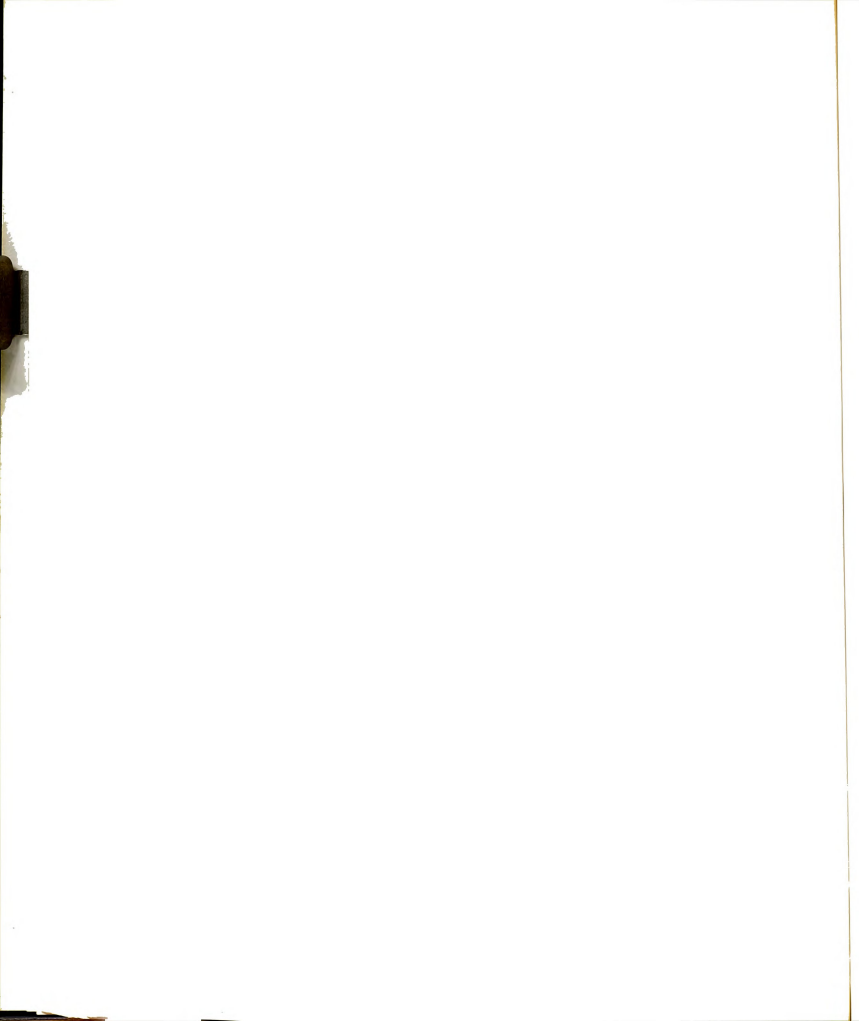


Figure 13.--Separation Factor, α , Versus Feed Rate (scfm) for $\text{SO}_2\text{-N}_2$ with Laminar Velocity Profiles, $\omega = 10000$ RPM, $R_w = 4$ Inches, $R_m/R_w = 0.5625$, $L = 18$ and 36 Inches, and Total Reflux.



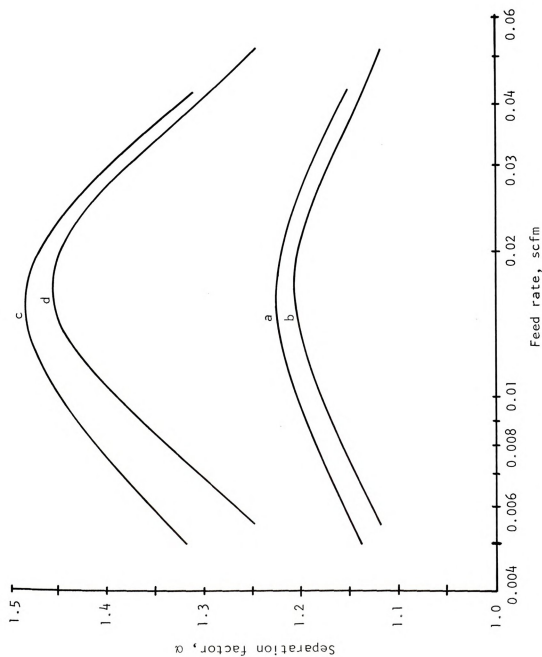
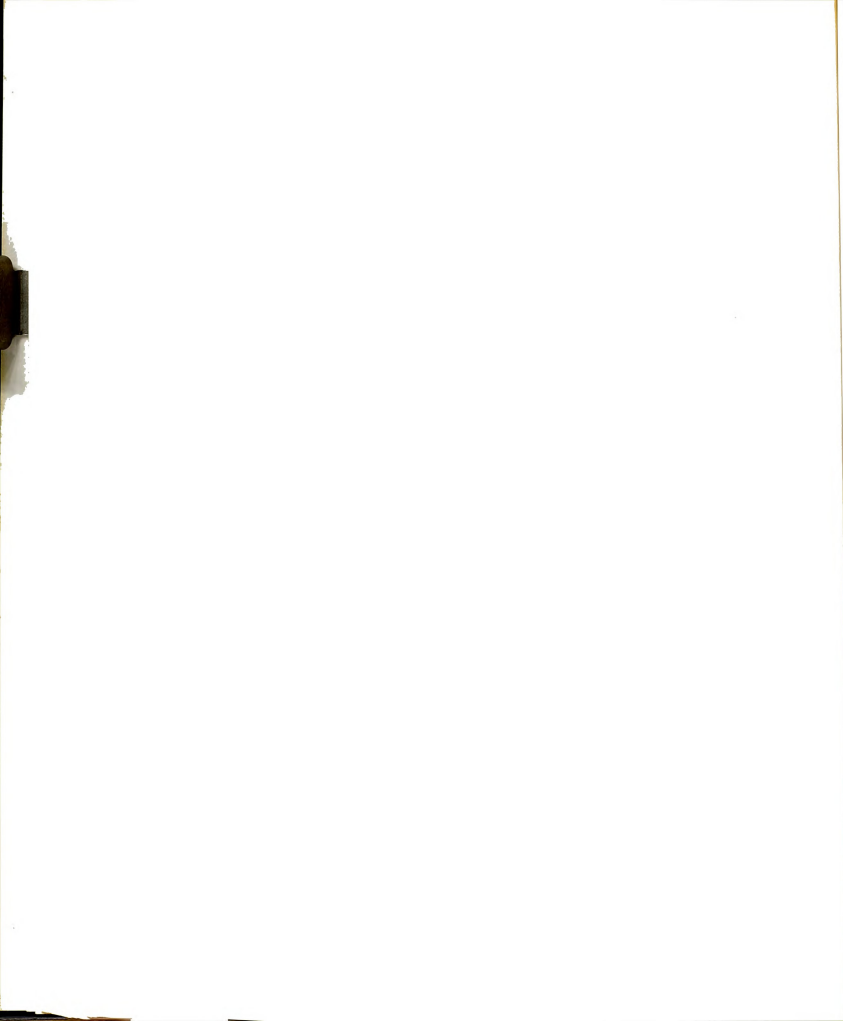


Figure 14. --Separation Factor, α , Versus Feed Rate (scfm) for $S_{O_2}-N_2$ With Plug Type Flow, $\omega = 10000$ RPM, $R_w = 4$ inches, $R_m/R_w = 0.5625$, $L = 18$ and 36 inches, and Total Reflux.



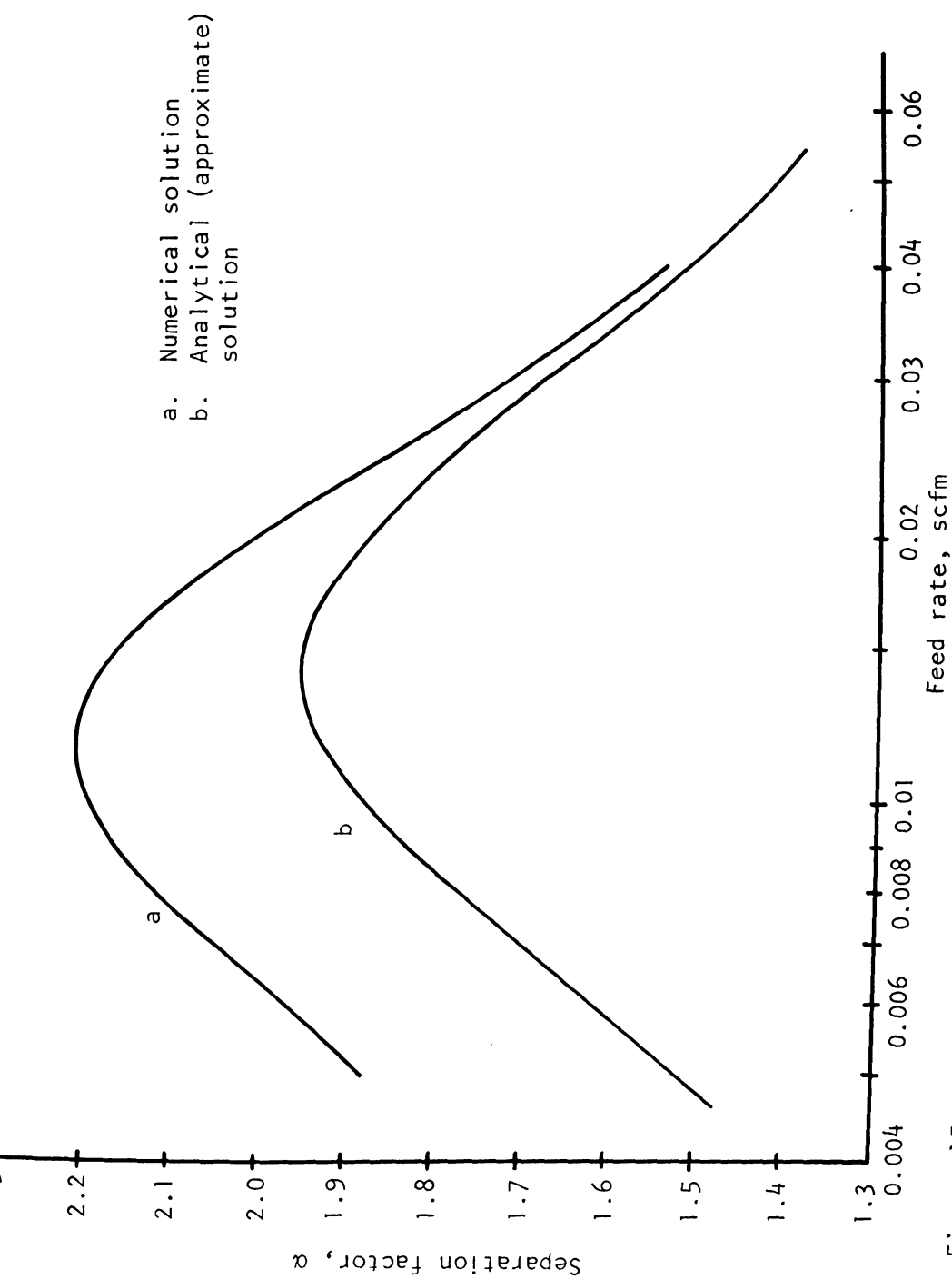
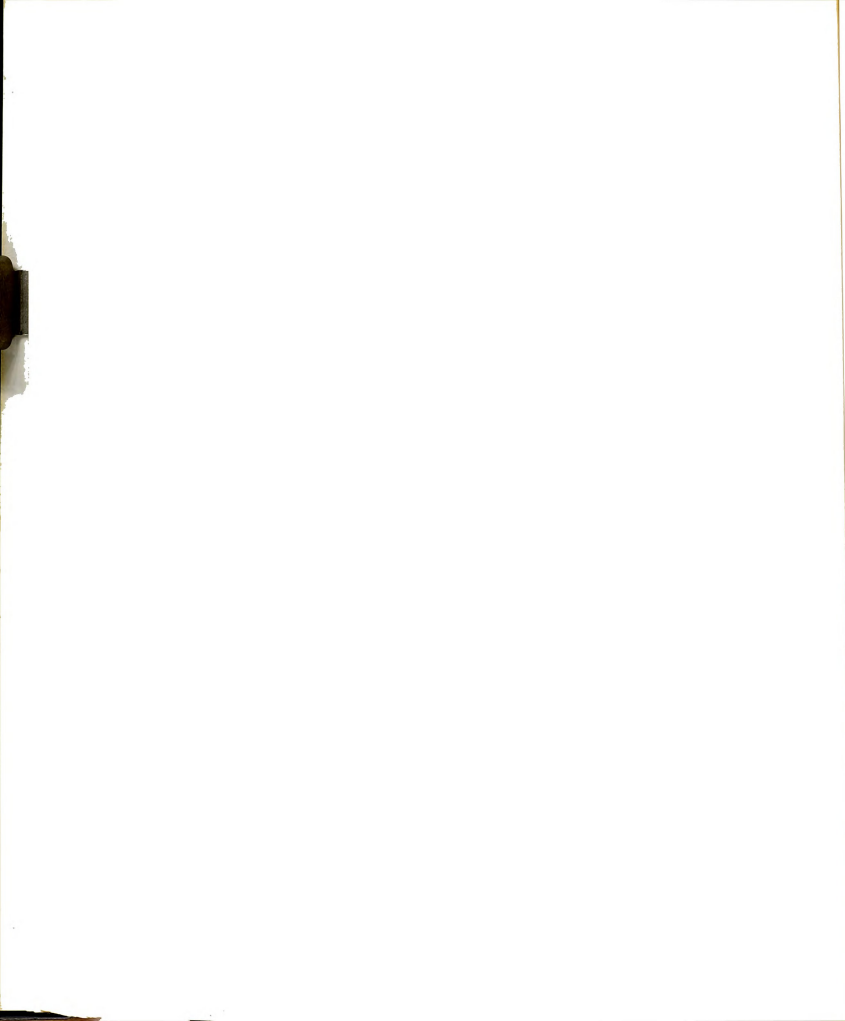


Figure 15.--Separation Factor, α , Versus Feed Rate (scfm) for $\text{SO}_2\text{-N}_2$ With Laminar Velocity. Profiles, $\omega = 20000$ RPM, $R_w = 4$ Inches, $R_m/R_w = 0.5625$, $L = 18$ Inches and Total Reflux.



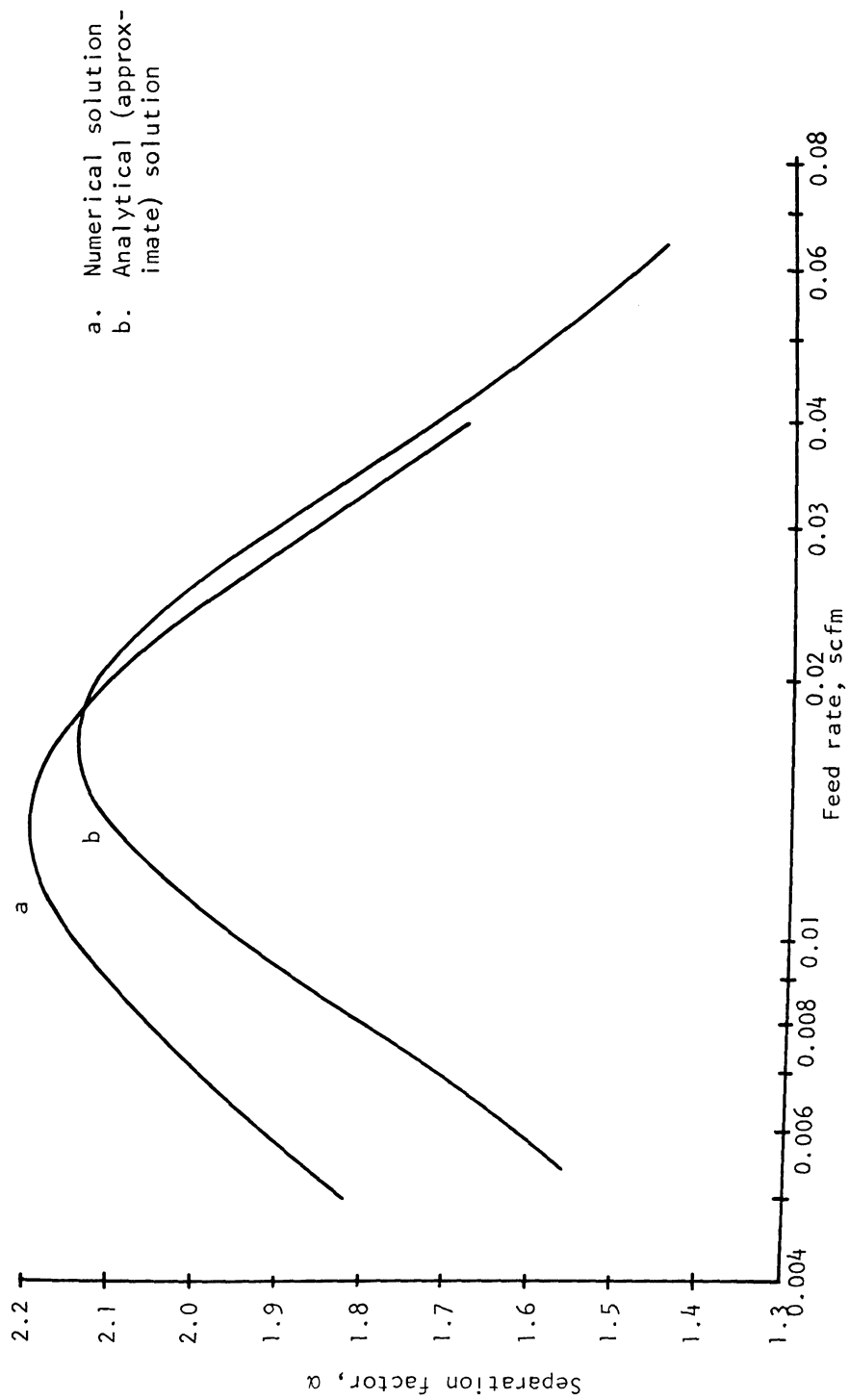
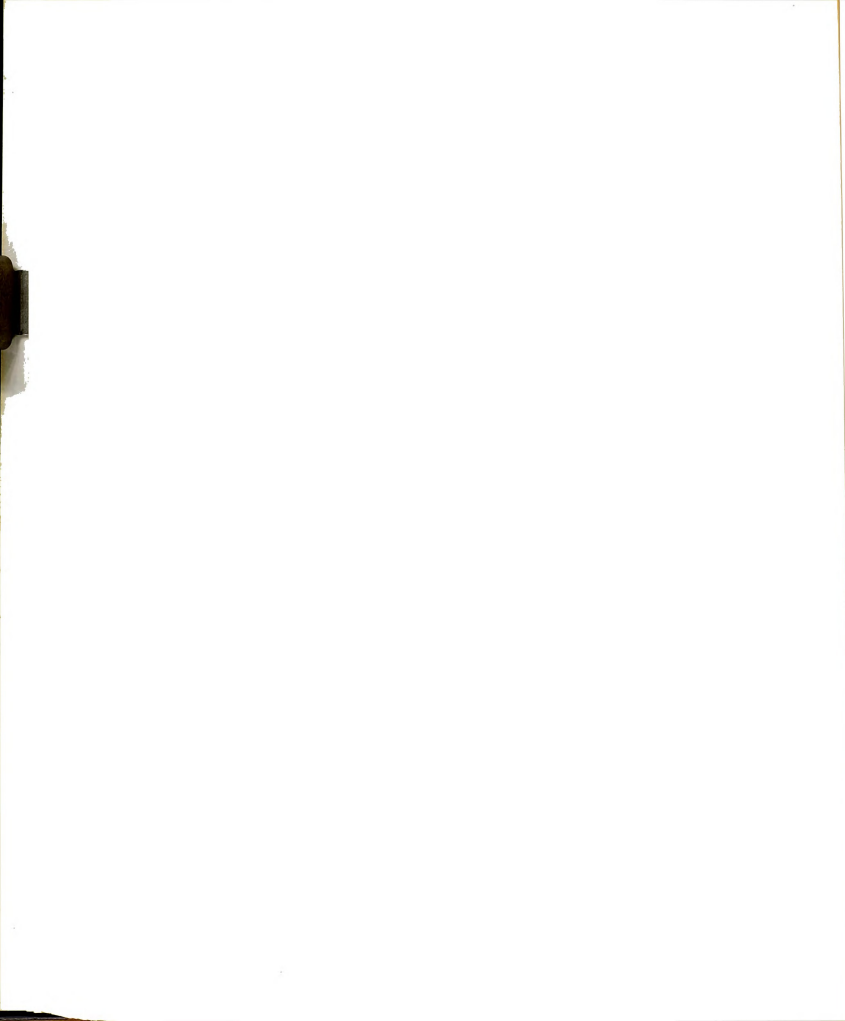


Figure 16.---Separation Factor, α , Versus Feed Rate (scfm) for $\text{SO}_2\text{-N}_2$ With Plug Type Flow, $\omega = 20000$ RPM, $R_w = 4$ Inches, $R_m/R_w = 0.5625$ Inches, $L = 18$ Inches and Total Reflux.



situation where the greatest separations will occur, hence amplifying any differences between the separations computed by the two solutions at a given feed rate.

As can be seen from the figures for either laminar or plug type flow, at either 10000 or 20000 RPM, the numerical solution always gives higher maximum separations. Also, these maximum separations occur at feed rates lower than those corresponding to the maximum separations computed analytically. These observations are listed for convenience in Table 12. It should be noted that even though the curves in each figure do not coincide, their shapes are essentially identical. Also, the sides of the curves at feed rates higher than the optimum agree very well. And, finally, that the numerical and analytical (approximate) solutions agree best, overall, when a plug type flow profile is used.

For illustration purposes, the following two tables were constructed from the results of two selected numerical solutions. Table 13 contains the radial mole fraction, y , and $\partial y / \partial z$ profiles at the axial mid-point of the 36-inch long centrifuge, rotating at 10000 RPM used in Comparison No. 1 with a feed rate of 0.0125 scfm. Also, Table 14 contains the radial mole fraction, y , and $\partial y / \partial z$ profiles at the axial mid-point of the 18-inch long centrifuge, rotation at 20000 RPM used in Comparison No. 2 with a feed rate of 0.02 scfm.

The fact that the analytically computed optimum flow rates are larger and the magnitude of the separations are smaller than those computed numerically can be explained in terms of the variance in the mole fraction profile. The analytical (approximate) solution assumes

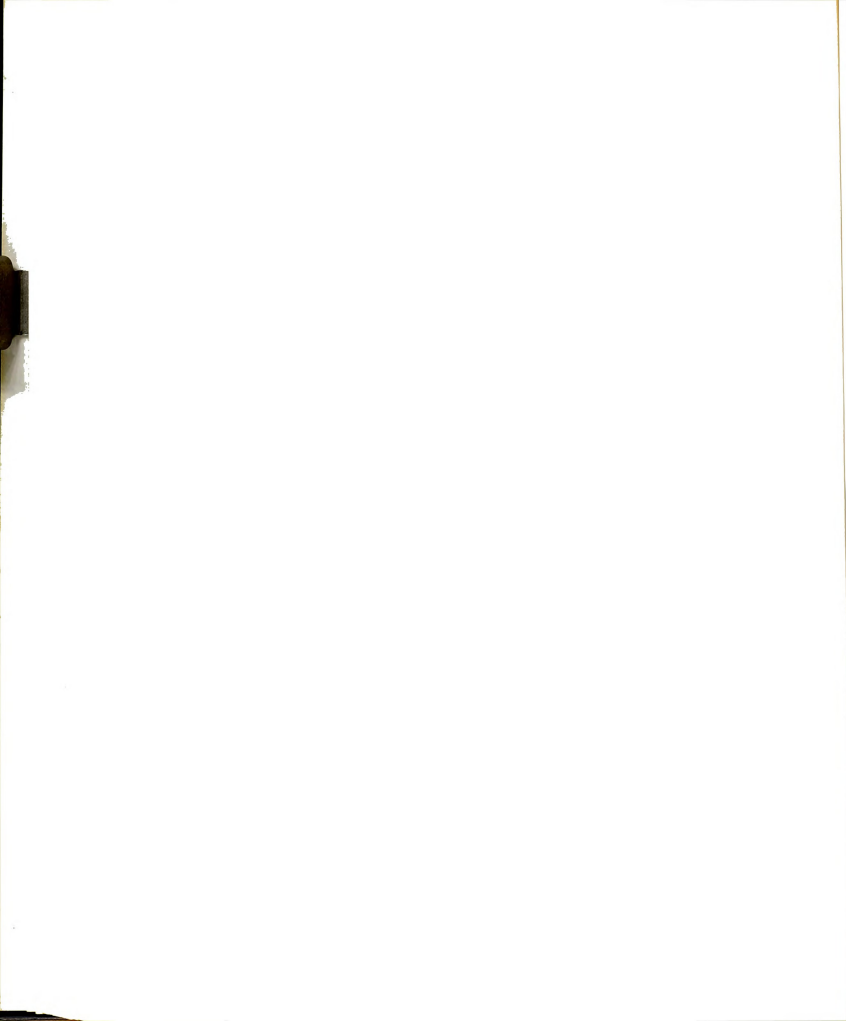


TABLE 12.--Maximum Separation Factors and Their Corresponding Feed Rates Found During the Comparison of the Numerical and Analytical (Approximate) Solutions: $\text{SO}_2\text{-N}_2$.

Velocity Profile	Rotational Speed and Length	Solution	Feed Rate, scfm	Separation Factor, α
laminar	10000 RPM 18 and 36 inches	numerical	0.0138, 0.0130	1.196, 1.472
plug	10000 RPM 18 and 36 inches	numerical	0.0167, 0.0164	1.228, 1.487
laminar	20000 RPM 18 inches	numerical	0.0117	2.204
plug	20000 RPM 18 inches	numerical	0.0136	2.193
laminar	10000 RPM 18 and 36 inches	analytical (approximate)	0.0141, 0.0141	1.180, 1.392
plug	10000 RPM 18 and 36 inches	analytical (approximate)	0.0169, 0.0169	1.207, 1.456
laminar	20000 RPM 18 inches	analytical (approximate)	0.0141	1.947
plug	20000 RPM 18 inches	analytical (approximate)	0.0168	2.136



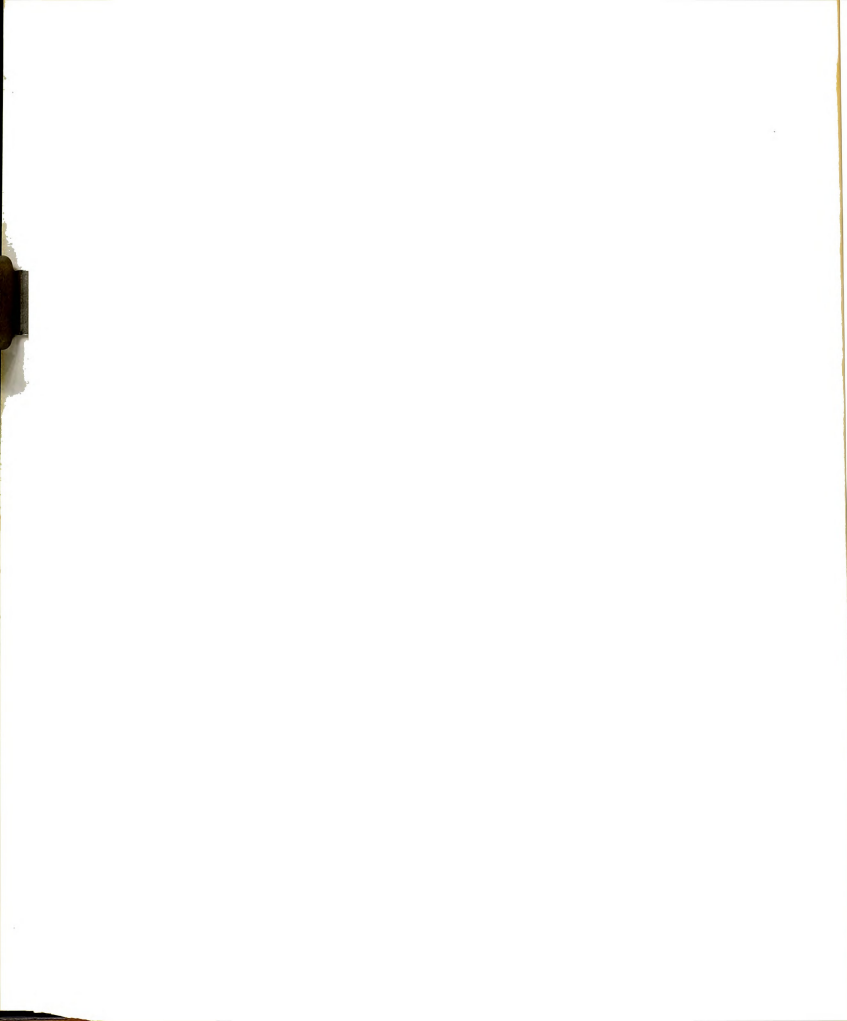
TABLE 13.--Mole Fraction, y , and $\partial y/\partial z$ Profiles at Various Radial Positions for Laminar and Plug Type Flow With a Feed Rate of 0.0125 scfm: $\text{SO}_2\text{-N}_2$.

Radius (inches)	10000 RPM, Length = 36 inches			
	Laminar Velocity Profile		Plug Type Flow	
	$y \times 10^2$	$\partial y/\partial z \times 10^3$	$y \times 10^2$	$\partial y/\partial z \times 10^3$
0.000	.6018	.8022	.5862	.8091
0.321	.6017	.8022	.5863	.8091
0.643	.6015	.8022	.5867	.8089
0.964	.6011	.8023	.5872	.8087
1.286	.6009	.8026	.5880	.8083
1.607	.6010	.8033	.5890	.8079
1.929	.6014	.8046	.5902	.8073
2.250 (R_m)	.6026	.8069	.5917	.8068
2.500	.6042	.8096	.5935	.8074
2.750	.6066	.8132	.5961	.8094
3.000	.6099	.8178	.5994	.8128
3.250	.6139	.8235	.6034	.8174
3.500	.6188	.8301	.6081	.8232
3.750	.6245	.8377	.6136	.8302
4.000	.6307	.8460	.6197	.8389



TABLE 14.--Mole Fraction, y , and $\partial y/\partial z$ Profiles at Various Radial Positions for Laminar and Plug Type Flow at Feed Rate of 0.02 scfm: $\text{SO}_2\text{-N}_2$.

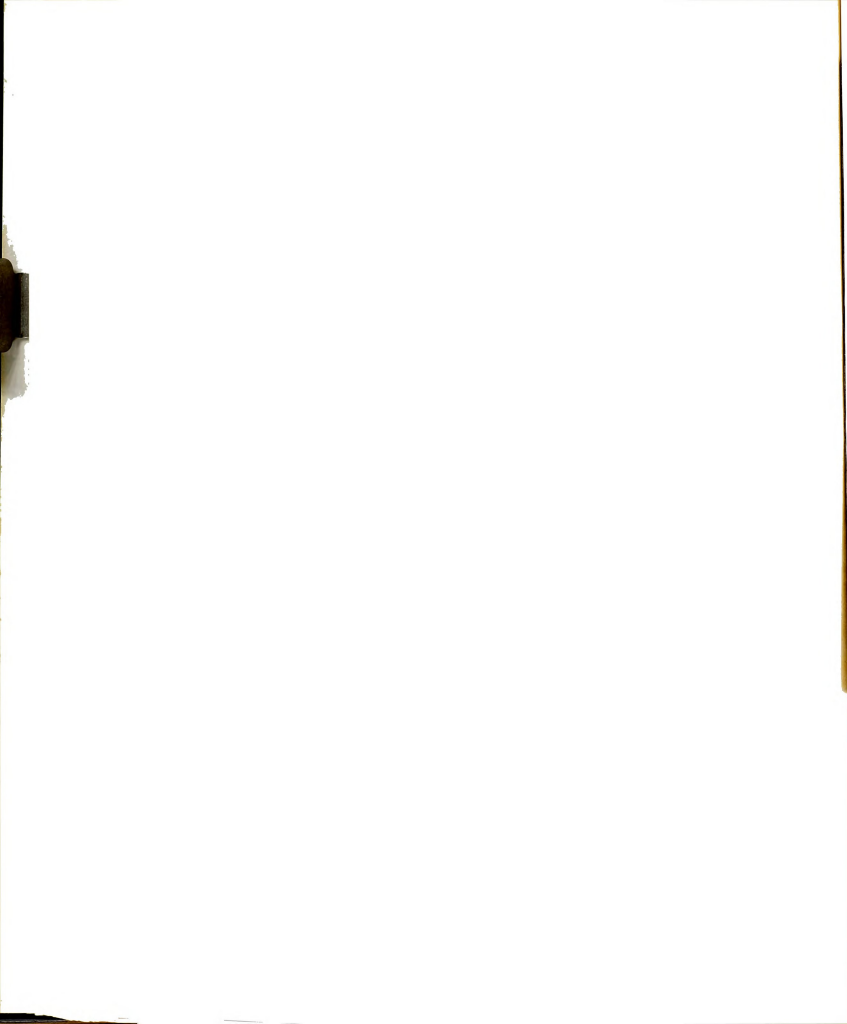
Radius (inches)	20000 RPM, Length = 18 inches			
	Laminar Velocity Profile		Plug Type Flow	
	$y \times 10^2$	$\partial y/\partial z \times 10^3$	$y \times 10^2$	$\partial y/\partial z \times 10^3$
0.000	.7141	.3391	.6922	.3768
0.321	.7125	.3386	.6921	.3767
0.643	.7091	.3375	.6921	.3764
0.964	.7040	.3359	.6920	.3758
1.286	.6979	.3342	.6917	.3751
1.607	.6920	.3327	.6914	.3740
1.929	.6875	.3320	.6909	.3727
2.250 (R_m)	.6864	.3329	.6905	.3713
2.500	.6893	.3353	.6938	.3721
2.750	.6964	.3396	.7016	.3755
3.000	.7083	.3461	.7139	.3815
3.250	.7254	.3549	.7307	.3899
3.500	.7476	.3659	.7521	.4010
3.750	.7747	.3792	.7784	.4147
4.000	.8061	.3944	.8097	.4313



that radial changes in $\partial y/\partial z$ are small and can be neglected. That is, at any axial position, the rate of change of the composition with axial position is the same all across the radius. However, as was seen in the operation of the unsteady state simple centrifuge (Chapter III), near the wall the mole fraction profile increased the fastest with time. This is also the case with the countercurrent rectifying centrifuge as shown in Tables 13 and 14, where the composition changes fastest with axial position near the wall. Thus, with this extra capacity of the outer stream, allowed for in the numerical solution, maximum separations would be expected to be larger.

In the inner stream, however, where the assumptions imposed by the analytical (approximate) solution are best approximated (almost constant y and $\partial y/\partial z$), the radial flux is essentially the same as computed by both the analytical (approximate) and numerical solutions. That is, the radial flux is essentially maximized being equal to that caused by pressure diffusion, since almost no radial gradient exists. Hence, to allow for the extra capacity of the outer stream, but yet being restricted to a given rate of flux from the inner stream, the optimum flows computed by the numerical solution would necessarily be expected to be lower.

The fact that agreement between the analytical (approximate) and numerical solutions is best for plug type flow can best be explained in terms of the velocity profiles. Figure 17 illustrates the shape of the laminar and plug type velocity profiles for a feed rate of 0.0125 scfm and centrifuge rotational speed of 10000 RPM. In the case of laminar flow, the velocity goes to zero in a continuous



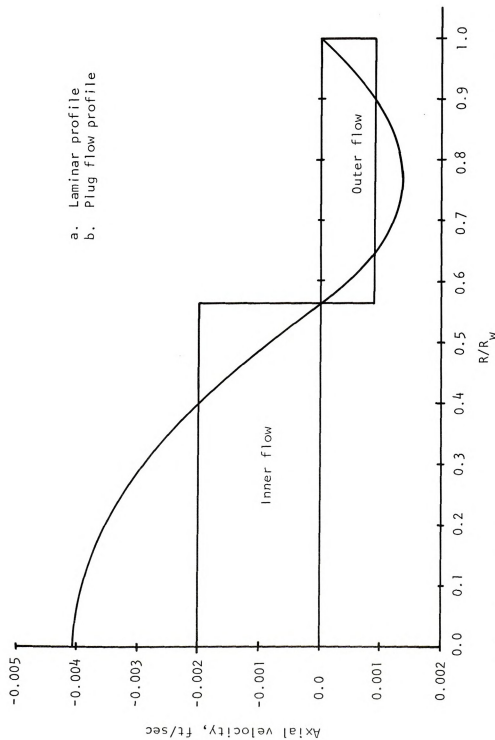
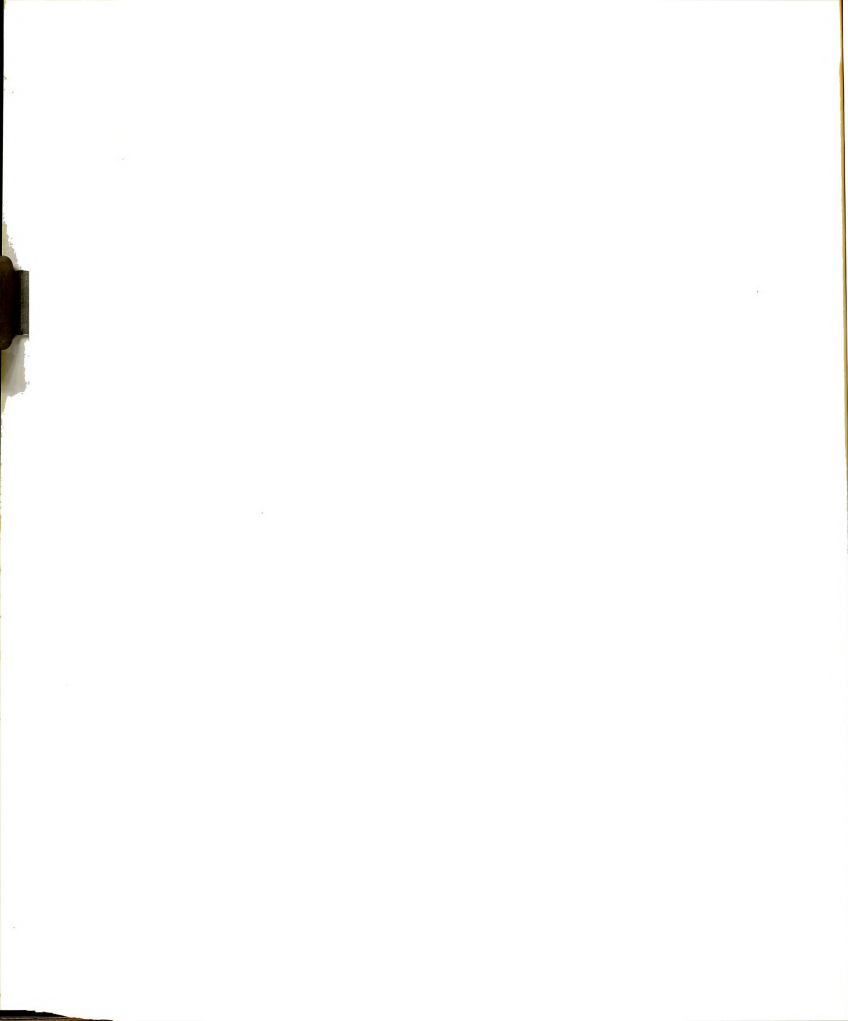


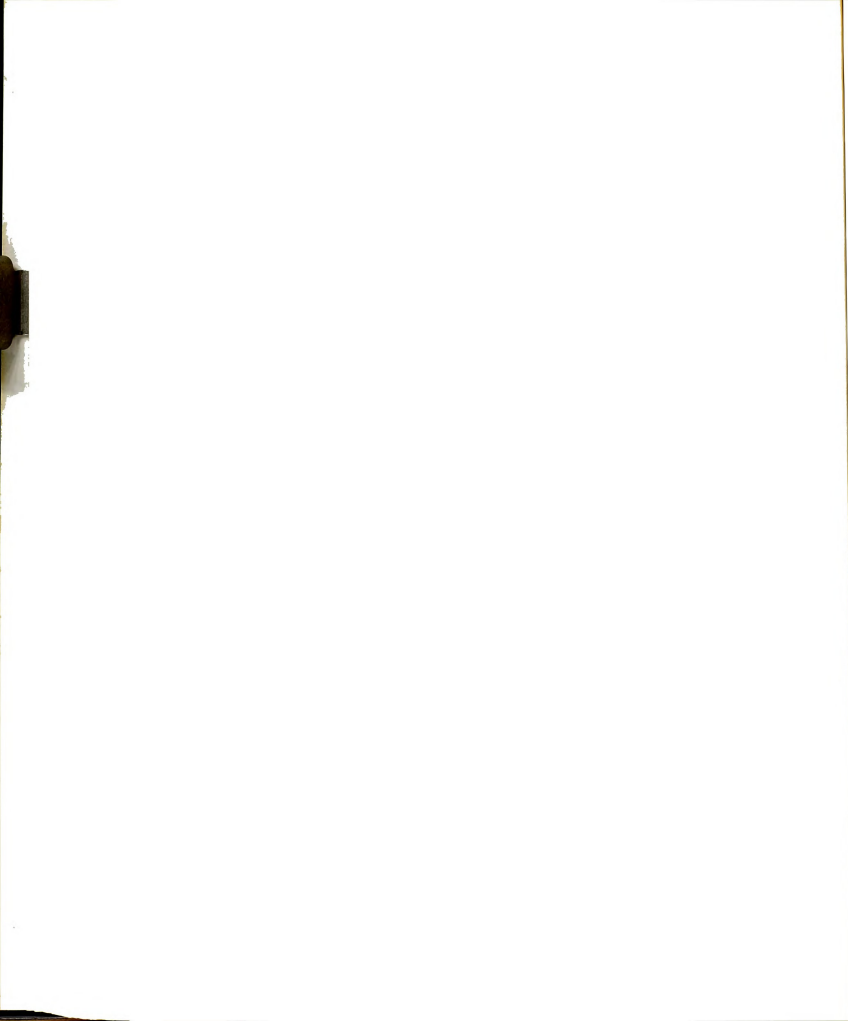
Figure 17.--Assumed Laminar and Plug Flow Velocity Profiles for a Feed Rate of 0.0125 scfm in a Countercurrent Rectifying Centrifuge With $R_m = 2.25$ Inches, $R_w = 4.0$ Inches, $\omega = 10000$ RPM and Total Reflux.



fashion as the wall is approached. This slower moving region near the wall will allow an even greater concentration buildup when the solution is computed numerically. But, as mentioned above, this increase in allowable separation must be accompanied by a decrease in the flow rates of the inner and outer streams. For plug type flow, however, the velocity profile is assumed constant over to the wall where it immediately goes to zero. With all the gas moving uniformly there is a lesser tendency for a radial mole fraction buildup near the wall, hence, a closer approximation to the assumptions made to obtain the analytical (approximate) solution. However, even for plug flow, as the rotational speed is increased from 10000 to 20000 RPM, the agreement becomes worse. At these speeds the centrifugal forces are becoming so great that the tendency for the heavy species to be "piled" up at the wall is seen regardless of the shape of the velocity profile.

Using feed rates higher than the optimum (increases the magnitudes of the velocity profiles) at a given rotational speed, inhibits the buildup of the heavy species near the wall (tends to diminish radial changes in y and $\partial y/\partial z$). Hence, there exists good agreement between the numerical solutions in this feed range. On the other hand, the opposite is true when feed rates less than the optimum are used. The slow moving gas, which not only allows the composition to build up near the wall, but farther into the outer stream, gives large deviations between the two solutions.

It may be concluded, then, by this analysis, that the optimum separation should always be higher than that predicted by the analytical



(approximate) solution, but occur at a lower flow rate than predicted analytically. Also that the agreement between the analytical (approximate) solution and the expected results will be determined by how well the operating conditions approximate the assumptions made to obtain the analytical (approximate) solution. That is, velocity profiles which have slow moving regions, high rotational speeds, and large molecular weight differences are typical parameters which enhance radial mole fraction gradients. Large diffusion coefficients, on the other hand, tend to erase a concentration gradient. By making a comparison of the gas pair and the operating conditions desired with the analysis presented above for $\text{SO}_2\text{-N}_2$, an estimation of the accuracy of the results predicted analytically can be made. For example, consider the system $\text{SO}_2\text{-H}_2$ in a countercurrent rectifying centrifuge with the operating conditions as fixed in Comparison No. 1 (length = 36 inches). Though the molecular weight difference is 1.72 times greater, the diffusion coefficient (see Appendix B) is 3.93 times greater; hence fairly good agreement is expected between the analytical (approximate) and numerical solutions. A comparison of the two solutions may be found in Figure 18 which illustrates the expected good agreement.

One last comparison to be made between the numerical and analytical (approximate) solutions is the effect of removing a product stream. Returning to the gas pair $\text{SO}_2\text{-N}_2$ with the operating conditions as given in Comparison No. 1, agreement between the solutions was found to be quite good at total reflux with a feed rate of 0.02 scfm (higher



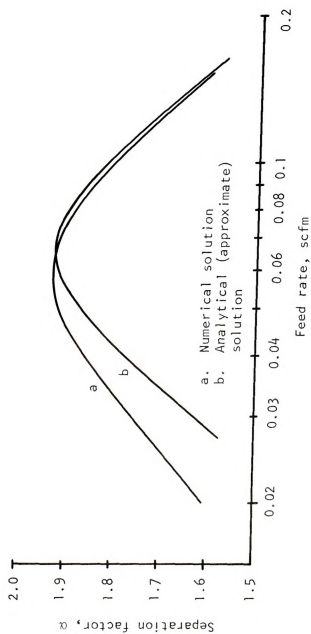
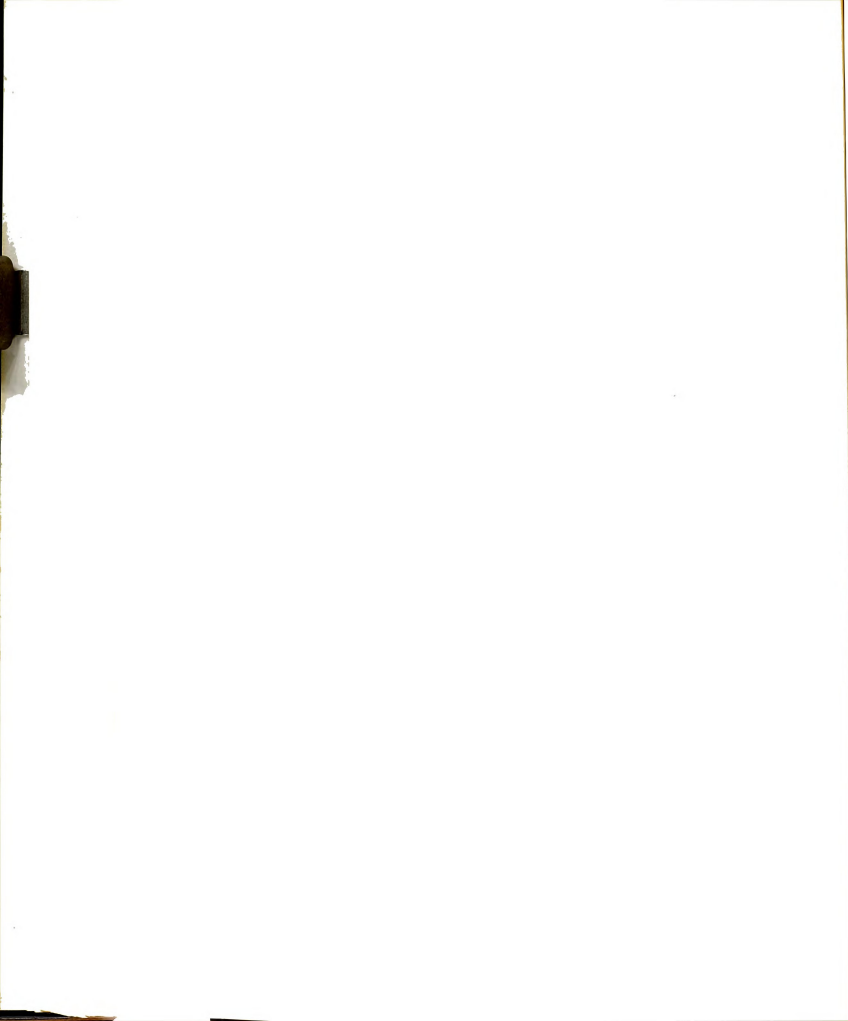


Figure 18.--Separation factor, α , Versus Feed Rate, scfm, for SO_2/H_2 , With Plug Type Flow, $\omega = 10000$ RPM, $R_w = 4$ inches, $R_m/R_w = 0.5625$, $L = 36$ inches, and Total Reflux.

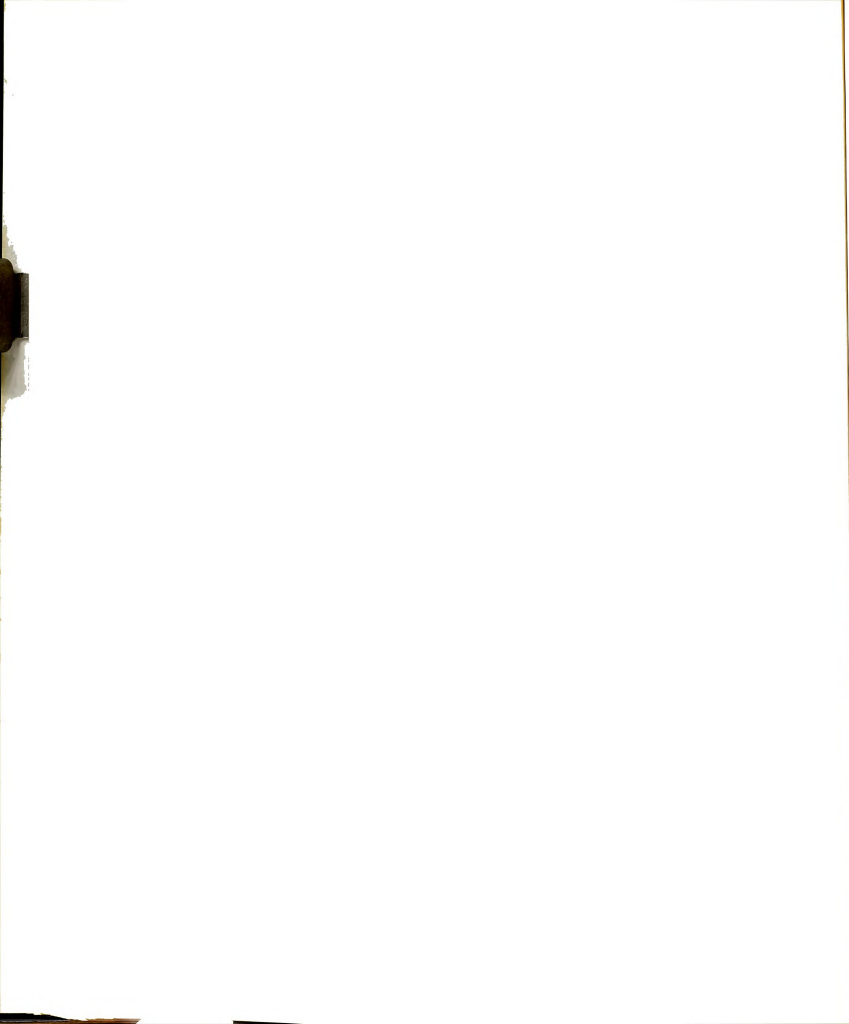


than the optimum). Table 15 illustrates the effect on this agreement when various percentages of the feed stream are taken off as product.

As it has been pointed out, the assumption that changes in y in the radial direction could be neglected, which was used to obtain the analytical (approximate) solution, must necessarily be violated when a product stream is taken off. Since the product stream is richer in the heavy species than is the feed, the leaving inner stream must necessarily be leaner than the feed. Although the error does become greater as the value of R/F is increased from 0 to 0.2, it is not large (maximum of -4.7%). This is due to the rather rapid decrease in the separation factor (-19.5% at $R/F = .2$) which, of course, decreases the expected composition difference (only 5.2% at $R/F = 0.2$) between the leaving lean stream and the entering feed. Hence, without the expected

TABLE 15.--Separation Factors for the Gas Pair $\text{SO}_2\text{-N}_2$ at Various Ratios of the Rich Stream to the Feed Stream (R/F) as Computed from the Numerical and Analytical (Approximate) Solutions. Feed Rate = 0.02 scfm, $R_w = 4$ Inches, $R_m/R_w = 0.5625$, $\omega = 10000$ RPM, $L = 36$ Inches, and Plug Type Flow.

R/F	Separation Factors		% Error	Average Mole Fraction of the Leaving Inner Stream, $y_f = 0.005$
	Numerical Solution	Analytical (Approximate) Solution		
0.00	1.470	1.448	-1.5	0.00500
0.05	1.361	1.327	-2.5	0.00491
0.10	1.284	1.239	-3.5	0.00484
0.15	1.227	1.175	-4.2	0.00479
0.20	1.184	1.128	-4.7	0.00474



composition differences the agreement between the numerical and analytical (approximate) solutions is maintained at approximately the level seen at total reflux. Discussion regarding the rapid decrease in separation with product removed will be presented in Chapter VI-E.

Several areas of disagreement and their causes have been pointed out between the numerical and analytical (approximate) solutions. These points of disagreement should be taken into account when investigating the potential of a gas centrifuge design and especially when comparing calculated results to experimental data. From this point on in this work, however, with attention being returned to the overall goal of analyzing the gas centrifuge and determining its key parameters, the analytical (approximate) solution will be used. The analytical (approximate) solution exhibits properties similar to the numerical solution and is certainly more convenient to evaluate. Although it should be remembered that while certain phenomena and trends can be predicted by the analytical (approximate) solution, their actual magnitudes may be in slight error.

With reference to Table 12, it should be noted that the difference between the maximum separations obtained using a laminar or plug type velocity profile differ at most by 9%. Also, the optimum feed rates differ at most by 16%. This is true for both the numerical and analytical (approximate) solutions. Furthermore, while this agreement as taken from Table 12 was obtained for $\text{SO}_2\text{-N}_2$, even better agreement is seen for $\text{SO}_2\text{-H}_2$. Hence, as long as it can be shown that the velocity profiles lie between laminar and plug type flow in an



actual centrifuge, knowing the exact shape of the profiles is not necessary. However, due to the better agreement between the numerical and analytical (approximate) solutions when plug type flow is assumed, it will be used in the remainder of this work. Also, when possible, feed rates greater than the optimum will be used.

B. The Effect of the Position of the Intersection
of the Inner and Outer Streams on the Maximum
Separation Factor and the Optimum Feed Rate

The separation in the countercurrent centrifuge depends on the heavy species moving from the inner to the outer stream. This movement is due to the centrifugal force in the form of pressure diffusion. With the flow intersection very near the axis, the inner stream is subjected to very little centrifugal force. Thus, the radial flux from the inner stream is reduced giving poorer separation factors. Also, as the flow intersection moves nearer to the axis the decreasing area available for the inner stream means higher velocities for a given mass flow rate. This has the effect of reducing the optimum feed rate.

On the other hand, moving the flow intersection nearer the wall allows a greater portion of the inner stream to be subjected to larger centrifugal forces. This increases the maximum separation factor, and with the increase in area for flow, increases the optimum flow rate. The fact that the outer stream is now moving faster does not hinder the separation since it (outer stream) serves merely to carry away the heavy species coming from the inner stream.

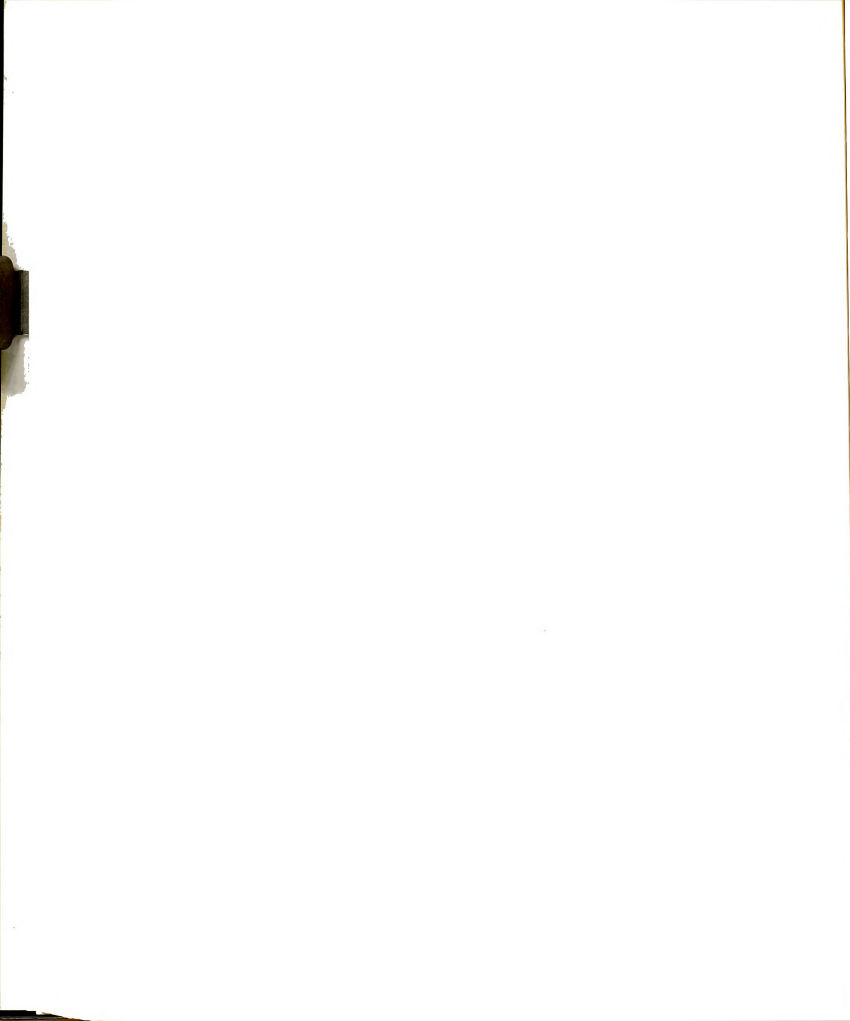


Figure 19 was constructed illustrating the effect of varying the flow intersection position. The following operating conditions were used:

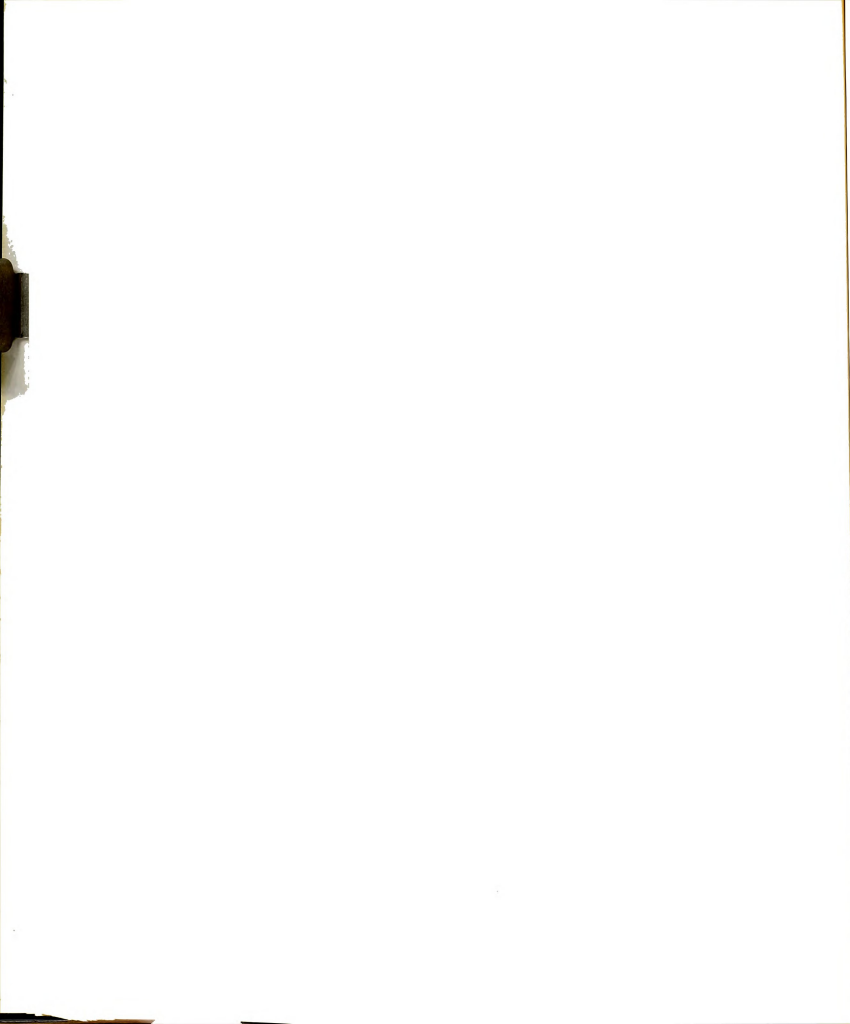
Gas pair = $\text{SO}_2\text{-N}_2$,
 Temperature = 530°R ,
 Pressure (axis), $P(0) = 14.7$ psia,
 $y_f = 0.005$,
 Centrifuge radius = 4 inches,
 Centrifuge length = 36 inches,
 Centrifuge RPM = 10000,
 Plug type flow and total reflux.

Data used to construct Figure 19 may be found in Appendix A.

As expected, the maximum separation factor becomes poorer and the optimum feed rate less as the intersection is moved toward the axis. Increasing R_m/R_w from 0.125 to 0.875 increases the separation factor by 32% while increasing the optimum feed rate by 137%.

C. The Effect of the Centrifuge Radius on the Maximum Separation Factor and the Optimum Feed Rate

Analysis of the simple centrifuge indicated that as long as the peripheral speed was maintained constant, the simple separation factor did not change by changing the size of the centrifuge (Chapter 11-B). If this was true for the countercurrent centrifuge it would be a definite "plus" factor. Since, by increasing the radius, and thereby increasing the area for flow of each stream, the optimum feed rate would increase. Also, by maintaining a constant peripheral speed, one is not operating any nearer the bursting point and by increasing the



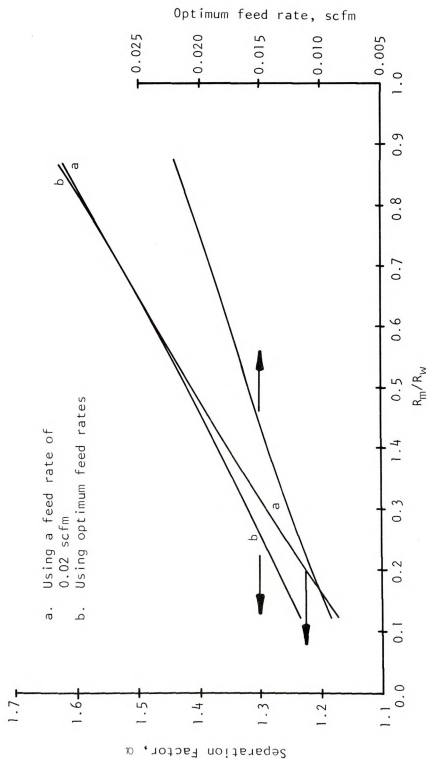
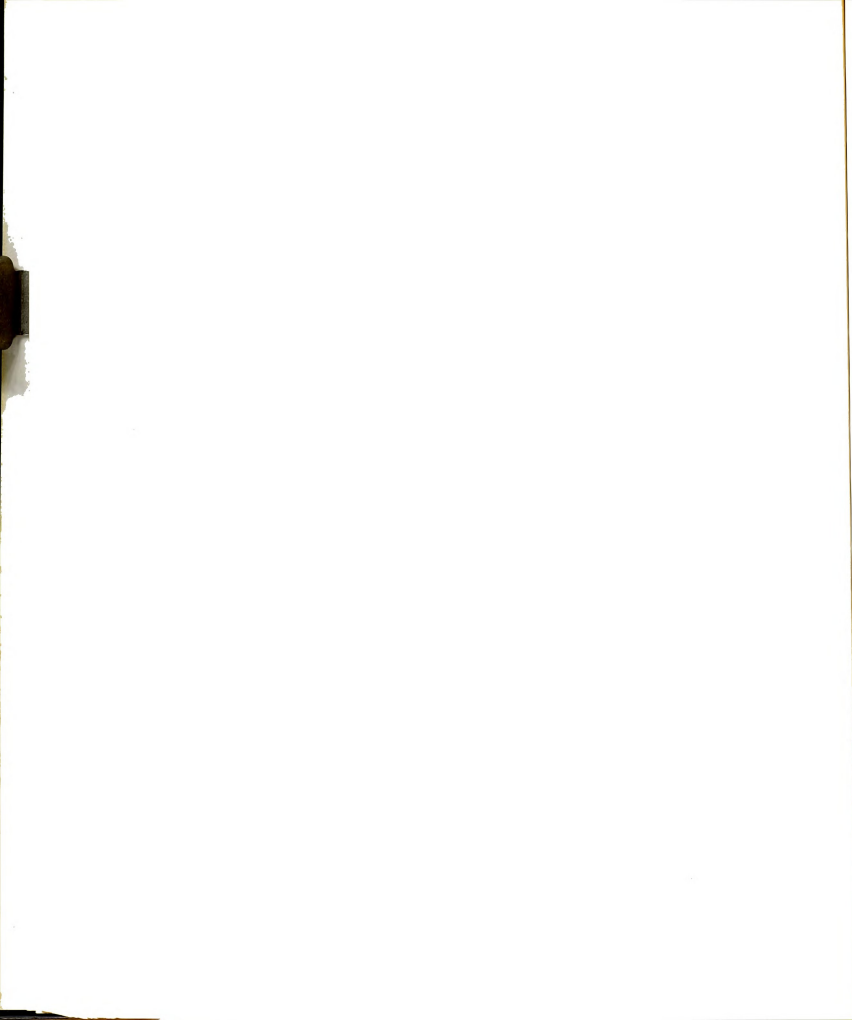


Figure 19.--Separation Factors, α , and Optimum Feed Rates Versus the Ratio of the Radius of the Flow Intersection to the Centrifuge Radius, R_m/R_w , for $\text{SO}_2\text{-N}_2$ With Plug Type Flow, $\omega = 10000$ RPM, $R_w = 4$ inches, $L = 36$ inches and Total Reflux.



radius (decreasing L/D), the first whirling speed is increased (Chapter IV, A and B).

To analyze the effect of different radii on the maximum separation factor and the optimum feed rate the following operating conditions were used:

Gas pair = SO_2-N_2 ,

Temperature = $530^\circ R$,

Pressure (axis), $P(0) = 14.7$ psia,

$y_f = 0.005$,

Centrifuge length = 36 inches,

$R_m/R_w = 0.5625$,

Plug type flow and total reflux.

Peripheral speeds of 350 and 700 feet/sec were used for the different radii investigated. Table 16 contains the results of varying the radius from 2 to 7 inches for the two peripheral speeds.

The undesirable reduction in the maximum separation factor accompanying an increase in the radial size of the centrifuge can be explained with some reflection on the factors which create a maximum separation factor. The optimum feed rate is such that the gas is moving axially fast enough to prevent excessive axial diffusion, but slow enough so that the heavy species may move from the inner to the outer stream. Thus, by doubling the radius, but maintaining a constant value of R_m/R_w , the optimum feed rate must necessarily increase to avoid excessive axial diffusion. The increase, however, is not by 4 times even though 4 times the area is available for flow. The reason for a smaller increase in the feed rate is that for the gas

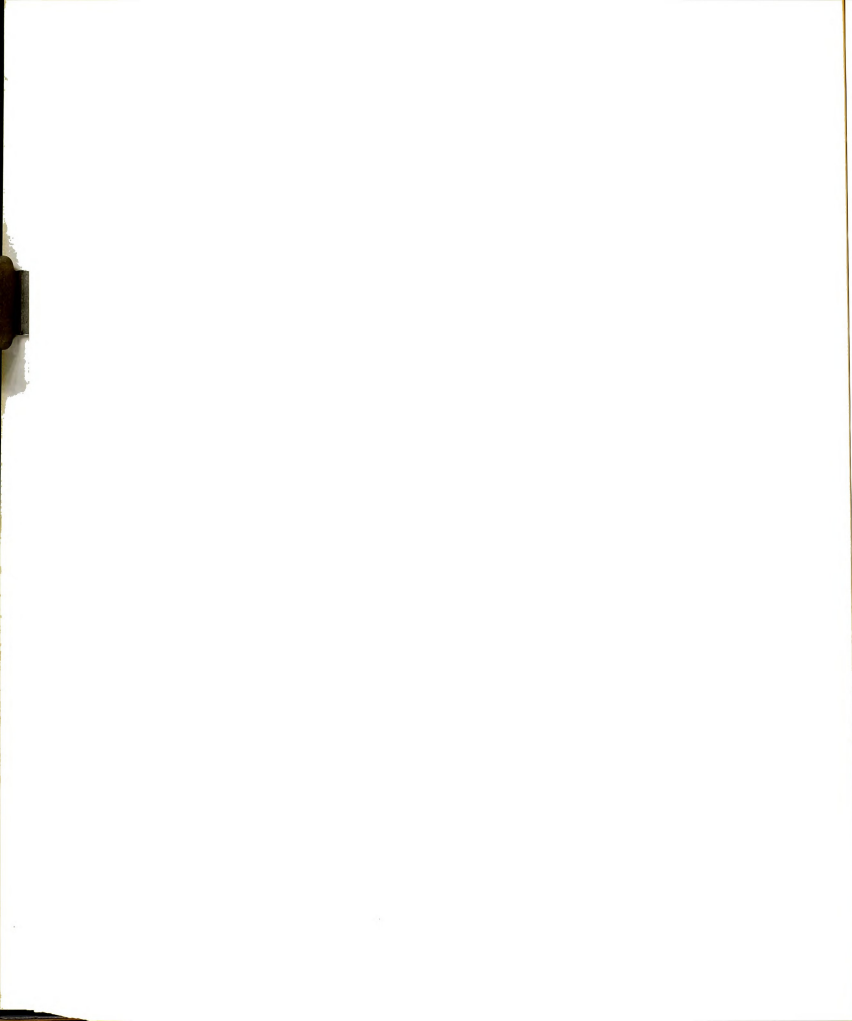


TABLE 16.--Maximum Separation Factors and Optimum Feed Rates Obtained for Various Centrifuge Radii for $\text{SO}_2\text{-N}_2$ With Plug Type Flow, $L = 36$ Inches, $R_m/R_w = 0.5625$, Peripheral Speeds of 350 and 700 ft/sec, and Total Reflux.

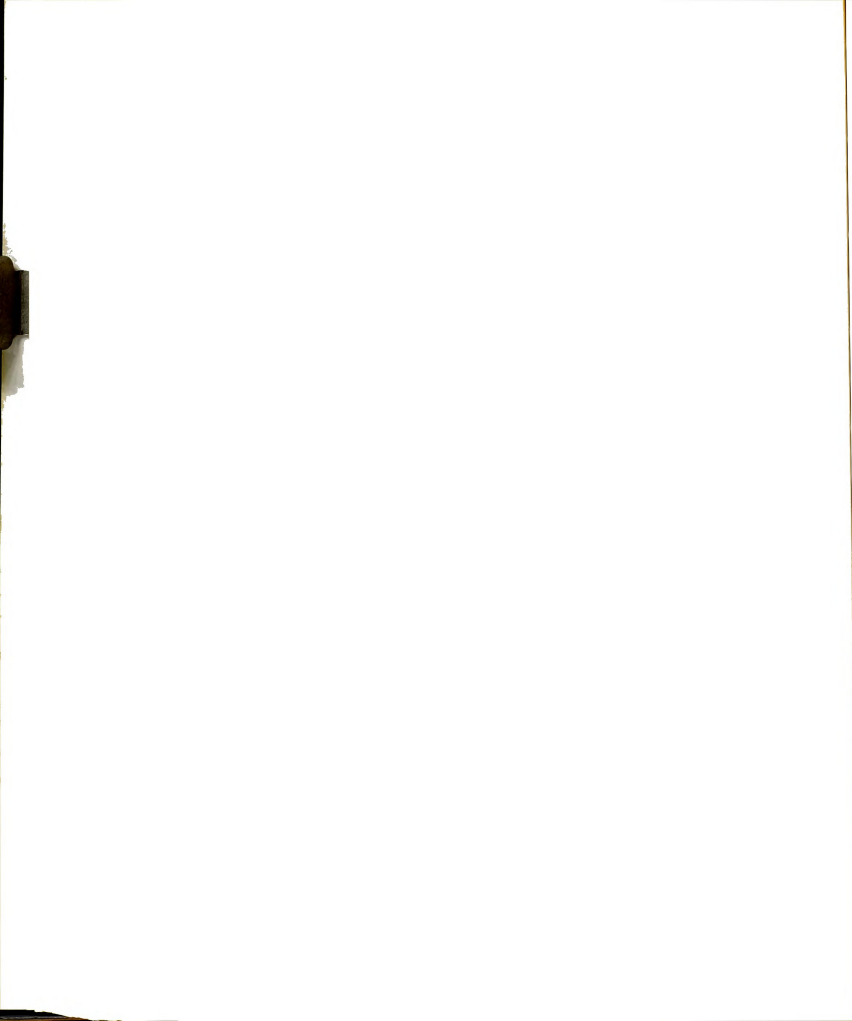
Centrifuge radius (inches)	Peripheral Speed = 350 ft/sec		Peripheral Speed = 700 ft/sec	
	Separation Factor	Optimum Feed Rate (scfm)	Separation Factor	Optimum Feed Rate (scfm)
2	2.120	0.0084	20.815	0.0084
3	1.651	0.0127	7.581	0.0126
4	1.456	0.0169	4.562	0.0169
5	1.351	0.0211	3.368	0.0211
6	1.285	0.0253	2.753	0.0253
7	1.240	0.0295	2.382	0.0295

molecules to move radially to the same dimensionless radial position (r/R_w), they must travel twice the distance. Thus, a longer residence time (smaller flow rate) is required.

Using these ideas and given the optimum feed rate for a particular centrifuge diameter, the optimum feed rate can be computed for any other diameter for the same operating conditions by the "simple minded" expression

$$\text{Feed}' = \text{Feed} \left(\frac{\text{Area}'}{\text{Area}} \right) \left(\frac{\text{Radius}}{\text{Radius}'} \right),$$

where the first multiplier accounts for the increased area for flow and the second multiplier accounts for the increased radial distance that must be traveled. Thus, for example doubling the radius of the



countercurrent centrifuge only doubles the optimum feed rate. This is illustrated in Table 16 where the values contained therein were computed using the analytical (approximate) solution.

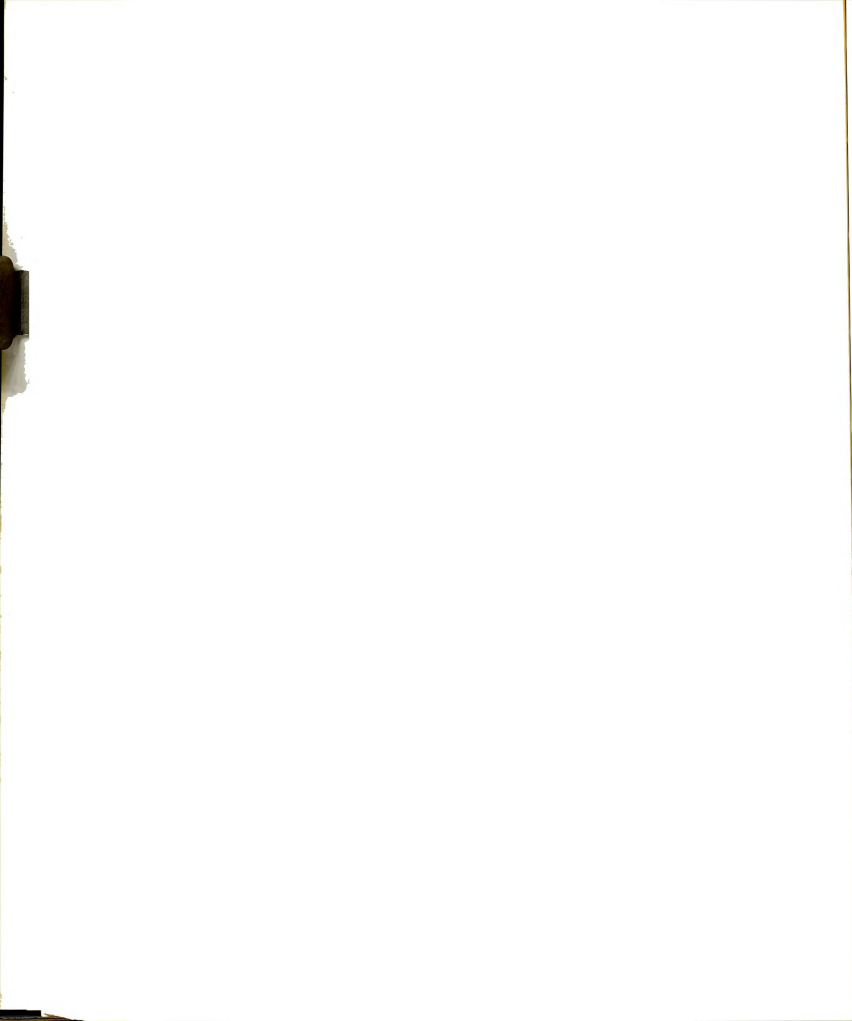
Remembering that the flux due to pressure diffusion was given by

$$F_{1P} = 2\pi \frac{P}{RT} D_{12} A r^2 (1-y)y ,$$

explains the reduction in the maximum separation factor. Since the value of R_m/R_w was maintained constant, the radial flux at the flow intersection, regardless of the centrifuge radius, is essentially a constant (assuming small mole fraction changes) for a given peripheral speed. Hence, while the flux from the inner to the outer stream is essentially constant, the throughput for optimum conditions, as shown above, must increase. Thus, the degree of separation must necessarily become worse when increasing the radius but maintaining a constant peripheral speed. These points are illustrated in Table 16.

D. The Effect of Rotational Speed and Temperature
on the Maximum Separation Factor and the
Optimum Feed Rate

In Chapter V-D-2 it was pointed out by analyzing the analytical (approximate) solution that changing the rotation speed would have very little effect on the optimum feed rate. This was expected from the analysis of the unsteady state simple centrifuge where it was found that while increasing the rotational speed improved the separation, the time required for the equilibrium mole fraction profile to develop essentially did not vary.



Increasing the temperature, however, did significantly reduce the time required for the equilibrium mole fraction profile to develop in the unsteady state simple centrifuge. The reduction in the time required is due to the strong dependence of the diffusion coefficient on temperature (~ 1.5 power, Appendix B). In the countercurrent gas centrifuge, increasing the diffusivity via increasing the temperature is expected to increase the optimum feed rate.

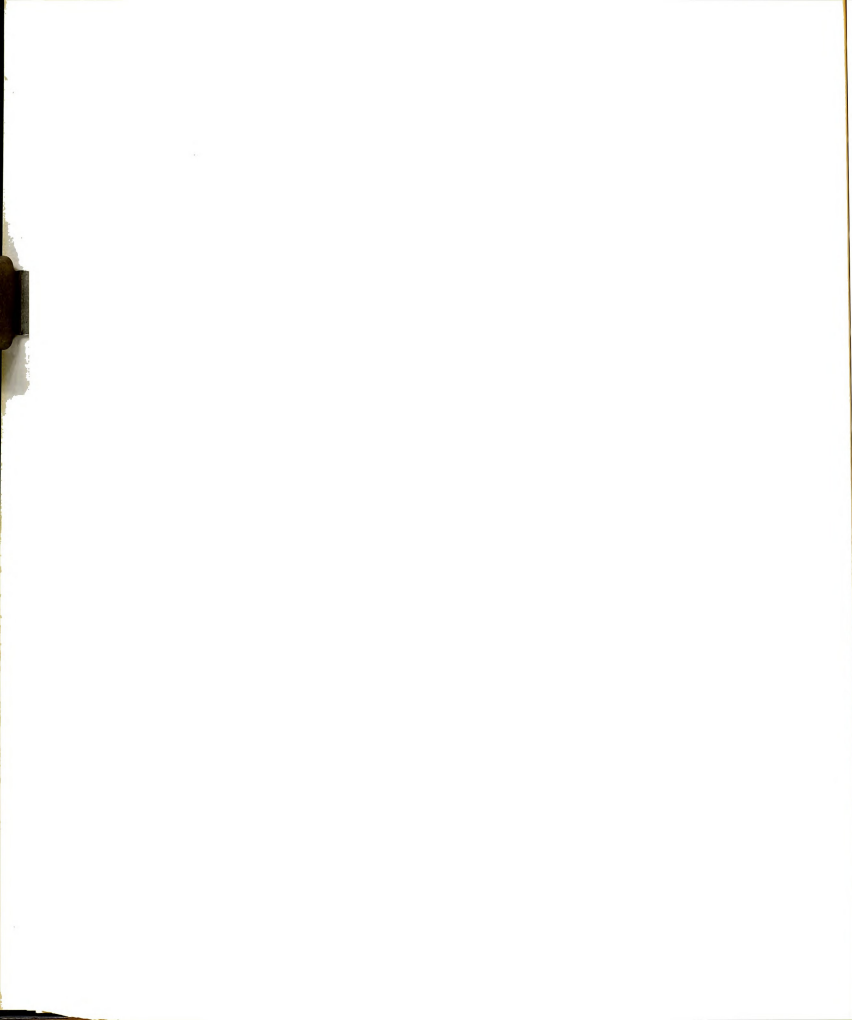
To clarify the effect of changing the diffusivity, consider for a moment a hypothetical situation in which the diffusivity of a gas pair in a countercurrent gas centrifuge operating at optimum condition could be doubled without altering the temperature. Doubling the diffusivity would necessarily double the magnitude of the net radial flux. However, it would also double the effect of axial diffusion. Hence, under this new condition, the optimum flow rates would have to be twice as great in order to compensate for twice the radial flux, yet keeping the ratio of axial flow to axial diffusion the same. The maximum separation factor would thus also be the same.

Increasing the diffusion coefficient via increasing the temperature, while giving higher optimum flow rates as discussed above, does not maintain the same maximum separation factor. This is due to the fact that the increase in temperature effectively decreases the molecular weight difference of the species as shown in Chapter II-A.

These points are illustrated with the following set of operating conditions:

$$\text{Gas pair} = \text{SO}_2\text{-N}_2,$$

$$y_f = 0.005,$$



Axis pressure, $P(0) = 14.7$ psia,

Centrifuge radius = 4 inches,

Centrifuge length = 36 inches,

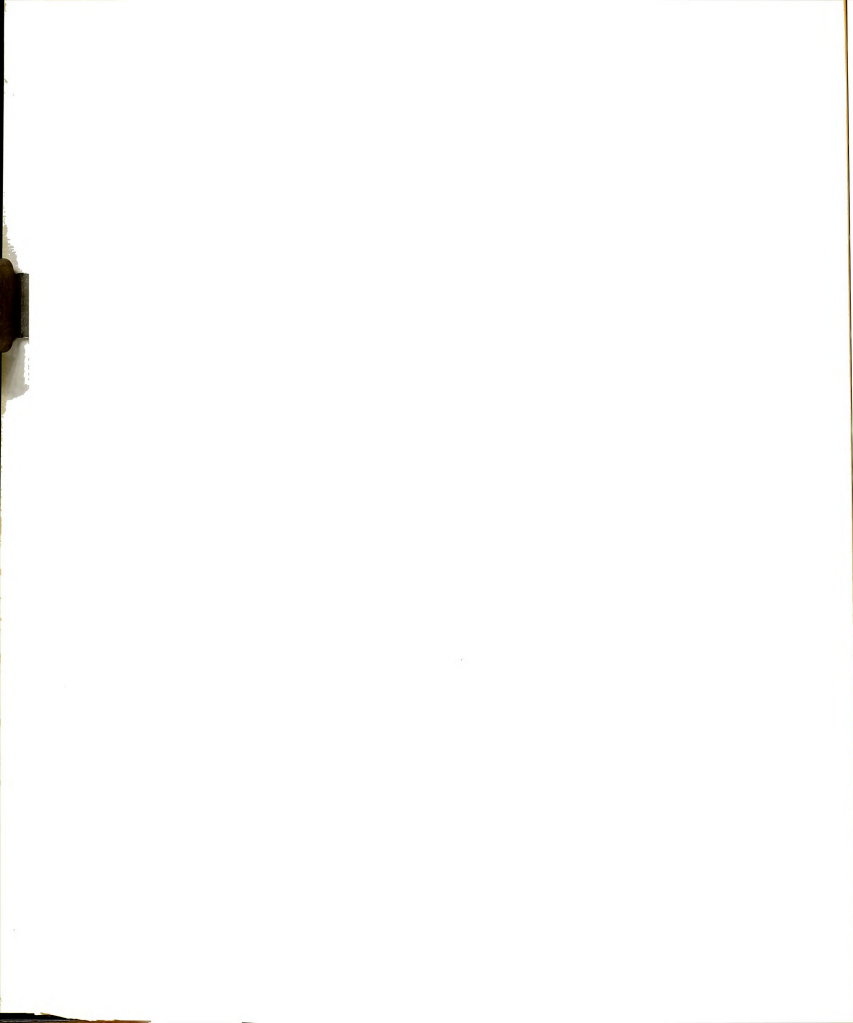
$R_m/R_w = 0.5625$,

Plug type flow and total reflux.

Table 17 contains the optimum feed rates at temperatures of 70 and 300°F for centrifuge speeds ranging between 10000 and 20000 RPM. Also included is the estimated increase in the optimum feed rates by raising the ratio of the temperatures to the 1/2 power and multiplying by the optimum feed rate at 70°F (from Chapter V-D). Figure 20 illustrates the effect of increasing the rotational speed and the temperature

TABLE 17.--The Effect of Increasing Rotational Speed and Increasing Temperature on the Optimum Feed Rate for the Gas Pair SO_2-N_2 . $R_w = 4$ Inches, $L = 36$ Inches, $R_m/R_w = 0.5625$, Plug Type Flow and Total Reflux.

ω , RPM	Optimum Feed Rates (scfm)		
	Temperature		
	70°F	300°F (estimated)	300°F
10000	0.01686	0.02019	0.02264
12000	0.01686	0.02019	0.02264
14000	0.01685	0.02018	0.02263
16000	0.01685	0.02018	0.02263
18000	0.01684	0.02017	0.02263
20000	0.01683	0.02015	0.02261



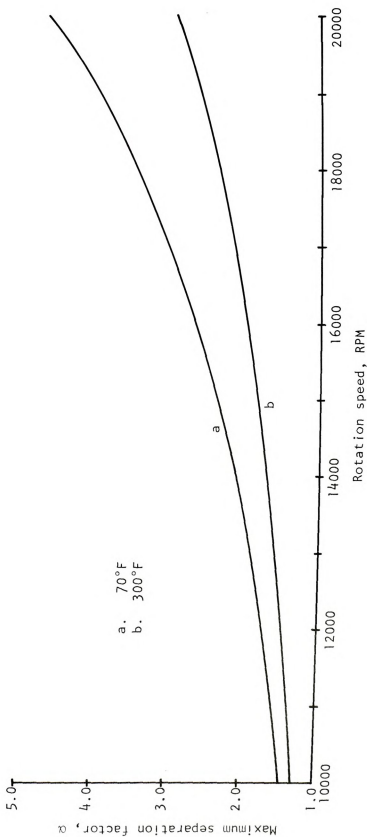
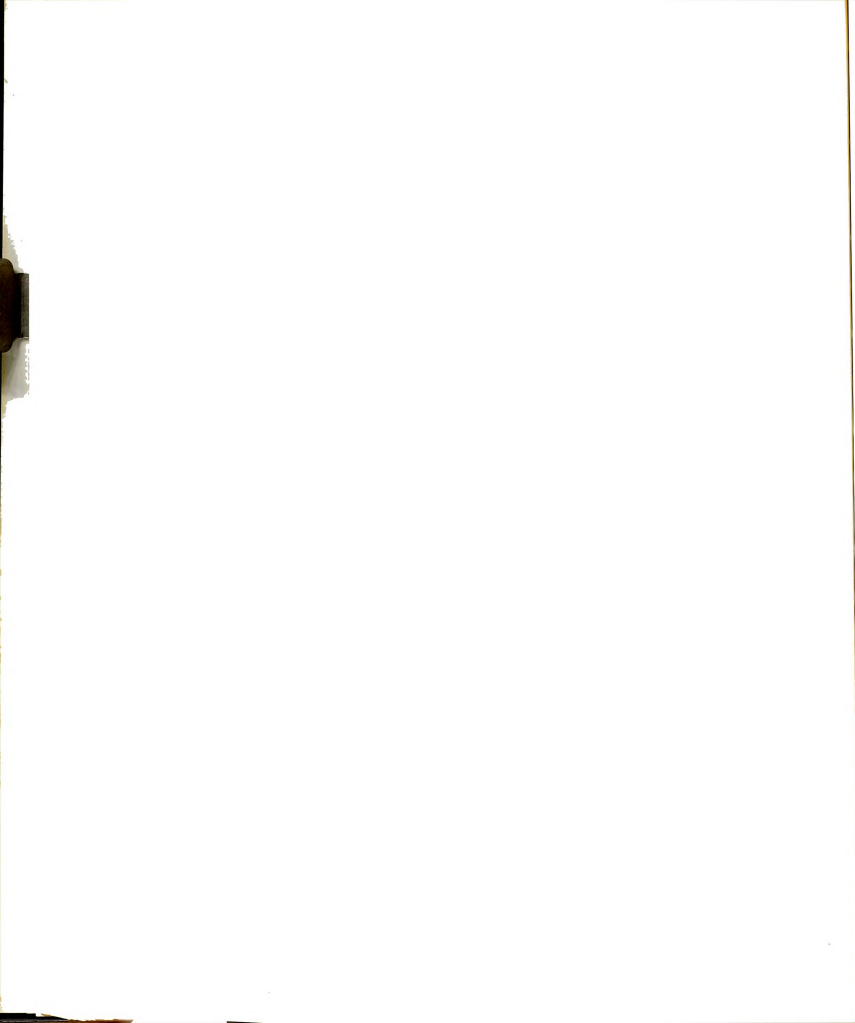


Figure 20. --Maximum Separation Factors Versus Centrifuge Rotational Speed for the Gas Pair $\text{SO}_2\text{-N}_2$ at 70 and 300°F. $R_w = 4$ Inches, $L = 36$ Inches, $R_m/R_w = 0.5625$, Plug Type Flow and Total Reflux.



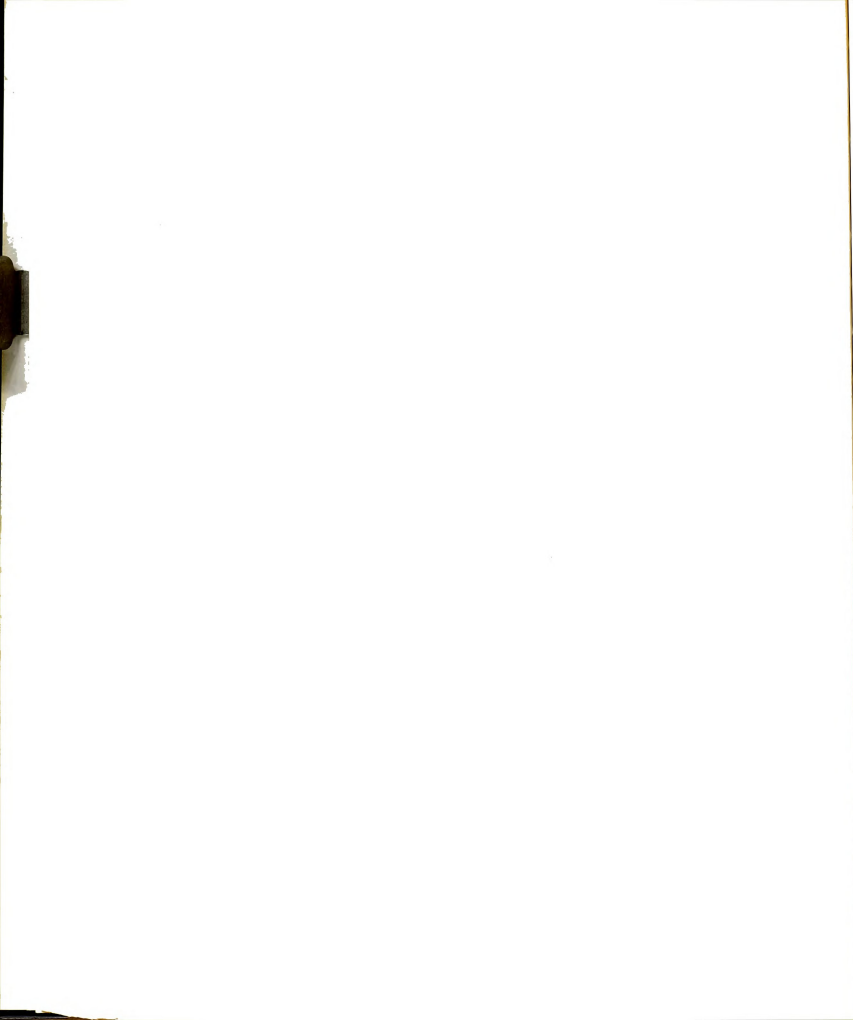
on the maximum separation factor. Data used to construct Figure 20 can be found in Appendix A.

As can be seen from Table 17 the reduction in the optimum flow rate going from 10000 to 20000 RPM is less than 0.2% at either 70 or 300°F. However, increasing the temperature from 70 to 300°F increases the optimum feed rate by approximately 34%. The fact that the estimation of the increase in the optimum feed rate is only 20% is due to a further dependence of the diffusion coefficient on temperature through the collision integral (see Appendix B). Had this factor been taken into account the estimate of the optimum feed rate at 300°F would have been 0.02264 scfm (10000 RPM) which is identical to that computed analytically.

Increasing the temperature from 70 to 300°F has the effect of decreasing the flux due to pressure diffusion by approximately 30%, which has a very significant effect on the separation factor. The reduction in the magnitude of the separation factor going from 70 to 300°F is as great as 37% at a centrifuge rotation speed of 20000 RPM. This, of course, explains why even though the diffusivity increases by 92.4% in going from 70 to 300°F that the optimum feed rate needed only to increase by 34%.

E. The Effect of Removing a Rich Product Stream on
the Maximum Separation Factor and
the Optimum Feed Rate

Consider a countercurrent rectifying centrifuge operating at total reflux with the optimum feed rate. As has been discussed previously, the optimum feed rate exists since a very slow flow rate allows



axial diffusion to destroy the separation and a high flow rate does not allow enough residence time for the heavy species to move from the inner to the outer stream. Both cases yield poor separations. By maintaining the optimum feed rate, but now removing a rich product stream, means the inner stream must necessarily be moving slower than the optimum. Hence, on this basis alone the degree of separation must fall.

If the ratio of the rich stream to the feed stream is held constant, the feed rate can be increased until the inner stream flow rate is equal to its value at the total reflux condition above. Since it is the inner stream which is controlling the separation a maximum separation should be realized at or very near this feed rate.

To illustrate these points the following operating conditions are used:

Gas pair = $\text{SO}_2\text{-N}_2$,

$y_f = 0.005$,

Axis pressure, $P(0) = 14.7$ psia,

Temperature = 530°R ,

Centrifuge radius = 4 inches,

Centrifuge length = 36 inches,

$R_m/R_w = 0.5625$,

Centrifuge speed = 15000 RPM,

Plug type flow.

Table 18 contains the maximum separation factors based on the feed and lean streams and the optimum feed rate for various ratios of the rich to the feed stream.

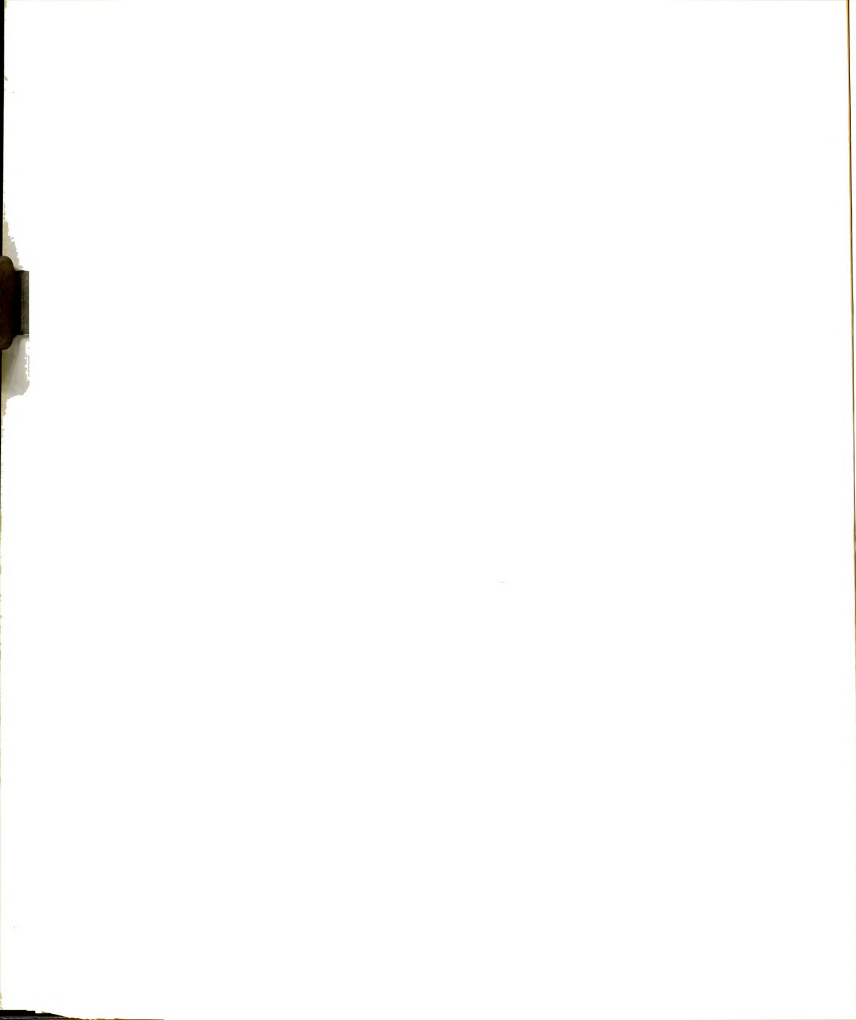


TABLE 18.--Maximum Separation Factors and Optimum Feed Rates for Various Ratios of the Rich Stream to the Feed Stream (R/F) for the Gas Pair $\text{SO}_2\text{-N}_2$, $\omega = 15000$ RPM, $R_W = 4$ Inches, $L = 36$ inches, $R_m/R_W = 0.5625$, and Plug Flow.

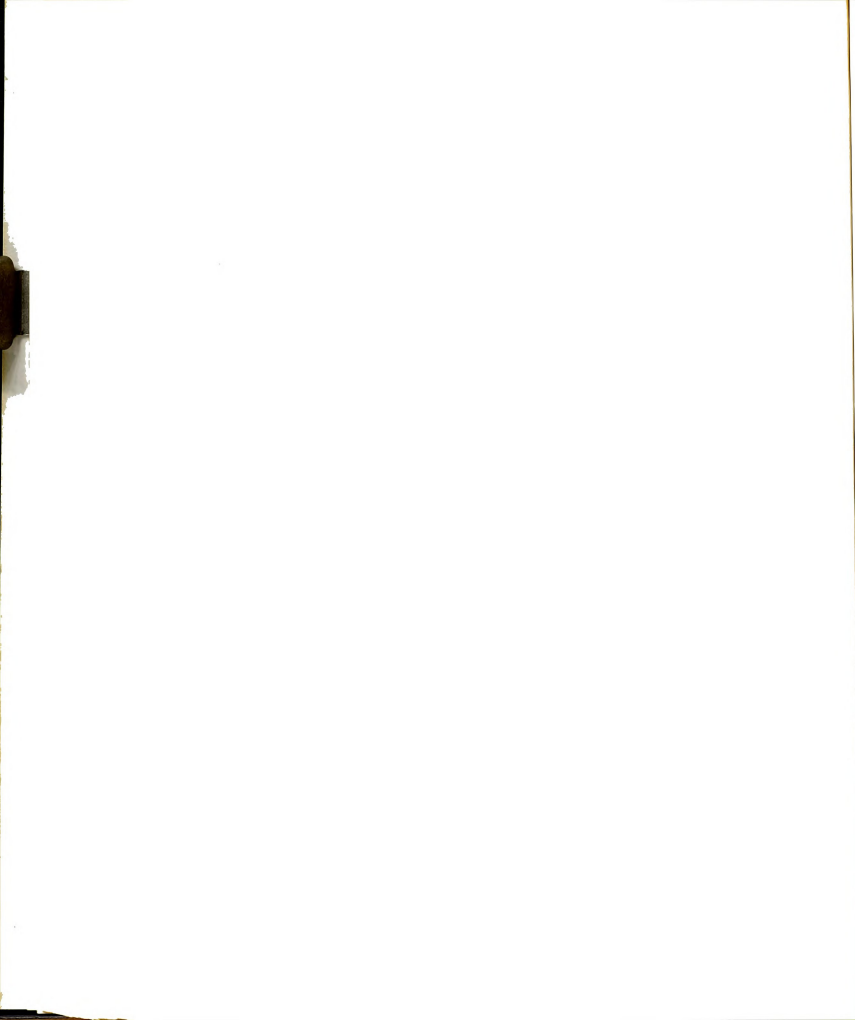
R/F	Inner Stream Flow Rate (scfm)	Outer Stream Feed Rate (scfm)	Separation Factors	
			Based on Feed Stream	Based on Lean Stream
0.00	0.0169	0.0169	2.337	2.337
0.05	0.0170	0.0179	1.860	1.947
0.10	0.0172	0.0191	1.586	1.696
0.15	0.0173	0.0204	1.413	1.523
0.20	0.0175	0.0219	1.296	1.400

The separation factor in Table 18 which is based on the composition of the rich (y_r) and lean (y_l) streams was computed by using the following equations:

$$y_l = \frac{y_r^{\text{FEED}} - y_r^{\text{RICH}}}{\text{LEAN}} \quad \text{and} \quad \alpha = \frac{y_r}{(1-y_r)} \frac{(1-y_l)}{y_l}$$

where FEED, RICH and LEAN are the flow rates of the feed, rich and lean streams, respectively.

The fact that the maximum separation factor drops rapidly as a rich product stream is removed can be explained in terms of the radial fluxes. At total reflux, mass balance requires the average compositions of the inner and outer streams to be equal at every axial position. Furthermore, at total reflux the maximum separation is only restricted by the length of the centrifuge. This is illustrated in

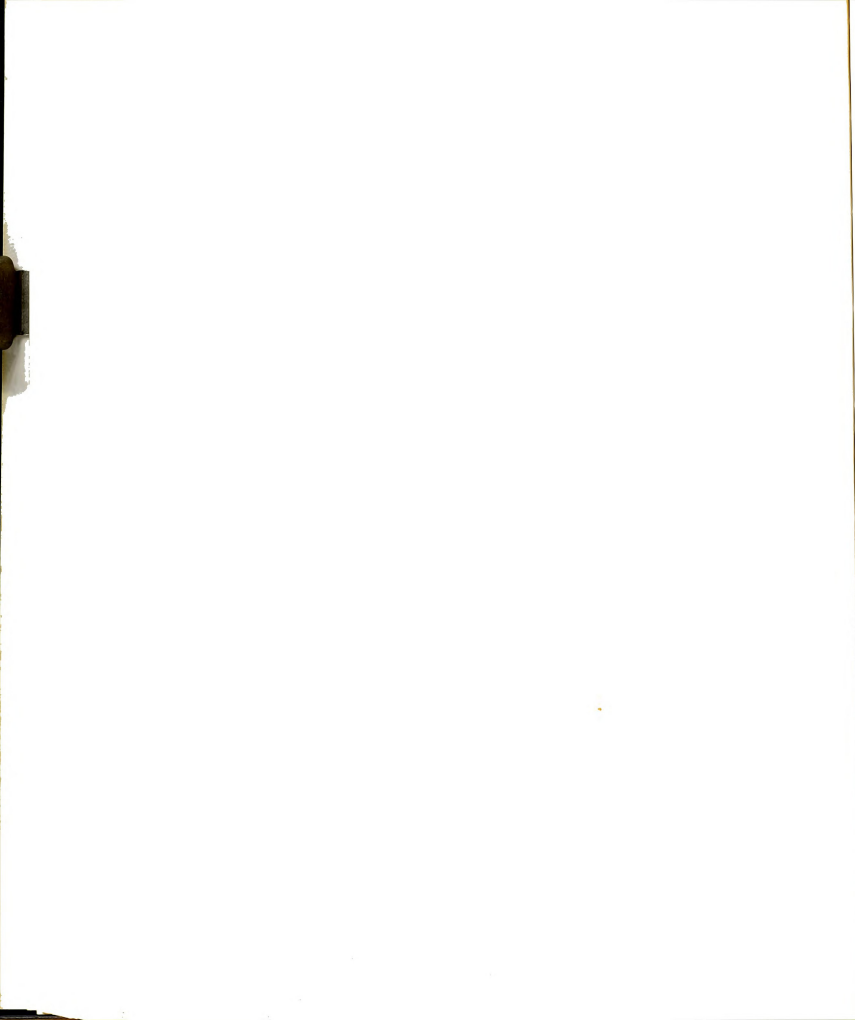


in Table 19 which contains the maximum separation factors at total reflux for different centrifuge lengths using the operating conditions given above. When a rich product stream is removed the average composition of the inner stream must by mass balance be less than the average composition of the outer stream. However, the problem that arises here is just how much less can the average inner stream composition be.

Consider, for a moment, the top of the centrifuge where the outer stream is the entering feed. Using the above operating conditions, the composition of the outer stream at this point is $y_f = 0.005$. From Chapter II-B (simple centrifuge) it was determined that knowing the axis composition, the equilibrium mole fraction profile could be computed by using the following expression:

TABLE 19.--Maximum Separation Factors for Various Centrifuge Lengths at Total Reflux for the Gas Pair $\text{SO}_2\text{-N}_2$, Feed Rate = 0.0169 scfm (optimum), $\omega = 15000$ RPM, $R_w = 4$ Inches, $L = 36$ Inches, $R_m/R_w = 0.5625$, and Plug Flow.

Centrifuge Length	Separation Factor (Based on Feed)
0.0	1.000
7.2	1.185
14.4	1.404
21.6	1.664
28.8	1.972
36.0	2.337
43.2	2.769
50.4	3.282
57.6	3.889
64.8	4.608
72.0	5.461



$$y(r) = \frac{\alpha y(0)}{y(0)(\alpha-1) + 1},$$

where $\alpha = \exp (Ar^2/2)$.

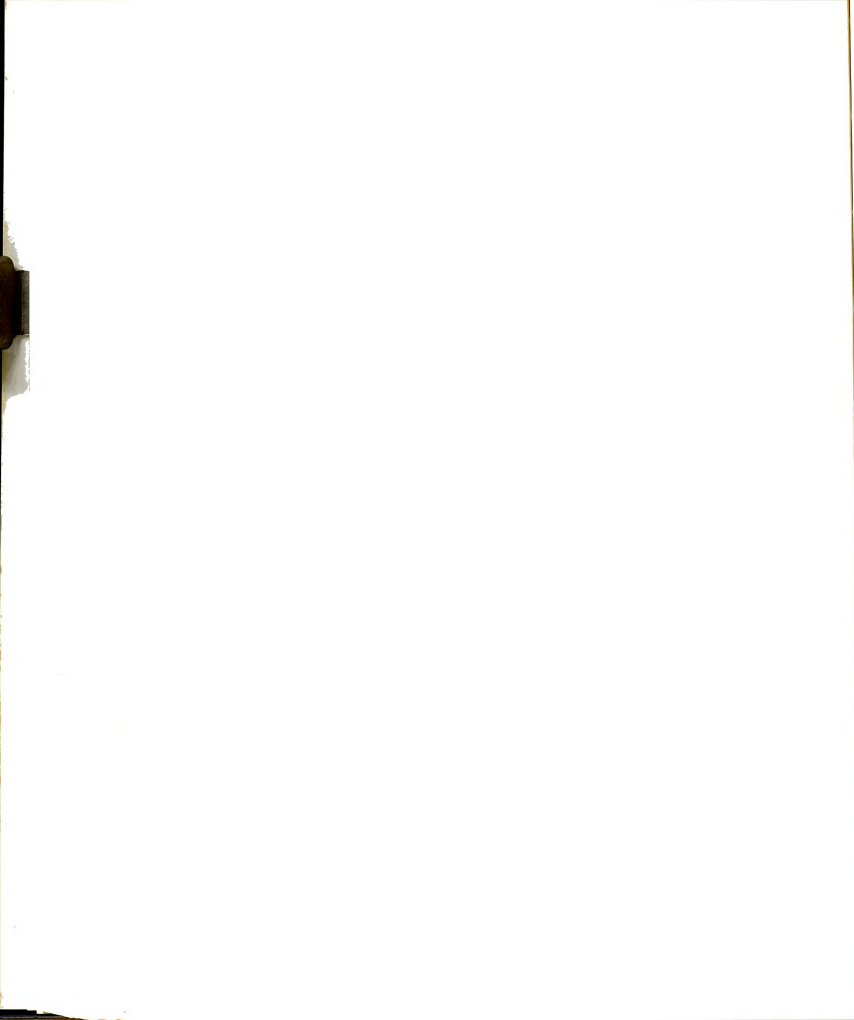
However, since the composition is known at the flow intersection, $R_m = 2.25$ inches, to be $y_f = 0.005$, the composition at the axis can be found by rearranging the expressions giving

$$y(0) = \frac{y_f}{\alpha - y_f(\alpha-1)}.$$

Using the operating conditions given above, $y(0)$ is found to be 0.00471.

As commented on in Chapter III, the equilibrium mole fraction profile results from a no net flux condition. That is, the concentration and pressure diffusion fluxes are equal in magnitude but opposite in direction. Herein lies the reason for the rapid decrease in the separation as a product stream is removed, since the mole fraction profile of the leaving inner stream cannot ever be any less in composition than the equilibrium mole fraction profile. (This is, of course, true at any axial position but is most easily seen at the top, since the feed composition is known.) Furthermore, the composition profile of the leaving stream can only approach the equilibrium profile, since the closer it gets the smaller the net radial flux and hence, the smaller the separation. The leaving inner stream mole fraction profile is in essence trapped between the feed composition and equilibrium composition profile.

This situation is much like the case of a binary distillation (assume constant molar overflow) in a rectifying column containing a



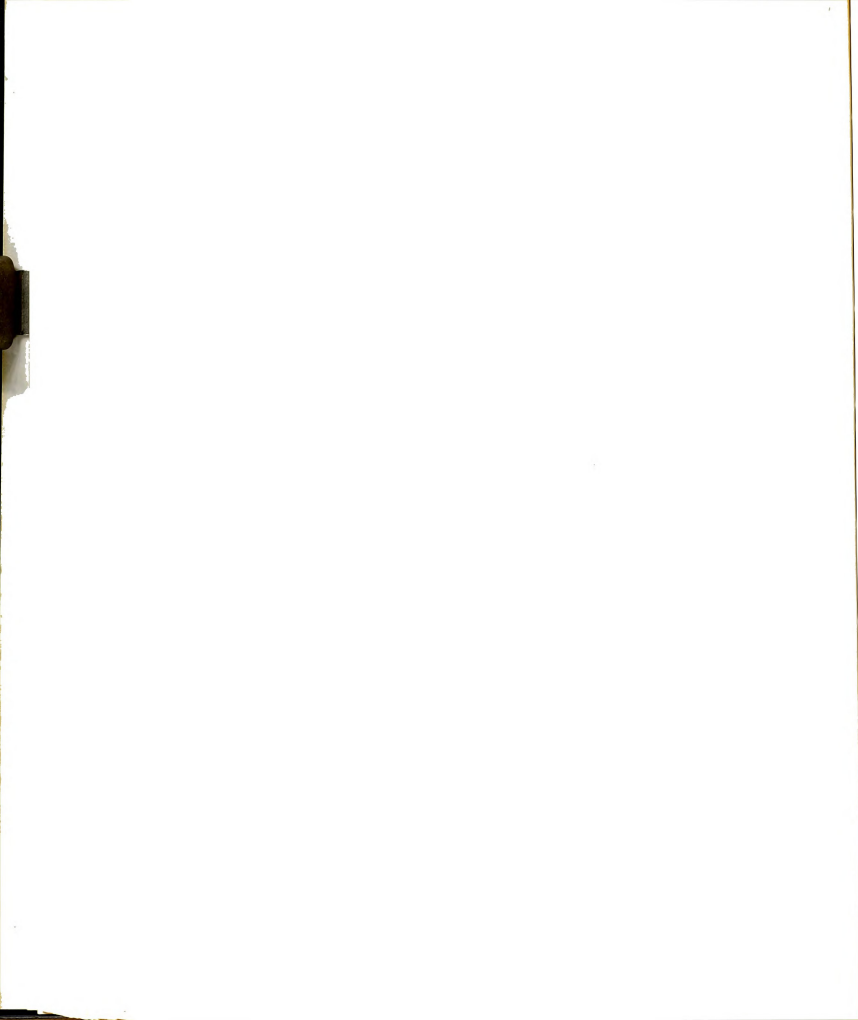
fixed number of trays. If the equilibrium curve lies very close to the "45° line," then removal of any overhead product causes a significant decrease in the separation per tray at the base of the column. Hence, as compared to total reflux, the overhead composition would be markedly reduced.

Further discussions regarding the limitations imposed on gas centrifugation by the results presented above will be contained in Chapter VII. However, Figure 21 is included in this section to further illustrate the reduction in the maximum separation factor with product removal and also how the maximum separation factor varies with feed rate at a given ratio of the rich to the feed stream. The operating conditions used are as given above and the data used to construct Figure 21 may be found in Appendix A.

F. Simple Power Requirements and Efficiencies of the Countercurrent Centrifuge

Before leaving this chapter attention will be turned for the moment to the development of expressions for the power required to rotate the gas as it is being fed through the centrifuge and the thermodynamic energy (entropy) required for the separation. This information will provide further insight when comparing the gas centrifuge to conventional gas separating equipment.

The power that must be supplied to rotate the gas can be computed by integrating the product of the kinetic energy and the mass flow rate profile over the radius of flow, i.e.,



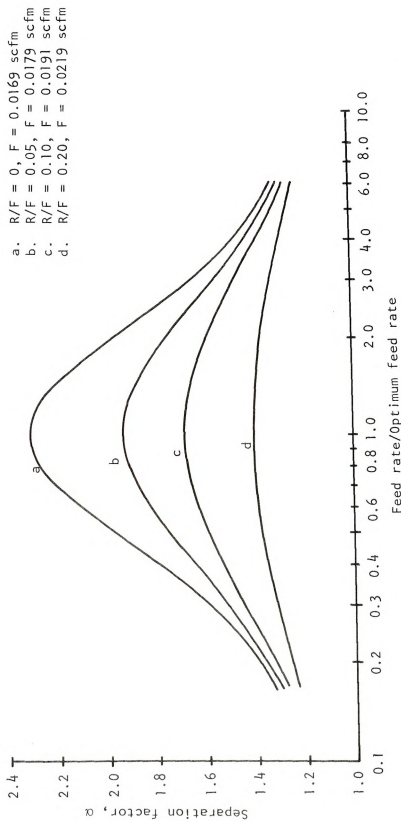
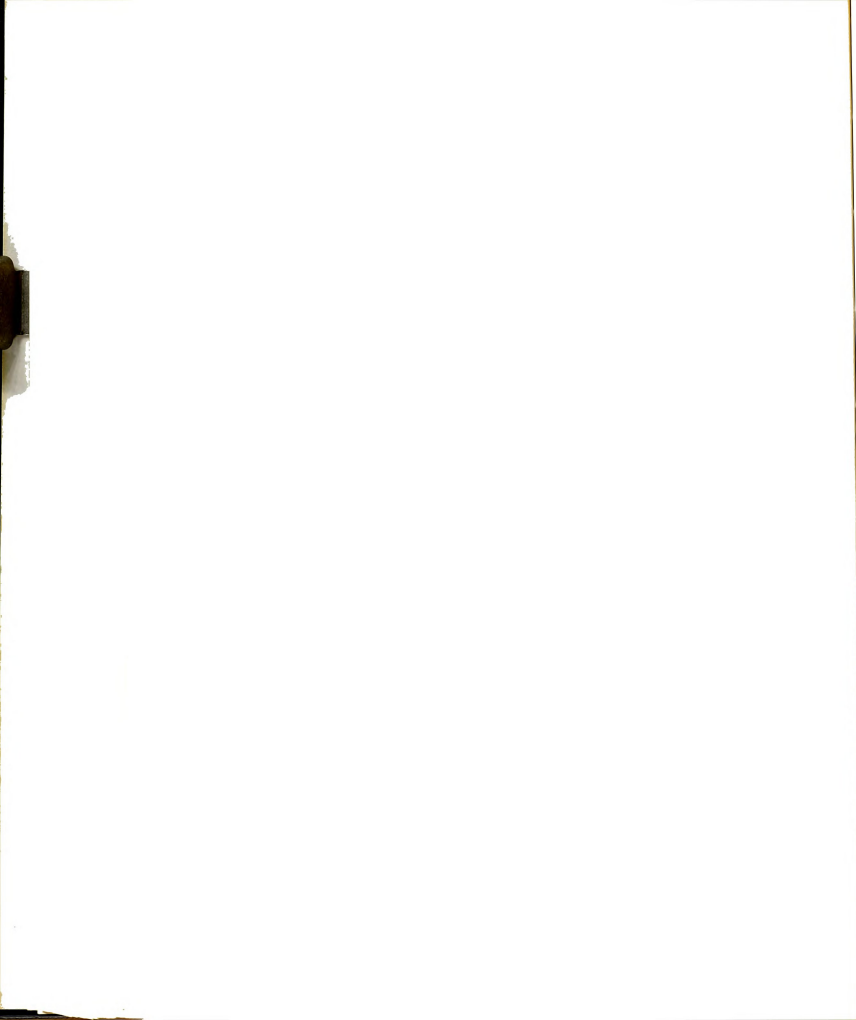


Figure 21.--Separation Factors Based on the Rich and Lean Streams Versus Feed Rate for Various Ratios of the Rich Stream to the Feed Stream for the Gas Pair $\text{SO}_2\text{-N}_2$. $\omega = 1500$ RPM, $R_w = 4$ Inches, $L = 36$ Inches, $R_{\text{opt}}/R_w = 0.5625$ and Plug Type Flow.



$$\text{Power} = \frac{2\pi}{RT} MW_a \int_0^R [Pv(r)] \frac{\omega^2 r^2}{2g_c} dr ,$$

where MW_a is the average molecular weight of the gas. For plug type flow, the integral is easily evaluated giving

$$\begin{aligned} \text{Power} = \frac{\pi MW_a P(0) \omega^2}{RTg_c} & \left[-v_i \left[\frac{R_m^2 e^a}{A} - \frac{2}{A^2} (e^a - 1) \right] \right. \\ & \left. + v_o \left[(R_w^2 e^b - R_m^2 e^a)/A - \frac{2}{A^2} (e^b - e^a) \right] \right] \end{aligned}$$

where $a = A R_m^2/2$,

$b = A R_w^2/2$, and

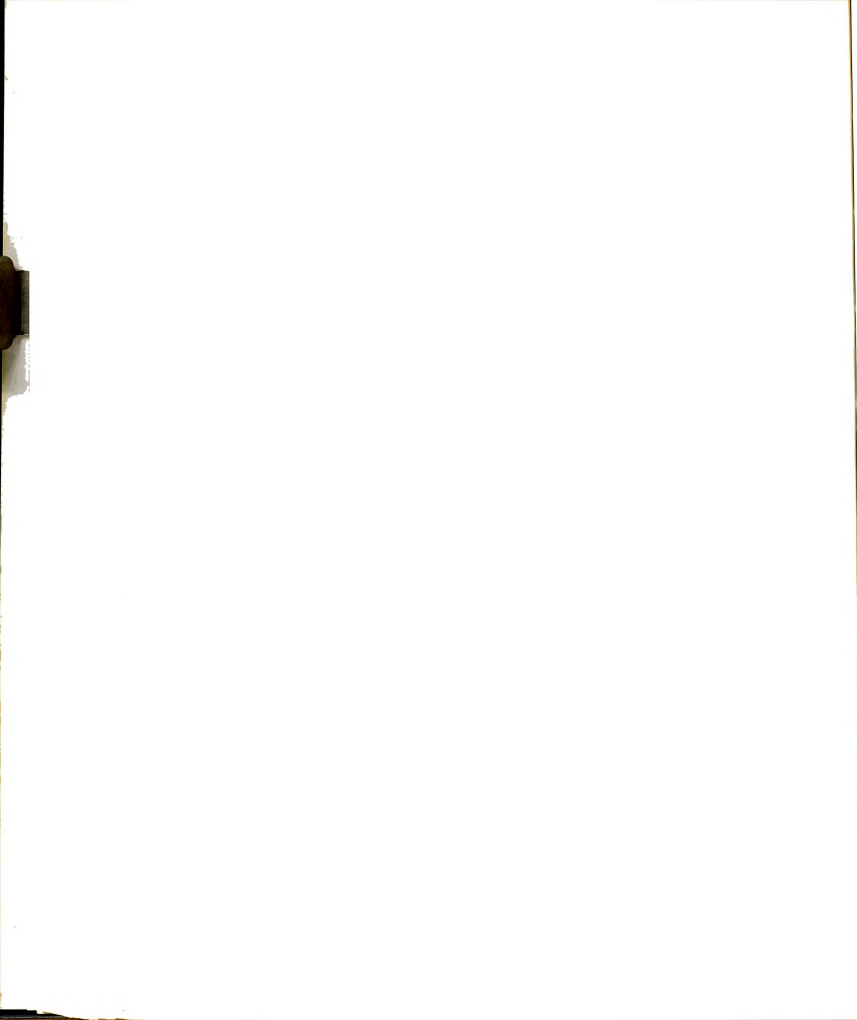
$$A = \frac{MW_a \omega^2}{RTg_c} .$$

The minus sign appears in front of v_i to account for the fact that the inner flow is taken as negative. For laminar flow the integral becomes difficult to evaluate analytically and a numerical integration technique such as the trapezoidal rule may instead be used, i.e.,

$$\text{Power} = \frac{\pi MW_a \omega^2 P(0)}{RTg_c} \sum_{i=1}^{n+1} \left[e \frac{A r_{i-1}^2}{2} v(r_{i-1}) r_{i-1}^3 + e \frac{A r_i^2}{2} v(r_i) r_i^3 \right] \frac{\Delta r}{2} ,$$

where the subscript i refers to incremental radial positions of which there are $n + 1$.

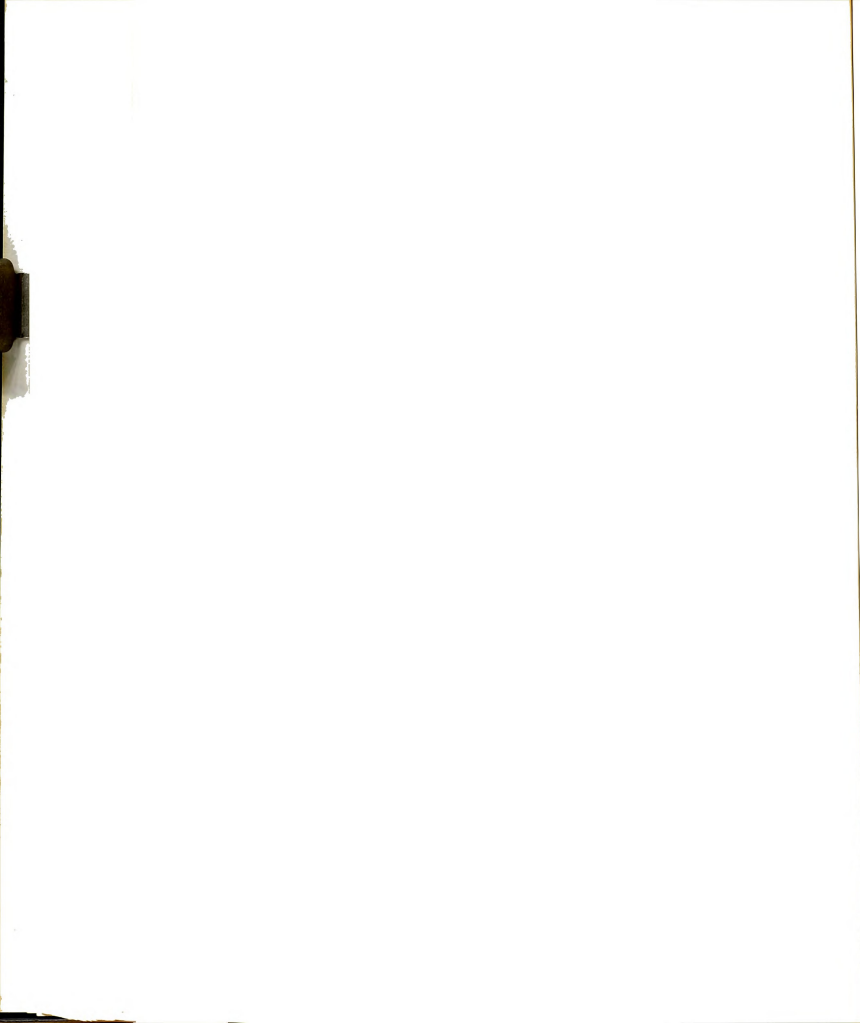
The power computed above is by no means the power required to operate the centrifuge where losses such as driver inefficiency,



windage losses, and bearing losses would be far greater in magnitude. However, the above expressions do give an idea as to how much power is actually required to simply rotate the gas. For example, from Chapter VI-B above, in which the effects of varying the flow inter-section was investigated, change in power requirements to rotate the gas can also be observed. The effect on the power requirements are presented in Table 20 for operating the conditions as stated in Chapter VI-B and with a feed rate of 0.02 scfm. As can be seen from Table 20 the simple power requirements vary from 1.75 watts/scfm (629 watts/lb-mole) at $R_m/R_w = 0.125$ to 4.25 watts/scfm (1527 watts/lb-mole) at $R_m/R_w = 0.875$. The increase, of course, being due to

TABLE 20.--The Power Required to Simply Rotate the Gas Being Fed to a Countercurrent Centrifuge for Different Flow Inter-sections: Feed Rate = 0.02 scfm, Radius = 4 Inches, $\omega = 10000$ RPM, Plug Type Flow and Total Reflux.

R_m/R_w	Power (Watts)
0.125	0.035
0.250	0.038
0.375	0.043
0.500	0.051
0.5625	0.055
0.625	0.060
0.750	0.072
0.875	0.085



more gas being near the periphery (higher angular velocities) as

R_m/R_w approaches 1.

For an ideal binary gas mixture, the entropy lost when the gases are separated at a given temperature and pressure is given by

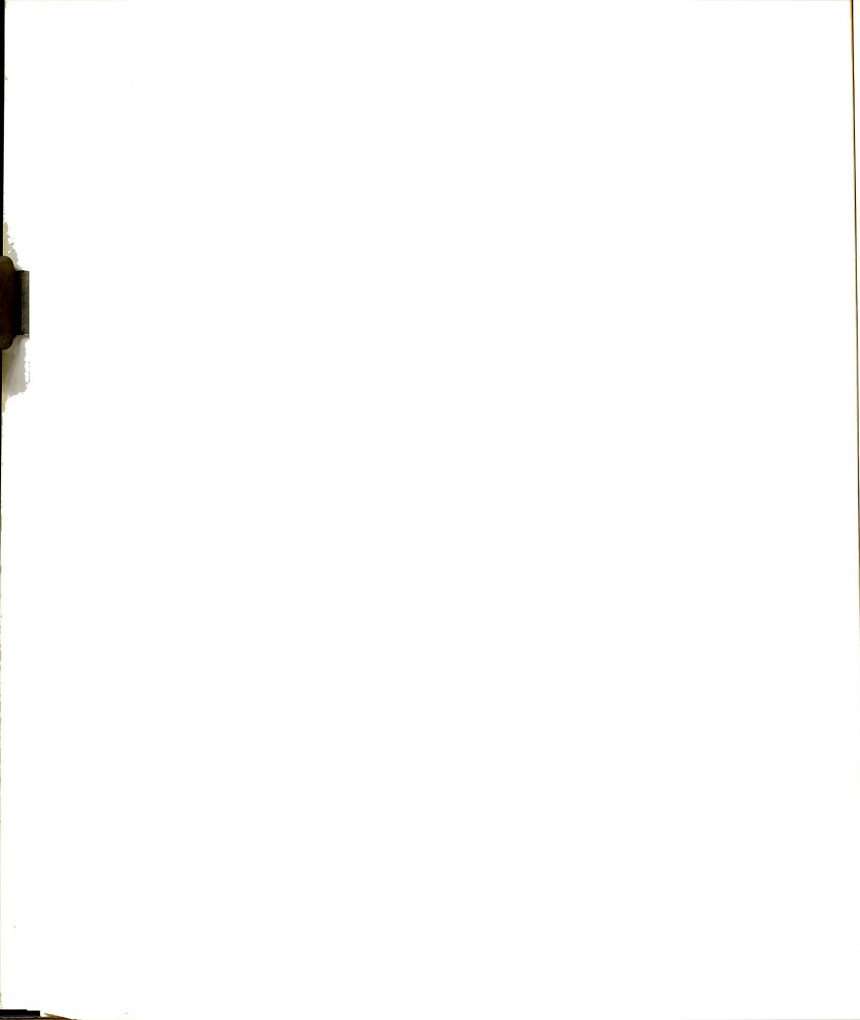
$$\Delta S = R[y \ln y + (1-y) \ln (1-y)] ,$$

where R is the gas constant. In the case of the countercurrent rectifying centrifuge where there are feed, rich and lean streams the entropy lost in the separation is then given by

$$\begin{aligned} \Delta S_s = & R \left(\text{RICH} [y_r \ln y_r + (1-y_r) \ln (1-y_r)] \right. \\ & + \text{LEAN} [y_l \ln y_l + (1-y_l) \ln (1-y_l)] \\ & \left. - \text{FEED} [y_f \ln y_f + (1-y_f) \ln (1-y_f)] \right) \end{aligned}$$

where all streams are referenced to the same temperature and pressure.

Pointed out in Chapter VI-A above was the fact that error between the analytical (approximate) and numerical solutions did not significantly change when a rich product stream was removed. This was found to be due to a rather rapid decrease in separation accompanying the removal of a rich product stream keeping the leaving inner stream composition at approximately the feed composition. With this good agreement, even though the analytical (approximate) solution assumes very little change in the mole fraction profile radially, a lean stream composition (y_l) was computed by using the expression given in Chapter VI-E, i.e.,



$$y_l = \frac{y_f \text{ FEED} - y_r \text{ RICH}}{\text{LEAN}} .$$

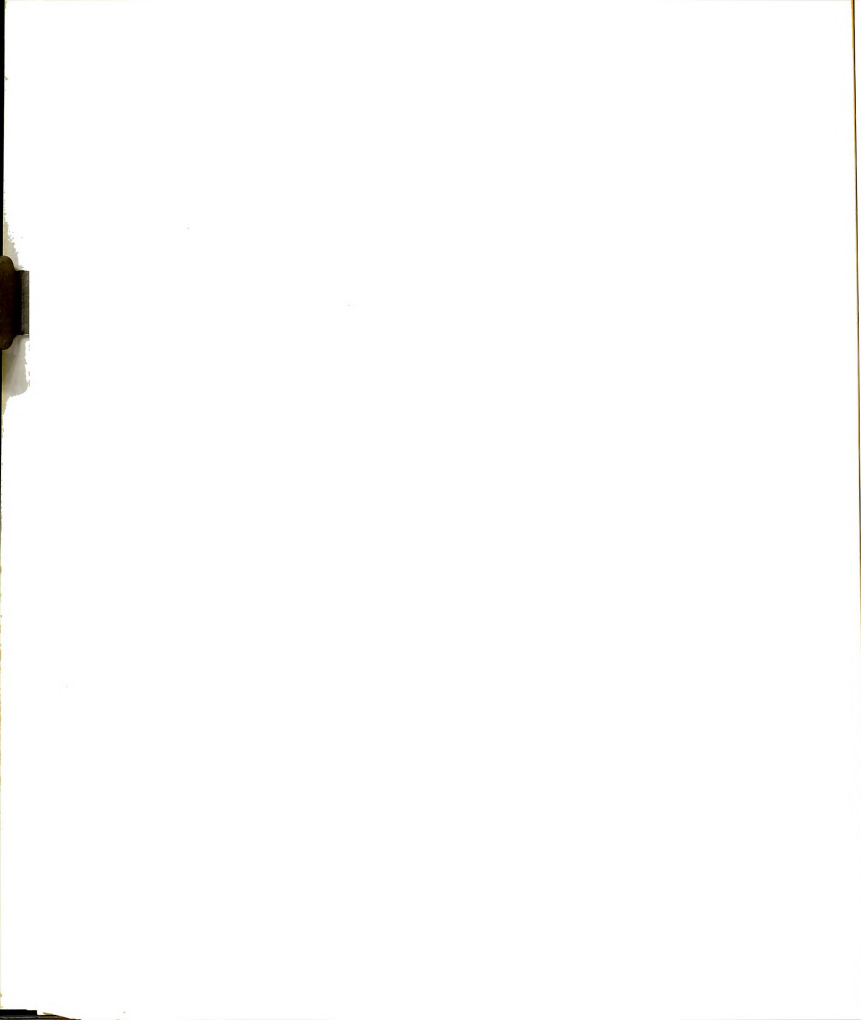
This expression cannot be in great error since y_r computed both numerically and analytically are in good agreement (Chapter VI-A).

Using the above expression to compute a lean stream composition from the analytical (approximate) solution allows the calculation of the entropy lost in a separation and an efficiency based on the simple power requirements. Entropy losses and the resulting efficiencies for the operating conditions specified in Chapter VI-A are contained in Table 21.

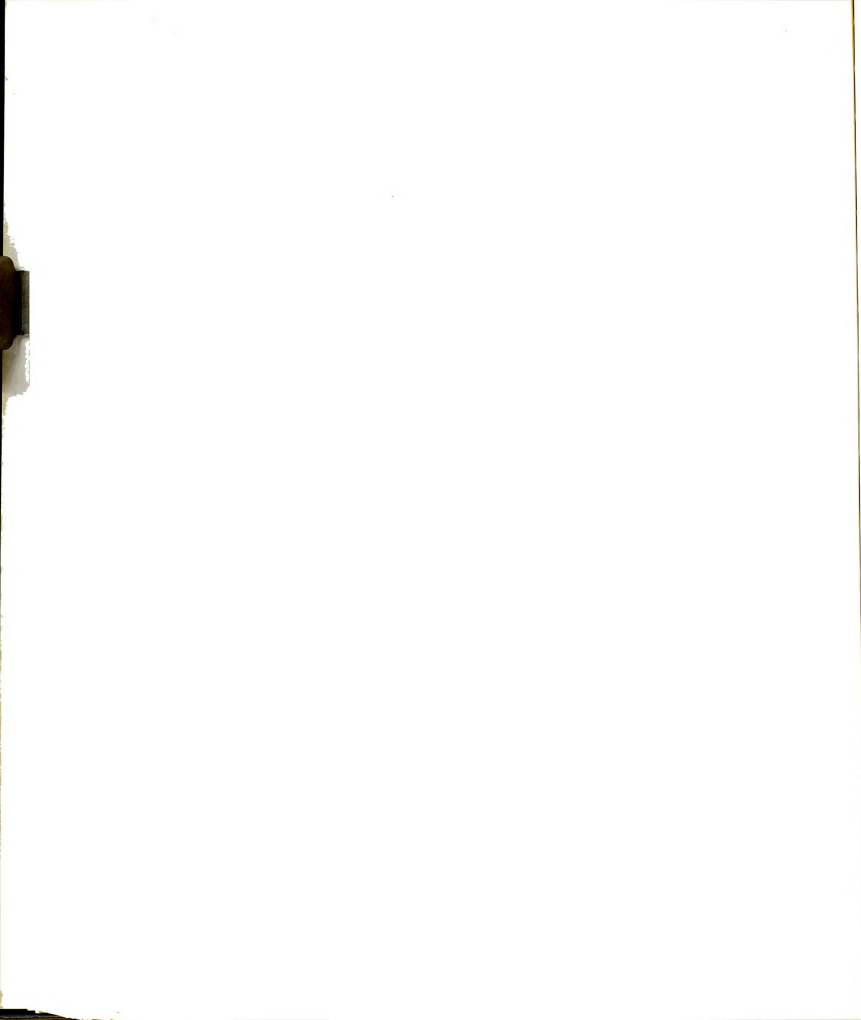
The gradual decrease in simple power required is due to less and less gas being recycled. On the other hand, the entropy lost must

TABLE 21.--Simple Power Requirements, Entropy Losses and Resulting Efficiencies for the Separation of the Gas Pair $\text{SO}_2\text{-N}_2$ at Various Ratios of the Rich Stream to the Feed Stream (R/F). Feed Rate = 0.02 scfm, $R_w = 4$ inches, $R_m/R_w = 0.5625$, $\omega = 10000$ RPM and Plug Type Flow.

R/F	Separation Factor	Simple Power Required (watts)	Entropy Lost (watts)	Efficiency
0.00	1.448	0.0550	0.0	0.0
0.05	1.327	0.0544	1.30×10^{-5}	2.40×10^{-4}
0.10	1.239	0.0539	1.51×10^{-5}	2.81×10^{-4}
0.15	1.175	0.0534	1.32×10^{-5}	2.47×10^{-4}
0.20	1.128	0.0529	1.02×10^{-5}	1.92×10^{-4}



be equal to zero for total reflux ($R/F = 0$) and also for no recycle ($R/F = 1.0$), hence there exists a maximum in the entropy lost column. The fact that there exists a maximum in the efficiency column is by itself significant, but loses its relevance when the absolute values of the efficiencies are considered. Furthermore, these already very small efficiencies would be further reduced (perhaps by magnitudes) if the entries in the entropy lost column were divided by the power required by the centrifuge driver instead of the simple power required.

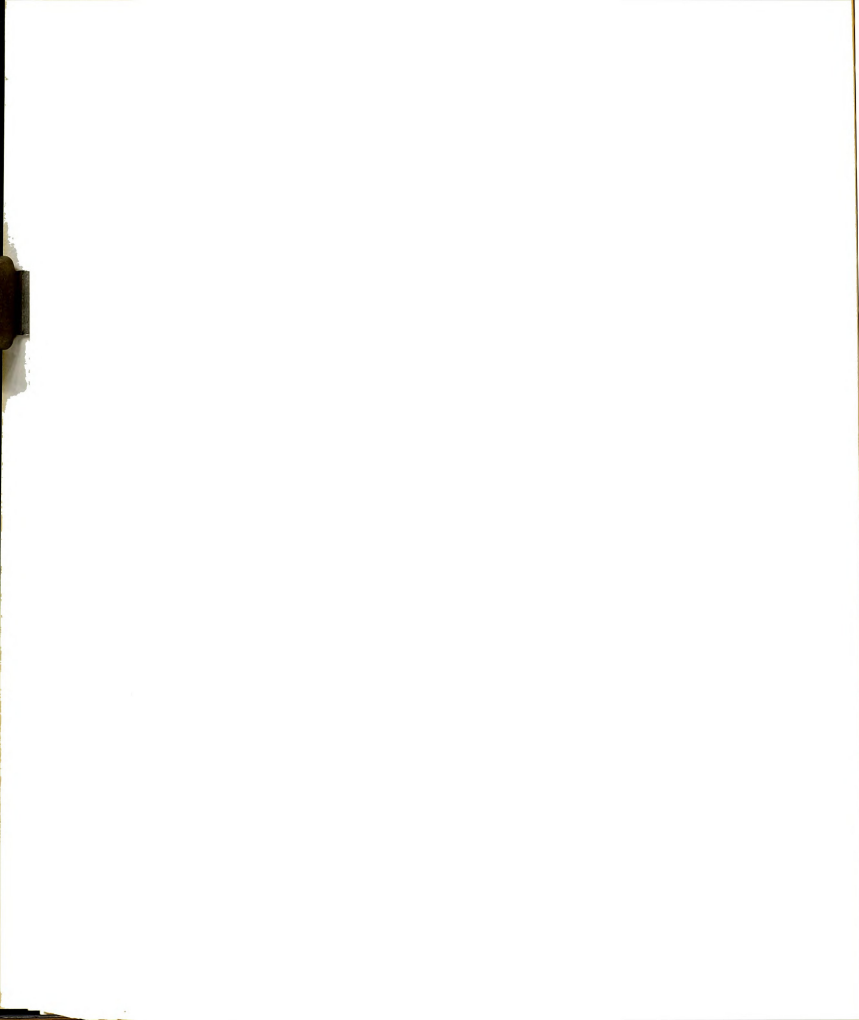


CHAPTER VII

CONCLUSIONS

The purpose of this work was to analyze the countercurrent gas centrifuge and determine its applicability for the separation of common gas mixtures in industrial situations with emphasis on the viability of gas centrifugation as a means for removing SO_2 from power plant stack gas. Analyses of the steady and unsteady state simple centrifuge (Chapters II and III) provided information regarding the equilibrium separations possible for different gas species, and the times required for such separations to develop. It was found that while large molecular weight differences and high rotational speeds controlled the magnitude of the separation, the diffusivity, as would be expected, directly controlled the time required for the separation to occur. The limitations of gas centrifuges began to be seen at this point, with times required for the axis composition to move to within 50% of its equilibrium value, being 49.5 seconds for SO_2 in N_2 and 12.6 seconds for SO_2 in H_2 at 70°F in an 8-inch diameter centrifuge rotating at 10000 RPM. (Both the ratio of the times required and the diffusivities for the two gas pairs are 3.93.)

The small radial flux in the gas centrifuge indicated long residence times would be required to realize the separating potential of the countercurrent production centrifuge. The mechanical limitations



(size and rotational speeds) were investigated by developing expressions which allowed the calculation of both the bursting speed and the first whirling speed of a rotating cylinder (Chapter IV). It was shown that only alloys of Aluminum or Magnesium (as compared to other common metals) were acceptable for the construction of a centrifuge. Furthermore, while it was shown that a peripheral speed of 700 ft/sec was well below the bursting speed, the length to diameter ratio had to be less than 5 for safe operation under the first whirling speed.

The equation of continuity for the heavy species in the counter-current centrifuge was developed and solved both numerically and, by making certain assumptions, analytically (Chapter V). It was shown that many different operating variables could be used to somewhat alter the maximum separation factor and optimum feed rate for the separation of a gas pair in a countercurrent centrifuge. Table 22 contains a list of many operating variables and their qualitative effect on the maximum separation factor and the optimum feed rate. At the optimum feed rate, the actual magnitude of the separation for a given gas pair was found to be controlled by their molecular weight difference, the operating temperature, and the length and the rotational speed of the centrifuge. The optimum feed rate, on the other hand, which may be more important when deciding on the applicability of the gas centrifuge, was found to be directly related to the diffusion coefficient for the gas pair and the diameter of the centrifuge. That is, all things being held constant in the operation of the countercurrent rectifying centrifuge, switching to a new gas pair having twice the diffusion coefficient will double the optimum feed

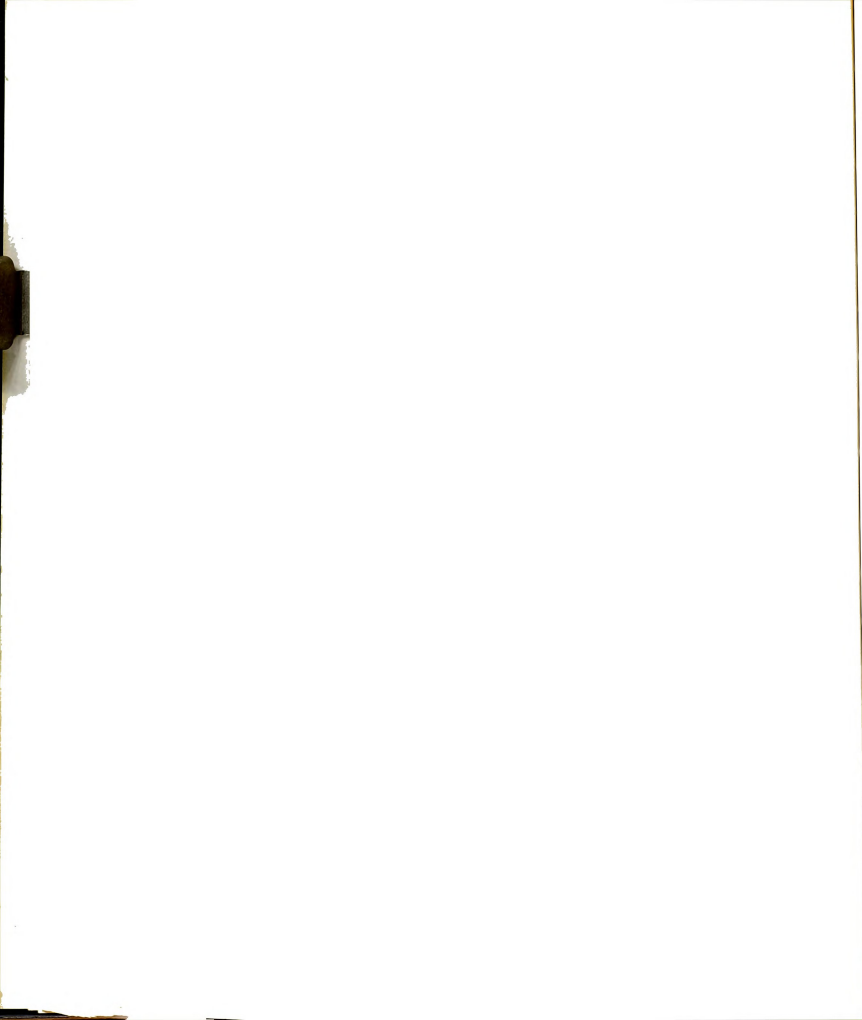
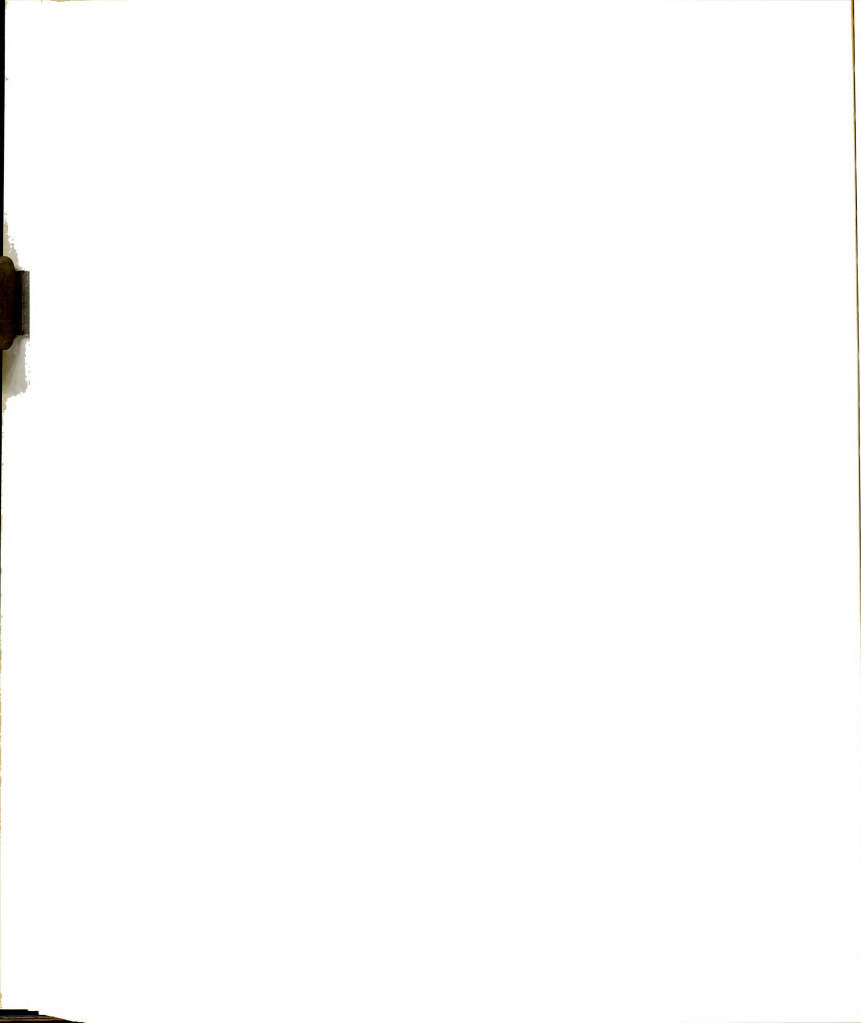


TABLE 22.--Operating Variables and Their Effect on the Maximum Separation Factor and the Optimum Feed Rate for the Separation of a Binary Gas Mixture in a Countercurrent Rectifying Centrifuge.

Operating Variable Changed	Given the maximum separation factor and optimum feed rate at a given set of conditions, the qualitative changes expected by varying indi- vidual operating conditions are:	
	Optimum Feed Rate	Maximum Sepa- ration Factor
Using the analytical solution instead of the numerical solution	Decreases	Increases
Increase centrifuge radius (constant peripheral speed)	Increases	Decreases
Increase centrifuge length	No effect	Increases
Going from plug to laminar flow	Decreases	Decreases
Moving flow intersection closer to the wall	Increases	Increases
Increase rotational speed	No effect	Increases
Increase molecular weight difference	No effect	Increases
Increase temperature	Increases	Decreases
Increase axis pressure	No effect	No effect



rate. The fact that the new gas pair will have a different molecular weight and thus a different pressure profile will be compensated for by the magnitude of the velocity profile. Likewise, doubling the diameter of the centrifuge but maintaining the same peripheral speed doubles the optimum feed rate. In this case, however, the positive effect of increased feed rate is negated by a rapid reduction in the maximum separation factor (Chapter VI, Table 16). This is due to the fact that while doubling the diameter at a constant peripheral speed (constant radial flux) and constant R_m/R_w doubles the throughput, twice the centrifuge length will be required (twice the moles to be moved from the inner to the outer stream) to obtain the same separation factor. Hence, if acceptable separations are shown to be possible in a 2-inch diameter by 10-inch long centrifuge at a given peripheral speed, increasing the diameter to 12 inches to obtain 6 times the throughput means the length must be at least 72 inches to sustain the desired level of separation. That is, when scaling up a centrifuge, L/D must be constant.

It was also shown that neither the optimum feed rate nor the maximum separation factor is affected by the operating pressure.

As an illustration, at 70°F and 1 atmosphere the gas pair SO_2-N_2 has a diffusion coefficient of $0.1345 \text{ cm}^2/\text{sec}$ while the gas pair SO_2-H_2 has a diffusion coefficient of $0.5282 \text{ cm}^2/\text{sec}$. Table 23 contains the maximum separation factors along with the optimum feed rates for the above two gas pairs for several ratios of the rich to the feed stream.

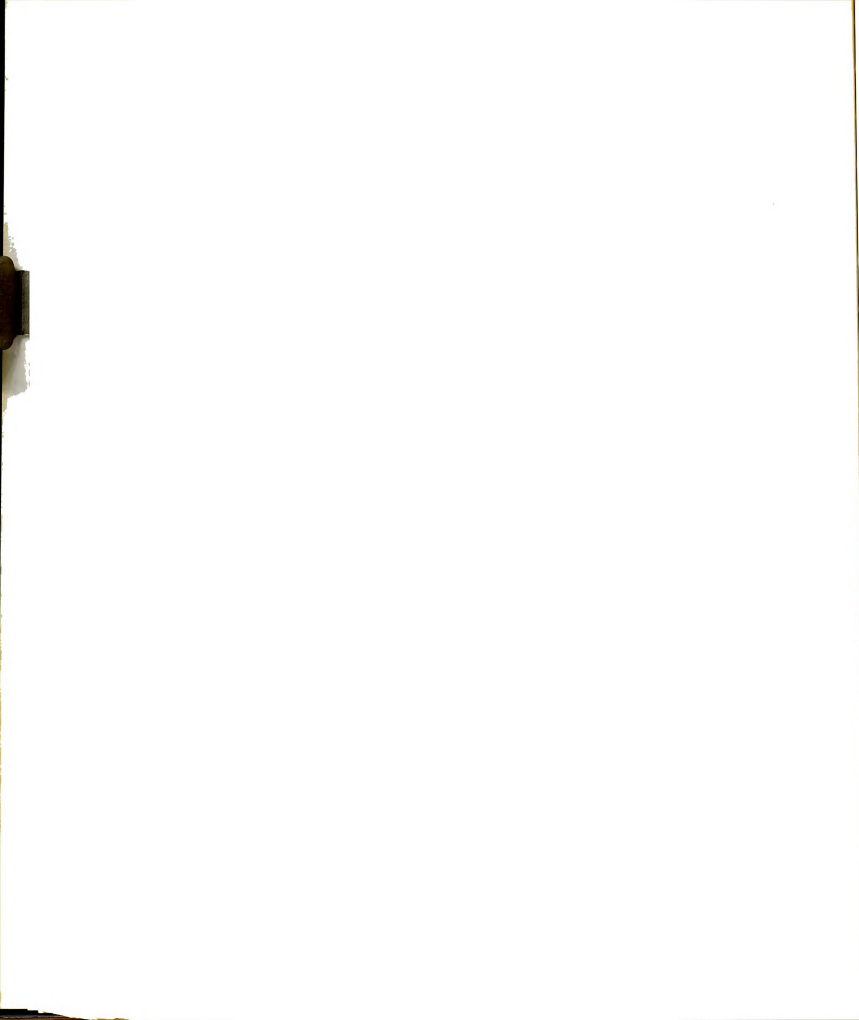


TABLE 23.--Maximum Separation Factors and Optimum Feed Rates for Various Ratios of the Rich to the Feed Stream (R/F) for the Gas Pairs $\text{SO}_2\text{-N}_2$ and $\text{SO}_2\text{-H}_2$. $\omega = 15000$ RPM, $R_w = 4$ Inches, $L = 36$ Inches, $R_m/R_w = 0.5625$, Plug Type Flow.

R/F	$\text{SO}_2\text{-N}_2$		$\text{SO}_2\text{-H}_2$		
	Maximum	Optimum	Maximum	Optimum	
	Separation Factor (Rich to Feed)	Feed Rate, scfm	Separation Factor (Rich to Feed)	Rate, scfm Estimated	Actual
0.00	2.337	0.0169	4.270	0.0663	0.0662
0.05	1.860	0.0179	2.742	0.0703	0.0704
0.10	1.586	0.0191	2.089	0.0750	0.0750
0.15	1.413	0.0204	1.734	0.0801	0.0802
0.20	1.296	0.0219	1.514	0.0859	0.0860

The following operating conditions were used:

$$Y_f = 0.005$$

$$\text{Temperature} = 530^\circ\text{R}$$

$$\text{Axis pressure} = 14.7 \text{ psia}$$

$$\text{Centrifuge radius} = 4 \text{ inches}$$

$$\text{Centrifuge length} = 36 \text{ inches}$$

$$R_m/R_w = 0.5625$$

$$\omega = 15000 \text{ RPM}$$

and Plug type flow.

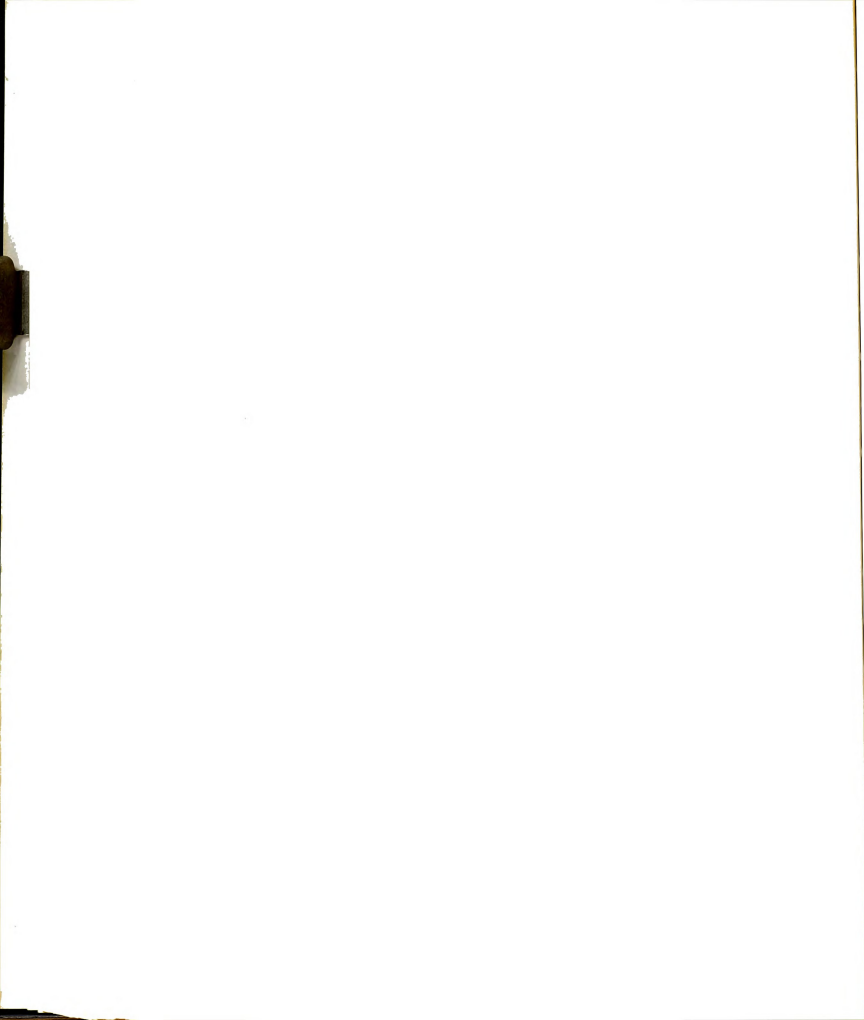
The estimated optimum feed rates for the gas pair $\text{SO}_2\text{-H}_2$ were computed by multiplying the respective optimum feed rates for the gas pair $\text{SO}_2\text{-N}_2$ by the ratio of the two diffusivities. The excellent agreement between the estimated and actual optimum feed rates illustrates the unimportance of the very different molecular weights of the feed gas (2.3 versus 28.2) on the optimum feed rate.



Since almost all common gas pairs have diffusion coefficients ranging between 0.05 and 1.5 cm^2/sec at 70°F and 1 atmosphere (Perry's Chemical Engineers' Handbook [13]), the possibility of an optimum feed rate being as great as 1/2 scfm is very remote for an 8-inch diameter centrifuge. While increasing the centrifuge diameter was shown to increase (linearly) the optimum feed rate, the separation factor was found to decrease unless the peripheral speed is increased. However, the increase in driver power requirements resulting from an increase in the centrifuge size and rotational speed would certainly make the only significant means on increasing the optimum feed rate less appealing. Figure 22 contains, for convenience, a plot of estimated optimum flows (scfm) versus diffusivities for different centrifuge sizes at an operating temperature of 70°F with $R_m/R_w = 0.5625$, plug type flow and total reflux.

Coupled with the small optimum feed rates to the gas centrifuge smaller than hoped for maximum separation factors are predicted. And to make the situation worse, when a rich product stream amounting to only 5% of the feed stream is removed, the maximum separation factor decreases dramatically. As discussed in Chapter VI, this rapid decrease in the maximum separation factor with product removal is fundamental and unavoidable and perhaps the most serious limitation of the gas centrifuge.

Increasing the length of the centrifuge at a constant diameter (increases L/D) gives very large separation factors at total reflux as illustrated in Table 19 (Chapter VI) for the gas pairs $\text{SO}_2\text{-N}_2$ and $\text{SO}_2\text{-H}_2$ using the operating conditions stated above. At total reflux



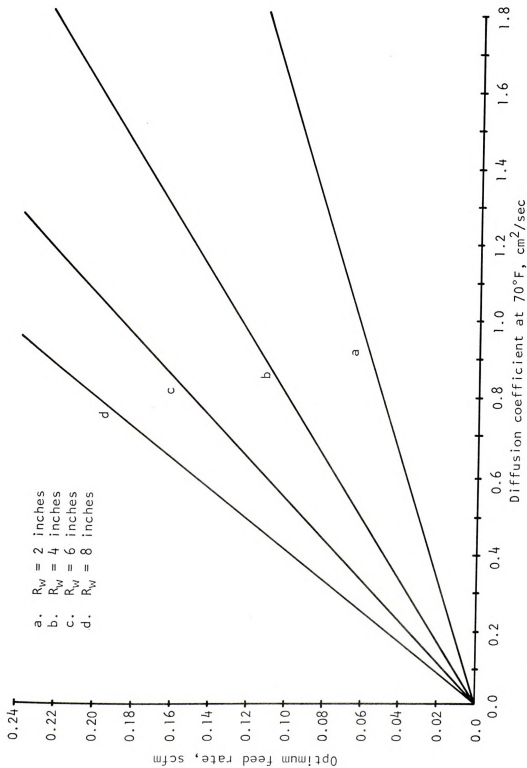
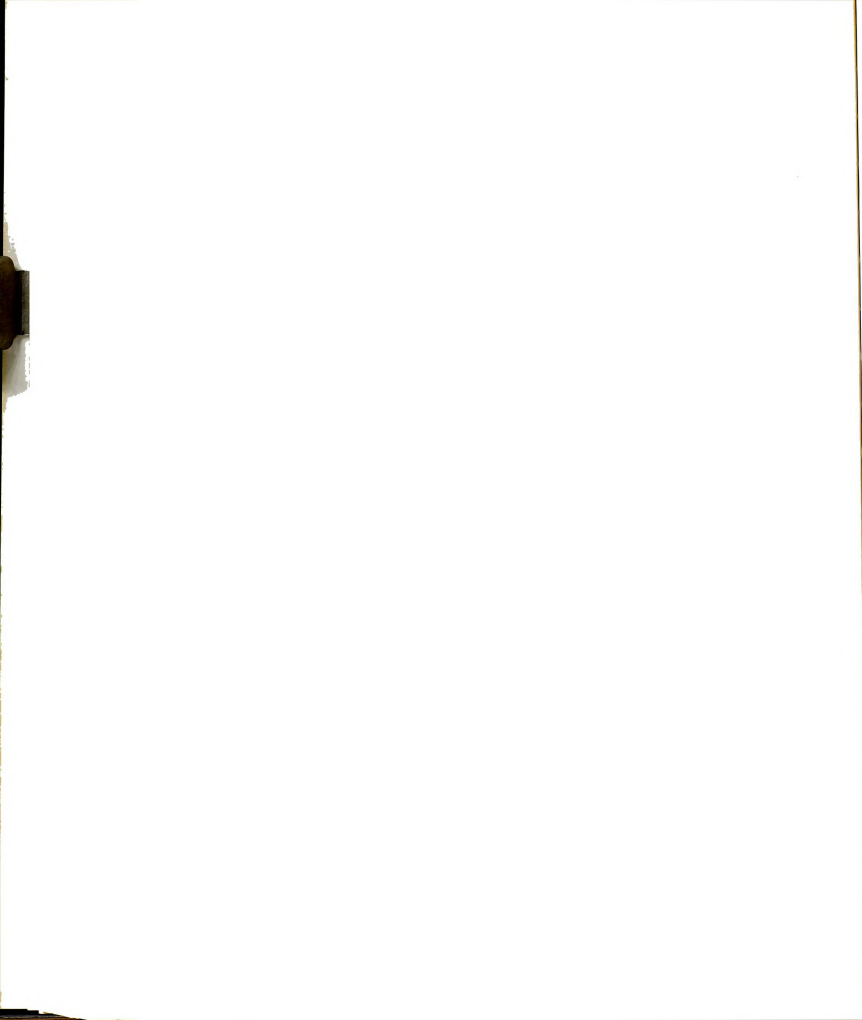


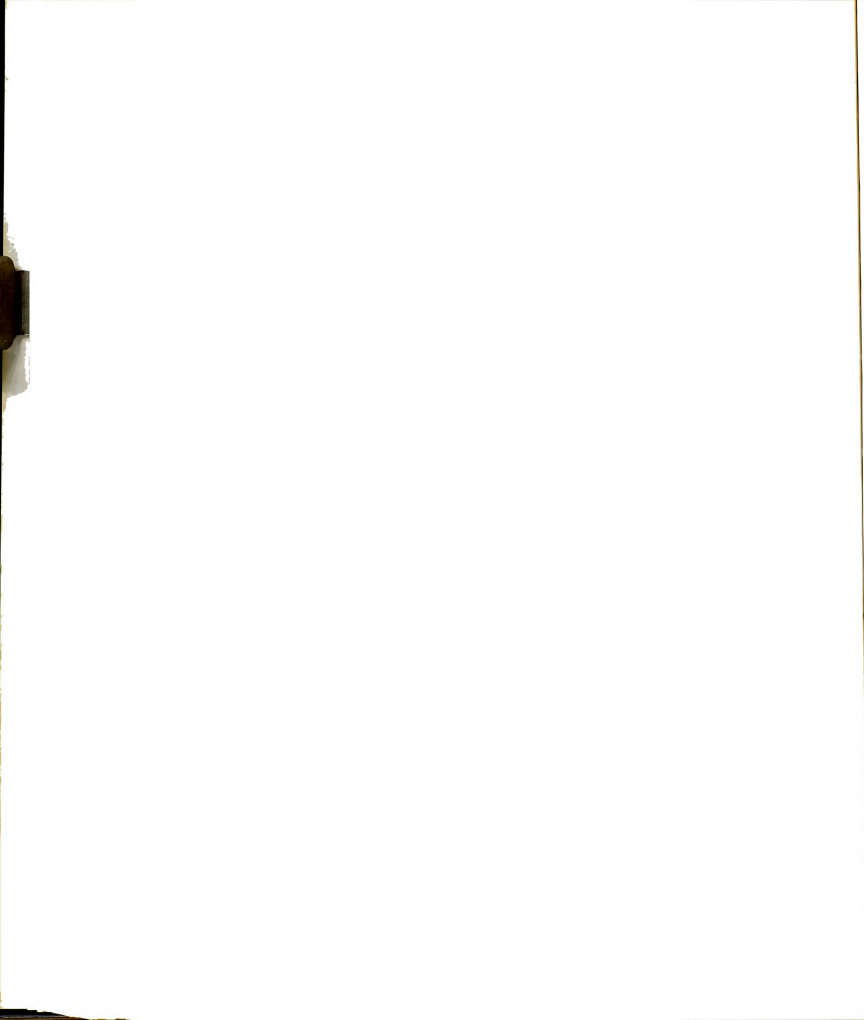
Figure 22.--Optimum Feed Rate Versus Diffusion Coefficient in a Countercurrent Rectifying Centrifuge at 70°F with $R_m/R_w = 0.5625$, Plug Type Flow and Total Reflux.



the difference in lengths (36 and 72 inches) significantly affects the maximum separation factor with 134% increase for $\text{SO}_2\text{-N}_2$ and 327% increase for $\text{SO}_2\text{-H}_2$. However, by removing 10% of the feed streams as a rich product stream, the maximum separation factor increases by only 10.6% for $\text{SO}_2\text{-N}_2$ and only 14.5% for $\text{SO}_2\text{-H}_2$ by doubling the length. This observation is expected since regardless of the length, the restriction on the composition of the leaving inner stream is always present. That is, in the case of the countercurrent rectifying centrifuge, the mole fraction profile of the leaving inner stream is trapped between the feed composition and the equilibrium mole fraction profile. Increasing the length merely increases the degree of closeness that the leaving inner stream profile may get to the equilibrium profile. Thus, there is no advantage to having a very long centrifuge, which necessarily must operate above the first whirling speed, if anything other than a very minute quantity of product is to be removed.

TABLE 24.--Maximum Separation Factors for the Gas Pairs $\text{SO}_2\text{-N}_2$ and $\text{SO}_2\text{-H}_2$ for Various Ratios of the Rich to the Feed Stream. $\omega = 15000$ RPM, $R_w = 4$ inches, $R_m/R_w = 0.5625$, and Plug Type Flow.

R/F	Maximum Separation Factors				
	SO ₂ -N ₂		SO ₂ -H ₂		
	Length, inches	36	72	36	72
0.00		2.337	5.461	4.270	18.234
0.05		1.860	2.430	2.742	3.738
0.10		1.586	1.754	2.360	2.703
0.15		1.413	1.468	1.733	1.804
0.20		1.296	1.315	1.514	1.536



At this point the effect of all the operating parameters on the optimum feed rate (OFR) and the corresponding maximum separation factor (MSF) may be summarized in equation form based on the above analyses. These equations may be used to obtain a quick estimate of the OFR and the MSF for any gas pair in any size centrifuge given the calculated performance of any other gas pair in a similar type centrifuge. The estimating equations are

$$\text{OFR}_{\text{new}} \approx \text{OFR}_{\text{old}} \cdot \frac{(\text{diffusivity times pressure}_{\text{new}})}{(\text{diffusivity times pressure}_{\text{old}})} \cdot \frac{(\text{diameter}_{\text{new}})}{(\text{diameter}_{\text{old}})}, \text{ and}$$

$$\text{MSF}_{\text{new}} \approx \exp \left\{ \ln(\text{MSF}_{\text{old}}) \cdot \frac{\Delta \text{MW}_{\text{new}}}{\Delta \text{MW}_{\text{old}}} \cdot \frac{(\text{rotational speed}_{\text{new}})^2}{(\text{rotational speed}_{\text{old}})^2} \right. \\ \left. \cdot \frac{(L/D)_{\text{new}}}{(L/D)_{\text{old}}} \cdot \frac{(\text{temperature}_{\text{old}})}{(\text{temperature}_{\text{new}})} \right\}.$$

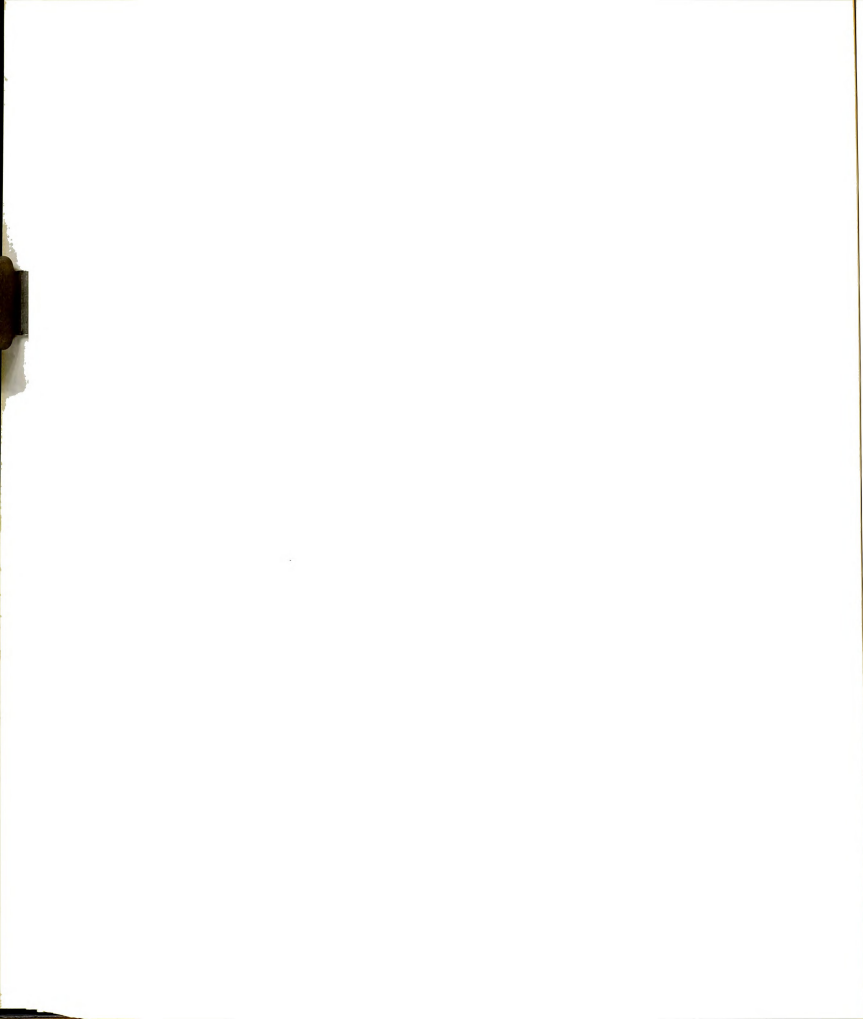
For example, using the performance computed for the gas pair $\text{SO}_2\text{-N}_2$ at total reflux and with a rich to feed stream ratio of 0.1 (Table 23), the equations may be simplified to

$$\text{OFR} \approx a \cdot (\text{diffusivity times pressure, cm}^2 \cdot \text{atm/sec}) \cdot (\text{diameter, inches}),$$

and

$$\text{MSF} \approx \exp[b \cdot (\text{rotational speed, ft/sec})^2 \cdot (\Delta \text{MW})$$

$$\cdot (L/D) / (\text{temperature, } ^\circ\text{R})],$$

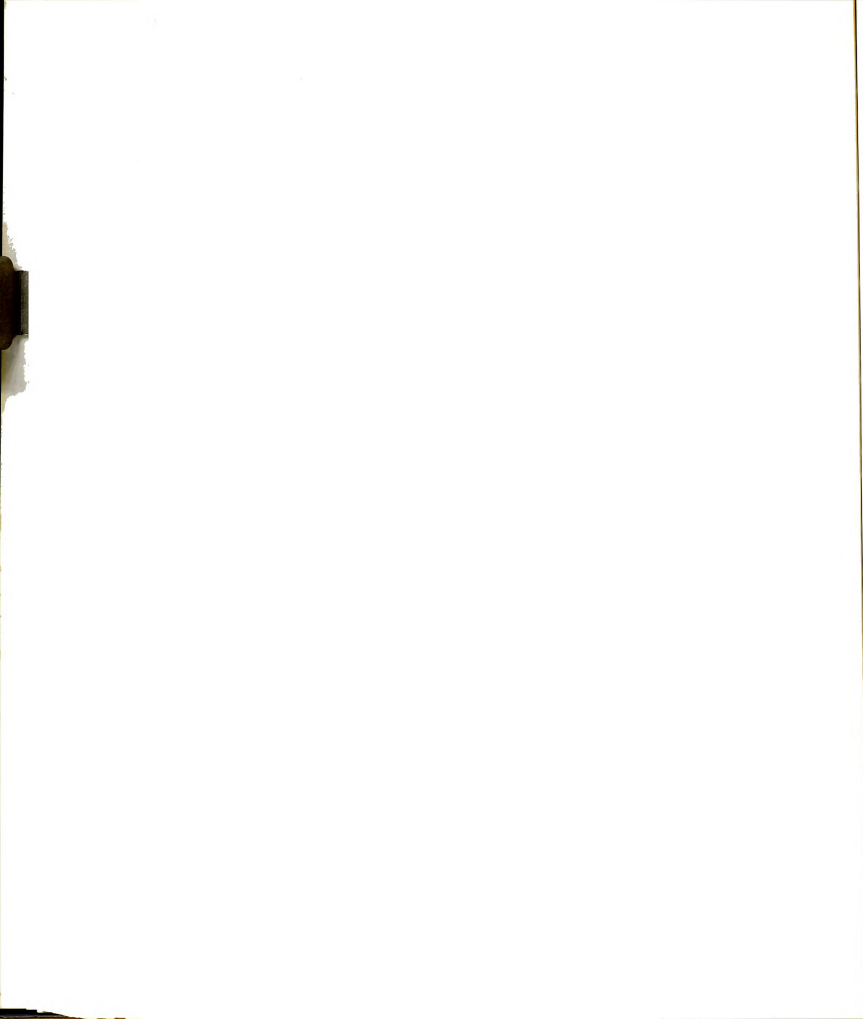


where $a = .0157$ and $b = 1.013 \times 10^{-5}$ at total reflux, and

$a = .0178$ and $b = 6.304 \times 10^{-6}$ where the ratio of the rich to the feed stream is 0.1.

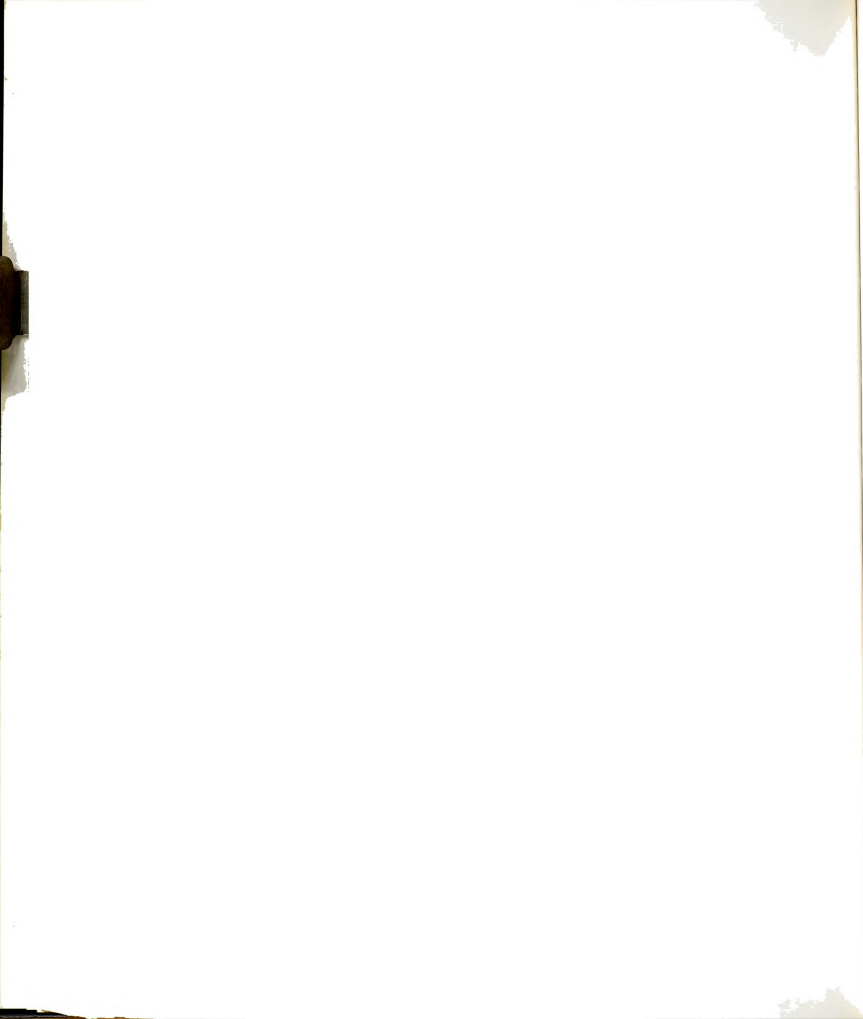
It should be remembered that throughout the analysis of the counter-current centrifuge it was assumed that the internal velocities were only in the axial direction. It was further assumed that these velocities were only a function of radial position. This represents an ideal situation giving the greatest separations. Since, if bulk movements existed, for example, in the radial direction (short circuiting) the separations would necessarily decrease. Thus, if the gas centrifuge is decided to have potential in a given situation, more research is needed to analyze the velocity profiles detailing, if possible, how to make them closest resemble the ideal velocity profiles.

Embodied in this work is a rather in-depth study of the gas centrifuge. Although the applicability of the gas centrifuge is not as general as had been hoped, its limitations as a gas separating device are now realized. For example, the gas centrifuge cannot be considered a viable means for separating SO_2 from power plant stack gas. The millions of standard cubic feet of gas produced by power plants and the high degree of SO_2 removal required are incompatible with the very small optimum feed rates (0.0169 scfm for an 8-inch diameter centrifuge) and small separations predicted for the gas centrifuge under ideal conditions. On the other hand, in the case of the enrichment of Uranium where the small predicted optimum flows and the separation factors are relatively large as compared to

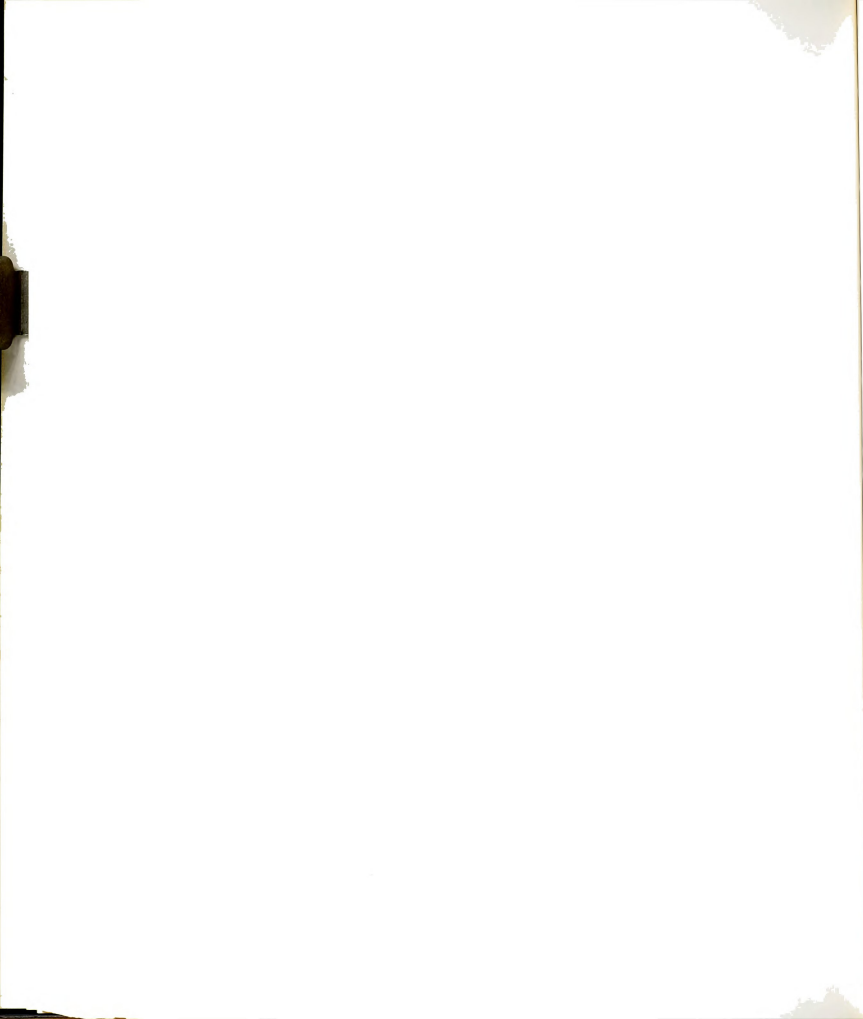


those obtained by other enriching techniques, the gas centrifuge is quite attractive.

In a situation where the gas centrifuge may be applicable, the computational tools, in the form of the general FORTRAN computer programs, NCENTRI and CENTRI, plus the analysis of all operating variables affecting the performance of the gas centrifuge, which are contained in this work, should prove to be a valuable aid to the investigator.

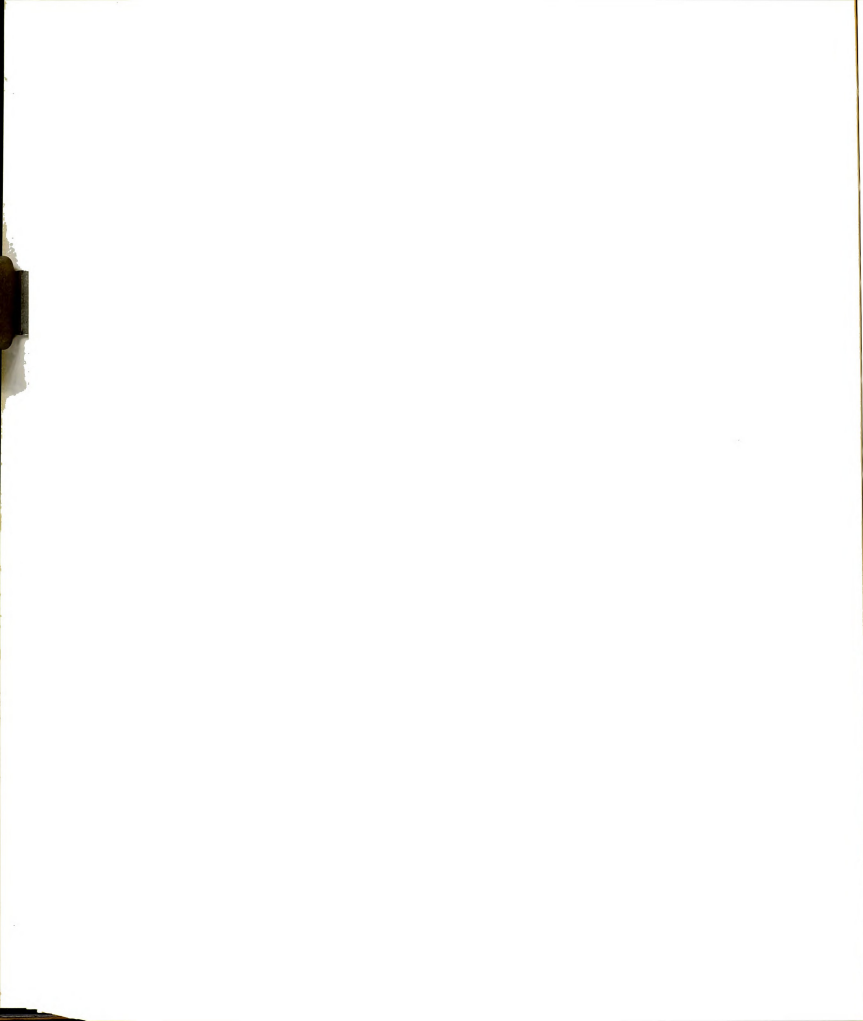


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NOMENCLATURE

$$A = (MW_1 - MW_2) \omega^2 / RTg_c$$

D_{12} = diffusion coefficient for a binary gas mixture

E = modulus of elasticity

e_r, e_θ, e_z = strains in the radial, angular and axial directions in a rotating cylinder

F_{1y}, F_{1p} = flux of species 1 due to concentration and pressure diffusion, respectively

$g(g_c)$ = acceleration due to gravity, 32.174 ft/sec^2
 $(32.174 \text{ lb}_m \text{ ft/lb}_f \text{ /sec}^2)$

h = height

i, j = subscripts denoting species i and j

$k = R_{cp} / R_w$

L = length

MW = molecular weight

P = pressure

$$Q_i = MW_i \omega^2 / RT / g_c$$

R = gas constant, $10.7315 \text{ lb}_f \text{ /in}^2 \cdot \text{ft}^3 \text{ /lb mole} \cdot ^\circ R$

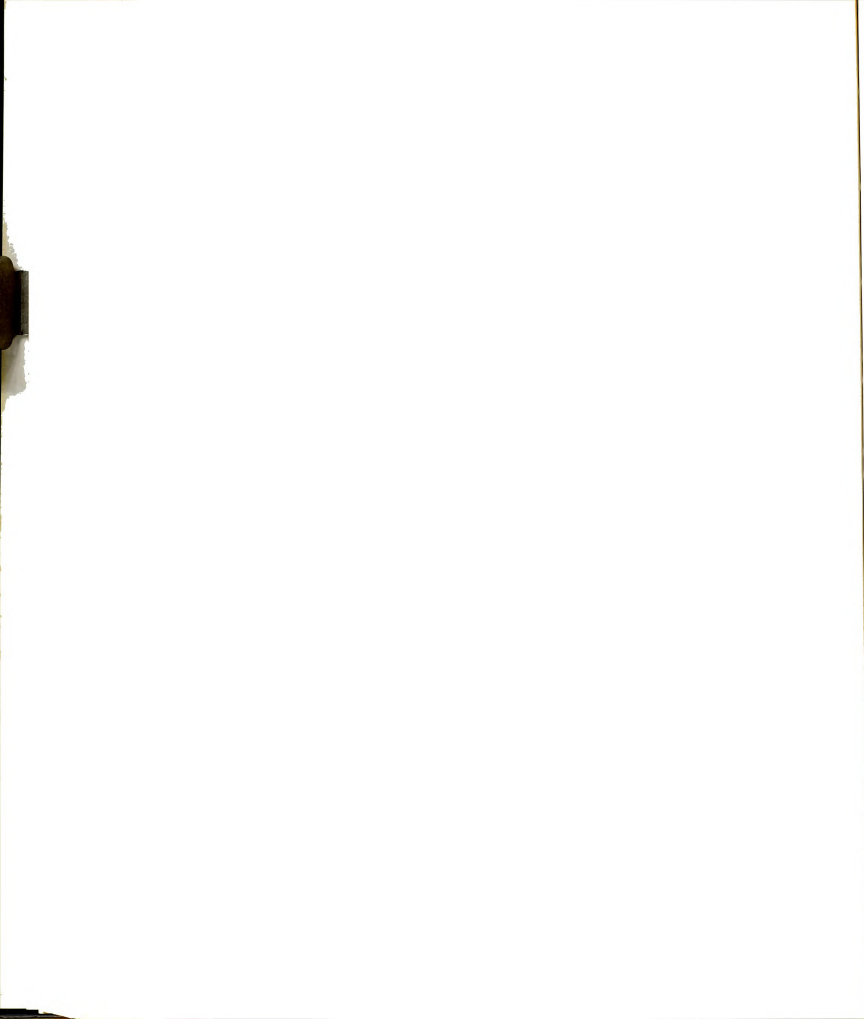
R_{cp}, R_w, R_o = radius of centerpipe, inner radius and outer radius, respectively

r = radial position

S = entropy

S_r, S_θ, S_z = stresses in the radial, angular, and axial directions in a rotating cylinder

s, s_o = inner and outer peripheral speeds



T = absolute temperature

t = time

$\bar{V}$ = partial molar volume

Y = Young's modulus

y = mole fraction of species 1 (heavy species) and also used as the deflection in the whirling speed analysis

z = axial position

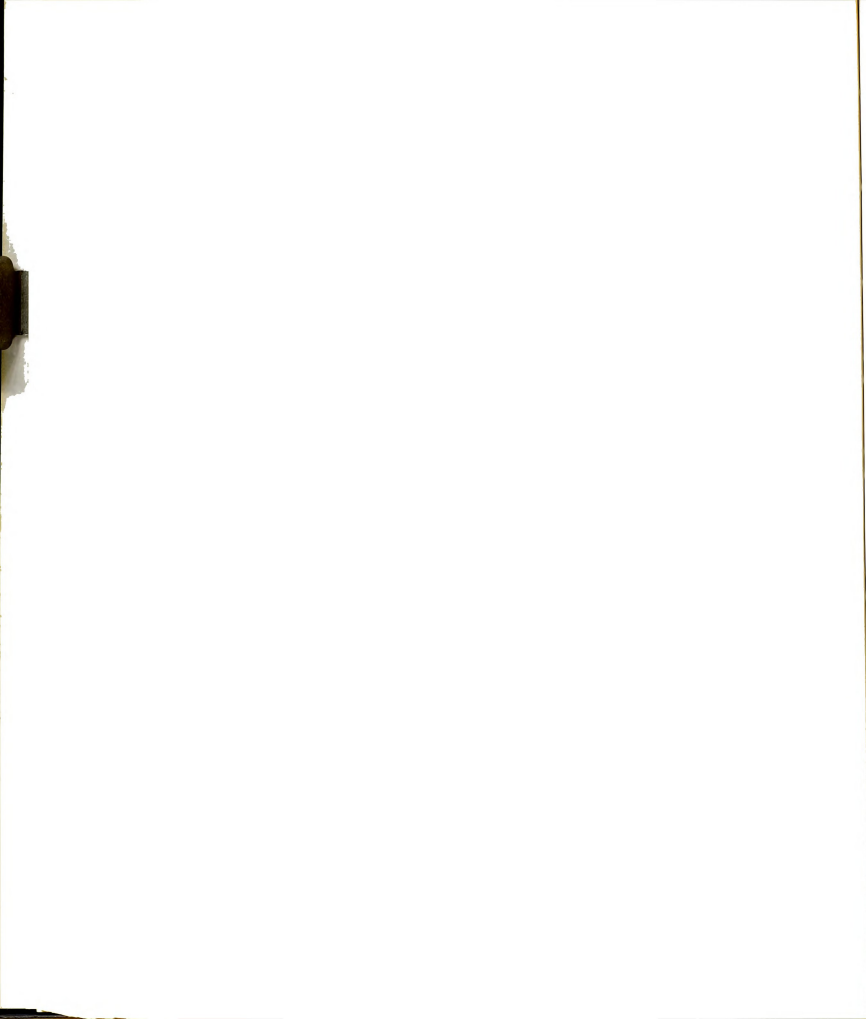
α = separation factor

$\alpha = y(R_w)/[1-y(R_w)] \cdot [1-y(0)]/y(0) = \exp (AR_w^2/2)$ for the simple centrifuge

ρ = density

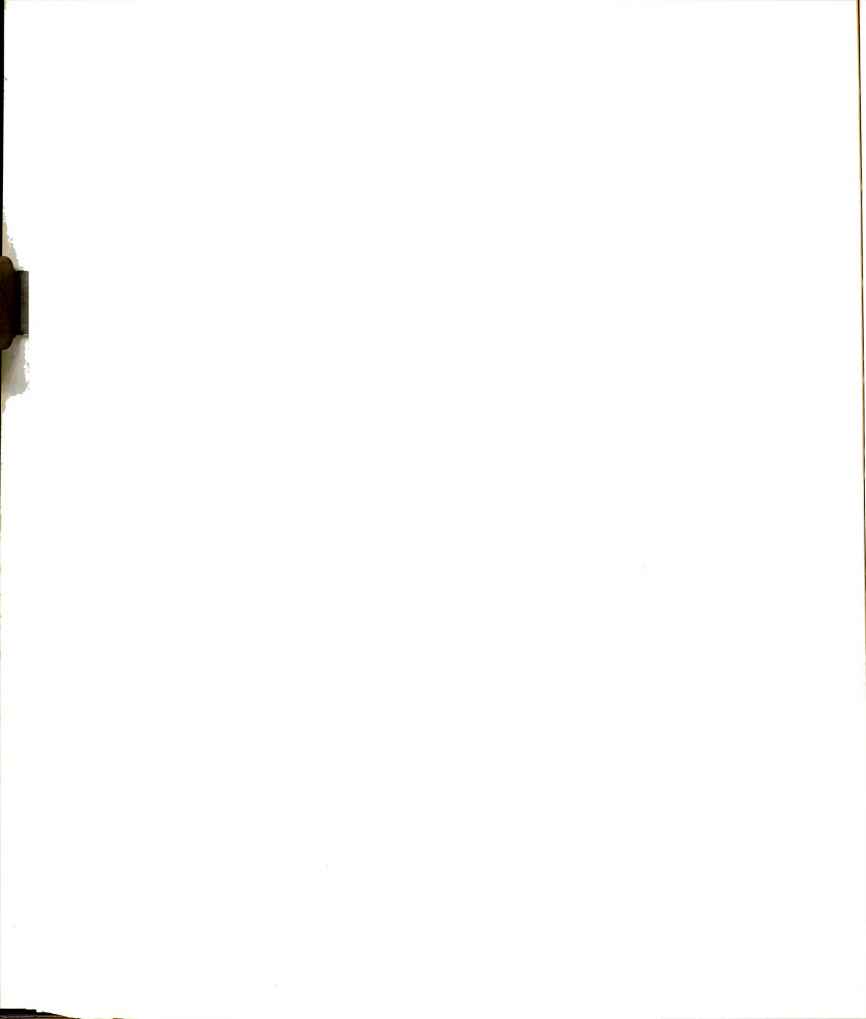
μ = viscosity

ω = angular speed



APPENDIX A

EQUATIONS AND CALCULATED DATA USED
TO CONSTRUCT ALL FIGURES



APPENDIX A

EQUATIONS AND CALCULATED DATA USED

TO CONSTRUCT ALL FIGURES

A. Calculated Data Used to Construct Figure 1: Wall to Axis Pressure Ratios Minus 1 vs. Peripheral Speed for Various Molecular Weights Between 2 and 100 and Figure 2: Wall to Axis Pressure Ratios vs. Peripheral Speed for Various Molecular Weights Between 100 and 400

The equation used to calculate the data is

$$P(\text{wall})/P(\text{axis}) = \exp \left(\frac{MW s^2}{2RTg_c} \right)$$

where MW = molecular weight

s = peripheral speed, ft/sec

R = gas constant, 10.731469 lb_f ft³/in² lb-mole °R

T = absolute temperature, 530°R

g_c = gravitational constant, 32.174 lb_m/lb_f ft/sec²

Units check:

lb _m	ft ²	in ² lb-mole °R	ft ²	lb _f sec ²
lb-mole	sec ²	lb _f ft ³	144 in ² °R	lb _m ft

Table A-1 contains values of wall to axis pressure ratios minus 1 at various peripheral speeds and for molecular weights between 2 and 100. Table A-2 contains values of wall to axis pressure ratios at various peripheral speeds and for molecular weights between 100 and 400.

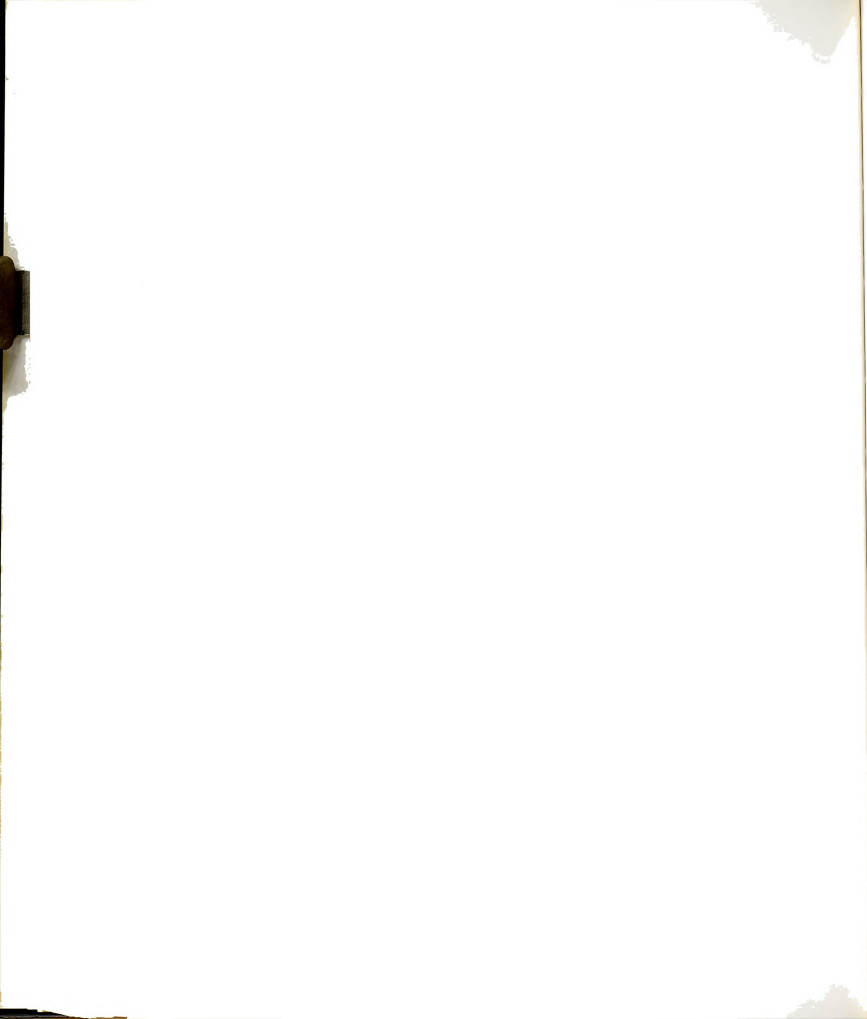


TABLE A-1.--Data Used to Construct Figure 1.

Peripheral Speed (s) ft/sec	P (wall)/P (axis) - 1							
	MW=2	MW=5	MW=10	MW=20	MW=40	MW=60	MW=80	MW=100
200	.00152	.00380	.00762	.01530	.0382	.04654	.06260	.07885
300	.00347	.00858	.01722	.03474	.07069	.10789	.14639	.18622
400	.00609	.01530	.03082	.06260	.12912	.19980	.27491	.35471
500	.00953	.02400	.04858	.09952	.20894	.32925	.46154	.60698
600	.01376	.03474	.07069	.14639	.31420	.50659	.72713	.97996
700	.01877	.04758	.09743	.20436	.45048	.74691	1.1039	1.5339
800	.02458	.06260	.12912	.27491	.62538	1.0722	1.6419	2.3681
900	.03122	.07988	.16613	.35986	.84923	1.5147	2.4197	3.6503
1000	.03868	.09952	.20894	.46154	1.1361	2.1220	3.5629	5.6688
1100	.04699	.12164	.25808	.58278	1.5052	2.9651	5.2759	8.9334
1200	.05617	.14639	.31420	.72713	1.9830	4.1520	7.8982	14.368

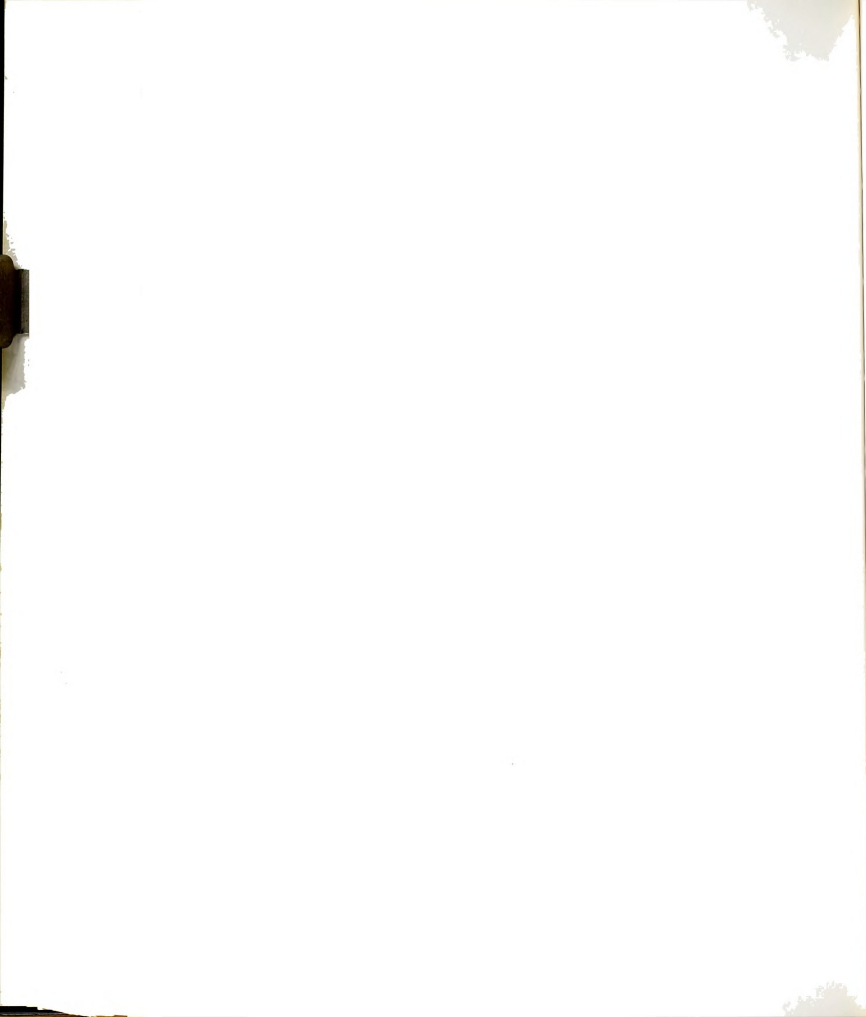


TABLE A-2.--Data Used to Construct Figure 2.

Speed (s) ft/sec	P(wall)/P(axis)				
	MW=100	MW=150	MW=200	MW=300	MW=400
200	1.0789	1.1206	1.1639	1.2557	1.3547
300	1.1862	1.2920	1.4071	1.6691	1.9800
400	1.3547	1.5768	1.8353	2.4862	3.3681
500	1.6070	2.0371	2.5824	4.1494	6.6688
600	1.9800	2.7860	3.9203	7.7619	15.368
700	2.5339	4.0334	6.4205	16.269	41.222
800	3.3681	6.1814	11.344	38.209	128.69
900	4.6503	10.028	21.625	100.56	467.64
1000	6.6686	17.221	44.473	296.58	1977.8
1100	9.9334	31.037	98.672	980.14	9736.1
1200	15.368	60.248	236.19	3629.8	55783.

B. Calculated Data Used to Construct Figure 3:

Effective Molecular Weights vs. Actual
Molecular Weights at Temperatures
Between 0 and 300°F

The equation used to calculate the data is

$$MW_e = MW_a \left(\frac{530}{460 + T_f} \right)$$

where $T_f = ^\circ F$

MW_e = effective molecular weight

MW_a = actual molecular weight

With the aid of this information the curves appearing in Figures 1 and 2 can be used for temperatures other than 70°F by using the effective molecular weight. Table A-3 contains the values of 530/(460 + T_f) at various values of T_f used to construct Figure 3.

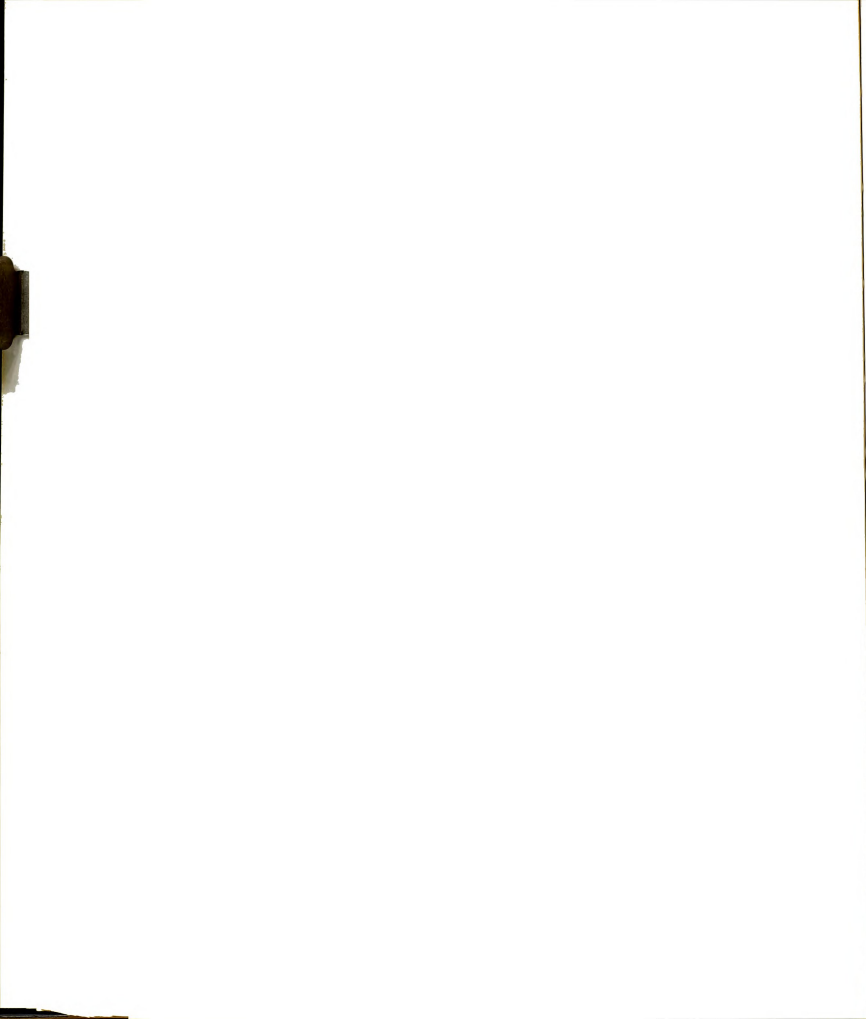


TABLE A-3.--Data Used to Construct Figure 3.

Temperature °F	530/(460 + T _f)	Temperature °F	530/(460 + T _f)
0	1.152	160	.8548
20	1.104	180	.8281
40	1.060	200	.8030
60	1.019	220	.7794
80	.9815	240	.7571
100	.9464	260	.7361
120	.9138	280	.7162
140	.8833	300	.6974

C. Calculated Data Used to Construct Figure 4:
 $[y(R_w) - y(0)]/y(0)$ Versus $y(0)$ for Values of α

The equation used was

$$\frac{[y(R_w) - y(0)]}{y(0)} = \frac{\alpha}{y(0)(\alpha - 1) + 1} - 1$$

where α is the simple separation factor. Table A-4 contains the calculated data used to construct Figure 4.

D. Calculated Data Used to Construct Figure 5: Mole Fraction
Profiles Developed in a Simple Centrifuge with a Peripheral
Speed of 500 ft/sec for the Gas Pairs: SO_2-H_2 , SO_2-N_2
and UF_6 (235, 238 isotopes) at 70°F

The equation used to compute $y(0)$ was

$$y(0) = \frac{y_f \frac{Q_1}{Q_2} C}{1 + y_f \left(\frac{Q_1}{Q_2} C - 1 \right)},$$

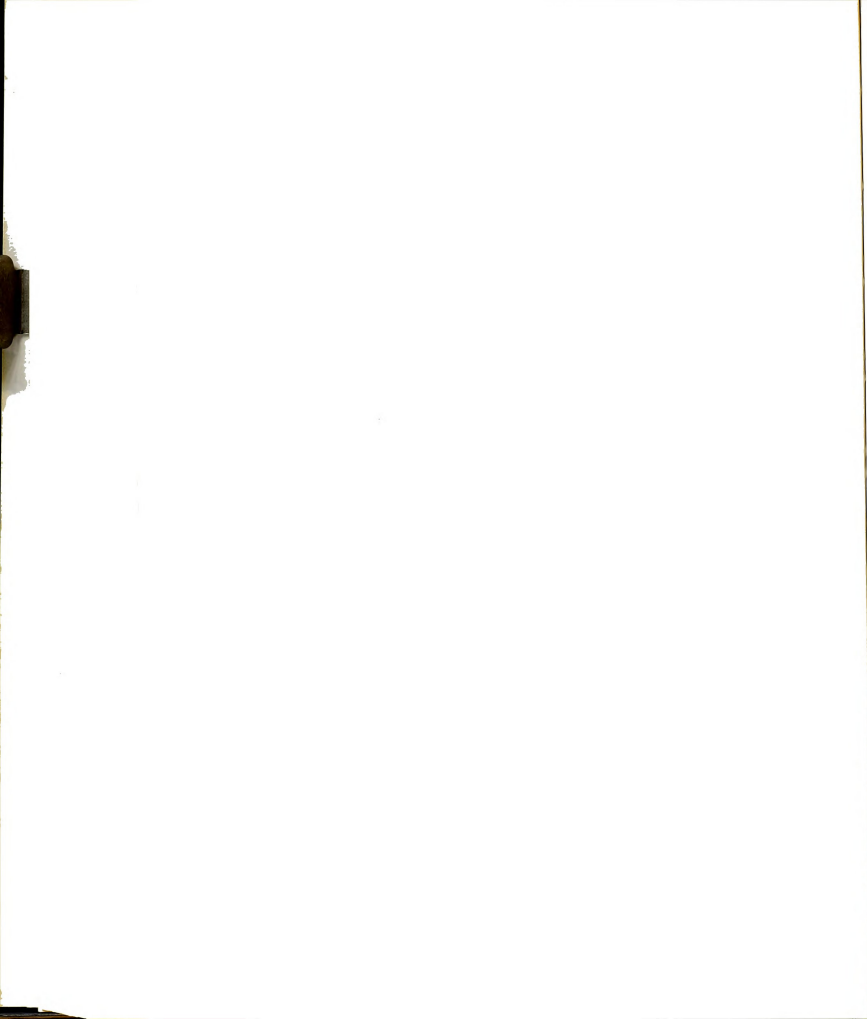
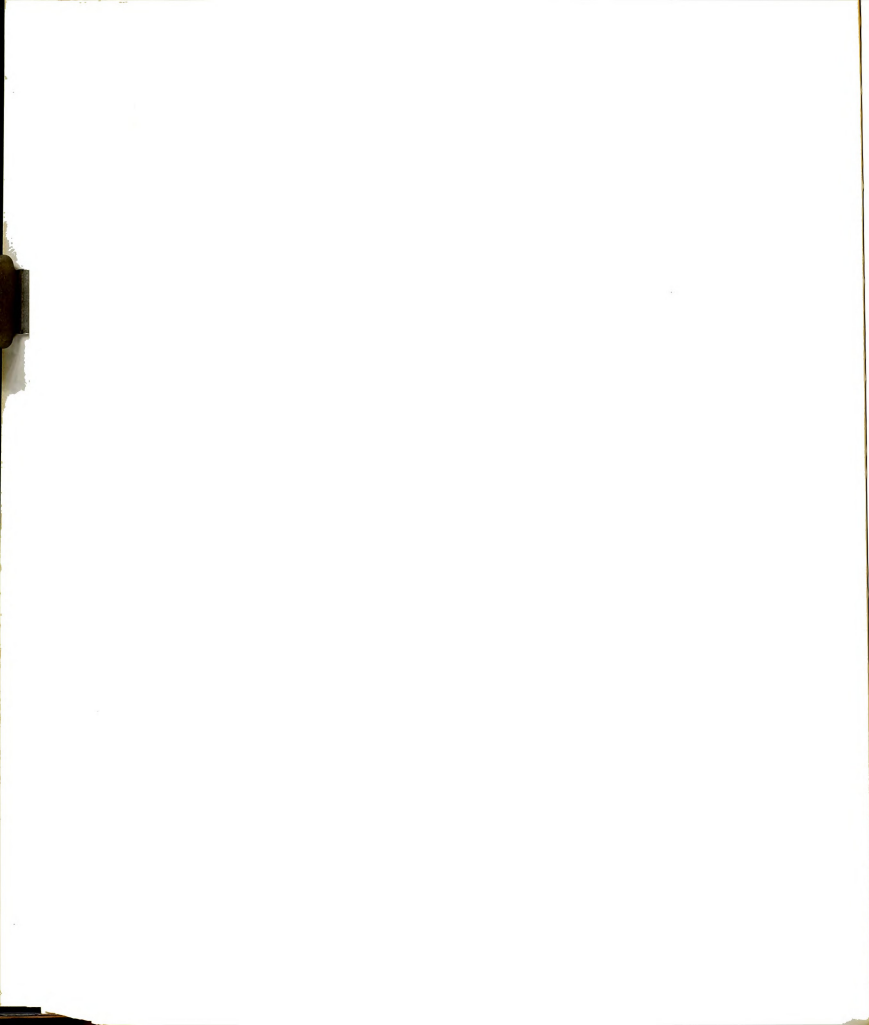


TABLE A-4.--Data Used to Construct Figure 4.

α	$y(0) = 0.0$	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
	$[y(R_w) - y(0)]/y(0)$										
1.05	.0500	.0448	.0396	.0345	.0294	.0244	.0194	.0145	.0096	.0048	0.0
1.10	.1000	.0891	.0784	.0680	.0577	.0476	.0377	.0280	.0185	.0092	0.0
1.25	.2500	.2195	.1905	.1628	.1364	.1111	.0870	.0638	.0417	.0204	0.0
1.50	.5000	.4286	.3636	.3043	.2500	.2000	.1538	.1111	.0714	.0345	0.0
1.75	.7500	.6279	.5217	.4286	.3462	.2727	.2069	.1475	.0938	.0448	0.0
2.00	1.000	.8182	.6667	.5385	.4286	.3333	.2500	.1765	.1111	.0526	0.0
5.00	4.000	2.571	1.778	1.273	.9231	.6667	.4706	.3158	.1905	.0870	0.0
10.0	9.000	4.263	2.571	1.703	1.174	.8182	.5625	.3699	.2195	.0989	0.0
20.0	19.000	5.897	3.167	1.985	1.326	.9048	.6129	.3986	.2346	.1050	0.0
very large		9.000	4.000	2.333	1.500	1.000	.6667	.4286	.2500	.1111	0.0



$$\text{where } C = \frac{\exp(Q_2 R_w^2/2) - 1}{\exp(Q_1 R_w^2/2) - 1}$$

$$Q_1 = \frac{MW_1 \omega^2}{RTg_c}, \text{ and } Q_2 = \frac{MW_2 \omega^2}{RTg_c}.$$

Calculations were done at 70°F in a simple centrifuge with a peripheral speed of 500 ft/sec.

$$1. \quad \underline{SO_2-H_2} \quad \quad \quad y_f(SO_2) = 0.002$$

$$\frac{Q_1 R_w^2}{2} = 0.30359, \quad \frac{Q_2 R_w^2}{2} = 0.0094872$$

$$y(0) = 0.00183$$

$$2. \quad \underline{SO_2-N_2} \quad \quad \quad y_f(SO_2) = 0.002$$

$$\frac{Q_1 R_w^2}{2} = 0.30359, \quad \frac{Q_2 R_w^2}{2} = 0.132821$$

$$y(0) = 0.00172$$

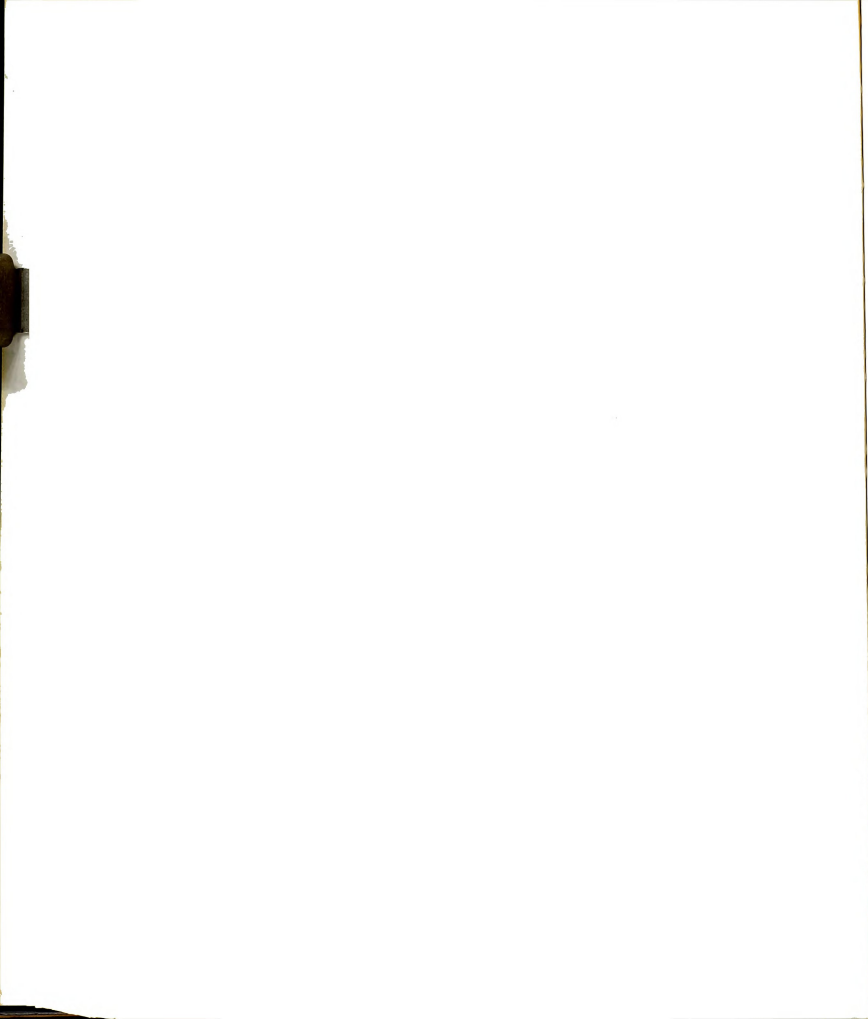
$$3. \quad \underline{UF_6 (235, 238)} \quad \quad \quad y_f(U_{238}) = 0.998$$

$$\frac{Q_1 R_w^2}{2} = 3.33949, \quad \frac{Q_2 R_w^2}{2} = 3.311028$$

$$y(0)(U_{235}) = y(0)(U_{238}) - 1 = 0.002018$$

The profiles were then computed by the following equation:

$$y(R_w) = \frac{y(0) \exp(Ar^2/2)}{y(0) [\exp(Ar^2/2) - 1] + 1}$$



where $A = \frac{MW^2}{RTg_c}$.

1. $\underline{SO_2-H_2}$ $\frac{A}{2\omega^2} = 1.176411 \times 10^{-6} \text{ sec}^2/\text{ft}^2$

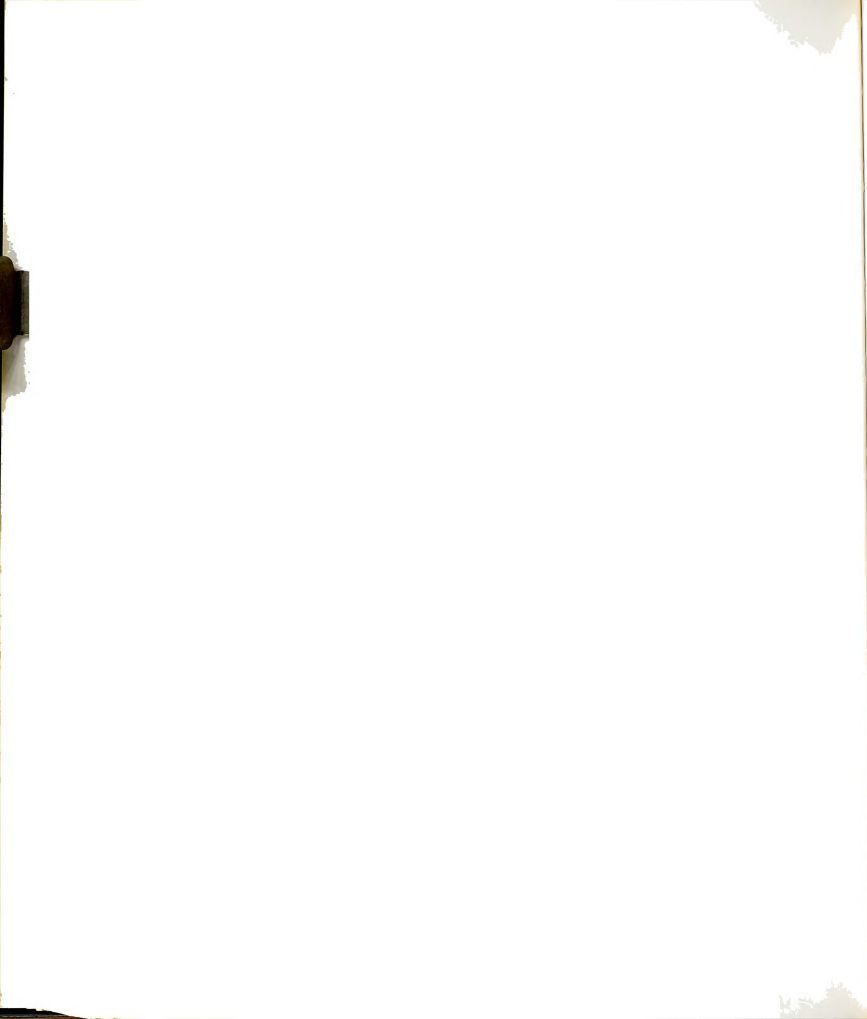
2. $\underline{SO_2-N_2}$ $\frac{A}{2\omega^2} = 6.830774 \times 10^{-7} \text{ sec}^2/\text{ft}^2$

3. UF_6 (235, 238 isotopes) $\frac{A}{2\omega^2} = 5.6923116 \times 10^{-8} \text{ sec}^2/\text{ft}^2$

The calculated data used to construct Figure 5 are found in Table A-5.

TABLE A-5.--Data Used to Construct Figure 5.

Dimensionless Radius (r/R_w)	SO_2-N_2 γ, SO_2	SO_2-H_2 γ, SO_2	UF_6 (235, 238 isotopes) γ, U_{235}
0.0	.001830	.001720	.0020180
0.1	.001833	.001725	.0020178
0.2	.001843	.001740	.0020169
0.3	.001858	.001776	.0020155
0.4	.001881	.001802	.0020135
0.5	.001909	.001851	.0020109
0.6	.001946	.001912	.0020078
0.7	.001989	.001986	.0020041
0.8	.002041	.002076	.0019998
0.9	.002101	.002182	.0019950
1.0	.002170	.002307	.0019896



E. Calculated Data Used to Construct Figure 6:
 θ Versus k for a Simple Centrifuge Containing a
Stationery Center Pipe

The equation used to compute θ was

$$\theta = \frac{(1/k^2 - k^2 + 4 \ln k)}{(1/k^2 + k^2 - 2)}.$$

Calculations were done varying k between its limits 0 and 1. Table A-6 contains the data used to construct Figure 6.

F. Calculated Data Used to Construct Figure 7: Mole
Fraction Profiles for SO_2 , y , Versus Dimensionless
Radius r/R_w ($R_w=4$ inches), at Various Times in the
Unsteady State Operation of a Simple Centrifuge
Containing SO_2-H_2 at $70^\circ F$, $RPM = 20000$

The equations used to compute the data were the equations describing the conservation of SO_2 , the total conservation of moles and the total pressure equation. These equations are described in detail in Appendix C and will not be repeated here. The data, however, representing the solution of these equations, and which was used to construct Figure 7, can be found in Table A-7.

G. Calculated Data Used to Construct Figure 10:
 $S_{\theta(max)}/(\rho/g_c)$ Versus Peripheral Speed, s_o , for
 k Values of 0.90, 0.95, and 1.00

The equation that was used to calculate the data is

$$\frac{S_{\theta(max)}}{\rho/g_c} = \frac{s_o^2}{8} (3 + 5k),$$

where $S_{\theta(max)}$ = the maximum circumferential stress (hoop tension),
 lb_f/in^2 ,

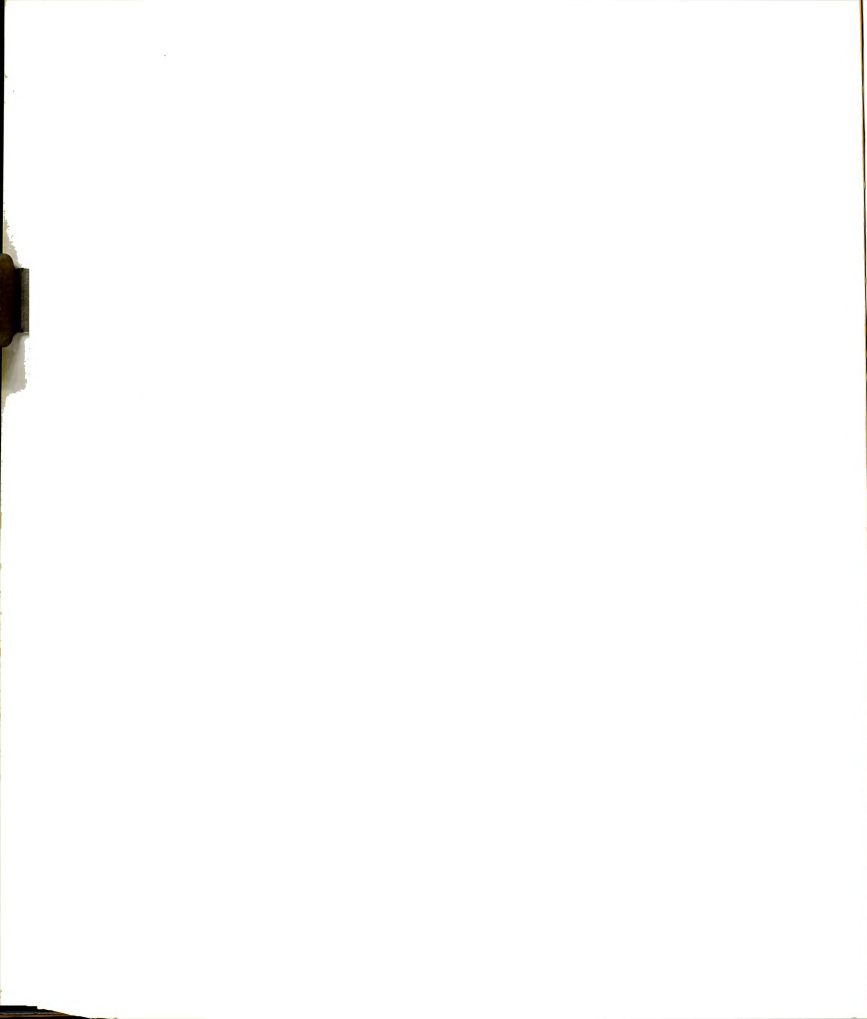
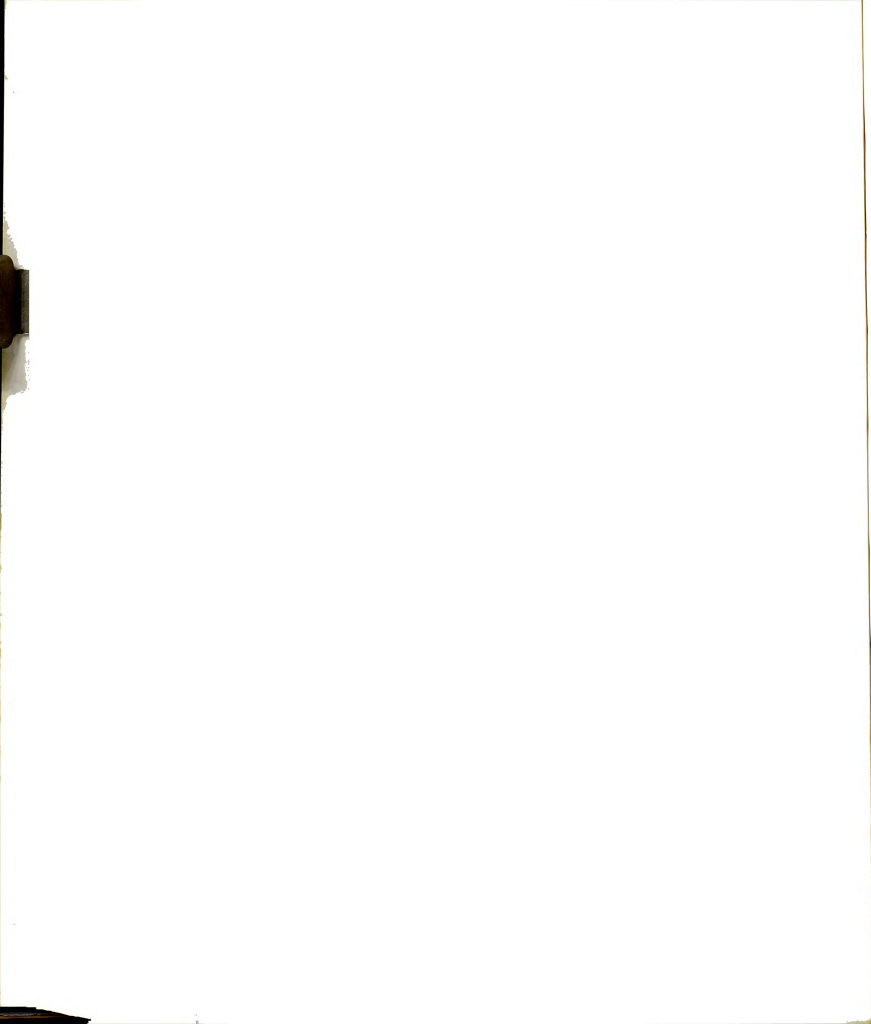


TABLE A-6.--Data Used to Construct Figure 6.

k	θ	k	θ
0.00	1.0000	0.55	0.3805
0.05	0.9749	0.60	0.3291
0.10	0.9262	0.65	0.2803
0.15	0.8673	0.70	0.2338
0.20	0.8039	0.75	0.1897
0.25	0.7390	0.80	0.1478
0.30	0.6744	0.85	0.1080
0.35	0.6111	0.90	0.0701
0.40	0.5498	0.95	0.0342
0.45	0.4909	1.00	0.0000
0.50	0.4344		

TABLE A-7.--Calculated Data Used to Construct Figure 7.

R/R _w	Time (sec)	3.6	Mole Fractions of SO ₂ × 10 ²		
			7.2	14.4	very large
0	0.1921		0.1841	0.1704	0.1481
0.05	0.1921		0.1841	0.1705	0.1483
0.10	0.1921		0.1841	0.1707	0.1489
0.15	0.1921		0.1841	0.1709	0.1500
0.20	0.1921		0.1842	0.1714	0.1515
0.25	0.1921		0.1843	0.1719	0.1535
0.30	0.1921		0.1844	0.1727	0.1559
0.35	0.1921		0.1845	0.1738	0.1588
0.40	0.1921		0.1848	0.1751	0.1623
0.45	0.1922		0.1853	0.1768	0.1663
0.50	0.1922		0.1859	0.1789	0.1708
0.55	0.1924		0.1869	0.1816	0.1761
0.60	0.1927		0.1884	0.1849	0.1819
0.65	0.1932		0.1904	0.1889	0.1886
0.70	0.1943		0.1932	0.1939	0.1960
0.75	0.1960		0.1970	0.1998	0.2043
0.80	0.1988		0.2020	0.2069	0.2136
0.85	0.2031		0.2085	0.2152	0.2239
0.90	0.2094		0.2168	0.2251	0.2354
0.95	0.2181		0.2270	0.2366	0.2482
1.00	0.2297		0.2395	0.2499	0.2624



ρ = metal or alloy density, lbm/m³

s_o = outer peripheral speed, ωR_o , ft/sec, and

k = inner radius/outer radius, R_w/R_o .

Calculations were done varying s_o from 200 to 1200 ft/sec for k values of 0.90, 0.95 and 1.00. Table A-8 contains the data used to construct Figure 10.

H. Calculated Data Used to Construct Figure 11: Critical Elastic Modulus over Density, $E/(\rho/g_c)$, Versus Peripheral Speed, s_o , for Length to Diameter Ratios, L/D_o , of 3, 4, 5 and 6

The equation that was used to calculate the data is

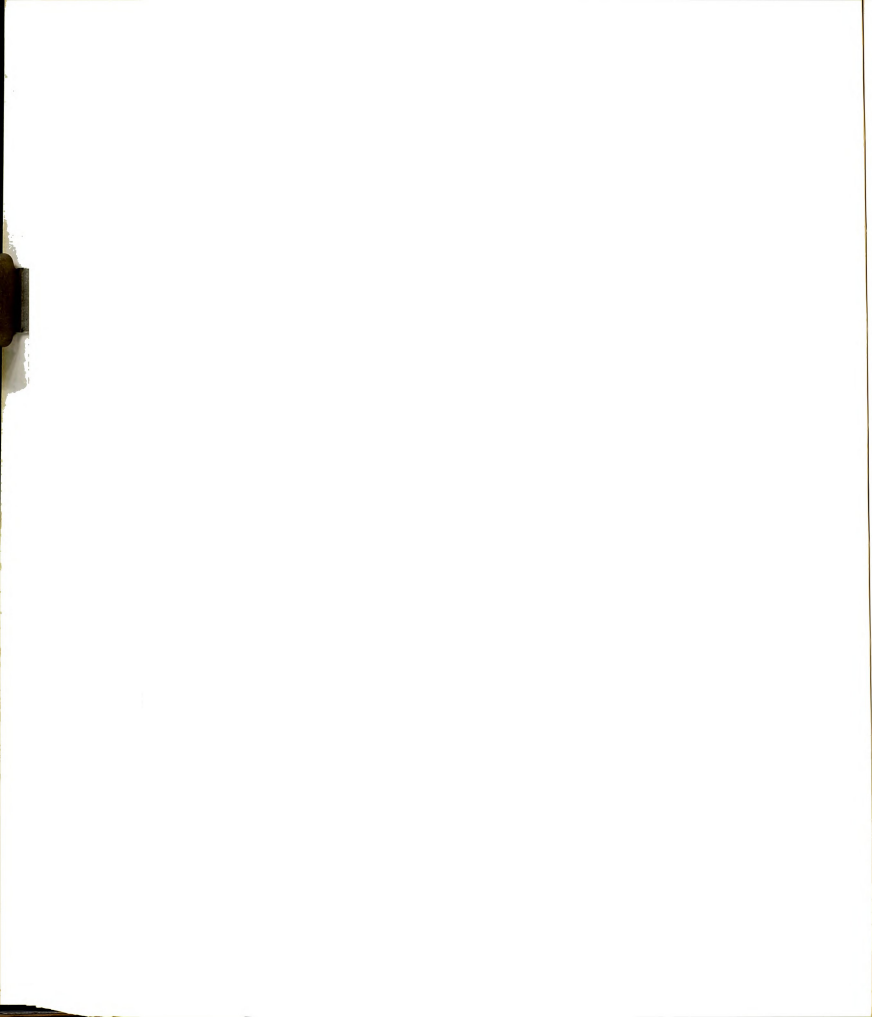
$$E/(\rho/g_c) = \frac{64}{(1+k^2)^4} \left(\frac{L}{D_o}\right)^4 s_o^2,$$

where E = the elastic modulus, lb_f/in²,

ρ = metal or alloy density, lb_m/in³,

TABLE A-8.--Data Used to Construct Figure 10.

s_o , ft/sec	$s_{(max)}/(\rho/g_c) \times 10^{-5}$, ft ² /sec ²		
	$k = 0.9$	$k = .95$	$k = 1.0$
200	.353	.376	.400
300	.793	.845	.900
400	1.41	1.50	1.60
500	2.20	2.35	2.50
600	3.17	3.38	3.60
700	4.32	4.60	4.90
800	5.64	6.01	6.40
900	7.14	7.61	8.10
1000	8.81	9.39	10.0
1100	1.07	1.14	12.1
1200	1.27	1.35	14.4



s_o = outer peripheral speed, ωR_o , ft/sec

L/D_o = length to diameter ratio, and

k = inner radius/outer radius, R_w/R_o .

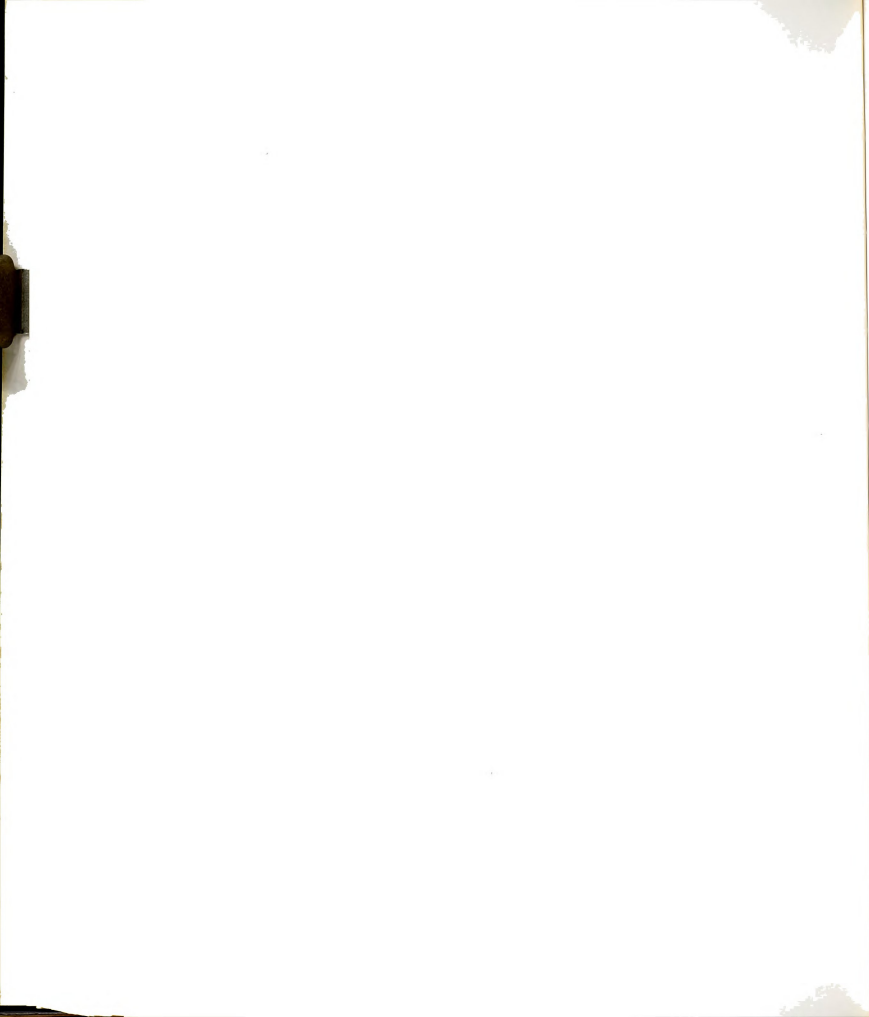
To perform the calculations a value of 0.95 was used for k . This simplified the above expression to

$$E/(\rho/g_c) = 0.34535 \left(\frac{L}{D_o}\right)^4 s_o^2.$$

Calculations were done varying s_o from 200 to 1200 ft/sec for L/D_o values of 3, 4, 5, and 6. Table A-9 contains the data used to construct Figure 11.

TABLE A-9.--Data Used to Construct Figure 11.

s_o	$L/D_o = 3$	$E/(\rho/g_c) \times 10^{-6}, \text{ ft}^2/\text{sec}^2$		
		$L/D_o = 4$	$L/D_o = 5$	$L/D_o = 6$
200	1.12	3.54	8.63	17.9
300	2.52	7.96	19.4	40.3
400	4.48	14.1	34.5	71.6
500	6.99	22.1	54.0	112.
600	10.1	31.8	77.7	161.
700	13.7	43.3	106.	219.
800	17.9	56.6	138.	286.
900	22.7	71.6	175.	363.
1000	28.0	88.4	216.	448.
1100	33.8	107.	261.	542.
1200	40.3	127.	311.	645.



I. Calculated Data Used to Construct Figure 13: Separation Factor, α , Versus Feed Rate (scfm) for $\text{SO}_2\text{-N}_2$ with Laminar Velocity Profiles, $\omega = 10000$ RPM, $R_w = 4$ Inches, $R_m/R_w = 0.5625$, $L = 18$ and 36 Inches and Total Reflux

The separation factor used is defined as

$$\alpha = \frac{y_r}{(1 - y_r)} \frac{(1 - y_f)}{y_f},$$

where y_r is the composition at the rich end of the centrifuge.

Table A-10 contains the data used to construct Figure 13.

J. Calculated Data Used to Construct Figure 14: Separation Factor, α , Versus Feed Rate (scfm) for $\text{SO}_2\text{-N}_2$ with Plug Type Flow, $\omega = 10000$ RPM, $R_w = 4$ Inches, $R_m/R_w = 0.5625$, $L = 18$ and 36 Inches and Total Reflux

The separation factor is defined as

$$\alpha = \frac{y_r}{(1 - y_r)} \frac{(1 - y_f)}{y_f},$$

where y_r is the composition at the rich end of the centrifuge. Table

A-11 contains the data used to construct Figure 14.

K. Calculated Data Used to Construct Figure 15: Separation Factor, α , Versus Feed Rate (scfm) for $\text{SO}_2\text{-N}_2$ with Laminar Velocity Profiles, $\omega = 20000$ RPM, $R_w = 4$ Inches, $R_m/R_w = 0.5625$, $L = 18$ Inches and Total Reflux

The separation factor used is defined as

$$\alpha = \frac{y_r}{(1 - y_r)} \frac{(1 - y_f)}{y_f},$$

where y_r is the composition at the rich end of the centrifuge.

Table A-12 contains data used to construct Figure 15.

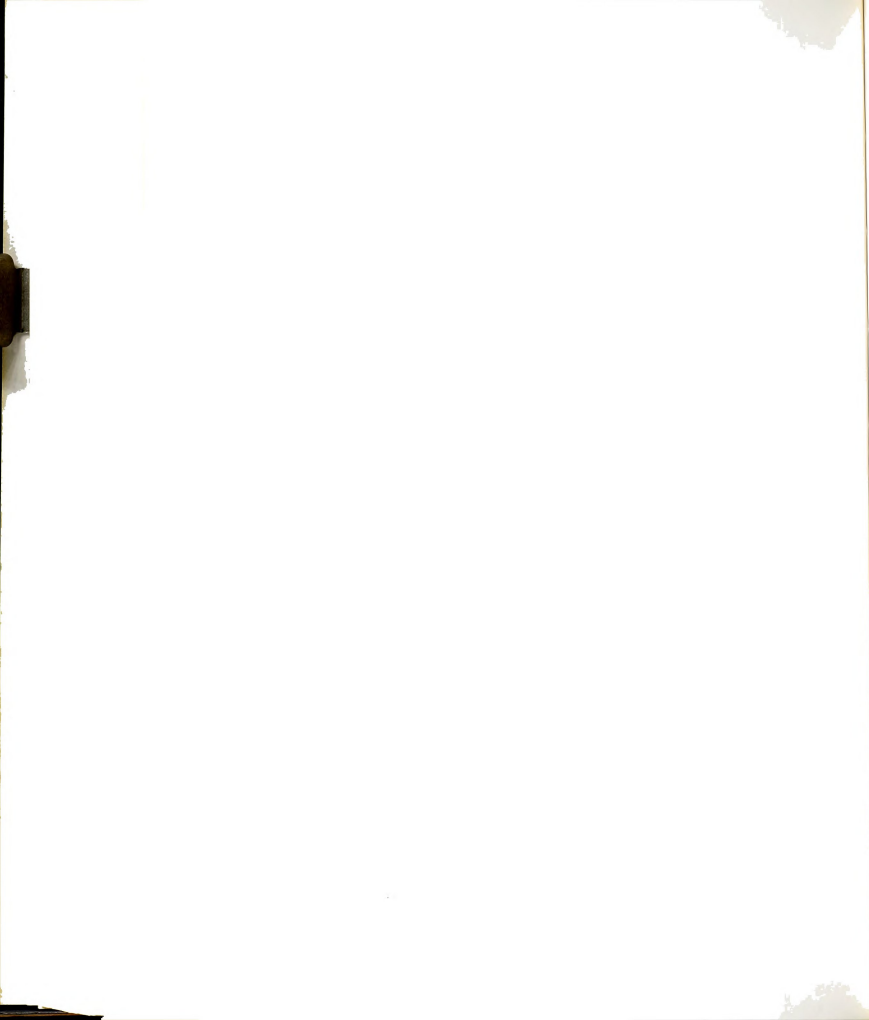


TABLE A-10.--Data Used to Construct Figure 13.

Feed Rate (scfm)	Numerical Solution Separation Factor		Feed Rate (scfm)	Analytical (Approximate) Solution Separation Factor	
	L=18 inches	L=36 inches		L=18 inches	L=36 inches
0.005	1.133	1.325	0.0046	1.103	1.216
0.0075	1.167	1.404	0.0072	1.144	1.308
0.01	1.187	1.456	0.009	1.162	1.350
0.01125	1.192	1.472	0.0113	1.175	1.381
0.0125	1.195	1.472	0.0141	1.180	1.392
0.01375	1.196	1.471	0.0176	1.175	1.381
0.015	1.195	1.467	0.0221	1.162	1.350
0.02	1.183	1.425	0.0276	1.144	1.308
0.03	1.146	1.325	0.0345	1.123	1.261
0.04	1.117	1.252	0.0431	1.103	1.216
			0.0538	1.084	1.176

TABLE A.11--Data Used to Construct Figure 14.

Feed Rate (scfm)	Numerical Solution Separation Factor		Feed Rate (scfm)	Analytical (Approximate) Solution Separation Factor	
	L=18 inches	L=36 inches		L=18 inches	L=36 inches
0.005	1.138	1.317	0.0055	1.118	1.249
0.0075	1.117	1.398	0.0086	1.165	1.356
0.010	1.203	1.449	0.0108	1.186	1.407
0.01125	1.213	1.465	0.0135	1.201	1.443
0.0125	1.219	1.476	0.0169	1.207	1.456
0.01375	1.224	1.482	0.0211	1.201	1.443
0.015	1.226	1.485	0.0263	1.186	1.407
0.0175	1.227	--	0.0329	1.165	1.356
0.020	1.224	1.470	0.0412	1.141	1.302
0.030	1.194	1.397	0.0515	1.118	1.249
0.040	1.162	1.327	0.0643	1.097	1.202

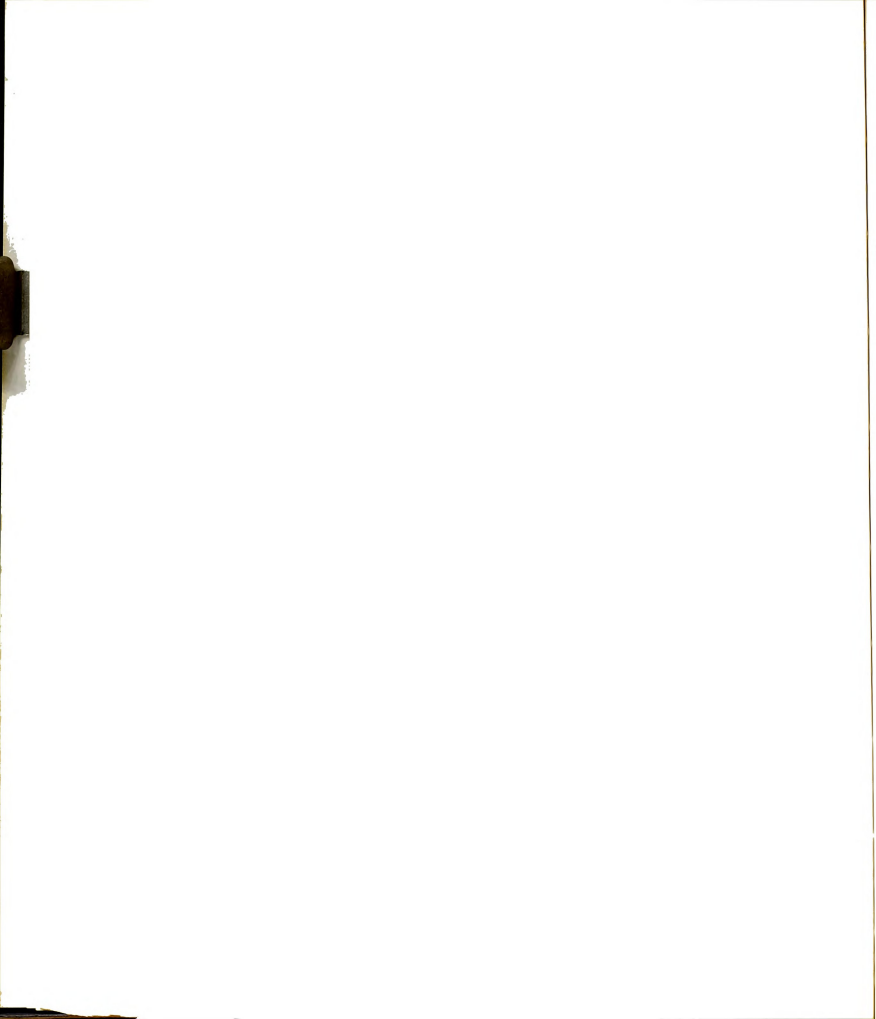


TABLE A-12.--Data Used to Construct Figure 15.

Feed Rate (scfm)	Numerical Solution Separation Factor	Feed Rate (scfm)	Analytical (Approximate) Solution Separation Factor
0.005	1.874	0.0046	1.483
0.0075	2.084	0.0058	1.596
0.010	2.187	0.0072	1.717
0.01125	2.203	0.0090	1.831
0.0125	2.201	0.0113	1.916
0.015	2.159	0.0141	1.947
0.020	2.008	0.0177	1.916
0.030	1.723	0.0221	1.831
0.040	1.541	0.0276	1.717
		0.0345	1.596
		0.0431	1.483
		0.0539	1.387

L. Calculated Data Used to Construct Figure 16: Separation Factor, α , Versus Feed Rate (scfm) for $\text{SO}_2\text{-N}_2$ with Plug Type Flow, $R_w = 4$ Inches, $R_m/R_w = 0.5625$, $\omega = 20000$ RPM, $L = 18$ Inches and Total Reflux

The separation factor used is defined as

$$\alpha = \frac{y_r}{(1 - y_r)} \frac{(1 - y_f)}{y_f},$$

where y_r is the composition at the rich end of the centrifuge. Table A-13 contains data used to construct Figure 16.

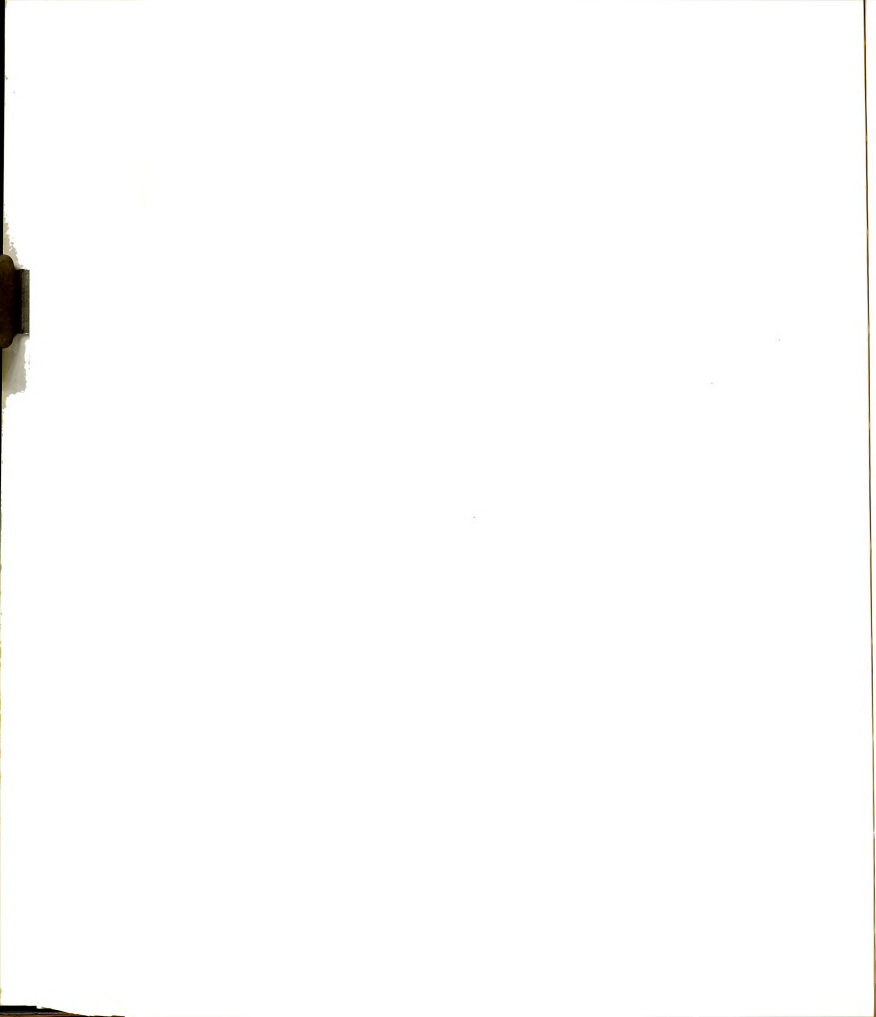


TABLE A-13.--Data Used to Construct Figure 16.

Feed Rate (scfm)	Numerical Solution Separation Factor	Feed Rate (scfm)	Analytical (Approximate) Solution Separation Factor
0.005	1.821	0.0055	1.567
0.0075	2.022	0.0069	1.703
0.010	2.141	0.0086	1.851
0.0125	2.189	0.0108	1.992
0.01375	2.193	0.0135	2.097
0.015	2.187	0.0168	2.136
0.020	2.102	0.0210	2.097
0.030	1.868	0.0263	1.992
0.040	1.683	0.0329	1.851
		0.0411	1.703
		0.0514	1.567
		0.0642	1.451

M. Calculated Data to Construct Figure 17: Assumed Laminar and Plug Flow Velocity Profiles for a Feed Rate of 0.0125 scfm in a Countercurrent Rectifying Centrifuge with $R_m = 2.25$ Inches, $R_w = 4.0$ Inches, $\omega = 10000$ RPM and Total Reflux

The magnitude of the profiles was computed so that the following integral was satisfied:

$$\text{Flow} = \frac{2\pi}{RT} \int_{r_1}^{r_2} P v(r) r dr ,$$

where Flow = the flow rate of the stream in lb-moles/sec,

P = the pressure profile,

$v(r)$ = the velocity profile, and

r_1 and r_2 are the radial boundaries for the flow.

With the top of the centrifuge chosen as the zero axial position the sign of the upward moving inner stream is taken as negative. Table A-14 contains data used to construct Figure 17.

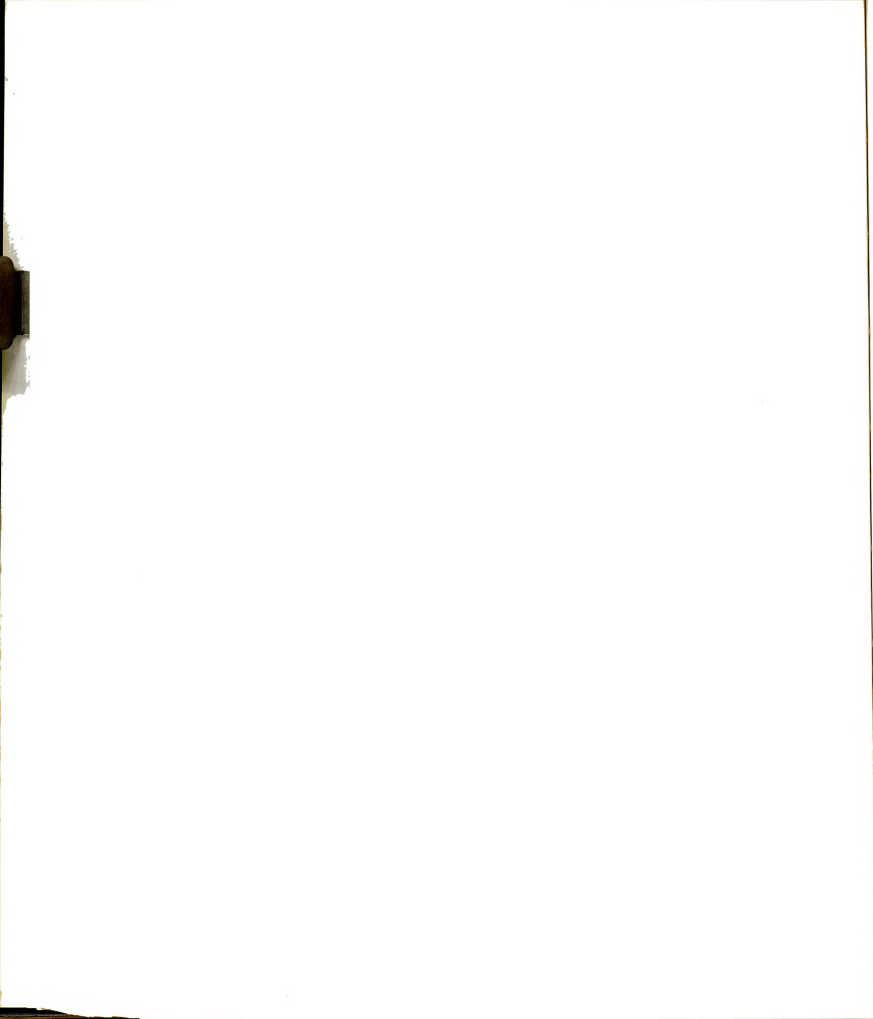


TABLE A-14.--Data Used to Construct Figure 17.

Radius (inches)	Velocities (ft/sec)	
	Laminar Profile $\times 10^2$	Plug Type Profile $\times 10^2$
0.00	-0.404	-0.201
0.321	-0.395	-0.201
0.643	-0.371	-0.201
0.964	-0.329	-0.201
0.286	-0.272	-0.201
1.607	-0.198	-0.201
1.929	-0.107	-0.201
2.25	0.0	0.0
2.50	0.072	0.90
2.75	0.116	0.90
3.00	0.135	0.90
3.25	0.131	0.90
3.50	0.107	0.90
3.75	0.063	0.90
4.00	0.0	0.0

N. Calculated Data Used to Construct Figure 18: Separation
 Factor, α , Versus Feed Rate, scfm, for $\text{SO}_2\text{-H}_2$ with Plug
 Type Flow, $\omega = 10000$ RPM, $R_w = 4$ Inches, $R_m/R_w =$
0.5625, L = 36 Inches and Total Reflux

The separation factor used is defined as

$$\alpha = \frac{y_r}{(1 - y_r)} \cdot \frac{(1 - y_f)}{y_f},$$

where y_r is the composition at the rich end of the centrifuge.

Table A-15 contains the data used to construct Figure 18.

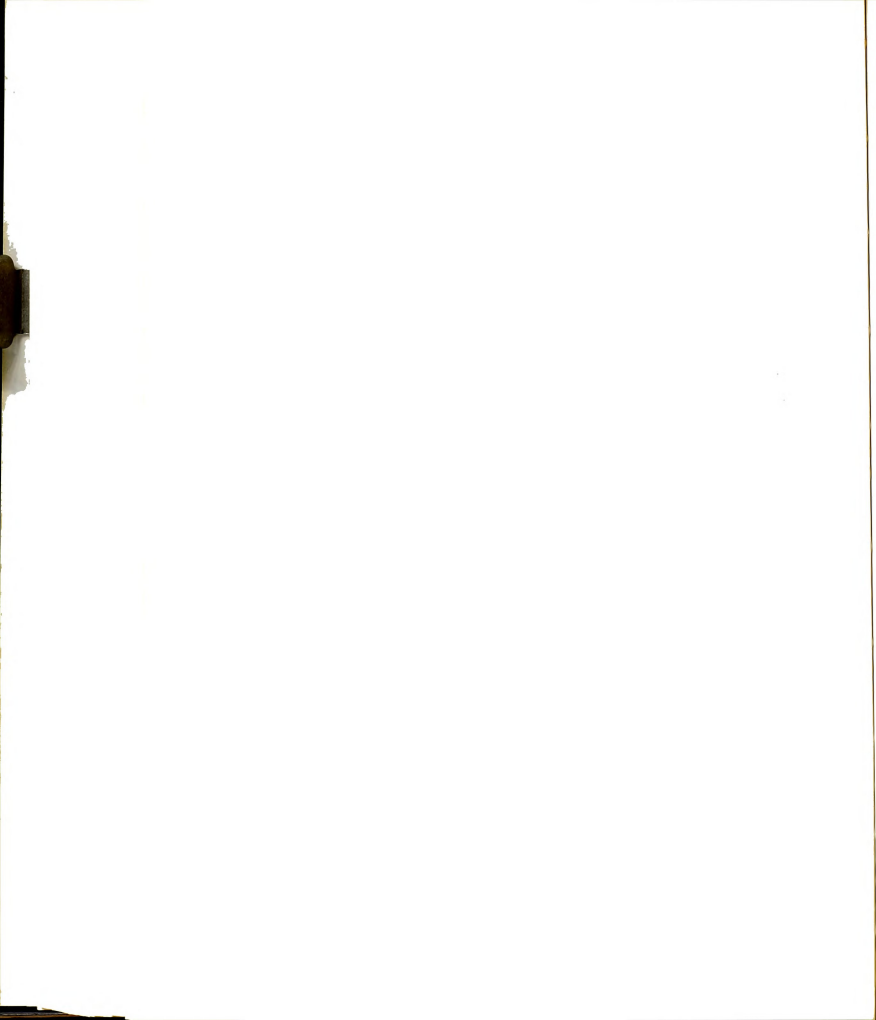


TABLE A-15.--Data Used to Construct Figure 18.

Feed Rate (scfm)	Numerical Solution Separation Factor	Feed Rate (scfm)	Analytical (Approximate) Solution Separation Factor
0.02	1.605	0.022	1.465
0.04	1.863	0.027	1.572
0.05	1.910	0.034	1.688
0.055	1.918	0.042	1.796
0.06	1.919	0.053	1.876
0.065	1.914	0.066	1.906
0.07	1.904	0.083	1.876
0.08	1.874	0.103	1.796
0.10	1.794	0.129	1.688
0.15	1.602	0.162	1.572

0. Calculated Data Used to Construct Figure 19: Separation Factors, α , and Optimum Feed Rates Versus the Ratio of the Radius of the Flow Intersection to the Centrifuge Radius, R_m/R_w , for SO_2-N_2 with Plug Type Flow, $\omega = 10000$ RPM, $R_w = 4$ Inches, $L = 36$ Inches, and Total Reflux

The separation factor used is defined as

$$\alpha = \frac{y_r}{(1 - y_r)} \frac{(1 - y_f)}{y_f},$$

where y_r is the composition at the rich end of the centrifuge. Table

A-16 contains the data used to construct Figure 19.

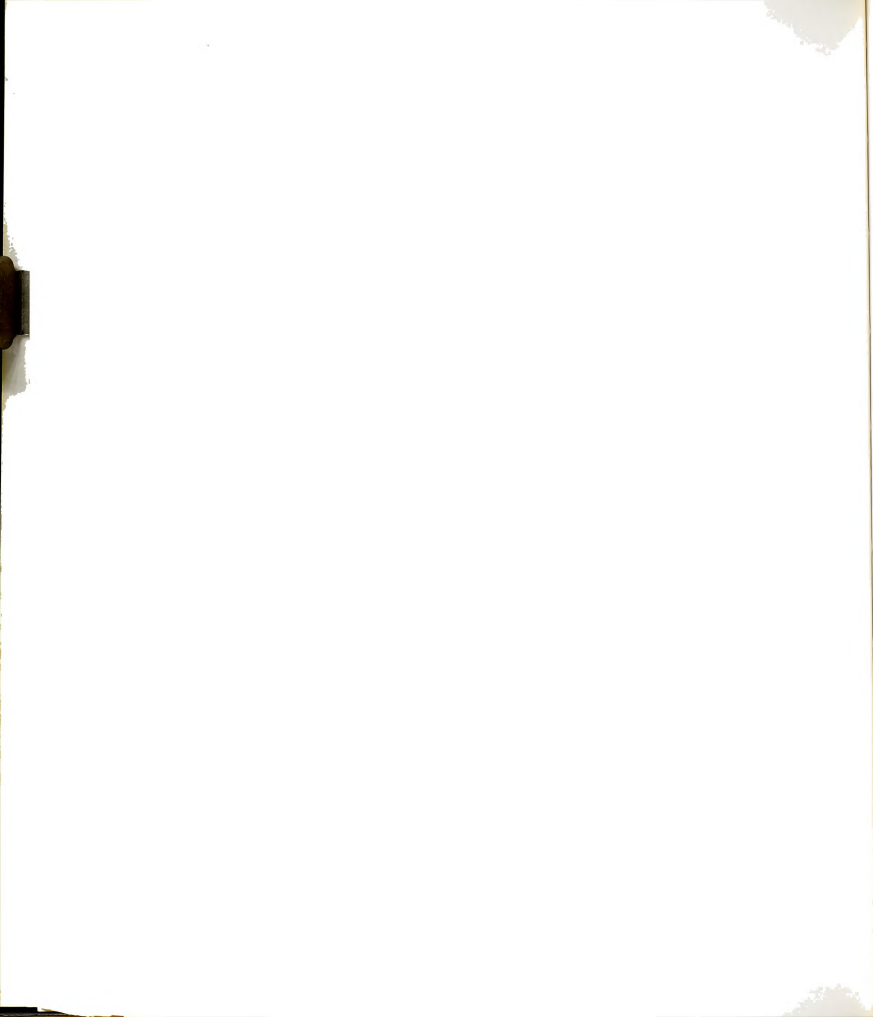


TABLE A-16.--Data Used to Construct Figure 19.

R_m/R_w	Separation Factor at a Feed Rate of 0.02 scfm	Separation Factor at the Optimum Feed Rate	Optimum Feed Rate (scfm)
0.125	1.173	1.232	0.0093
0.25	1.254	1.298	0.0116
0.375	1.333	1.361	0.0138
0.500	1.411	1.424	0.0159
0.5625	1.448	1.456	0.0169
0.625	1.485	1.489	0.0179
0.750	1.556	1.556	0.0200
0.875	1.622	1.626	0.0220

P. Calculated Data Used to Construct Figure 20: Maximum Separation Factors Versus Centrifuge Rotational Speed for the Gas Pair SO₂-N₂ at 70°F and 300°F. $R_w = 4$ Inches, $L = 36$ Inches, $R_m/R_w = 0.5625$, Plug Type Flow and Total Reflux

The separation factor used is defined as

$$\alpha = \frac{y_r}{(1 - y_r)} \frac{(1 - y_f)}{y_f},$$

where y_r is the composition at the rich end of the centrifuge. Table A-17 contains the data used to construct Figure 20.

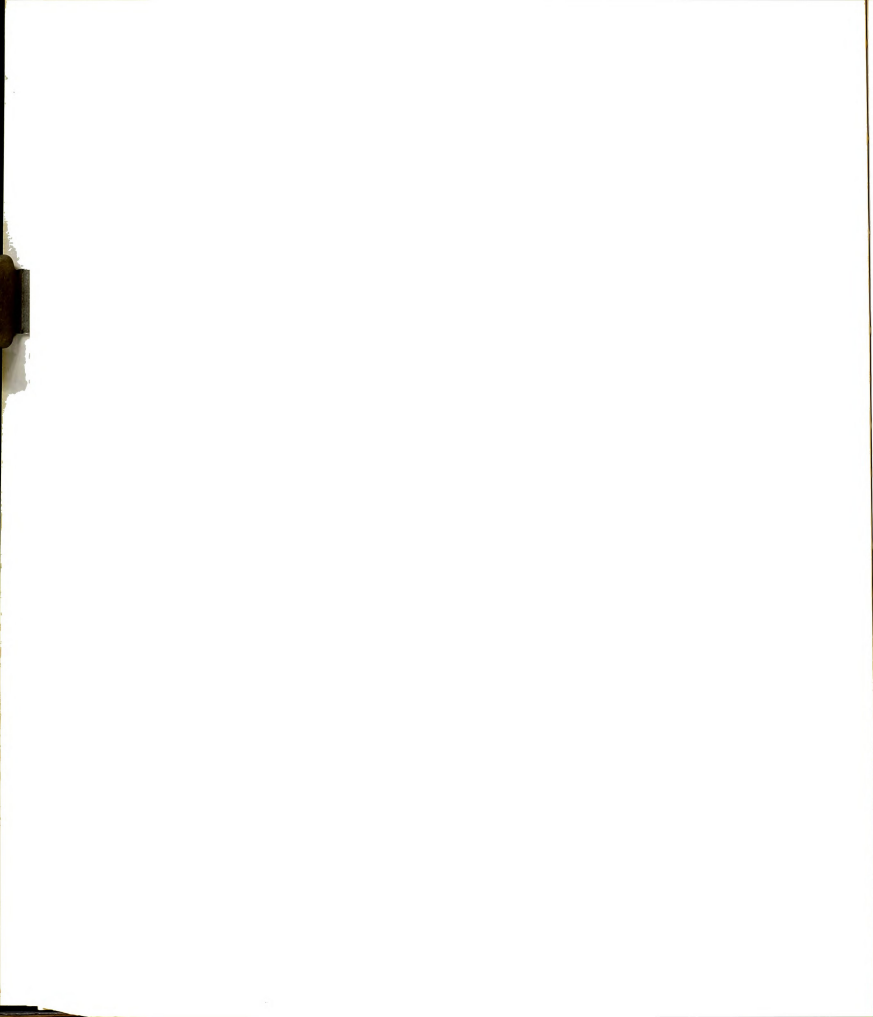


TABLE A-17.--Data Used to Construct Figure 20.

ω , RPM	Temperature = 70°F	Temperature = 300°F
	Maximum Separation Factor	Maximum Separation Factor
10000	1.456	1.299
12000	1.719	1.458
14000	2.093	1.672
16000	2.629	1.959
18000	3.409	2.345
20000	4.562	2.870

Q. Calculated Data Used to Construct Figure 21: Separation Factors Based on the Rich and Lean Streams Versus Feed Rate for Various Ratios of the Rich Stream to the Feed Stream for the Gas Pair $\text{SO}_2\text{-N}_2$. $\omega = 15000$ RPM, $R_w = 4$ Inches, $L = 36$ Inches, $R_m/R_w = 0.5625$, and Plug Type Flow

The separation factor used is defined as

$$\alpha = \frac{y_r}{(1 - y_r)} \cdot \frac{(1 - y_l)}{y_l},$$

where y_r is the rich stream composition and y_l is the lean stream composition. Table A-18 contains the data used to construct Figure 21.

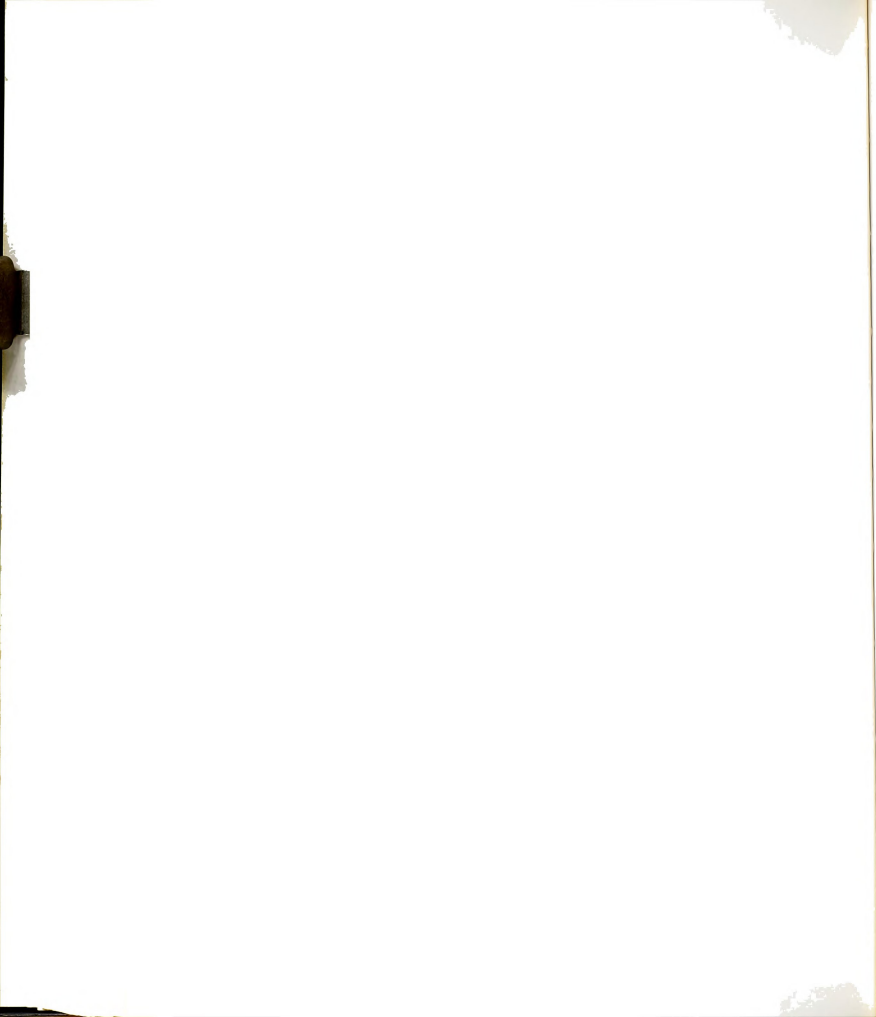
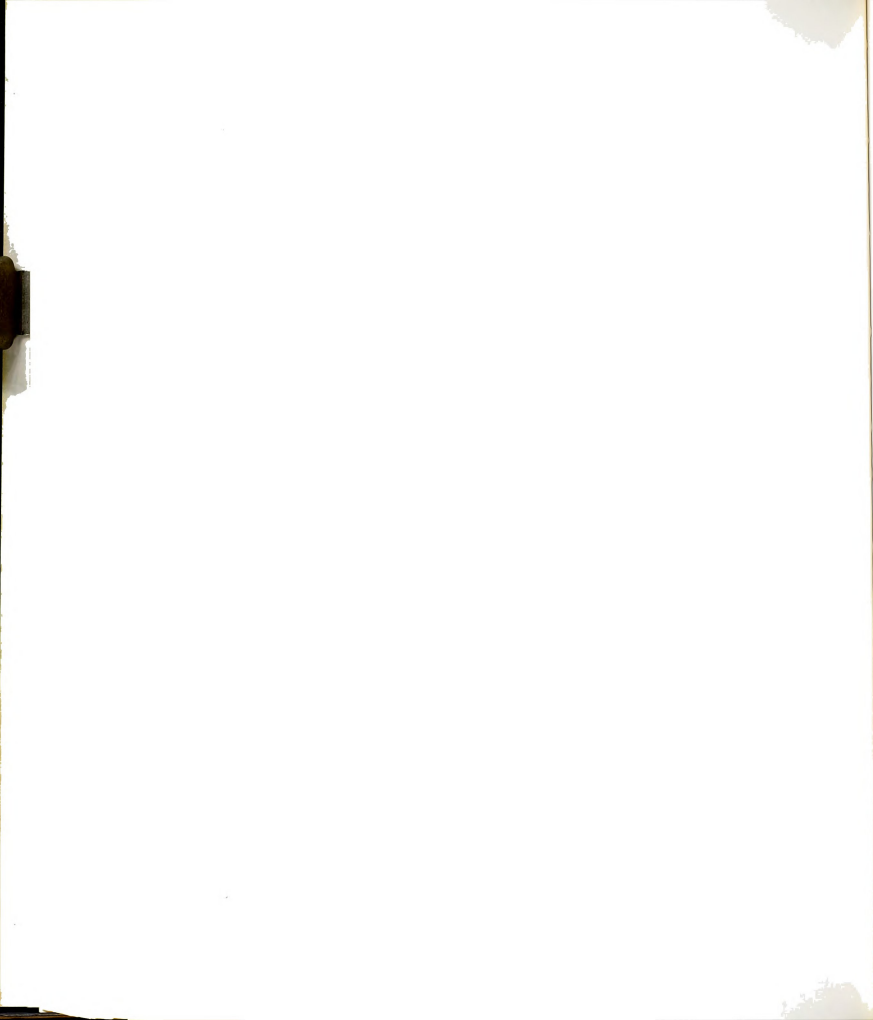


TABLE A-18.--Data Used to Construct Figure 21.

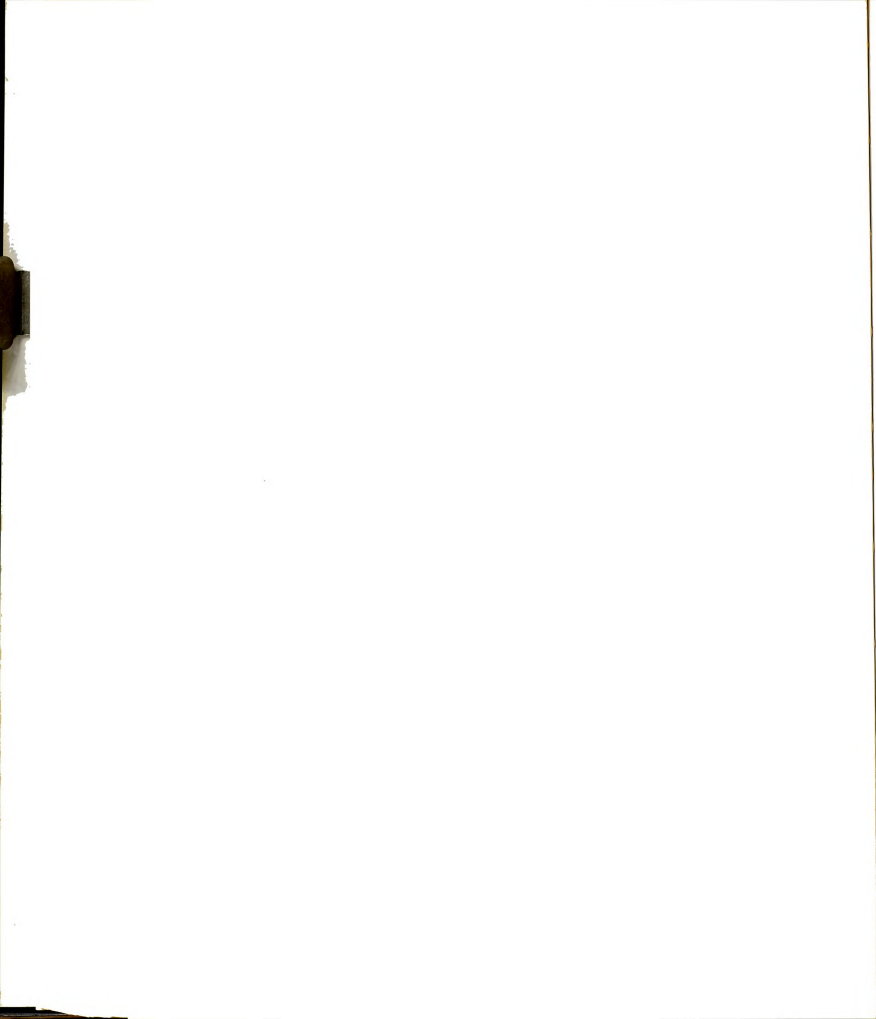
Feed Rate/ Optimum Feed Rate	Separation Factors			
	R/F = 0.0	R/F = 0.05	R/F = 0.10	R/F = 0.20
0.1678	1.319	1.300	1.281	1.234
0.2097	1.406	1.374	1.340	1.269
0.2621	1.517	1.461	1.406	1.304
0.3277	1.652	1.560	1.476	1.335
0.4096	1.814	1.667	1.545	1.360
0.5120	1.991	1.772	1.607	1.379
0.6400	2.161	1.863	1.655	1.391
0.8000	2.289	1.925	1.686	1.398
1.0000	2.337	1.947	1.696	1.400
1.2500	2.289	1.925	1.686	1.398
1.5625	2.161	1.863	1.655	1.391
1.9531	1.991	1.772	1.607	1.379
2.4414	1.814	1.667	1.545	1.360
3.0518	1.652	1.560	1.476	1.335
3.8147	1.517	1.461	1.406	1.304
4.7648	1.406	1.374	1.340	1.269
5.9605	1.319	1.300	1.281	1.234



APPENDIX B

DIFFUSIVITIES FOR THE GAS PAIRS $\text{SO}_2\text{-N}_2$,

$\text{SO}_2\text{-H}_2$ AND UF_6 (235, 238 ISOTOPES)



APPENDIX B

DIFFUSIVITIES FOR THE GAS PAIRS $\text{SO}_2\text{-N}_2$, $\text{SO}_2\text{-H}_2$ AND UF_6 (235, 238 ISOTOPES)

The diffusivities for the gas pairs $\text{SO}_2\text{-N}_2$ and $\text{SO}_2\text{-H}_2$ were computed by using the Wilke and Lee (17) modification of the equation by Hirschfelder, Bird and Spotz (11). The equation used was

$$D = \frac{BT^{1.5} \sqrt{1/MW_1 + 1/MW_2}}{P r_{12}^2 I_D},$$

where D = gas diffusivity, cm^2/sec ,

$$B = (10.7 - 2.46 \sqrt{1/MW_1 + 1/MW_2}) \times 10^{-4},$$

T = temperature, $^{\circ}\text{K}$,

MW_1, MW_2 = molecular weights,

P = absolute pressure, atm,

$$r_{12} = \frac{(r_o)_1 + (r_o)_2}{2} = \text{collision diameter, angstroms,}$$

I_D = collision integral a function of kT/ϵ_{12} , and

$$\epsilon_{12}/k = \sqrt{\left(\frac{\epsilon_1}{k}\right) \left(\frac{\epsilon_2}{k}\right)} = \text{force constant, } ^{\circ}\text{K}.$$

Values of the individual force constants and collision diameters were taken from a table prepared by Wilke and Lee (17). The collision integral was evaluated by using a table prepared by Hirschfelder, Bird and Spotz (11).

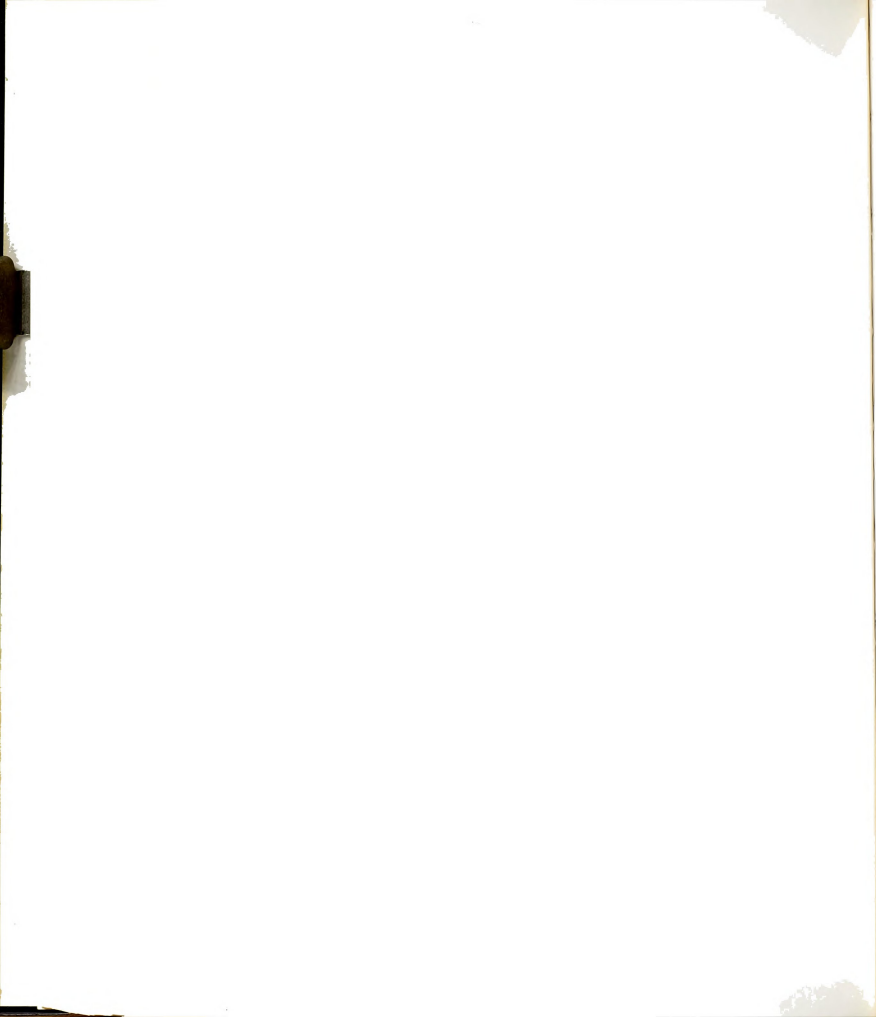
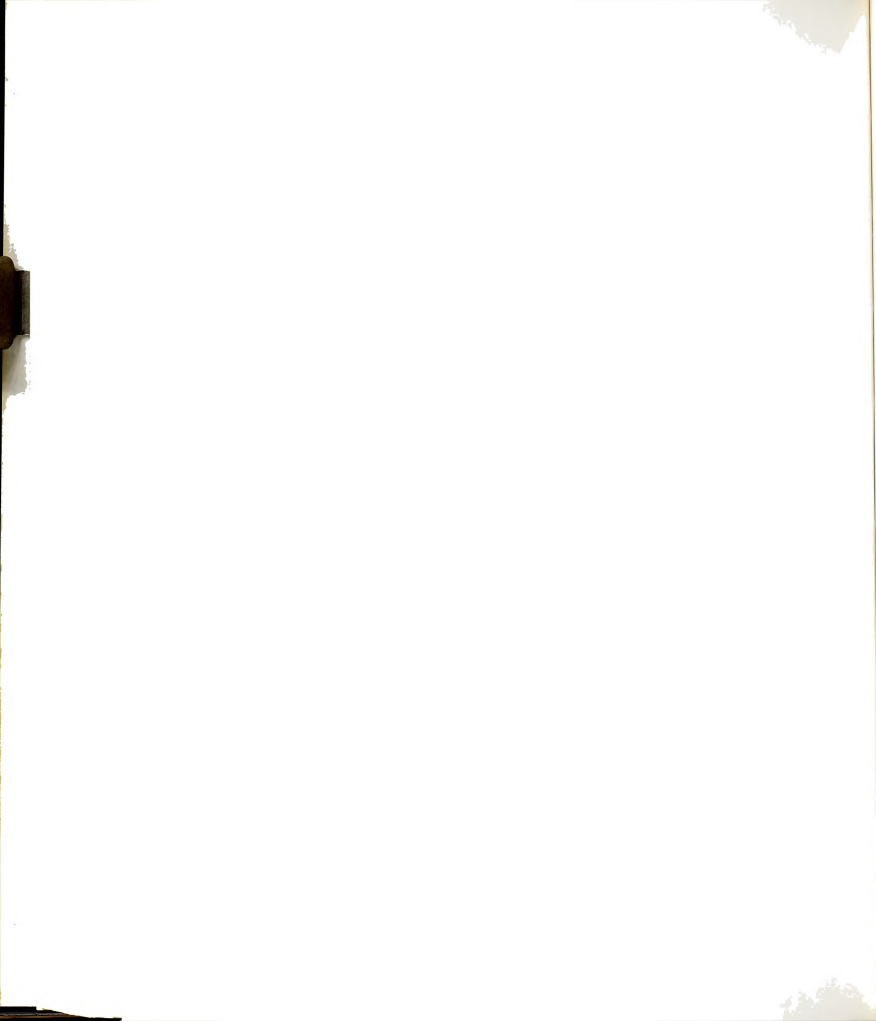


Table B-1 contains all the parameters along with intermediate values used in the calculations. All units are defined above.

The value used for the self diffusion of UF_6 was taken from Benedict and Pigford, Nuclear Chemical Engineering (16). At 80°F , D_p is given as 6.6×10^{-7} g-mole/cm²/sec. Using the ideal gas law and a pressure of 1/7 atm gives $D = .1135 \text{ cm}^2/\text{sec}$.

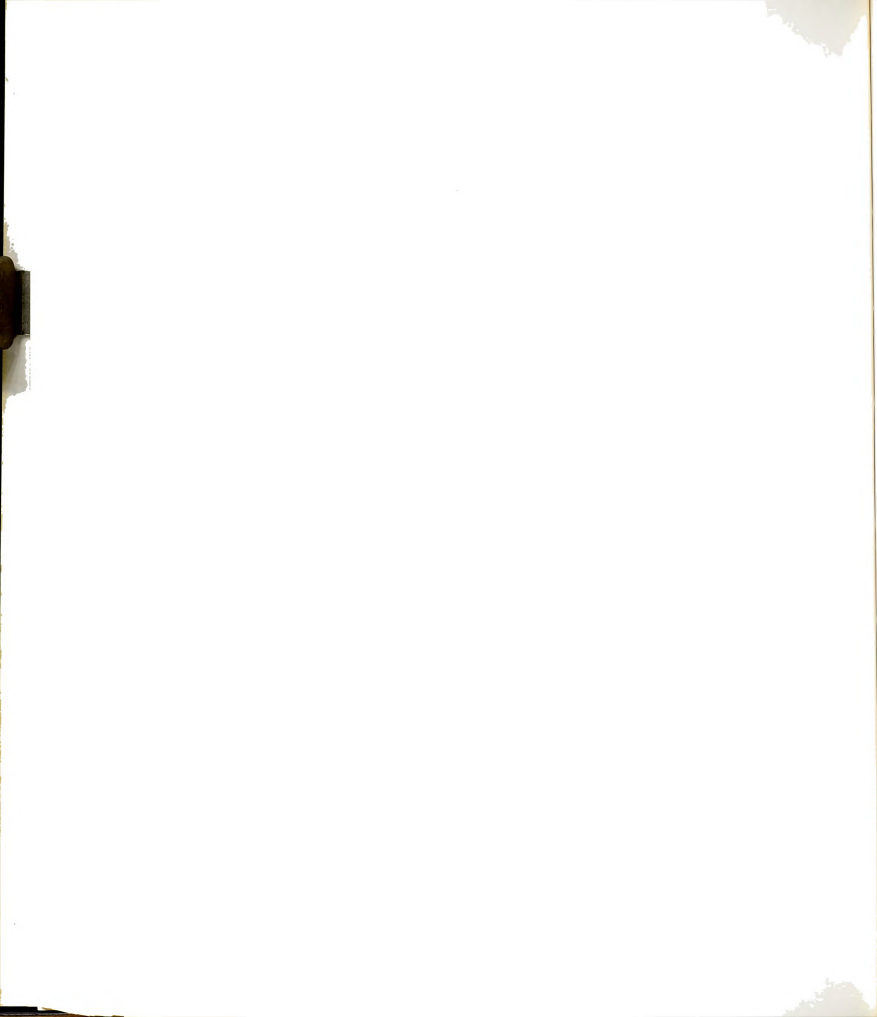
TABLE B-1.--Calculation of the Diffusivities of the Gas Pairs $\text{SO}_2\text{-N}_2$ and $\text{SO}_2\text{-H}_2$.

Parameter	$\text{SO}_2\text{-N}_2$	$\text{SO}_2\text{-H}_2$
temperature	294.4, 422.2	294.4, 422.2
MW_1, MW_2	64, 28	64, 2
$\sqrt{1/MW_1 + 1/MW_2}$	0.2266	0.71807
B	10.1426×10^{-4}	8.9335×10^{-4}
$(r_o)_1, (r_o)_2$	4.290, 3.681	4.290, 2.968
r_{12}	3.986	3.629
$\epsilon_1/k, \epsilon_2/k$	252, 91.5	252, 33.3
kT/ϵ_{12}	1.9391, 2.7806	3.2143, 4.6091
I_D	0.5433, 0.4846	0.4659, 0.4282
P	1	1
D	0.1346, 0.2590	0.5282, 0.9869



APPENDIX C

NUMERICAL METHOD AND FORTRAN PROGRAM
USED TO ANALYZE THE UNSTEADY
STATE SIMPLE CENTRIFUGE



APPENDIX C

NUMERICAL METHOD AND FORTRAN PROGRAM USED TO ANALYZE THE UNSTEADY STATE SIMPLE CENTRIFUGE

As established in Chapter III-B, the following three equations define the unsteady state simple centrifuge.

A. The Equation of Continuity for Species 1:

$$P \frac{\partial y}{\partial t} + y \frac{\partial P}{\partial t} + D_{12}P \left(2A y(1-y) + [Ar(1-2y) - \frac{1}{r}] \frac{\partial y}{\partial r} - \frac{\partial^2 y}{\partial r^2} \right) = 0,$$

where $\frac{\partial y}{\partial r} = 0$ at $r = 0$ and $\frac{\partial y}{\partial r} = A(1-y) y r$ at $r = R_w$.

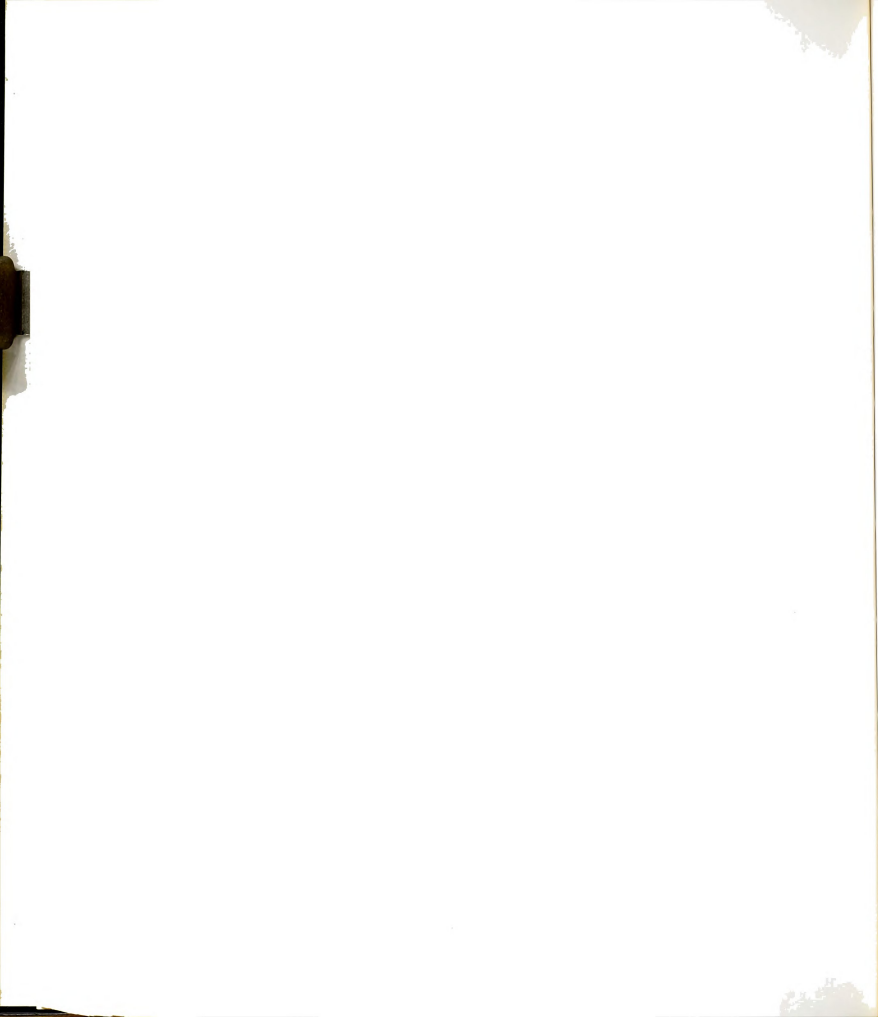
In Appendix A, Section A, it was determined that the units on A were ft^{-2} . This allows a quick units check to be made on the above equation as follows:

$$P \frac{\partial y}{\partial t} \text{ and } y \frac{\partial P}{\partial t}; \frac{\text{lb}_f}{\text{in}^2} \frac{1}{\text{sec}},$$

$$2A y(1-y); \frac{1}{\text{ft}^2},$$

$$[Ar(1-2y) - 1/r] \frac{\partial y}{\partial r}; \frac{1}{\text{ft}^2},$$

$$\frac{\partial^2 y}{\partial r^2}; \frac{1}{\text{ft}^2} \text{ and by using the fact that } D_{12}P \text{ has units } \text{ft}^2/\text{sec} \cdot \text{lb}_f/\text{in}^2 \text{ completes the check.}$$



B. The Total Pressure Equation:

$$\frac{\partial P}{\partial r} = \frac{P\omega^2}{RTg_c} (\Delta MW_y + MW_2) r,$$

where $P = P(0)$ at $r = 0$.

The units for this equation were checked in Appendix A, Section 1.

C. The Conservation of Moles Equation:

$$B/L = \frac{2\pi P(0)}{RT} \int_0^R r^w Pr dr,$$

where B/L are the moles/ft charged. The units of the left and right sides of this equation can easily be seen to be equal.

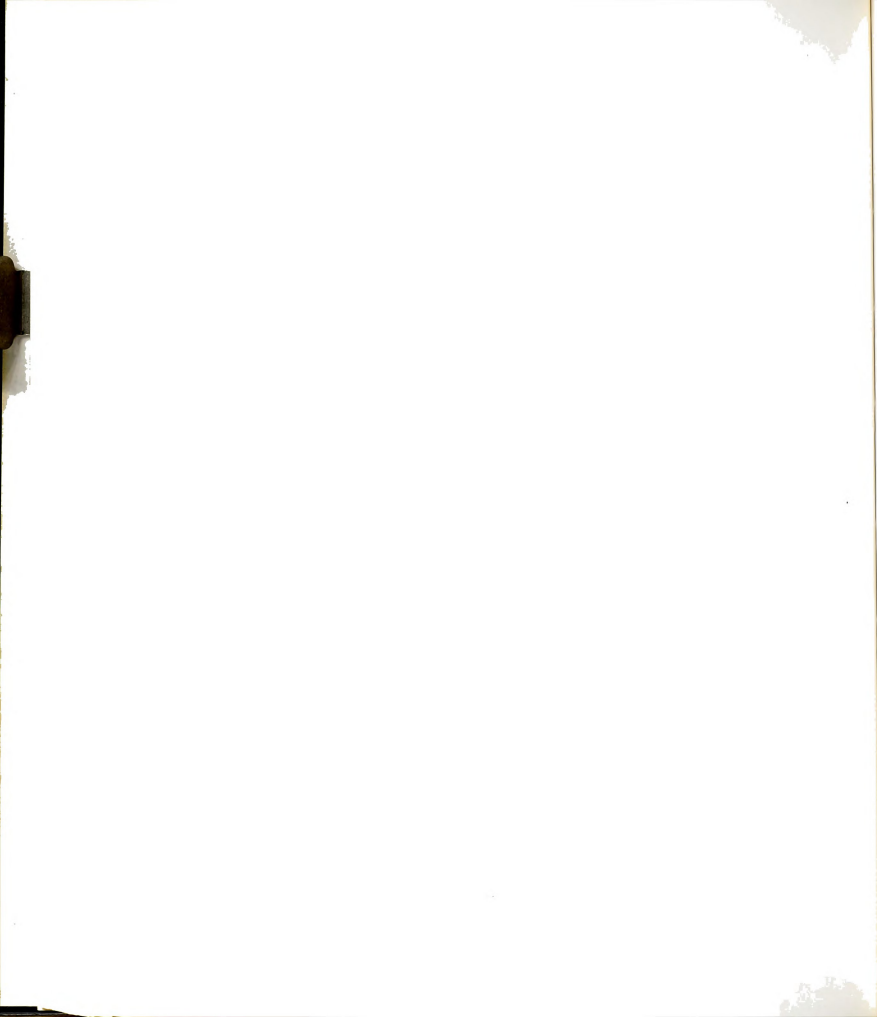
The initial value of y was given as the composition of the charge, y_f . This allowed the initial pressure profile to be computed analytically as

$$P(r)/P(0) = \exp(A r^2/2),$$

$$\text{where } P(0) = \frac{B/L}{\frac{2\pi}{RT} A \left[\exp\left(\frac{A R_w^2}{2}\right) - 1 \right]}, \text{ and}$$

$$A = \frac{\omega^2}{RT g_c} (\Delta MW y_f + MW_2).$$

With the values of y and P initialized at time zero, future values were computed using an implicit numerical approach. That is, all partial derivatives were approximated at the next increment in time which



resulted in a set of simultaneous equations which were then solved using the scientific subroutine ONEDIAG.

Table C-1 contains a collection of the finite difference approximations used for the various partial derivatives. The subscripts used are all referenced to the point about which the expansions are made, 1. From Table C-1, for example, the approximation used for the boundary condition $\partial y / \partial r = 0$ at the axis (subscript 1) is

$$\left[\frac{-y(0)}{4} - \frac{10}{12} y(1) + 1.5 y(2) - \frac{y(3)}{2} + \frac{y(4)}{12} \right] / Dr = 0 ,$$

where the use of the fictitious point $y(0)$ assumes the continuity of the function through the axis (method of images). For the approximation of the partial derivative $\partial y / \partial t$, four time grid points were used, giving the following formula (see Table C-1):

$$\frac{\partial y}{\partial t} = \left[\frac{22}{12} y(j) - 3y(j-1) + 1.5 y(j-2) - \frac{y(j-3)}{3} \right] / Dt .$$

Due to the nonlinear nature of the partial differential equations the values of y and P had to be estimated at the next position in time. This was accomplished by using the first term of Taylor's series, i.e.,

$$y(j+1) = y(j) + \frac{\Delta t \partial y(j)}{\partial t} , \text{ and}$$

$$P(j+1) = P(j) + \frac{\Delta t \partial P(j)}{\partial t} ,$$

where $\frac{\partial y(j)}{\partial t}$ was replaced by

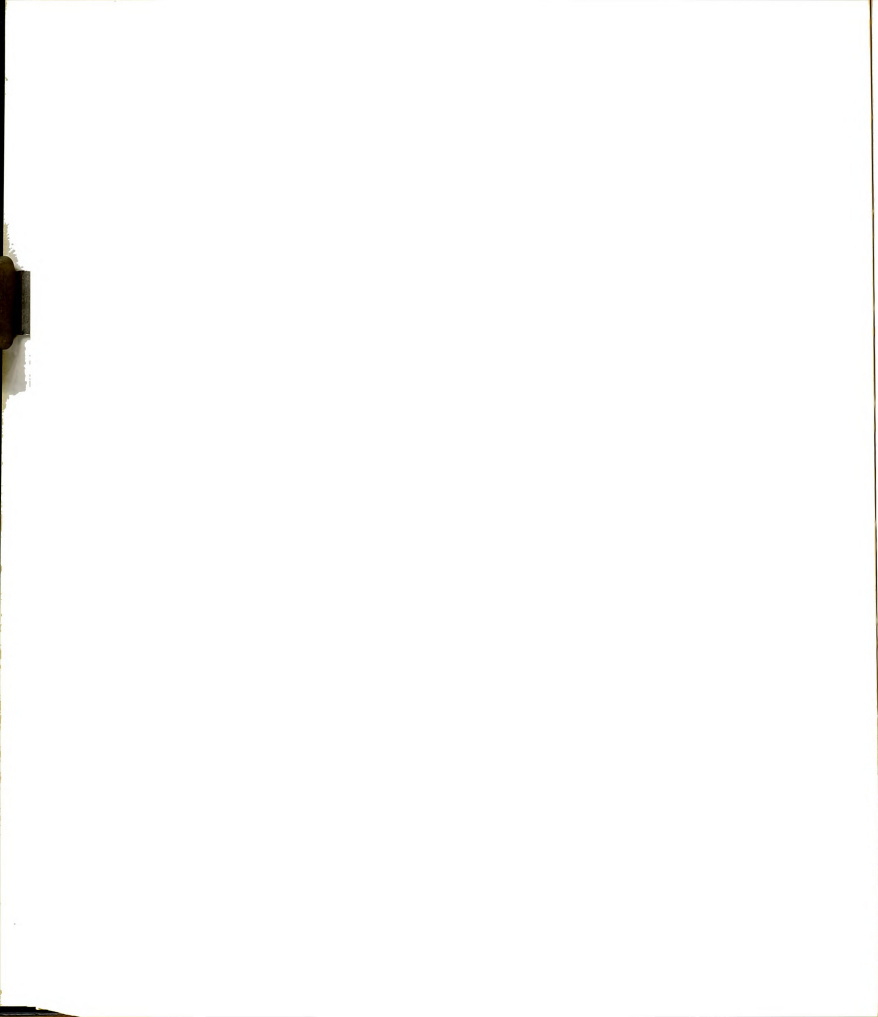
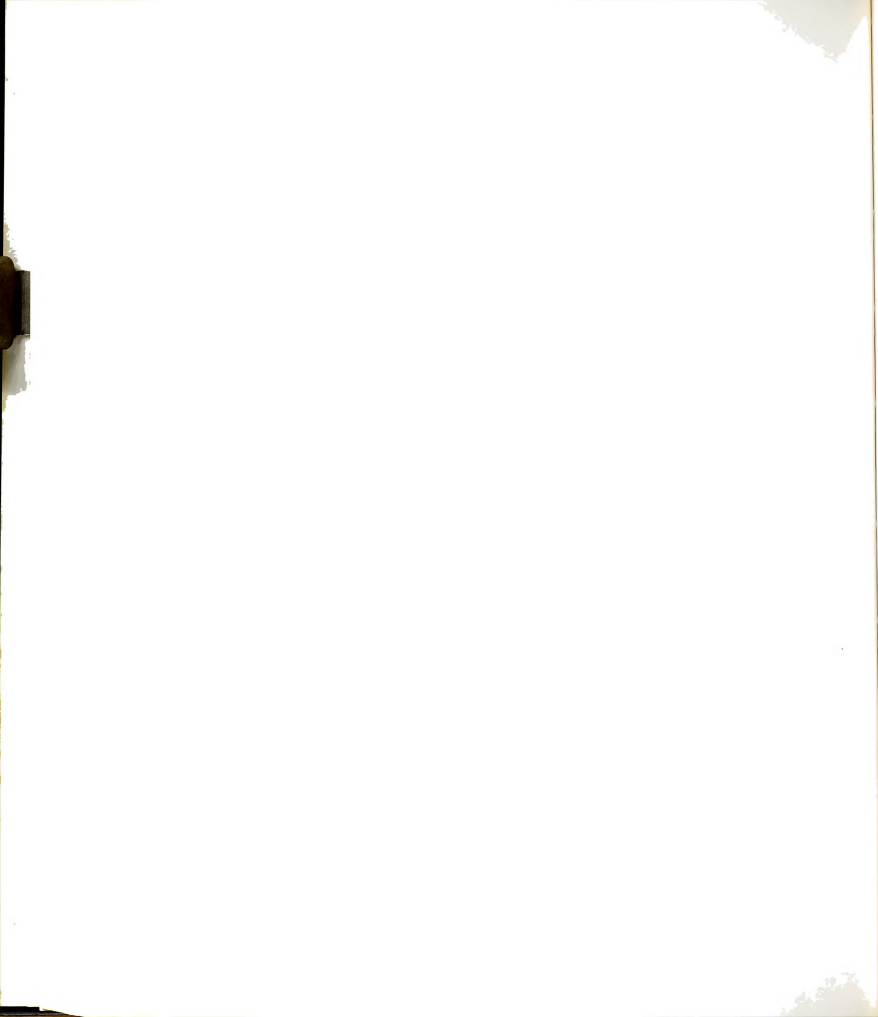


TABLE C-1.--Finite Difference Approximations Used for the Various Partial Derivatives.

Points Ahead and Behind Central Point	Increment Size = Δx	
	Derivative	Formula
0 points ahead 3 points behind	first	$\left[\frac{22}{12} u(1) - 3u(1-1) + 1.5 u(1-2) - \frac{u(1-3)}{3}\right]/\Delta x$
	first	$\left[-\frac{u(1-1)}{4} - \frac{10}{12} u(1) + 1.5 u(1+1) - \frac{u(1+2)}{2} + \frac{u(1+3)}{12}\right]/\Delta x$
3 points ahead 1 point behind	second	$\left[\frac{11}{12} u(1-1) - \frac{5}{3} u(1) + \frac{u(1+1)}{2} + \frac{u(1+2)}{3} - \frac{u(1+3)}{12}\right]/\Delta x^2$
	first	$\left[-\frac{u(1+1)}{4} + \frac{10}{12} u(1) - 1.5 u(1-1) + \frac{u(1-2)}{2} - \frac{u(1-3)}{12}\right]/\Delta x$
1 point ahead 3 points behind	second	$\left[\frac{11}{12} u(1+1) - \frac{5}{3} u(1) + \frac{u(1-1)}{2} + \frac{u(1-2)}{3} - \frac{u(1-3)}{12}\right]/\Delta x^2$
	first	$\left[\frac{u(1-2)}{12} - \frac{2}{3} u(1-1) + \frac{2}{3} u(1+1) - \frac{u(1+2)}{12}\right]/\Delta x$
2 points ahead 2 points behind	second	$\left[-\frac{u(1-2)}{12} + \frac{4}{3} u(1-1) - 2.5 u(1) + \frac{4}{3} u(1+1) - \frac{u(1+2)}{12}\right]/\Delta x^2$



$$[1/3 \ y(J+1) + \frac{y(J)}{2} - y(J-1) + \frac{y(J-2)}{6}]/Dt ,$$

and $\frac{\partial P(J)}{\partial t}$ by a similar expression.

The resulting expressions for the estimation of $Y(J+1)$ and $P(J+1)$ are

$$Y(J+1) = 2.25 \ Y(J) - 1.5 \ Y(J-1) + .25 \ Y(J-2)$$

and

$$P(J+1) = 2.25 \ P(J) - 1.5 \ P(J-1) + .25 \ P(J-2).$$

With these estimations the values of y and P could be computed from the approximations of the partial differential equations. Using these newly computed values of y and P as the estimates the calculations were repeated giving values of y and P varying only slightly from the estimates. Thus, only two iterations at each point in time were required to compensate for the nonlinearity.

To solve the unsteady state problem a general FORTRAN program, USTEADY, was written and executed on a Control Data Corporation 6500 Digital Computer. The general program USTEADY was aided in the solution of the above mentioned simultaneous equations by the scientific subroutine ONEDIAG. No other subprograms were required. The general program USTEADY along with ONEDIAG can be used to analyze any gas pair in any size centrifuge rotating at any speed. Table C-2 contains a list of the data that is required by USTEADY.

At the end of this appendix is a complete list of the program USTEADY and the subprogram ONEDIAG. The listings contain many comment cards which reiterate and in some cases further detail the information given above.

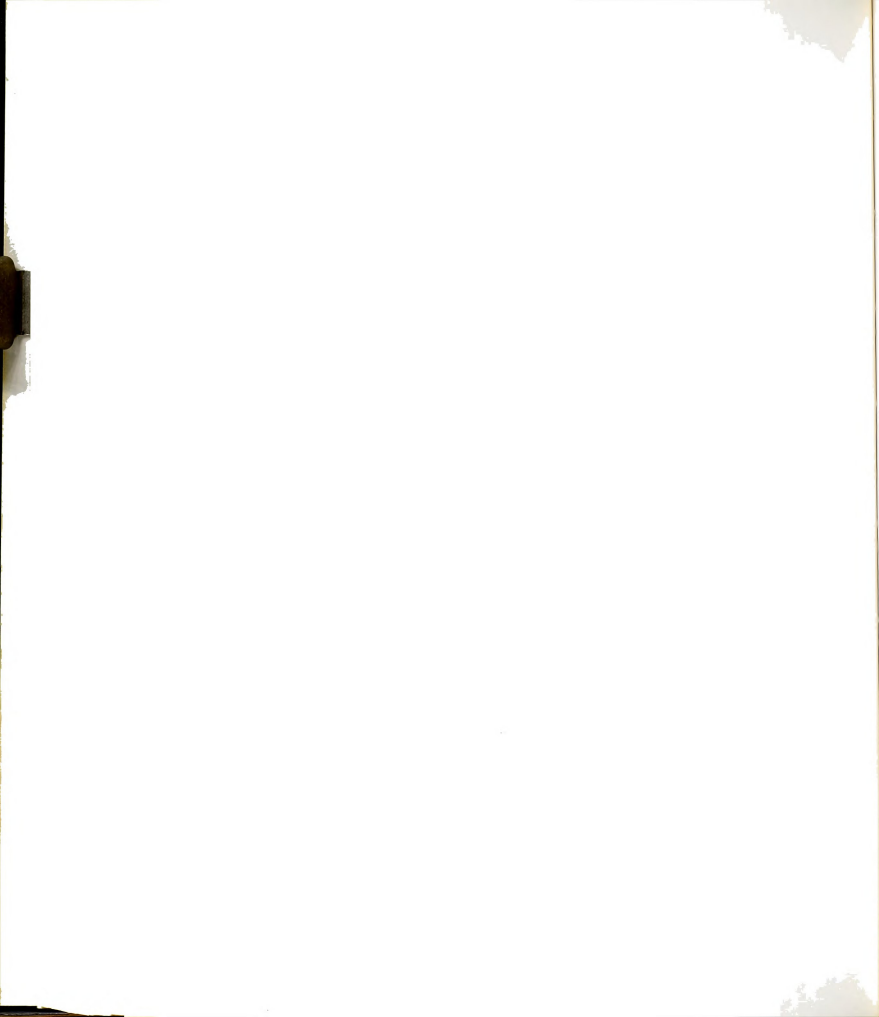
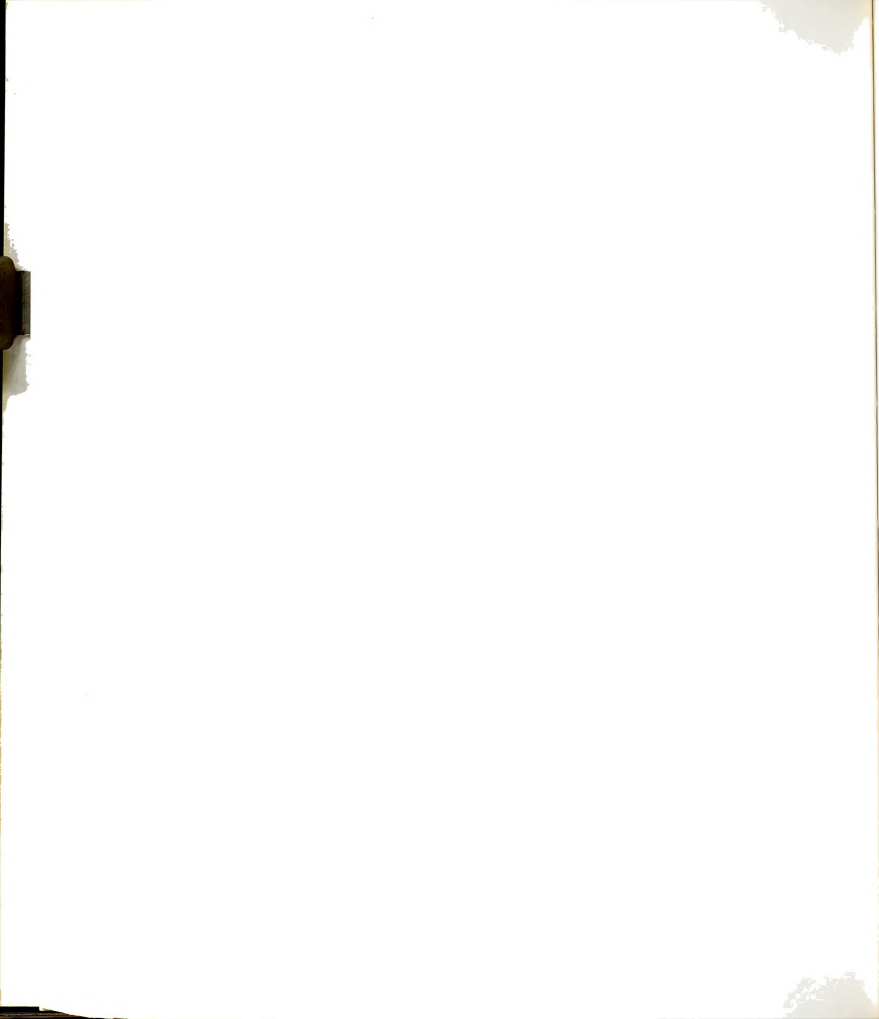
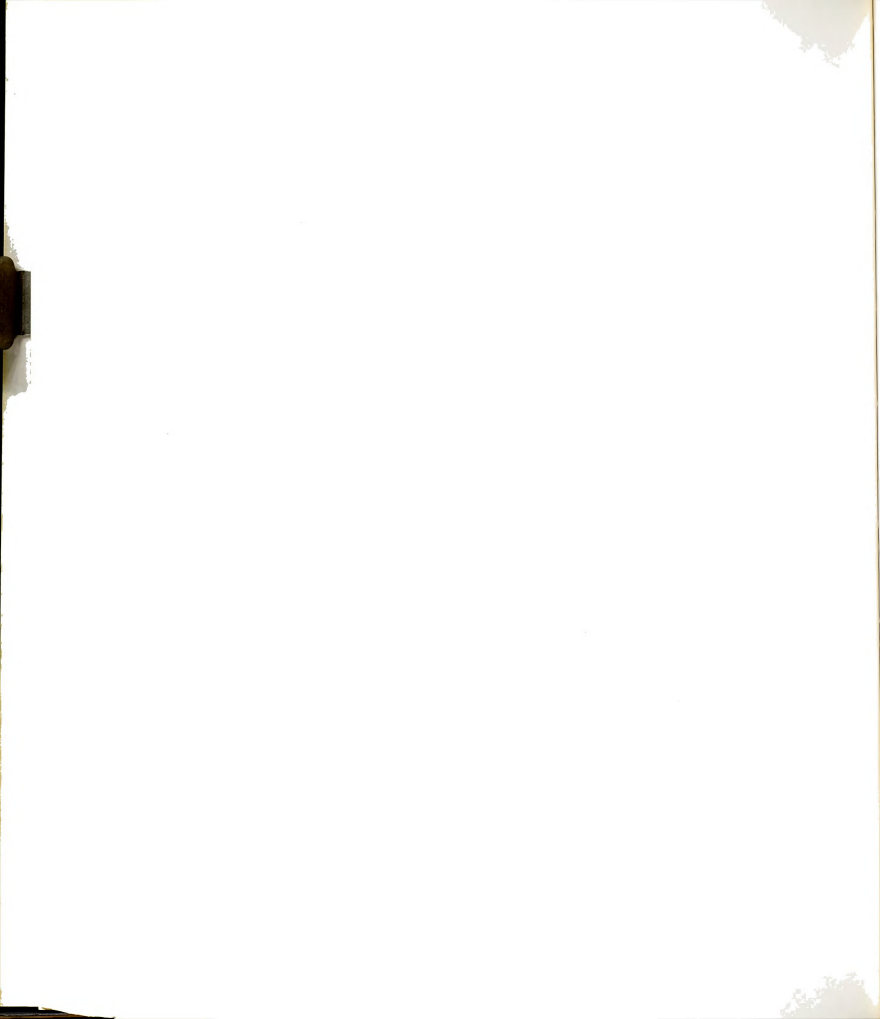


TABLE C-2.--Data Required by the Fortran Program USTEADY.

Parameter	Description	Units	Formating
TIME	Time period over which calculations will be carried out	Hours	
NT	Total time increments into which TIME will be divided	None	
IPRINT	Number of time increments between output	None	
(This completes the first data card.)			F10.0, 215
T	Absolute temperature	°F	
P0	Charge pressure	psia	
RPM	Centrifuge rev. per minute	rev/min	
RW	Centrifuge radius	inches	
N	Radial increments	None	
(This completes the first data card.)			4F10.0, 215
WM1	Molecular weight species 1	lb _m /lb-mole	
WM2	Molecular weight species 2	lb _m /lb-mole	
YF	Molecular weight species 1	None	
DP	Diffusivity times absolute pressure	$\frac{ft^2}{sec}$ psia	
(This completes the third and final data card.)			3F10.0, F20.0



In the analysis of the gas pairs, $\text{SO}_2\text{-N}_2$, $\text{SO}_2\text{-H}_2$ and UF_6 (235 , 238 isotopes) in a simple centrifuge with a radius of 4 inches, it was found that using twenty radial increments was sufficient. This number of radial increments was coupled with time increments chosen such that $D_{12}^P \Delta T \approx 0.5 \text{ lb}_f$. Any further increase in the number of radial and/or time increments gave essentially no change in the solutions.



```

PROGRAM USTEADY( INPUT, OUTPUT )
DIMENSION R(21), Y(4,21), P(4,21), C(23,8), ANS(23,1), DPDI(21)
DIMENSION VE(21)
DATA PIE, GC, RGAS/ 3.141592654, 32.174, 10.731469 /
DATA MD, KD / 23, 8 /

```

```

..... THIS PROGRAM COMPUTES THE UNSTEADY STATE MOLE FRACTION

```

```

AND PRESSURE PROFILES FOR THE SIMPLE CENTRIFUGE. THE
PROGRAM REQUIRES THE AID OF THE SCIENTIFIC
SUBROUTINE ONEGDIQ TO SOLVE THE SIMULTANEOUS EQUATIONS
ENCOUNTERED IN THE COURSE OF THE SOLUTION .....

```

```

..... INPUT DATA TO USED IN THIS CALCULATION .....

```

```

READ 5, TIME, NT, IPRINT
5 FORMAT( F10.0, 2I5 )
READ 10, I, PO, RPM, RW, N
10 FORMAT( 4F10.0, 2I5 )
READ 15, WM1, WM2, YF, DP
15 FORMAT( 3F10.0, F20.0 )

```

```

..... INITIALIZE CONSTANTS .....

```

```

DR = RW/12.0 / FLOAT( N ) $ DRDR = 1.0/DR/DR
DT = TIME/FLOAT(NT) $ RADPSEC = RPM * PIE / 30.0
DPH = 3600.0 * DP
A = (WM1-WM2) * RADPSEC/RADPSEC / RGAS / T / GC / 144.0
AA = A / (WM1-WM2) * WM2 $ NPI = N + 1

```

```

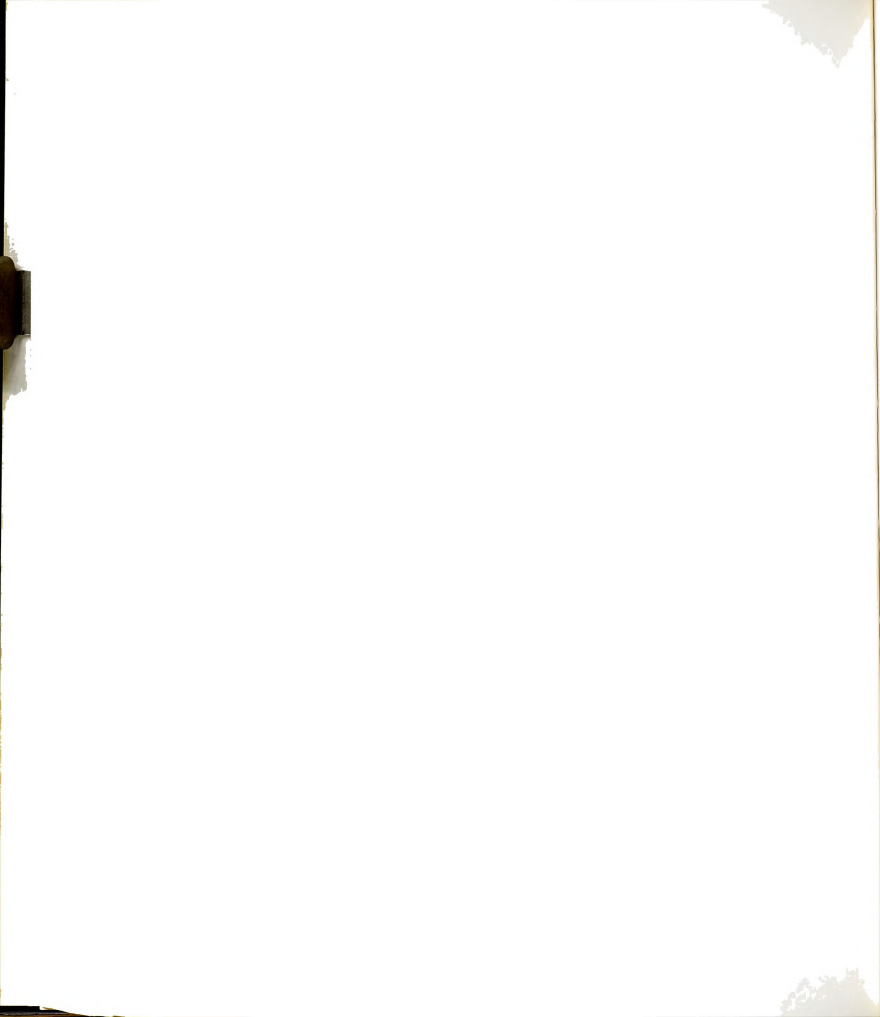
..... OUTPUT INFORMATION ABOUT THE CALCULATION .....

```

```

PRINT 8000, RW, N, DR, TIME, NT, DT
8000 FORMAT( '1$, //, 47X, *UNSTEADY STATE SIMPLE CENTRIFUGE ANALYSIS*
1, ///, 20X, *A, CENTRIFUGE RADIUS =*, F10.4, * INCHES*, //,
2 20X, *B, RADIAL INCREMENTS =*, I5, * GIVING DR =*, E15.6,
3 * FT*, //, 20X, *C, CALCULATION TIME LIMIT =*, F10.4, * HOURS*,

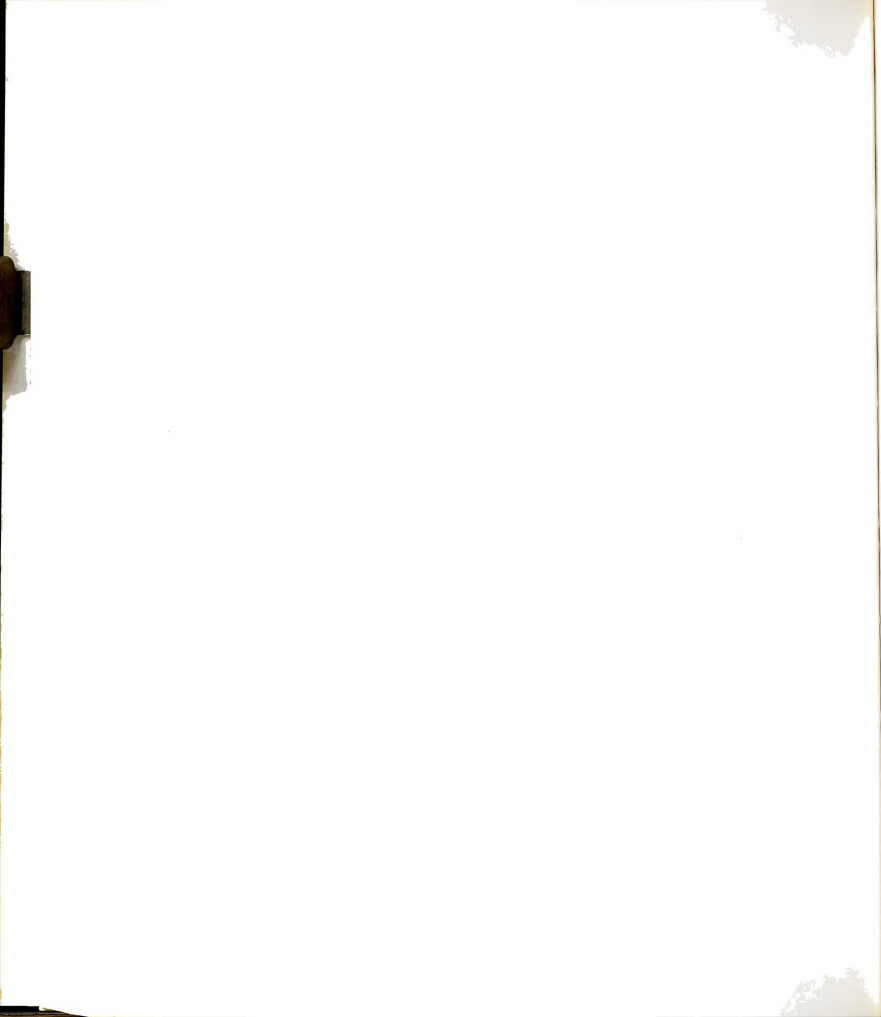
```



```

4 //, 20X, *D. TIME INCREMENTS =*, 15, * GIVING DT =*, E15.6,
5 * HOURS*, )
PRINT 8100, RPM, T, PO
8100 FORMAT( //, 20X, *E. CENTRIFUGE RPM =*, F10.1, //, 20X, *F. TEMPE
1RATURE =*, F12.3, * R*, //, 20X, *G. CHARGE PRESSURE =*, F15.6,
2 * PSIA*, )
PRINT 8200, WM1, WM2, YF, DP
8200 FORMAT( //, 20X, *H. HEAVY AND LIGHT SPECIE MOLECULAR WEIGHTS =*,
1 F12.4, //, 20X, *I. HEAVY SPECIE MOLE FRACTION =*, E13.5, //,
2 20X, *J. DIFFUSIVITY TIMES PRESSURE =*, E10.7, * F: FT/SEC PSI
3*, //, 20X, *K. EQUILIBRIUM MOLE FRACTION PROFILE* )
C
C ..... COMPUTE INCREMENTAL RADIAL DISTANCES AND INITIALIZE Y .....
C
R(1) = 0.0 $ Y(1,1) = Y(2,1) = Y(3,1) = YF
DO 20 I = 2, NP1
R(I) = R(I-1) + DR $ Y(1,I) = Y(2,I) = YF
20 Y(3,I) = YF
C
C ..... COMPUTE THE EQUILIBRIUM MOLE FRACTION PROFILE .....
C
CC = ( EXP( AA*(NP1)*R(NP1)/2.0 ) - 1.0 ) /
1 ( EXP( AA*(WM1/WM2)*R(NP1)*R(NP1)/2.0 ) - 1.0 )
YE(1) = YF * CC * WM1/WM2 / ( 1.0 + YF*( WM1/WM2*CC - 1.0 ) )
DO 2111 J = 2, NP1
DUM = EXP( A * R(J) * R(J) / 2.0 )
2111 YE(J) = YE(1) * DUM / ( YE(1) * ( DUM - 1.0 ) + 1.0 )
C
C ..... OUTPUT EQUILIBRIUM MOLE FRACTION PROFILE .....
C
PRINT 2112
2112 FORMAT( //, 55X, *RADIUS(FT)*, 8X, *MOLE FRACTIONS*, / )
DO 2113 J = 1, NP1
2113 PRINT 2114, R(J), YE(J)
2114 FORMAT( 48X, E17.5, 3X, E17.6 )
PRINT 2115

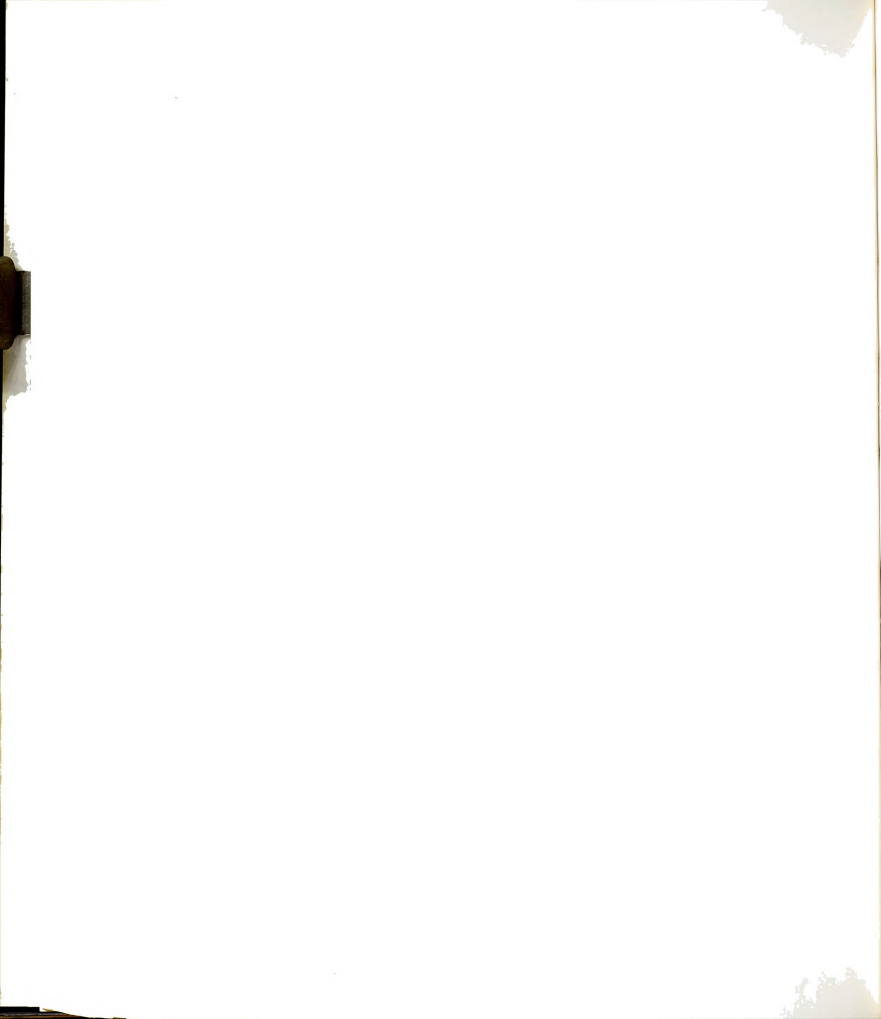
```



```

2115 FORMAT( *1*, 20X, *L. DY/DYE = (YF-Y)/(YF-YE) AND PRESSURE PROFILE
1S WITH TIME* )
C
C
C ..... COMPUTE THE MOLES PER FOOT FROM THE INITIAL CHARGE .....
C
C BOL = PIE / RGAS / T * P0 * R(NP1)*R(NP1)
C
C ..... COMPUTE THE PRESSURE AT THE AXIS .....
C
C AAA = *YF * AA
C PAXIS = BOL * RGAS * T / 2.0 / PIE * AAA / ( EXP( AAA *
1 R(NP1) * R(NP1) / 2.0 ) - 1.0 )
C
C ..... INITIALIZE THE PRESSURE PROFILE .....
C
C DO 30 I = 1, NP1
C P(1,I) = P(2,I) = PAXIS * EXP( AAA * R(I) * R(I) / 2.0 )
C 30 P(3,I) = P(2,I)
C
C ..... BEGIN CALCULATIONS .....
C
C NP1 = NT + 1
C NANS = NP1 + 2 $ NN = NP1 + 1 $ TS = 0.0
C JPRINT = IPRINT - 1
C DO 1000 I TIMES = 1, NP1
C JPRINT = JPRINT + 1
C IF( I TIMES .EQ. NP1 ) JPRINT = IPRINT
C IF( JPRINT .NE. IPRINT ) GO TO 1150
C
C ..... OUTPUT DY/DYE = (YF-Y)/(YF-YE) AND PRESSURE PROFILES .....
C
C JPRINT = 0 $ PRINT 1100, TS
1100 FORMAT( //, 10X, *TIME =, E15.4, * HRS*, / )
C MSTART = 1 $ MSTOP = 10
1160 IF( MSTOP .GT. NP1 ) MSTOP = NP1
C PRINT 1110, ( R(J), J = MSTART, MSTOP )

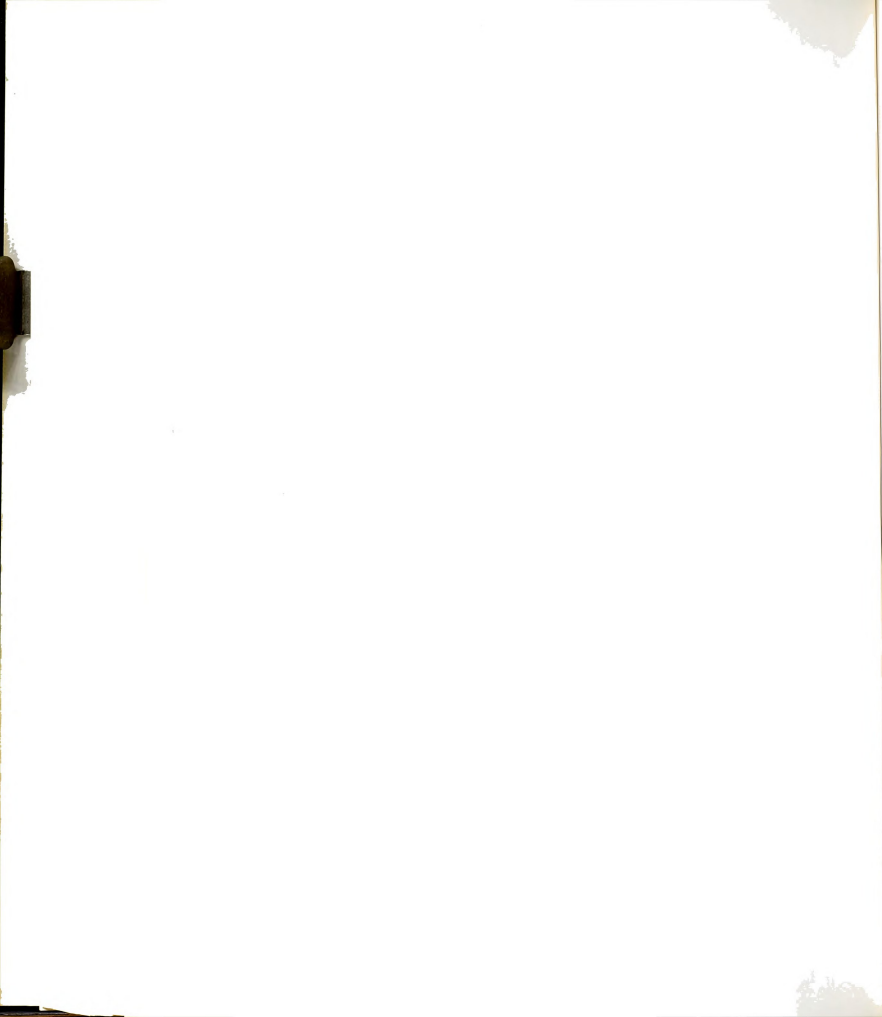
```



```

1110 FORMAT( 1X, 'RADII', 10E12.4 )
DO 2115 J = 1, NPI
2115 DPDI(J) = ( YF - Y(3*J) ) / ( YF - YE(J) )
PRINT 1120, ( DPDI(J), J = MSTART, MSTOP )
1120 FORMAT( 1X, 'DPDI', 9E11.4, 9E12.4 )
DO 1130 J = 1, NPI
1130 DPDI(J) = P(5,J) - P0
PRINT 1140, ( DPDI(J), J = MSTART, MSTOP )
1140 FORMAT( 1X, 'DPDI', 1X, 10E12.4 )
IF( MSTOP .EQ. NPI ) GO TO 1150
PRINT 1161
1161 FORMAT( / )
MSTART = MSTOP + 1 $ MSTOP = MSTOP + 10
GO TO 1160
1150 IF( I*TIMES .GT. NT ) STOP
C
C
C ..... ESTIMATE PRESSURES AND MOLE FRACTIONS AT NEW TIME .....
DO 60 I = 1, NPI
P(4,I) = 2.25*P(3,I) - 1.5*P(2,I) + P(1,I)/4.0
60 Y(4,I) = 2.25*Y(3,I) - 1.5*Y(2,I) + Y(1,I)/4.0
C
C ..... DUE TO THE NON LINEAR NATURE OF THE EQUATIONS EACH
POINT WILL BE ITERATED UPON TWICE .....
DO 9995 NOLIN = 1, 2
C
C ..... COMPUTE DP/DT .....
DO 70 I = 1, NPI
70 DPDI(I) = ( 22.0*P(4,I)/12.0 - 3.0*P(3,I) + 1.5*P(2,I) -
1 P(1,I)/3.0 ) / DT
C
C ..... CLEAR ARRAYS C AND ANS .....
DO 75 I = 1, NANS

```

```

      ANS(I,1) = 0.0
      DO 75 J = 1, 7
      75 C(I,J) = 0.0

      ..... COMPUTE NEW MOLE FRACTIONS .....

      ..... NO FLUX AT THE AXIS .....

      C(1,4) = -1.0/3.0 $ C(1,5) = -0.5
      C(1,6) = 1.0 $ C(1,7) = -1.0/6.0

      ..... NO FLUX AT THE WALL .....
      C(MANS,4) = 1.0/3.0 $ C(MANS,2) = -1.0 $ C(MANS,1)=1.0/6.0
      C(MANS,3) = 0.5 - DR * R(NP1) * A * ( 1.0 - Y(4,NP1) )

      ..... SPECIAL DIFFERENCE EQUATION AT THE AXIS .....

      I = 2 $ J = I - 1
      C(I,4) = ( P(4,J)/DT * 22.0/12.0 + DPDT(J) ) / DPH
      1 + 5.0/3.0 + DRDR * 2.0 * A * ( 1.0 - Y(4,J) )
      C(I,3) = -11.0/12.0*DRDR $ C(I,5) = -0.5 * DRDR
      C(I,6) = -DRDR/3.0 $ C(I,7) = DRDR/12.0

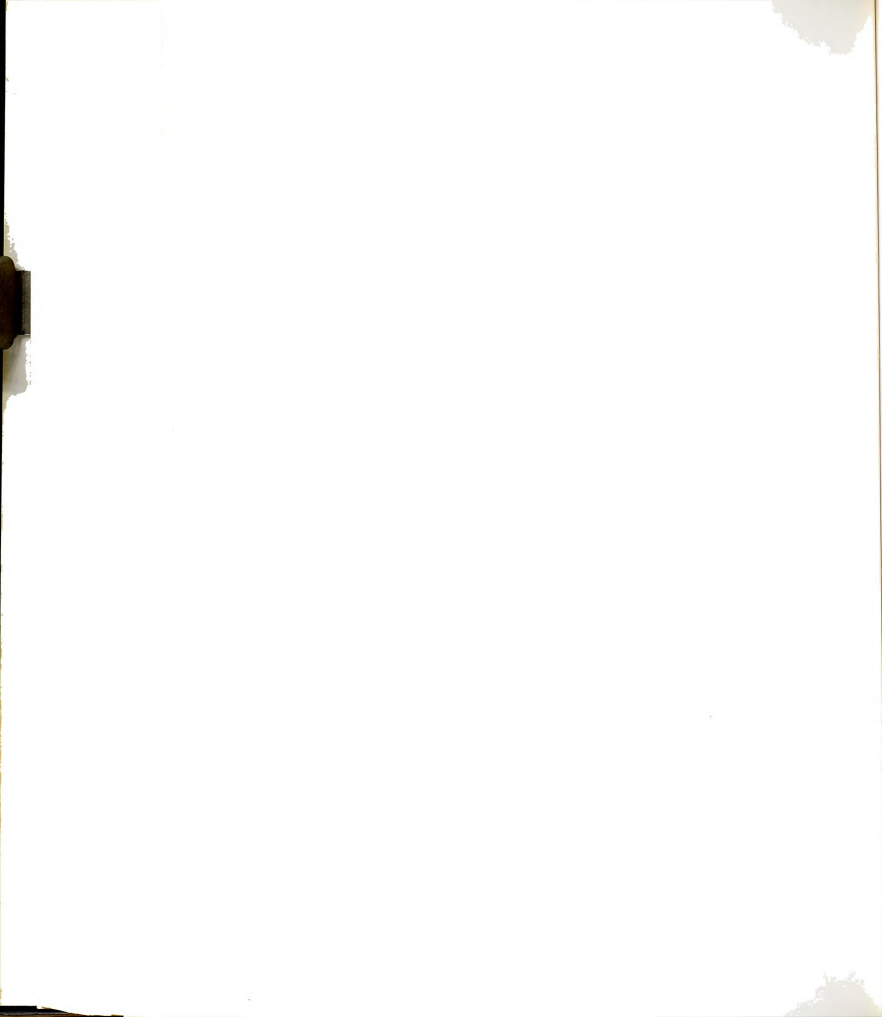
      ..... SPECIAL DIFFERENCE EQUATION AT THE WALL .....

      I = NW $ J = I - 1
      DUM = A * R(J) * ( 1.0-2.0*Y(4,J) ) - 1.0 / R(J)
      C(I,4) = ( P(4,J)/DT * 22.0/12.0 + DPDT(J) ) / DPH
      1 + 5.0/3.0 + DRDR * A * ( 1.0-Y(4,J) ) * ( DUM * R(J) + 2.0 )
      C(I,5) = -11.0/12.0 * DRDR $ C(I,3) = -DRDR / 2.0
      C(I,2) = -DRDR/3.0 $ C(I,1) = DRDR/12.0

      ..... INTERIOR POINTS .....

      DO 100 I = 3, NP1
      J = I - 1

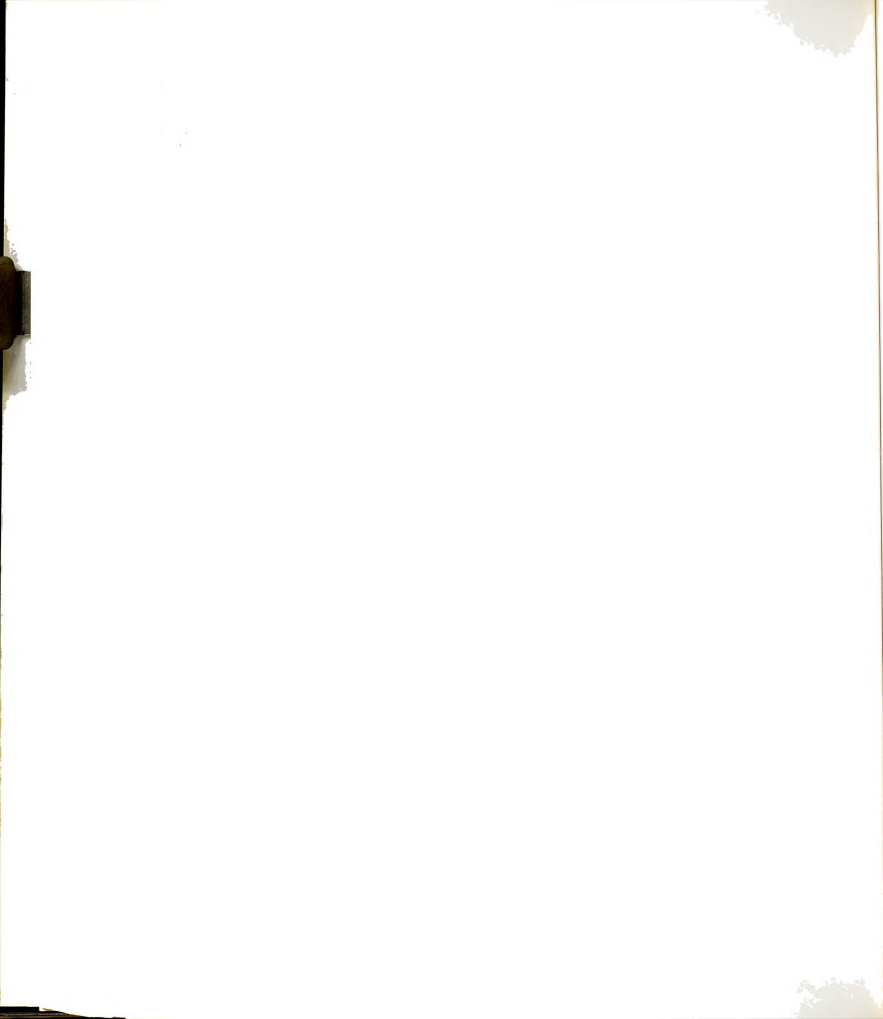
```



```

DUM = ( A * P(J) * ( 1.0-2.0*Y(4,J) ) - 1.0 / R(J) ) / DR
C(1,4) = ( P(4,J)/DT * 22.0/12.0 + DROT(J) ) / DPH + 2.5*DRDR
1  + 2.0 * A * ( 1.0 - Y(4,J) )
C(1,3) = -12.0*DUM*4.0*DRDR/3.0 $ C(1,2) = (DUM+DRDR)/12.0
C(1,5) = ( 2.0*DUM - 4.0*DEOR ) / 3.0
100 C(1,6) = (-DUM + DRDR) / 12.0
C
C ..... GIVE THE KNOWN TERMS FROM DY/DT TO ANS .....
C
DO 110 I = 2, NN
J = I - 1
110 ANS(I,1) = -P(4,J)/EPH/DT * ( -3.0*Y(3,J)+1.5*Y(2,J)-Y(1,J)/3.0 )
CALL ONEDIAG( C, ANS, 3, NANS, 1, DUM, XD, 1 )
C
C ..... GIVE THE ANSWERS TO Y .....
C
DO 120 I = 2, NN
J = I - 1
120 Y(4,J) = ANS(I,1)
C
C ..... NOW MUST INTEGRATE TO GET THE NEW PRESSURE PROFILE ----
C
C ..... WILL TEMPORARILY SET P(4,1) = 1.0 .....
C
C ..... CLEAR ARRAYS C AND ANS .....
C
DO 130 I = 1, NN
ANS(I,1) = 0.0
DO 130 J = 1, 7
130 C(I,J) = 0.0
C
C ..... WRITE EQUATIONS FOR THE AXIS AND THE INITIAL VALUE .....
C
C(1,4) = - 1.0/3.0 $ C(1,5) = -0.5
C(1,6) = 1.0 $ C(1,7) = -1.0/6.0
C(2,4) = 1.0 $ ANS(2,1) = 1.0
C

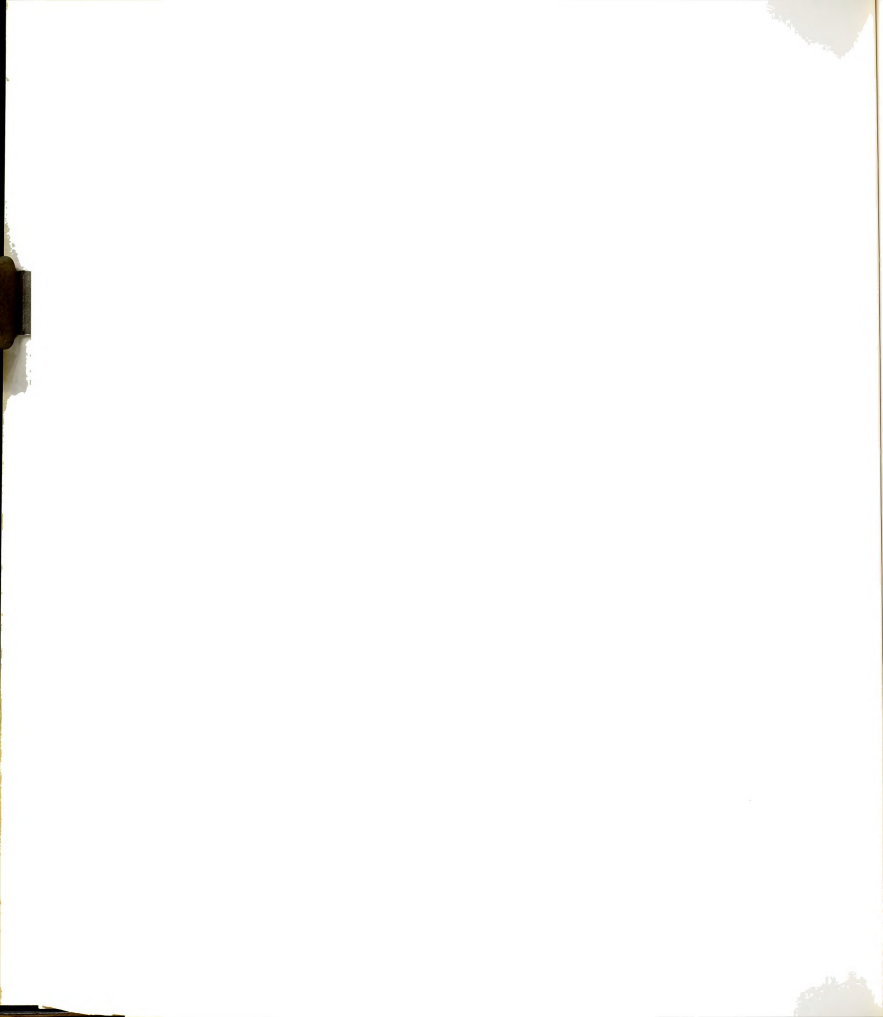
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```

C ..... WRITE EQUATIONS OVER TO TWO POINTS FROM THE BOUNDARY .....
C
DO 150 I = 3, N
  J = I - 1
  C(I,4) = -DR * ( A * Y(4,J) + AA ) * R(J)
  C(I,3) = -2.0/3.0 $ C(I,2) = 1.0/12.0 $ C(I,5) = 2.0/3.0
150 C(I,6) = - 1.0 / 12.0
C
C ..... ONE POINT BEFORE THE BOUNDARY .....
C
I = NP1 $ J = I - 1
C(I,4) = 10.0/12.0 - DR * ( A * Y(4,J) + AA ) * R(J)
C(I,5) = 0.25 $ C(I,3) = -1.5
C(I,2) = 0.5 $ C(I,1) = -1.0 / 12.0
C
C ..... EQUATIONS FOR THE WALL .....
C
I = NN $ J = I - 1
C(I,4) = 22.0/12.0 - DR * ( A * Y(4,J) + AA ) * R(J)
C(I,3) = -3.0 $ C(I,2) = 1.5 $ C(I,1) = -1.0/3.0
CALL ONEDIAG( C, ANS, 3, NN, 1, DUM, MD, KD, 1 )
C
C ..... GIVE THE ANSWERS TO P .....
C
DO 160 I = 2, NN
  J = I - 1
160 P(4,J) = ANS(I,1)
C
C ..... MUST NOW INTEGRATE TO FIND PAXIS .....
C
C ..... CLEAR ARRAYS C AND ANS .....
C
DO 200 I = 1, NN
  ANS(I,1) = 0.0
DO 200 J = 1, 7
200 C(I,J) = 0.0

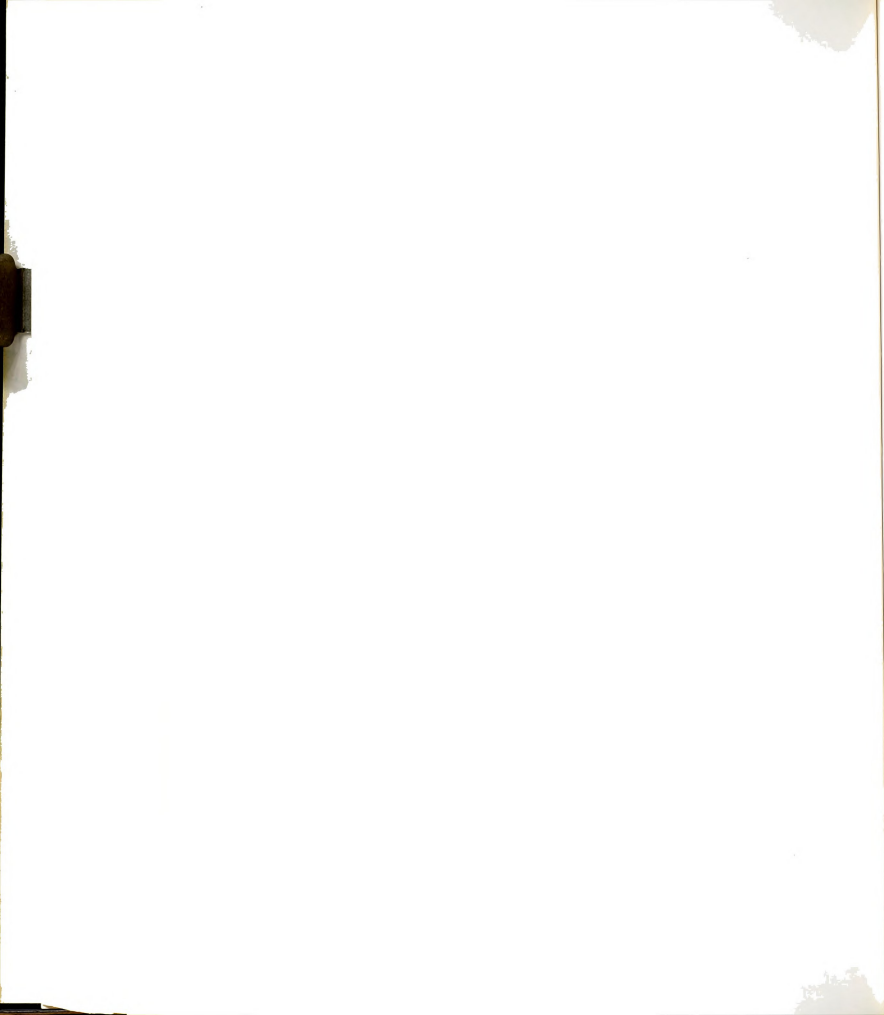
```



```

C      ..... WRITE EQUATIONS FOR THE AXIS AND THE INITIAL VALUE .....
C      C(1,4) = -1.0/3.0 $ C(1,5) = -0.5 $ C(1,6) = 1.0
C      C(1,7) = -1.0/6.0 $ C(2,4) = 1.0
C
C      ..... WRITE EQUATIONS UP TO TWO POINTS BEFORE THE BOUNDARY .....
C
C      DO 220 I = 3, N
C      J = I - 1
C      C(1,2) = 1.0 / 12.0 $ C(1,3) = -2.0/3.0
C      C(1,5) = 2.0 / 3.0 $ C(1,6) = -1.0/12.0
C      220 ANS(I,1) = P(4,J) * R(J) * DR
C
C      ..... SPECIAL DIFFERENCE EQUATION FOR ONE POINT BEFORE THE WALL ...
C
C      I = NP1 $ J = I - 1
C      C(1,4) = 10.0/12.0 $ C(1,5) = 0.25
C      C(1,3) = -1.5 $ C(1,2) = 0.5
C      C(1,1) = -1.0/12.0 $ ANS(I,1) = P(4,J) * R(J) * DR
C
C      ..... SPECIAL DIFFERENCE EQUATION AT THE WALL .....
C
C      I = NN $ J = I - 1
C      C(1,4) = 22.0/12.0 $ C(1,3) = -3.0 $ C(1,2) = 1.5
C      C(1,1) = -1.0/3.0 $ ANS(I,1) = P(4,J) * R(J) * DR
C      CALL ONEDIAG( C, ANS, 3, NN, 1, DUM, MD, KD, 1 )
C      PAXIS = BOL * RGAS * I / 2.0 / PIE / ANS(NN,1)
C
C      ..... COMPUTE THE PRESSURE PROFILE .....
C
C      DO 250 J = 1, NP1
C      250 P(4,J) = PAXIS * P(4,J)
C      9995 CONTINUE
C
C      ..... MOVE ALL VALUES OF Y AND P BACK A ROW FOR THE NEXT

```

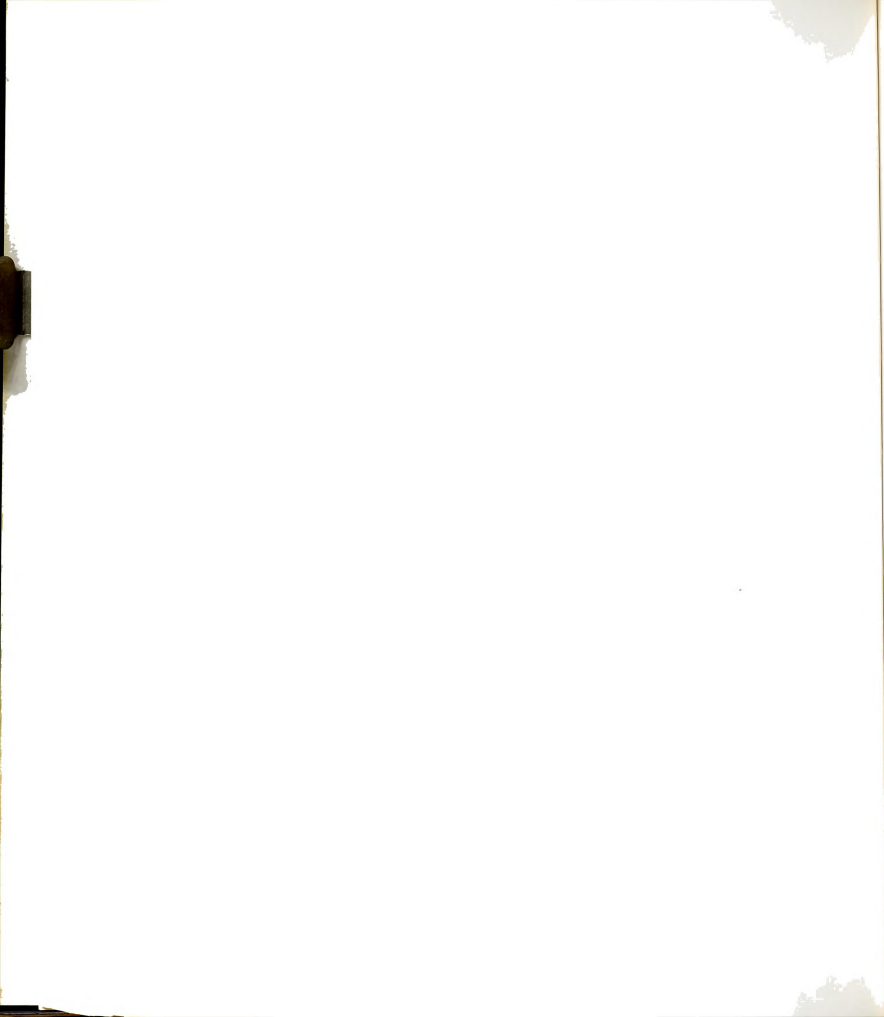



C INCREMENT IN TIME
C

```

DO 300 I = 2, 4
  K = I - 1
  DO 300 J = 1, NP1
    Y(K,J) = Y(I,J)
  300 P(K,J) = P(I,J)
  1000 TS = TS + DT
  END

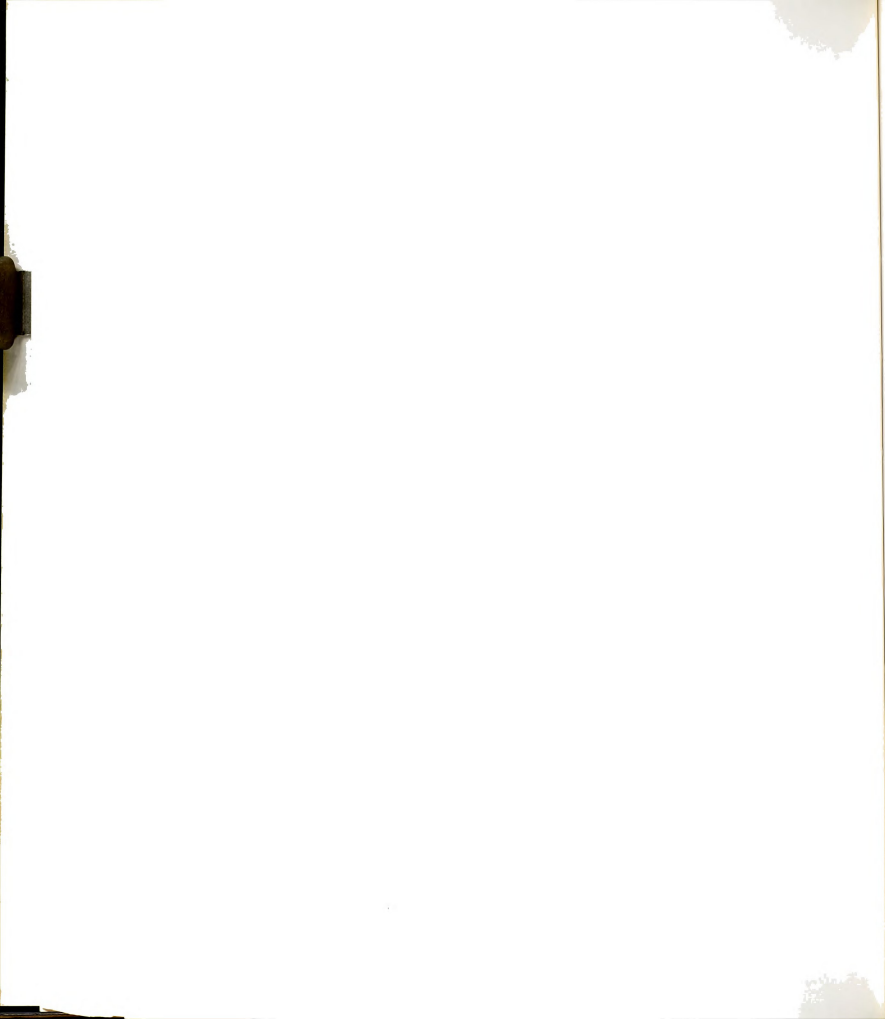
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```

SUBROUTINE ONEDIAG( COEFF, ANS, IM, IEQ, MSETS, DETERM, MD, KD, ND )
..... THIS SUBROUTINE SOLVES SIMULTANEOUS EQUATIONS WHICH HAVE
      A DIAGONAL COEFFICIENT MATRIX .....
DIMENSION COEFF(MD,KD), ANS(MD,ND)
DOUBLE PRECISION DUM, DUNNY, BD(50), E(10)
..... CHECK DIMENSIONS .....
IF( IEQ .LE. MD ) GO TO 1
PRINT 2, IEQ, MD
      $
2 FORMAT( '1*, 20X, 15, * EQUATIONS ARE SPECIFIED, BUT ONLY*, 15,
1* ARE PROVIDED FOR IN THE DIMENSION STATEMENT* )
..... IF MSETS = 0 ONLY THE DETERMINANT IS WANTED
      MSETS = 1-10 = THE SETS OF EQUALITIES ANYTHING
      ELSE TERMINATES THE PROGRAM .....
1 IF( MSETS .LE. ND ) GO TO 3
PRINT 4, MSETS, ND
      $
4 FORMAT( '1*, 10X, 15, * SETS OF EQUALITIES ARE SPECIFIED, BUT ONL
1Y*, 15, * ARE PROVIDED FOR IN THE DIMENSION STATEMENT* )
3 IF( MSETS .GE. 0 .AND. MSETS .LE. 10 ) GO TO 5
PRINT 7, MSETS
7 FORMAT( '1*, 20X, *MSETS CAN BE 0 THRU 10, YOU SPECIFIED*, 15 )
5 IF( KD .GE. IM+IM+2 ) GO TO 8
PRINT 6, IM, KD
      $
6 FORMAT( '1*, 20X, *YOU SPECIFIED A MAXIMUM OF*, 120, *MINOR DIAGO
1NALS*, //, 20X, *HOWEVER, KD IS ONLY*, 120 )
..... BEGIN SOLUTION .....
..... CHECK FOR INDEFINITE OR OUT OF RANGE ENTRIES .....

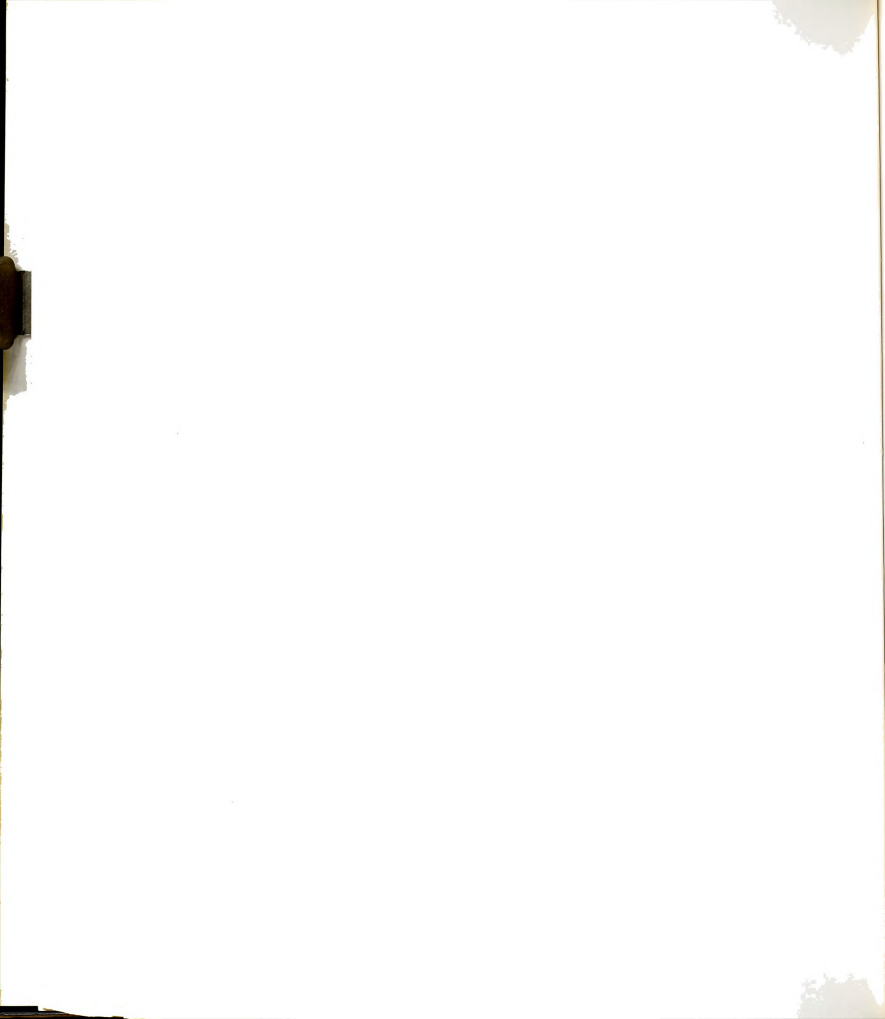
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```

      8 K = IM + IM + 1
      DO 2000 I = 1, K
      DO 2000 J = 1, IEQ
      L = LEQVAR( COEFF(J,I) )
      IF( L ) 2010, 2000, 2010
      2010 PRINT 2020 $ CALL MMOUT( COEFF, IEQ, 1, K, MD, KD )
      2020 FORMAT( '1*', 20X, 'ONE OR MORE ELEMENTS OF THE COEFF MATRIX IS OUT
      11 OF RANGE OR UNDEFINED*' )
      STOP
      2000 CONTINUE
      IF( MSETS .EQ. 0 ) GO TO 11
      DO 2030 I = 1, MSETS
      DO 2030 J = 1, IEQ
      L = LEQVAR( ANS(J,I) )
      IF( L ) 2040, 2030, 2040
      2040 PRINT 2025 $ CALL MMOUT( ANS, IEQ, 1, MSETS, MD, ND )
      2025 FORMAT( '1*', 20X, 'ONE OR MORE ELEMENTS OF MATRIX ANS IS OUT OF R
      11 RANGE OR UNDEFINED*' )
      STOP
      2030 CONTINUE
      11 DEIGN = 1.0 $ L = K+1 $ IMID = IM+1 $ SUM = 1.0E-07
      IMIDP1 = IMID + 1
      C ..... BEGIN UPPER TRIANGULATION .....
      DO 900 I = 1, IEQ
      C ..... THE CALCULATIONS NECESSARY TO UPPER TRIANGULATE THE RO
      C ARE DONE IN DOUBLE PRECISION .....
      C
      COEFF(I,L) = 0.0 $ ISIT = 0
      990 DO 910 J = 1, L
      910 RD(J) = DBLE( COEFF(I,J) )
      IF( MSETS .EQ. 0 ) GO TO 925
      DO 915 J = 1, MSETS

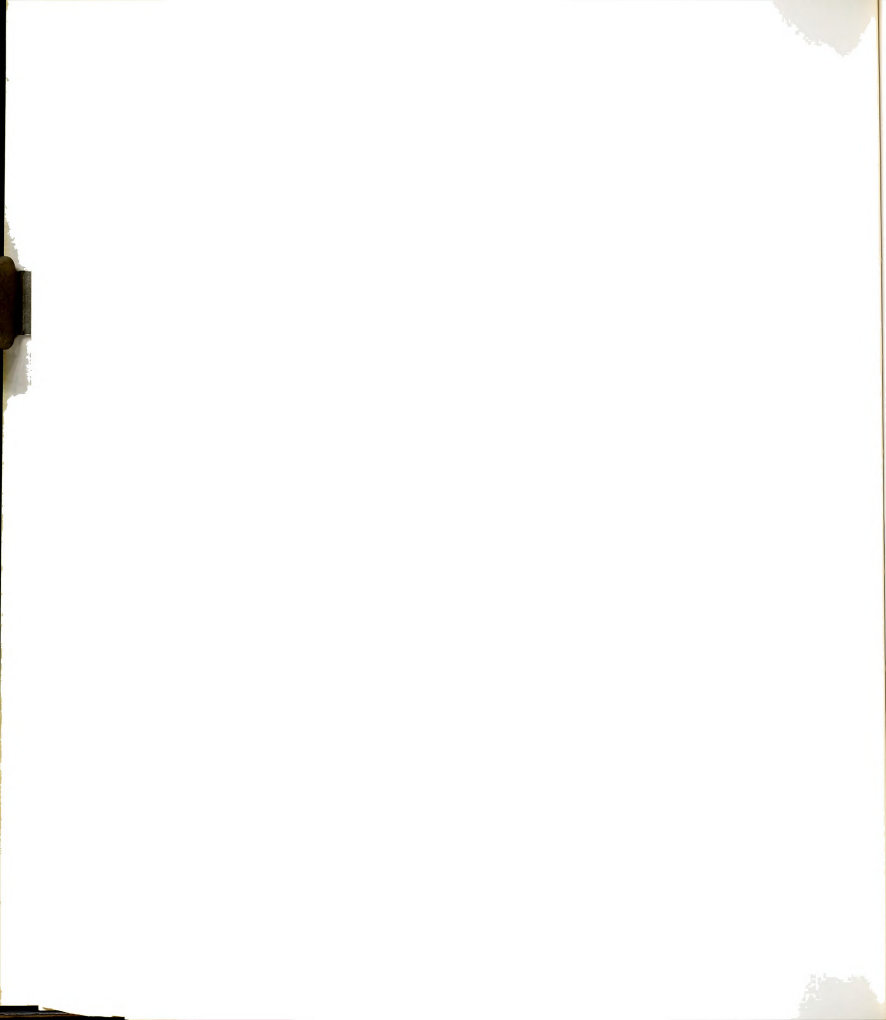
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```

915 E(J) = DBLE( ANS(I,J) )
925 DO 920 J = 1, IM
C
C      ..... CHECK FOR NON ZERO ENTRIES BEFORE THE DIAGONAL .....
C
IF( BD(J) ) 926, 920, 926      JJ = J
926 M = 1 - IMID + J          $
IF( M .LE. 0 ) GO TO 9000
C
C      ..... SUBTRACT DUM TIMES ROW M TO REDUCE AN ELEMENT TO ZERO .....
C
DUM = BD(J) / DBLE( COEFF(M,IMID) )
DO 930 LL = IMIDP1, L
JJ = JJ + 1
930 BD(JJ) = BD(JJ) - DUM * DBLE( COEFF(M,LL) )
IF( MSETS .EQ. 0 ) GO TO 935
DO 940 LL = 1, MSETS
940 E(LL) = E(LL) - DUM * DBLE( ANS(M,LL) )
935 COEFF(I,J) = 0.0
920 CONTINUE
C
C      ..... GIVE THE DOUBLE PRECISION UPPER TRIANGULATED ROW BACK
C      TO COEFF .....
C
DO 950 J = IMID, L
950 COEFF(I,J) = SNGL( BD(J) )
IF( MSETS .EQ. 0 ) GO TO 955
DO 960 J = 1, MSETS
960 ANS(I,J) = SNGL( E(J) )
C
C      ..... CHECK IF A RELATIVELY SMALL NUMBER IS LEFT ON THE DIAGONAL .
C
955 SUM = SUM + ABS( COEFF(I,IMID) )
IF( ABS( COEFF(I,IMID) ) / SUM * FLOAT( I ) .GT. 1.0E-08 )
1
GO TO 900
C

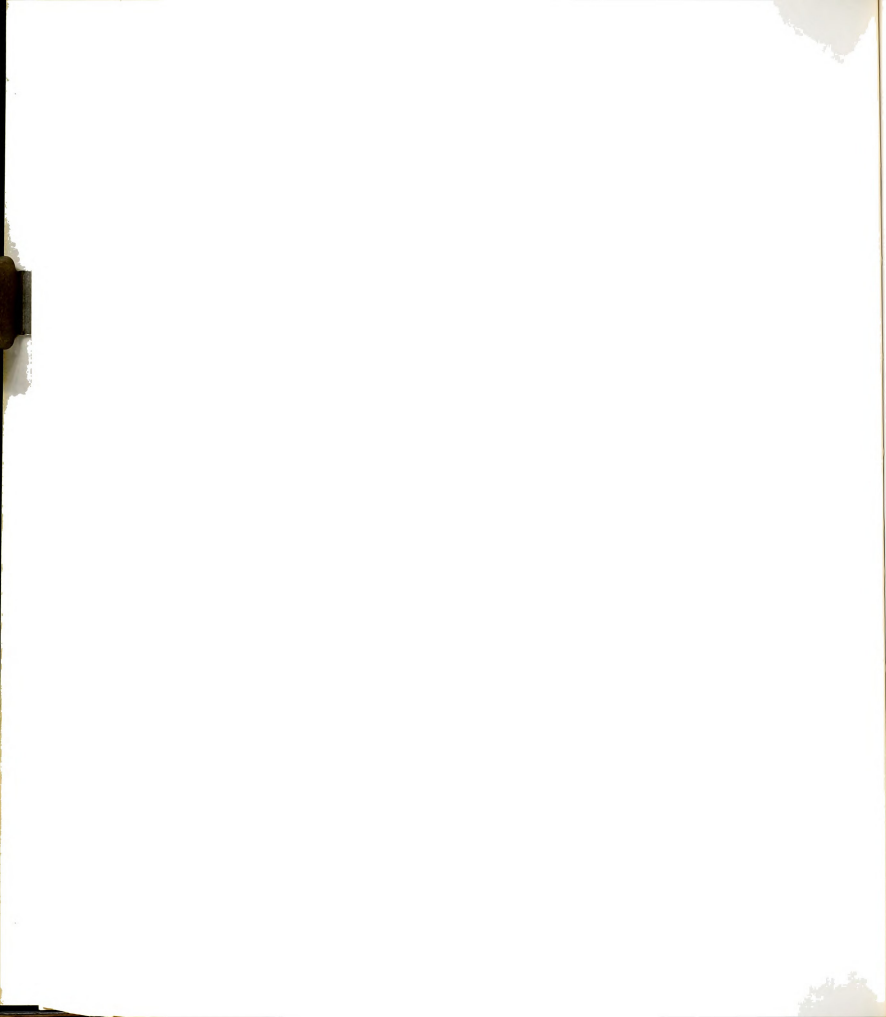
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C      ..... IF ISIT IS ONE IT MEANS THAT A ROW HAS ALREADY BEEN
C      SWITCHED AND THE SUBROUTINE CAN NOT CONTINUE .....
C
C      IF( ISIT .EQ. 1 )      GO TO 9200
C      IF( I .NE. IEQ )      GO TO 9410
C      IF( MSETS .NE. 0 )      GO TO 9400
C      GO TO 900
C
C      ..... SWITCH THE BAD ROW WITH THE ONE FOLLOWING IT .....
C
C      9410 ISIT = 1      $      II = I + 1      $      DETERM = -DETERM
C      DO 970 J = 1, K
C      X = COEFF(I,J+1)      $      COEFF(I,J+1) = COEFF(II,J)
C      970 COEFF(II,J) = X
C      IF( MSETS .EQ. 0 )      GO TO 990
C      DO 980 J = 1, MSETS
C      X = ANS(I,J)      $      ANS(I,J) = ANS(II,J)
C      980 ANS(II,J) = X
C
C      ..... GO BACK AND REUPPER TRIANGULATE ROW I .....
C
C      GO TO 990
C      900 DETERM = DETERM * COEFF(I,IMID)
C
C      ..... IF MSETS IS ZERO ONLY THE DETERMINANT IS WANTED .....
C
C      IF( MSETS .EQ. 0 )      RETURN
C
C      BEGIN THE BACK SUBSTITUTION .....
C
C      MIEQ = IEQ - 1
C      DO 1000 J = 1, MSETS
C      1000 ANS(IEQ,J) = SNGL( E(J) / BD(IMID) )
C
C      ..... CALCULATIONS ARE DONE IN DOUBLE PRECISION .....
C

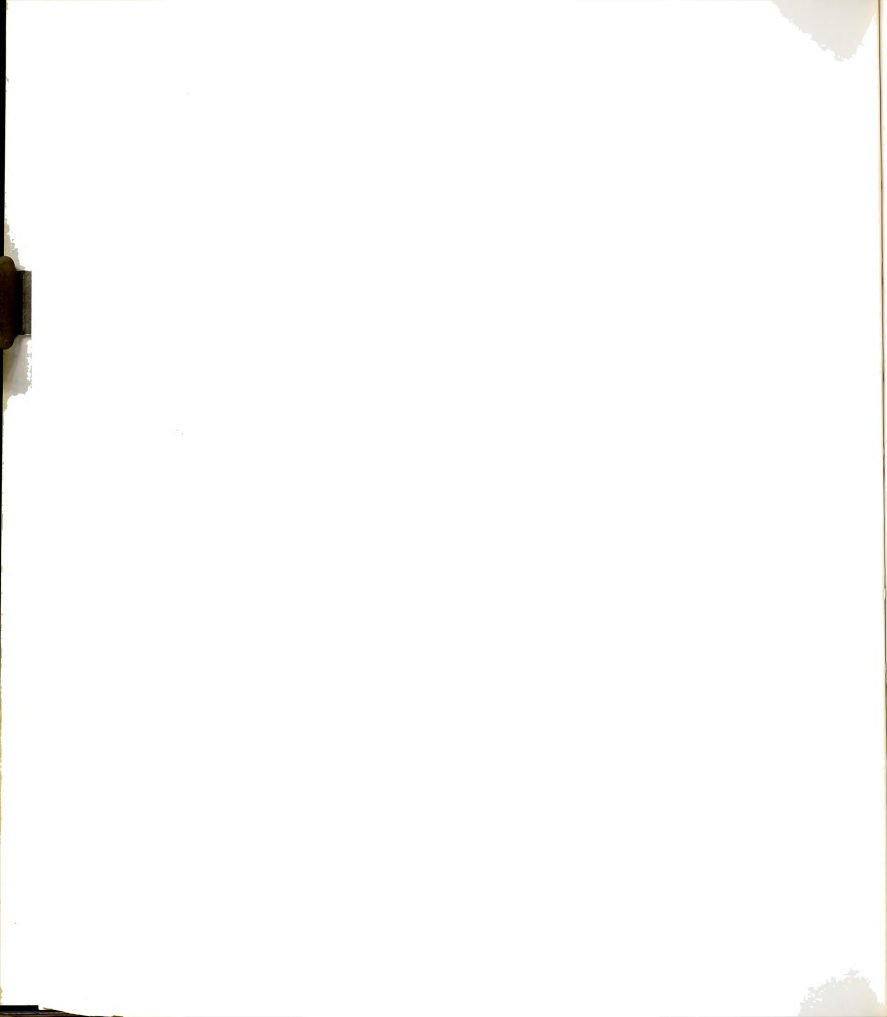
```



```

DO 1100 II = 1, MIEQ
I = IEQ - II
IF( II - IMID ) 1200, 1200, 1300
1200 IC = IMID + II
1300 DO 1350 LL = 1, MSETS
1350 E(LL) = DBLE( ANS(I,LL) )
DO 1400 JJ = IMID, IC
LL = I + JJ - IMID $ DUMMY = DBLE( COEFF(I,JJ) )
DO 1400 KK = 1, MSETS
1400 E(KK) = E(KK) - DUMMY * DBLE( ANS(LL,KK) )
C
C ..... GIVE DOUBLE PRECISION ANSWERS TO ANS .....
C
DO 1500 JJ = 1, MSETS
1500 ANS(I,JJ) = SNGL( E(JJ) / DBLE( COEFF(I,IMID) ) )
1100 CONTINUE
RETURN
C
C ..... OUTPUT IN THE CASE OF TROUBLE .....
C
9000 PRINT 9001 $ CALL MATOUT( COEFF, IEQ, 1, K, MD, KD )
9001 FORMAT( '1*, 20X, *THE FIRST IN EQUATIONS HAVE ENTRIES WHICH ARE
1 INCONSISTANT WITH THE DIAGONAL FORM* )
STOP
9200 PRINT 9201, I $ CALL MATOUT( COEFF, IEQ, 1, K, MD, KD )
9201 FORMAT( '1*, 20X, *A VERY SMALL NUMBER WAS ENCOUNTERED ON THE DIA
1GONAL AFTER UPPER TRIANGULATING*, //, 20X, *ROWS*, 15, * AND THE
2 FOLLOWING ROW OFFERS NO HELP --- THE EQUATIONS NEED BETTER ORDERIN
3G OR THEY ARE DEPENDENT* )
STOP
9400 PRINT 9401 $ CALL MATOUT( COEFF, IEQ, 1, K, MD, KD )
9401 FORMAT( '1*, 20X, *A VERY SMALL NUMBER WAS ENCOUNTERED ON THE DIA
1GONAL OF THE LAST EQUATION*, //, 20X, *BACK SUBSTITUTION WILL NOT B
2E MADE --- THE FIRST MATRIX IS COEFF AND THE SECOND IS ANS* )
CALL MATOUT( ANS, IEQ, 1, MSETS, MD, ND ) $ STOP
END

```

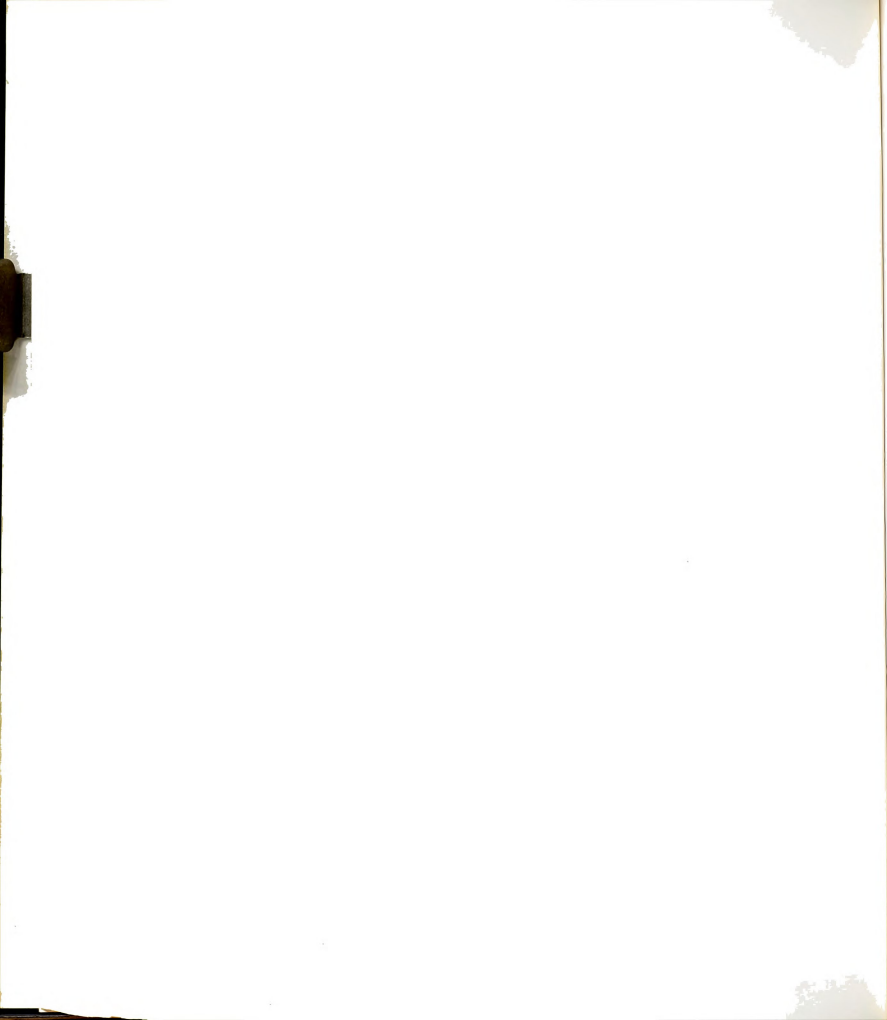


APPENDIX D

NUMERICAL METHOD AND FORTRAN PROGRAM

USED TO ANALYZE THE COUNTERCURRENT

RECTIFYING CENTRIFUGE



APPENDIX D

NUMERICAL METHOD AND FORTRAN PROGRAM USED TO ANALYZE THE COUNTERCURRENT RECTIFYING CENTRIFUGE

As established in Chapter V-B, the equation of continuity for Species 1 in the countercurrent rectifying centrifuge is

$$\frac{1}{r} \frac{\partial}{\partial r} [Ar^2 y(1-y) - r \frac{\partial y}{\partial r}] + \frac{Pv(r)}{D_{12}P} \frac{\partial y}{\partial z} - \frac{\partial^2 y}{\partial z^2} = 0 ,$$

where $v(r)$ is the axial velocity profile assumed to be only a function of r . The units for the above partial differential equation are ft^{-2} as computed in Appendix C.

The radial boundary conditions are those given for the unsteady state simple centrifuge, i.e.,

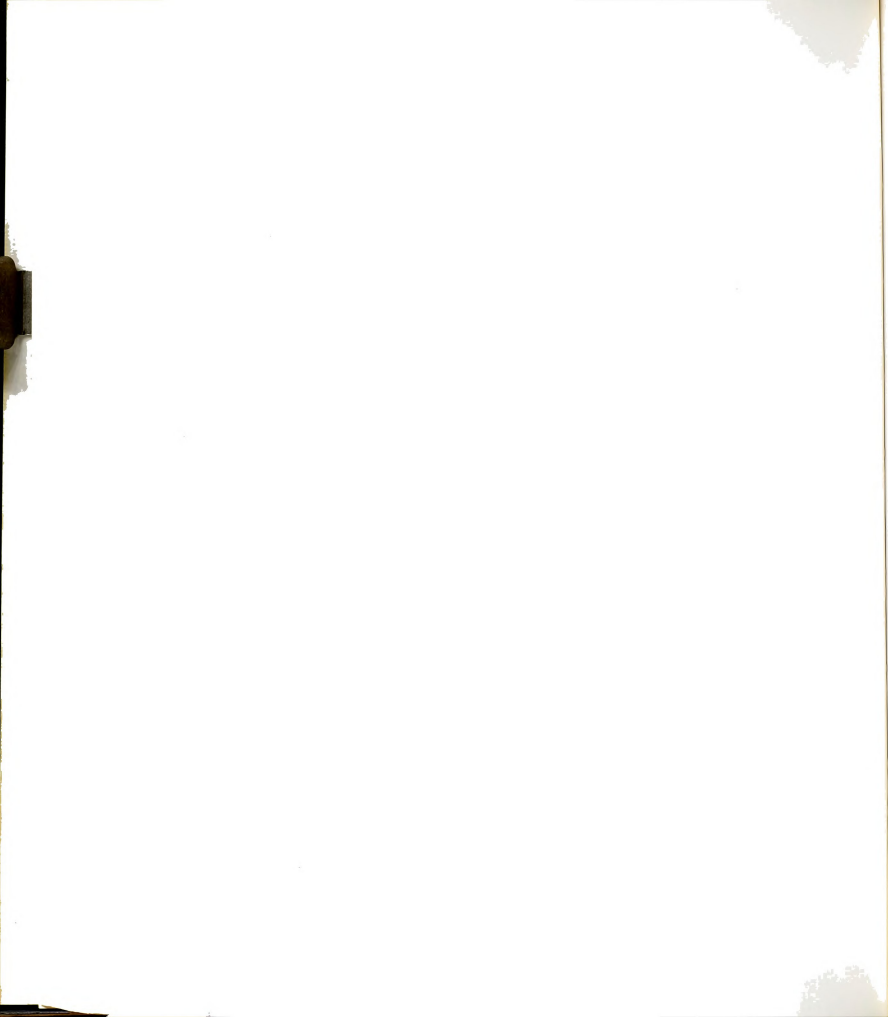
$$\frac{\partial y}{\partial r} = 0 \text{ at } r = 0 \text{ and}$$

$$\frac{\partial y}{\partial r} = Ar y(1-y) \text{ at } r = R_w.$$

The axial boundary conditions for the countercurrent rectifying centrifuge as given in Chapter V-B are that:

$$y = y_f \text{ for all } r \text{ in the interval } R_m \leq r \leq R_w \text{ at the top} \\ (z = 0), \text{ and}$$

$$y = y_r \text{ for all } r \text{ in the interval } 0 \leq r \leq R_m \text{ at the bottom} \\ (z = L),$$



where R_m is the radial position of the intersection of the inner and outer streams and

$$y_r = \frac{\frac{2\pi}{RT} \int_{R_m}^{R_w} [P_v(r) y - D_{12} P \frac{\partial y}{\partial r}] r dr}{\frac{2\pi}{RT} \int_{R_m}^{R_w} P_v(r) r dr}.$$

The quantity y_r is simply the average composition of the outer stream as it leaves the centrifuge representing the composition of the recycle stream.

To compute the pressure profile in the countercurrent rectifying centrifuge an average molecular weight equal to that of the feed was used. The pressure profile is then given by

$$P(r) = P(\text{axis}) \exp \left(\frac{A r^2}{2} \right),$$

$$\text{where } A = \frac{\omega^2}{RTg_c} [MW_1 y_f + MW_2 (1 - y_f)].$$

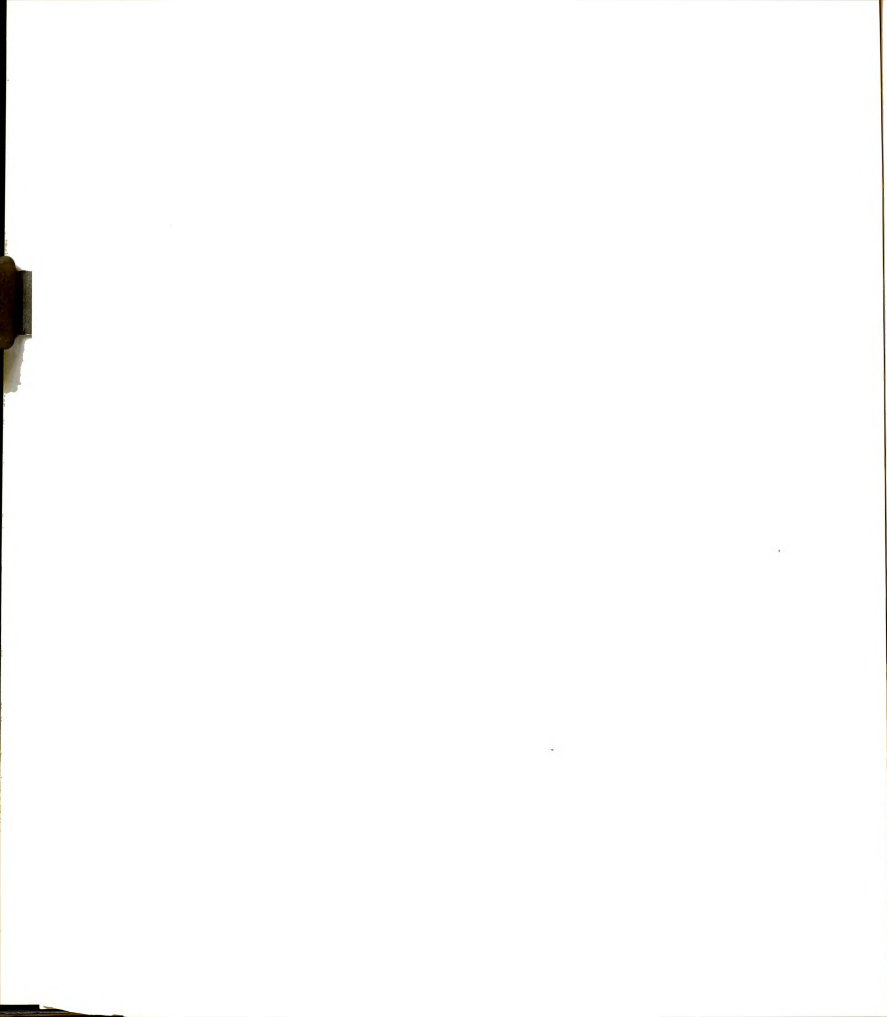
The units on this equation were checked in Appendix A.

The velocity profile, $v(r)$, was assumed to be either plug (rod) type flow or laminar flow. In either case, having assumed the shape of the profile, the magnitude of the velocity profile was computed so that the following integral was satisfied:

$$\text{Flow} = \frac{2\pi}{RT} \int_{r_1}^{r_2} P_v(r) r dr,$$

where Flow = the stream flow rate in lb-moles/sec, and

r_1, r_2 = the radial boundaries of the stream.



Using the above expression, the magnitudes of the assumed velocity profiles are computed as follows:

1. Plug type flow: Plug type flow by definition has a velocity profile which is constant with radial position. Thus, for the inner stream

$$v_i = \frac{\text{Flow}_i \text{ RT A}}{2\pi P(0)(e^a - 1)} \text{ for } 0 \leq r \leq R_m,$$

where $a = A R_m^2 / 2$.

For the outer stream

$$v_o = \frac{\text{Flow}_o \text{ RT A}}{2\pi P(0)(e^b - e^a)} \text{ for } R_m \leq r \leq R_w,$$

where $b = A R_w^2 / 2$. At the flow intersection and the centrifuge wall the velocities are taken as zero, i.e.,

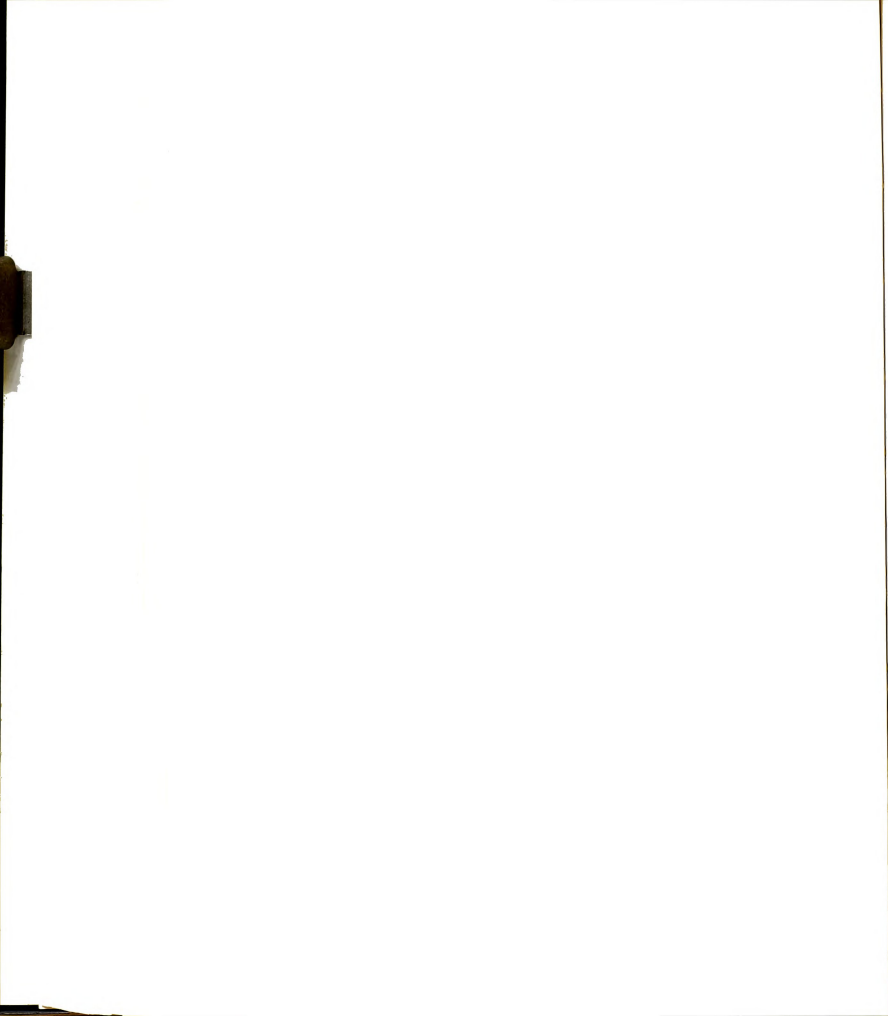
$$v_i = v_o = 0 \text{ at } r = R_m \text{ and } v_o = 0 \text{ at } r = R_w.$$

2. Laminar flow: The shape of the velocity profile for the inner stream was assumed to be that for laminar flow through a circular pipe, i.e.,

$$v_i(r) = v_i(\text{max})(1 - r^2/R_m^2).$$

The maximum velocity computed by using the above integral is

$$v_i(\text{max}) = \frac{\text{Flow}_i \text{ RT A}}{2\pi P(0)[(e^a - 1)/a - 1]}$$



where a is as defined above. The shape of the velocity profile for the outer stream was assumed to be that for laminar flow through an annulus, i.e.,

$$v_o(r) = \frac{v_o(\max)}{C} [1 - r^2/R_w^2 + d \ln(r/R_w)],$$

where $d = (1-k^2)/\ln(1/k)$,

$C = 1 - d[1 - \ln(d/2)]/2$, and

$$k = R_m/R_w.$$

The maximum velocity is given by

$$v_o(\max) = \frac{\text{Flow}_o \text{ CRT } A}{2\pi P(0) f},$$

$$\text{where } f = (e^b - e^a)/b - e^a(1-k^2) + d \ln(1/k)(e^a - 1) - \frac{d}{2} \sum_{n=1}^{\infty} \frac{b^n - a^n}{n \cdot n!},$$

and a and b are as defined above.

The numerical solution to the partial differential equation for the continuity of Species 1 was found using the FORTRAN program NCENTRI along with its ten associated FORTRAN subprograms. Table D-1 contains a list of the subroutines and their duties. The basic technique used to obtain the numerical solution was to approximate the partial derivatives in the equation of continuity by finite difference formulas. By numerically approximating the derivatives in the partial differential equation and in the boundary conditions an equation could be written for each grid point in the axial and radial directions. The resulting set of simultaneous equations upon solution

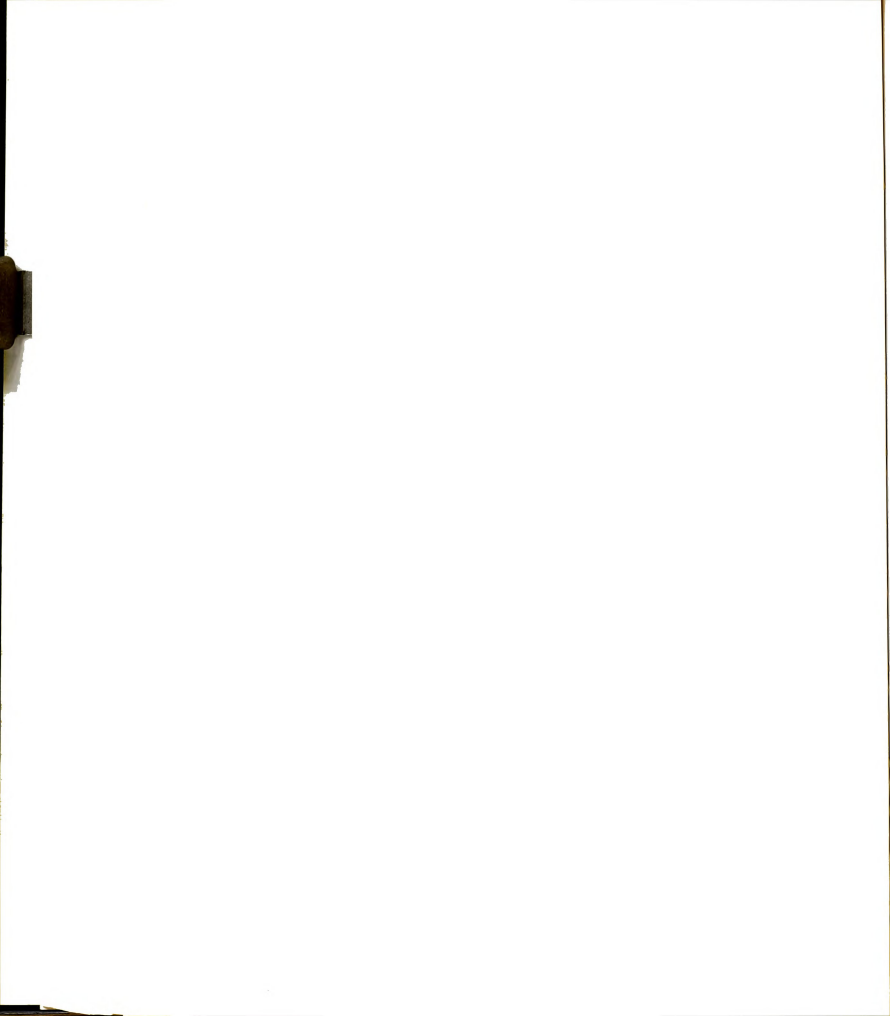
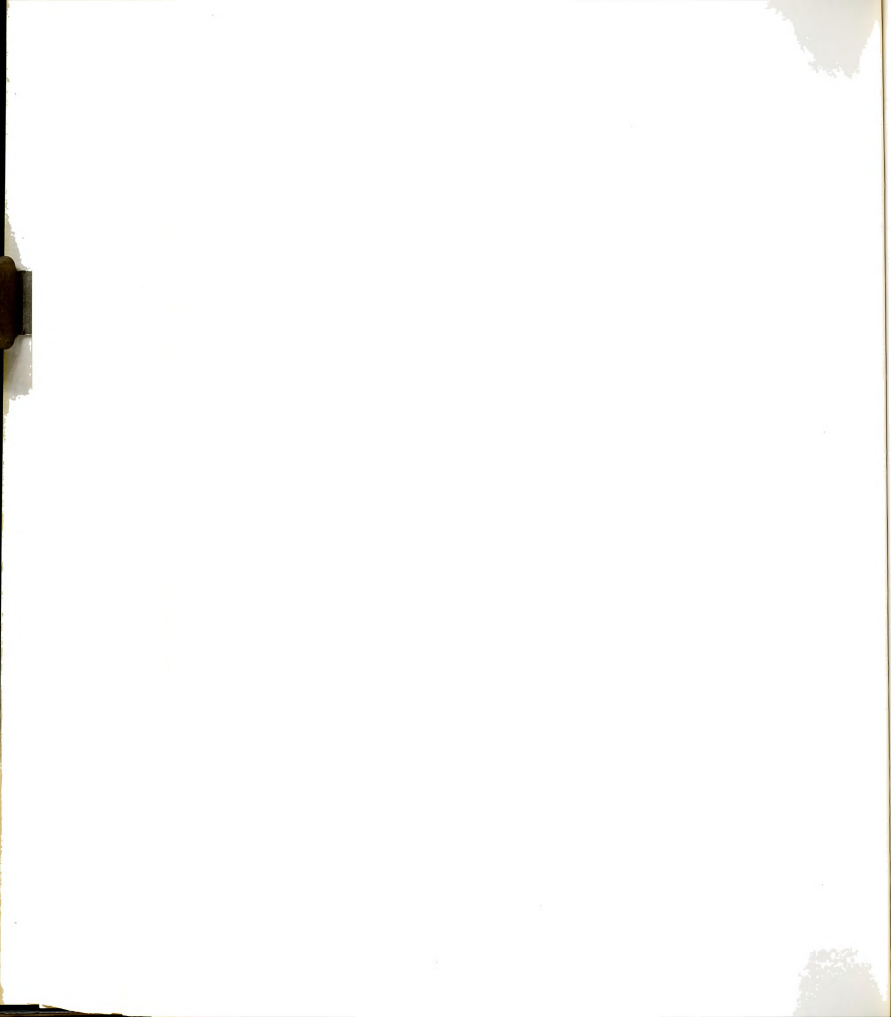


TABLE D-1.--Subprograms Associated With Program NCENTRI.

Subprogram	Duties
INITIAL	Input operating conditions, compute constants, and set up axial and radial incremental positions
VELS	Computes the pressure and velocity profiles
SUMVEL	Evaluates the infinite series needed by VELS
RDIFF	Computes the coefficients of all terms resulting from the approximation of r direction partial derivatives for the numerical approximation of the partial differential equation and/or boundary conditions at each grid point
SPECIAL	Used by RDIFF to compute the finite difference approximations (4'th order) for the first and second derivatives with respect to r at the flow intersection where the radial increment size changes
ZDIFF	Computes the coefficients of all terms resulting from the approximation of z direction partial derivatives for the numerical approximation of the partial differential equation and/or boundary conditions at each grid point
DIAG567	Solves the set of simultaneous equations resulting from the numerical approximation of the partial differential equation and the boundary conditions
UPPERT7	Used by DIAG567 to upper-triangulate equations
SWITCH7	Used by DIAG567 to switch equations
CONCOUT	Outputs the mole fraction matrix



gave the mole fraction profiles of the heavy species. These ideas are presented in the following sections describing program NCENTRI and its associated subprograms.

A. Inputting Data and Setting Up the Problem

Except for two computing options (read directly by NCENTRI) subroutine INITIAL inputs all operating conditions and initializes constants. The computing options and the data required by subroutine INITIAL along with the proper units can be found in Table D-2.

After all operating conditions have been read in by INITIAL and such things as the constant $(WM_1 - WM_2)\omega^2/RTg_c$, among others, and the radial and axial increments and incremental positions have been computed, subroutine VELs computes the pressure and velocity profiles. In the case of laminar flow, the equation for the maximum velocity of the outer stream contains an infinite series which must be evaluated. The value of the series is computed by subroutine SUMVEL.

Since the partial differential equation is nonlinear, initial estimates of the mole fraction profile are needed. Simply initializing the mole fraction profile with the feed composition was found to be too "crude." That is, calculation of mole fraction profiles had to be repeated at least four times using each newly computed mole fraction profile as the best estimate of the true values. This problem becomes obvious when it is realized that for a grid with 15 radial and 21 axial positions, approximately 15 seconds of central processor time (CDC 6500 Digital computer) are required for each iteration. To alleviate this problem a simplified version of the analytical solution was used to provide the estimates.

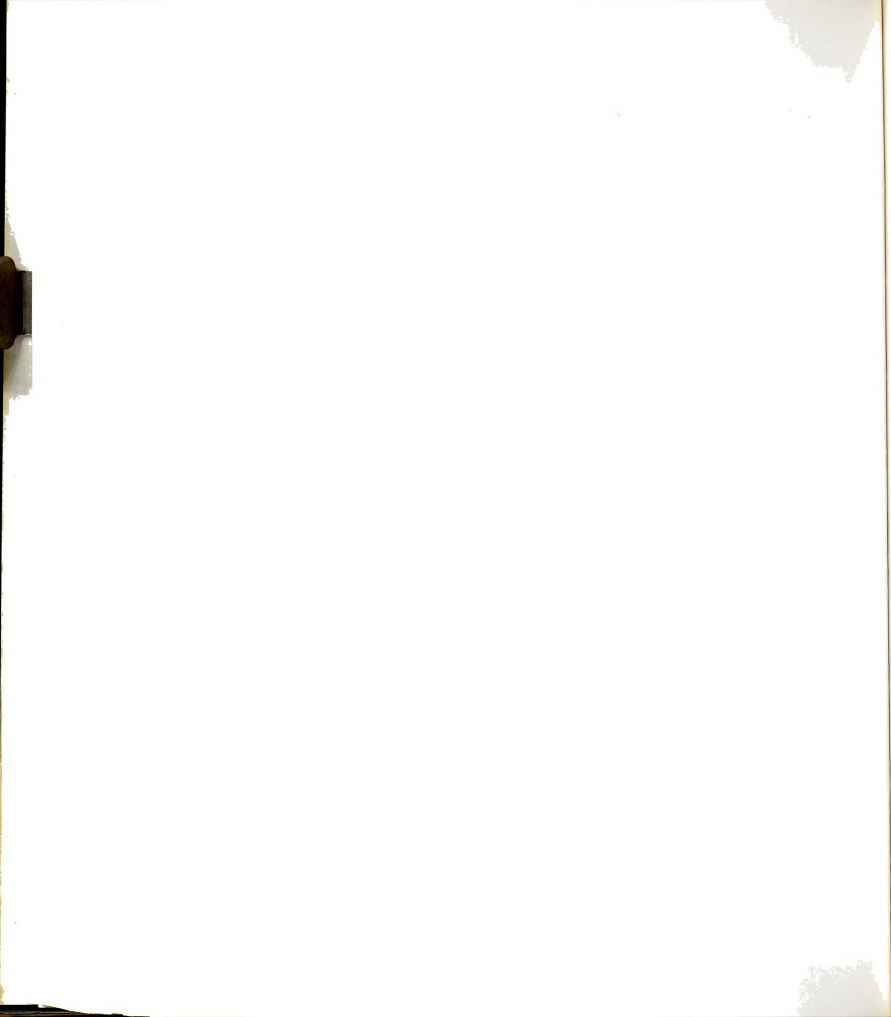
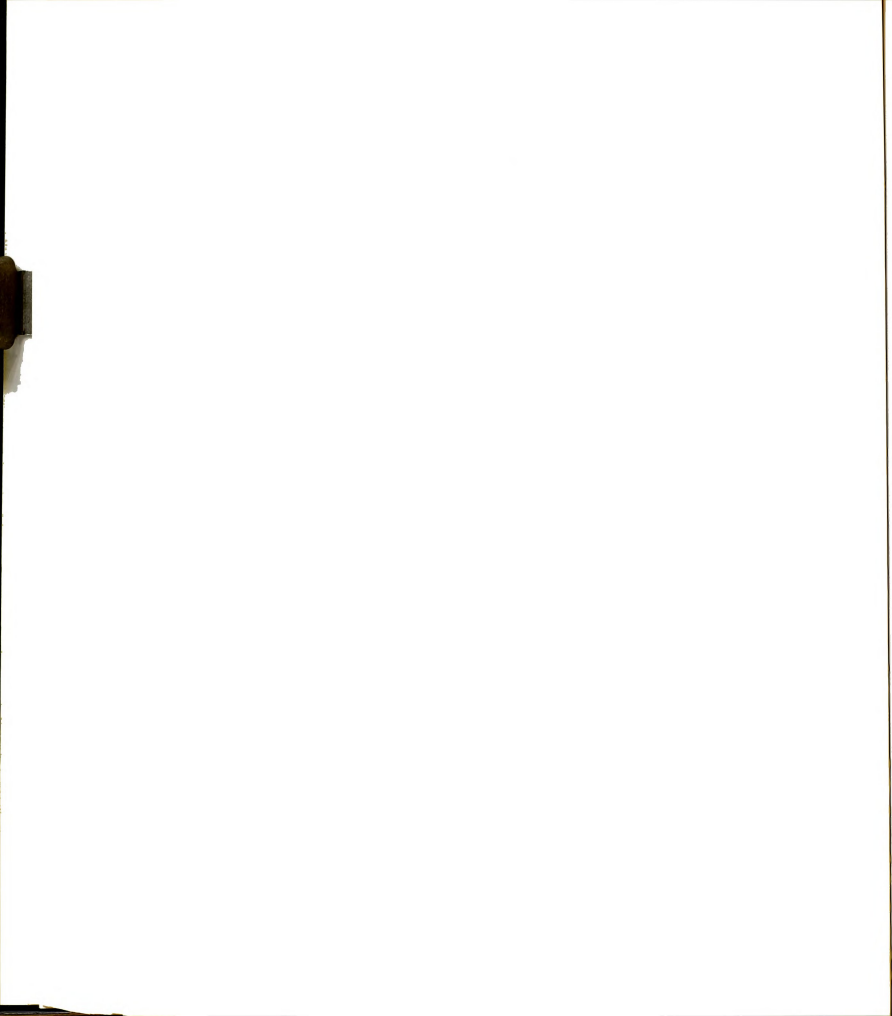


TABLE D-2.--Data Required by the FORTRAN Program NCENTRI.

Parameter	Description	Units	Formating
ITER	Controls iterations performed to compensate for the nonlinearity of the partial differential equation	None	
IZOPT	Option = 1; the first partial derivative of y with respect to z ($\partial y/\partial z$) is computed and printed Option = 0; $\partial y/\partial z$ is not computed	None	
(This completes the first data card.)			215
YF	Feed mole fraction (heavy species)	None	
WM1	Heavy species molecular weight	lb _m /lb-mole	
WM2	Light species molecular weight	lb _m /lb-mole	
T	Temperature	°R	
P0	Axis pressure	psia	
DP	Diffusivity at 1 atmosphere	cm ² /sec	
(This completes the second data card.)			6F10.0
RAD	Centrifuge radius	inches	
RM	Flow intersection	inches	
H	Centrifuge length	inches	
IW	Radial increments for each stream	None	
IH	Axial increments	None	
OMEGA	Rotational speed of the centrifuge	RPM	
(This completes the third data card.)			3F10.0, 215, F10.0
FSCFM	Feed rate	scfm	
FRAC	Ratio of the rich stream to the feed stream	None	
POWER	Option = 1 laminar flow Option = any other number; Plug type flow	None	
(This completes the fourth and final data card.)			6F10.0



The differential equation given in Chapter V-C-2 used to obtain the analytical (approximate) solution was

$$-C_5 \frac{dy}{dz} + [yQ - C_1 y(1-y)] = y_p Q,$$

where $C_5 = C_2 + C_3$,

$$C_1 = \frac{2\pi A}{RT} \int_0^R r dr \int_0^r P_v(r) r dr,$$

$$C_2 = \frac{2\pi}{RT} \frac{PD_{12} R_w^2}{2},$$

$$C_3 = \frac{2\pi}{RT} \frac{1}{PD_{12}} \int_0^R \frac{dr}{r} \left[\int_0^r P_v(r) r dr \right]^2, \text{ and}$$

$$Q = \frac{2\pi}{RT} \int_0^R P_v(r) r dr.$$

Letting $C_1' = C_1(1-y_f)$, the differential equation becomes linear,

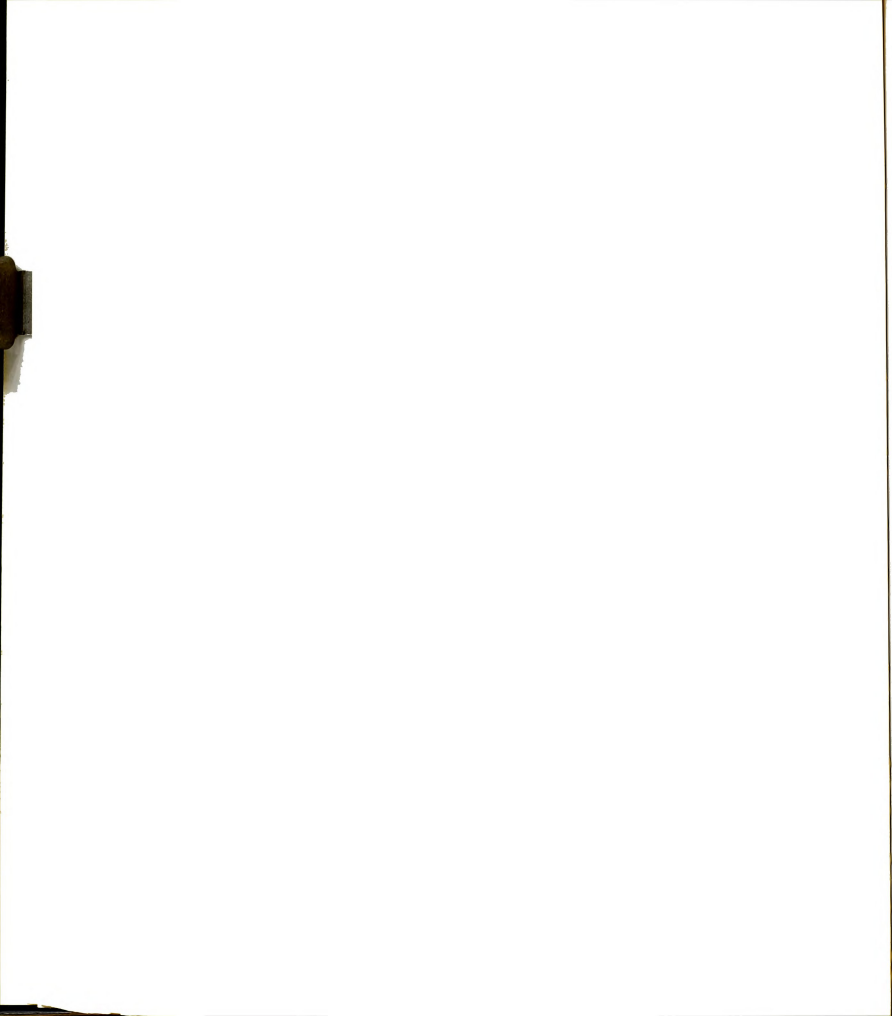
$$-C_5 \frac{dy}{dz} + (Q - C_1')y = y_p Q.$$

Its solution may be written as

$$y_p/y_f = \frac{(1 + Q/C_1')e^a}{1 + Q/C_1' e^a},$$

$$\text{where } a = \exp \left[\frac{C_1' Z}{(C_2 + C_3)} (1 + Q/C_1') \right].$$

By using the pressure and velocity profiles and the trapezoidal rule integration algorithm, the constants C_1 and C_3 can be evaluated.



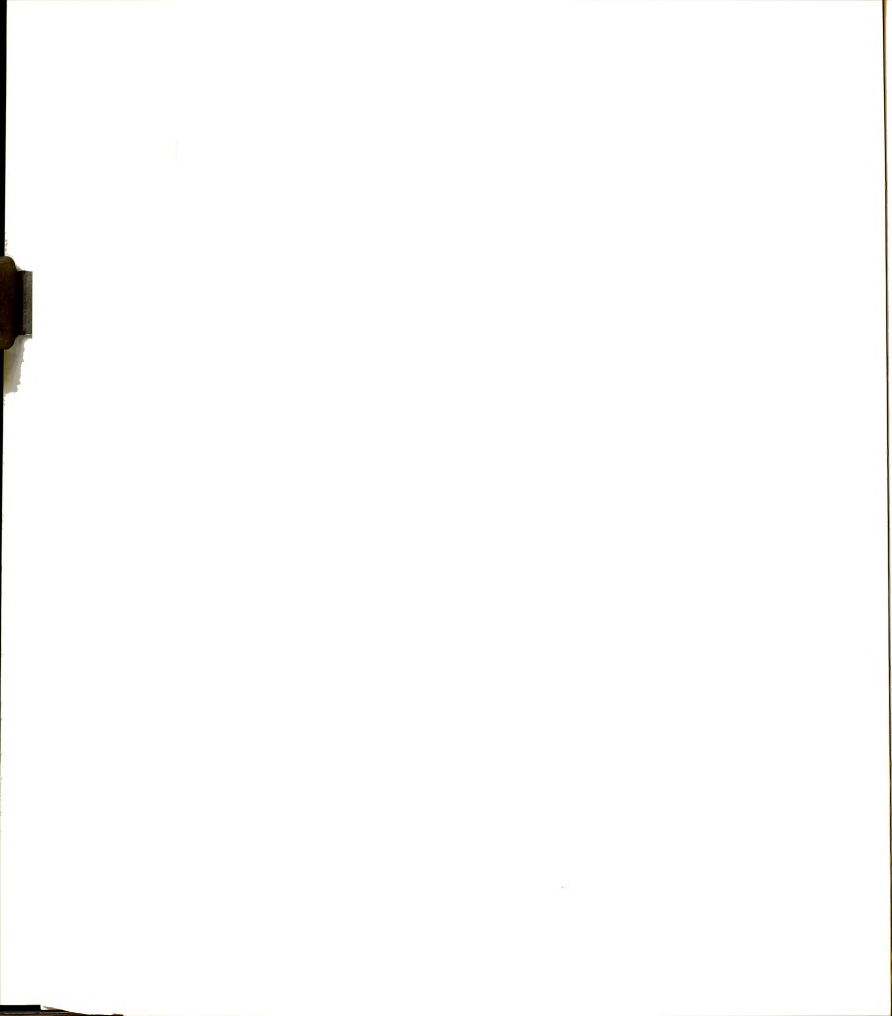
The mole fraction profile, although constant radially, can then be initialized with values which at least have an axial variance similar in form to the numerical solution. Using this approach only two successive iterations were required to compensate for the nonlinearity.

B. Writing the Numerical Approximation of the Partial Differential Equation

Finite difference formulas used to approximate partial derivatives can be found in Table C-1 in Appendix C. By using these formulas the partial differential equations and/or boundary conditions can be approximated at each grid point by a linear algebraic equation. Subroutine RDIFF is used to compute the coefficients of the equation at a grid point resulting from the approximation of any r direction derivatives, whereas subroutine ZDIFF is used to compute the coefficients of the equation resulting from the approximation of any z direction derivatives.

The integral boundary condition at the rich end of the centrifuge to determine the recycle stream composition is written as a linear algebraic equation by using Simpson's integration rule to reduce the integral to a summation. The radial boundary conditions are approximated by using the standard "method of images" technique.

By just dividing the radius into a given number of equally spaced increments, a problem arises when arbitrarily picking a flow intersection position. That is, if the flow intersection is chosen to be very near the wall, perhaps only one or two incremental positions may be included in the outer stream with the remainder in the inner stream. To avoid this situation the position of the flow intersection

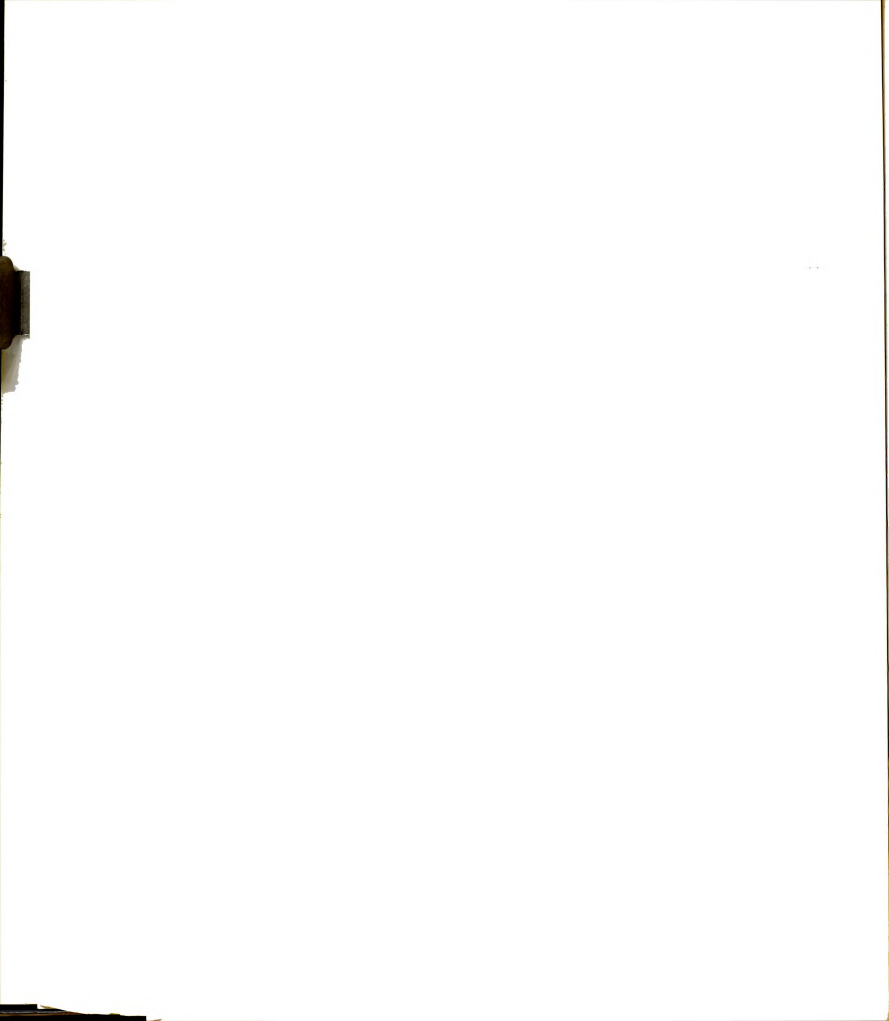


is always made to fall on a grid point. The inner and outer streams, regardless of their areas, are then divided into an equal number of increments. Thus, it is only coincidence if the increment size in the inner stream equals the increment size in the outer stream.

A problem then arises when subroutine RDIFF, while computing the coefficients of the approximating equation at each grid point resulting from the approximation of any r direction derivatives, crosses the flow intersection. This is due to the fact that RDIFF is using the finite difference formulas found in Table C-1 (Appendix C) which are for equal increments between grid points. To alleviate this situation subroutine SPECIAL is used by RDIFF to generate the necessary fourth order finite difference formulas for the grid point at the flow intersection plus one grid point before and one after it.

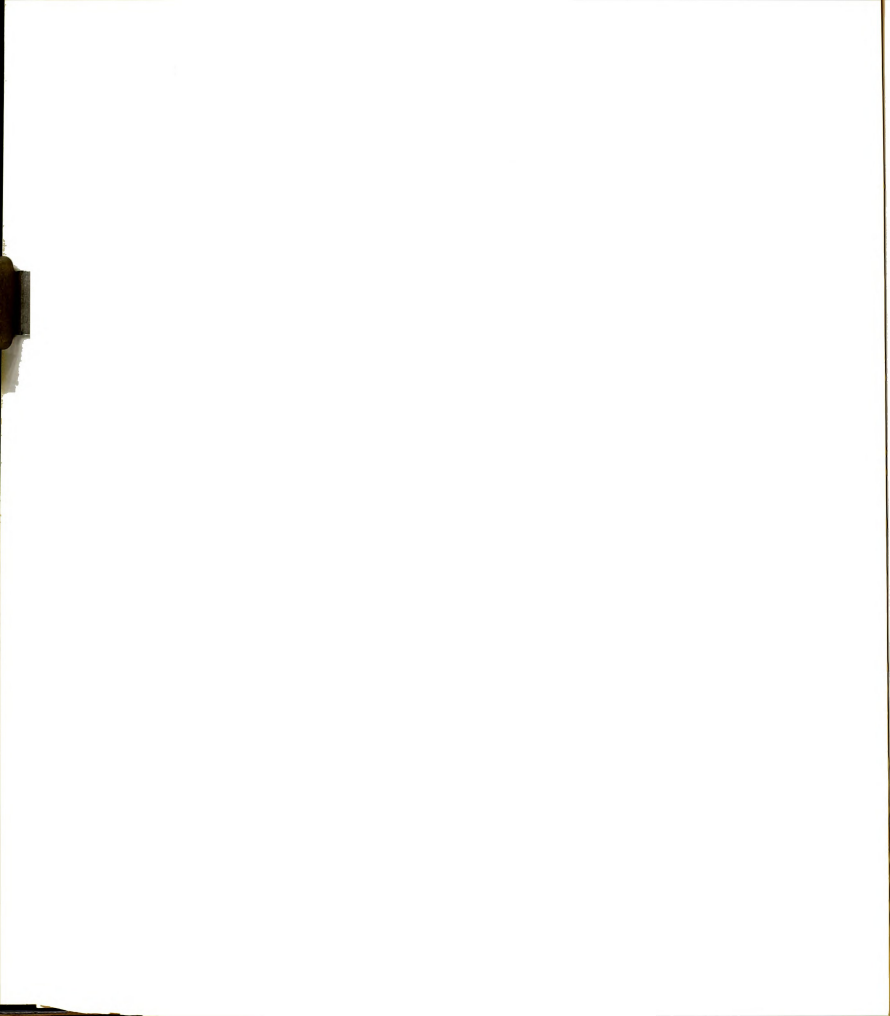
C. Solving the Set of Simultaneous Linear Equations

In essentially all the cases investigated using the program NCENTRI, 15 radial and 21 axial incremental positions were used. This, of course, results in 315 simultaneous linear equations. By making use of the fact that the coefficients of these equations create a matrix with the entries located on the main and off diagonals, the coefficient matrix expected to be (315×316) can be compressed to a (315×33) matrix. In this form subroutine DIAG567 can solve the equations simultaneously, both quickly and accurately. Subroutine DIAG567 uses subroutine UPPERT7 to upper-triangulate the equations and subroutine SWITCH7 to switch equations if necessary.



Once the mole fractions have been found they are printed by subroutine CONCOUNT and calculations are repeated if requested. After completing the mole fraction calculations if the proper option is given, the first derivative of y with respect to z is computed and printed.

Included in the remaining pages of this Appendix are a sample output and a complete listing (subroutines included) of program NCENTRI. The listing of the program and subprogram contains many comment cards which parallel and in some instances present in more detail the information given above.



GAS CENTRIFUGE ANALYSIS --- RECTIFYING NUMERICAL SOLUTION TO CASE

A. CENTRIFUGE DIMENSIONS AND SPEED

1. RADII (INCHES) = 4.000
2. ROTATING SPEED = 15.00
3. REV PER MINUTE = 20000.0

B. OPERATING CONDITIONS

1. TEMPERATURE (°R) = 530.0
2. AIRY AND LIGHT SPECIE MOLES/SEC = 14.7000
3. DIFFUSIVITY TIMES PRESSURE (FT²/SEC LB/IN/IN) = 64.3000
4. DIFFUSIVITY TIMES PRESSURE (FT²/SEC LB/IN/IN) = 28.0000
5. DIFFUSIVITY TIMES PRESSURE (FT²/SEC LB/IN/IN) = .212761E-02

C. STREAM FLOWS

1. FEED MOLE FRACTION HEAVY SPECIE = .5000E-02
2. FEED STREAM FLOW (LB MOLES/SEC) = .2000E-01
3. FEED STREAM FLOW (LB MOLES/SEC) = -0.0000
4. RICH AND LEAN STREAM FLOWS (LB MOLES/SEC) = 0.
5. RICH AND LEAN STREAM FLOWS (LB MOLES/SEC) = .92854E-06 RESPECTIVELY
6. RICH AND LEAN STREAM FLOWS (LB MOLES/SEC) = .92854E-06 RESPECTIVELY

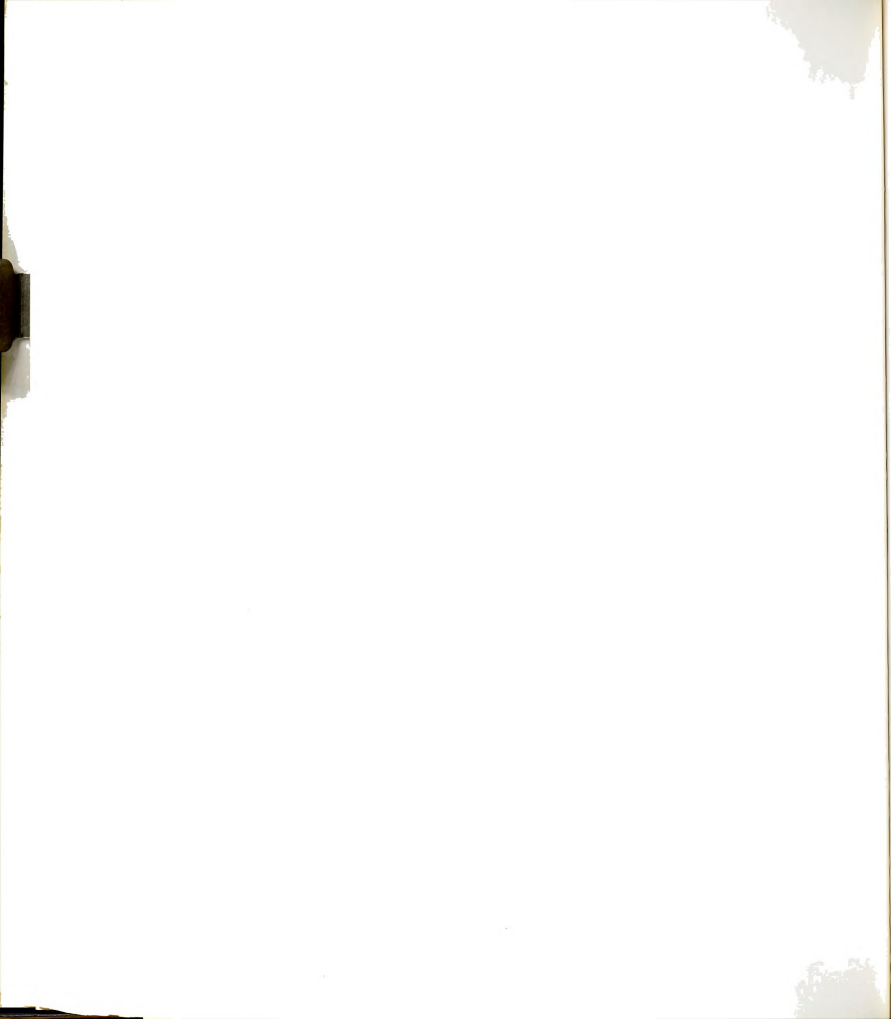
D. NUMERICAL PARAMETERS

1. FLOW INTERSECTION (INCHES) = 2.3500
2. FLOW INTERSECTION (INCHES) = 2.3500
3. OR FOR THE INNER AND OUTER STREAMS ARE EQUAL AT 7 EACH
4. THE LENGTH IS DIVIDED INTO 20 INCREMENTS
5. DL (INCHES) = .900000
6. THE LENGTH IS DIVIDED INTO 20 INCREMENTS
7. THE LENGTH IS DIVIDED INTO 20 INCREMENTS
8. THE LENGTH IS DIVIDED INTO 20 INCREMENTS
9. THE LENGTH IS DIVIDED INTO 20 INCREMENTS
10. THE LENGTH IS DIVIDED INTO 20 INCREMENTS
11. THE LENGTH IS DIVIDED INTO 20 INCREMENTS
12. THE LENGTH IS DIVIDED INTO 20 INCREMENTS
13. THE LENGTH IS DIVIDED INTO 20 INCREMENTS
14. THE LENGTH IS DIVIDED INTO 20 INCREMENTS
15. THE LENGTH IS DIVIDED INTO 20 INCREMENTS
16. THE LENGTH IS DIVIDED INTO 20 INCREMENTS
17. THE LENGTH IS DIVIDED INTO 20 INCREMENTS
18. THE LENGTH IS DIVIDED INTO 20 INCREMENTS
19. THE LENGTH IS DIVIDED INTO 20 INCREMENTS
20. THE LENGTH IS DIVIDED INTO 20 INCREMENTS

E. INITIAL PRESSURE AND VELOCITY DISTRIBUTIONS

RADIUS (INCHES)	PRESSURE (PSIA)	VELOCITY (FT/SEC)
0.000	14.70000	-.006323
.321	14.72478	-.006194
.643	14.79326	-.005807
.964	14.91851	-.005122
1.287	15.10150	-.004258
1.609	15.33214	-.003197
1.929	15.61842	-.001678
2.250	15.96455	0.000000
2.500	16.27959	.001013
2.750	16.62958	.001931
3.000	17.02472	.002762
3.250	17.46497	.003505
3.500	17.94897	.004151
3.750	18.48719	.004702
4.000	19.08039	0.000000

THE MAXIMUM INNER AND OUTER VELOCITIES ARE -.63230E-02 .19187E-02 FT/SEC RESPECTIVELY



F. THE RATIOS OF THE INTEGRATED TO ACTUAL FLOWS OF THE INNER AND OUTER STREAMS ARE
.99994

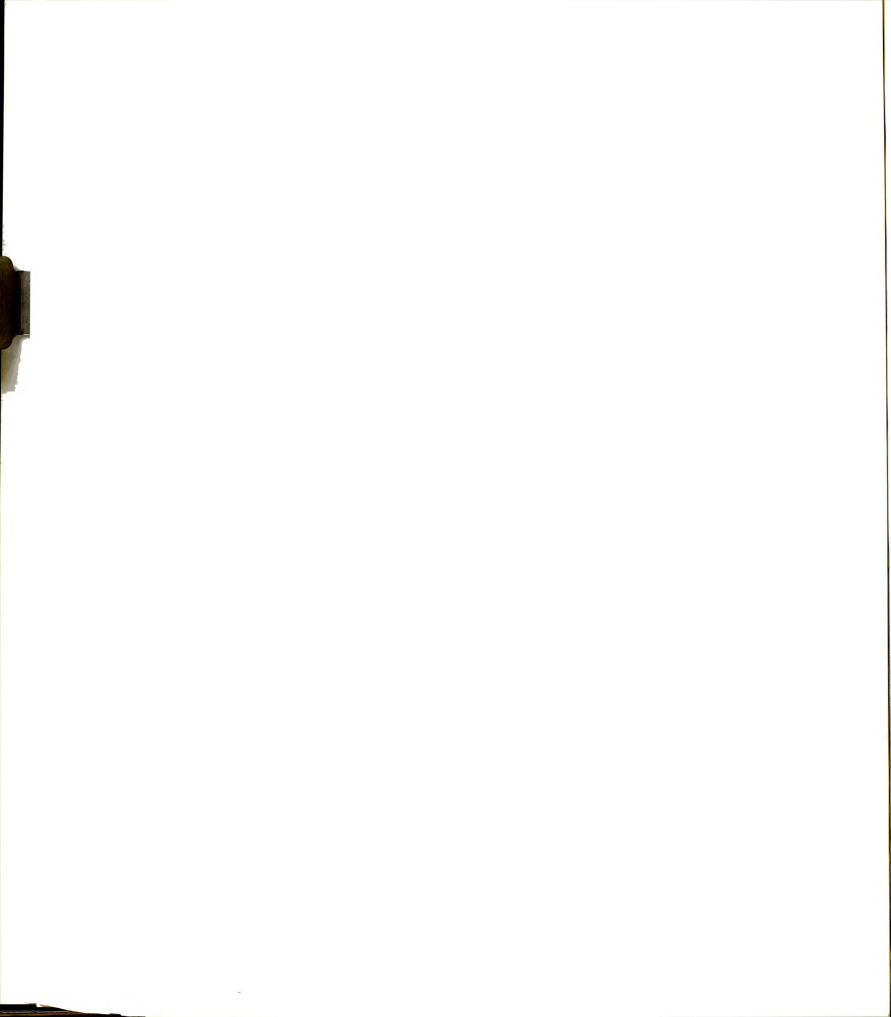
G. RESULTS

1. FEED, LEAN, AND RICH STREAM MOLE FRACTIONS
.50000E-02 .49710E-02 .99159E-02
2. SEPARATION FACTORS BASED ON THE LEAN AND FEED COMPOSITIONS
.19923E-01 .19530E-01
3. RATIOS OF RICH TO LEAN AND RICH TO FEED MOLE FRACTIONS
.12843E-01 .19431E-01

H. THE MOLE FRACTION PROFILES ARE GIVEN ON THE NEXT TWO PAGES

INNER STREAM MOLE FRACTIONS

Z (FT)	0.0000	.0260	.0536	.0804	.1071	.1339	.1607	.1875
0.0000	.49862E-02	.49710E-02	.49523E-02	.49378E-02	.49372E-02	.49587E-02	.49500E-02	
.0750	.51545E-02	.51195E-02	.50822E-02	.50465E-02	.50114E-02	.49683E-02	.49641E-02	
.1500	.53413E-02	.53010E-02	.52606E-02	.52272E-02	.51894E-02	.51299E-02	.51154E-02	
.2250	.55429E-02	.54978E-02	.54585E-02	.54232E-02	.53833E-02	.53120E-02	.52970E-02	
.3000	.57597E-02	.57171E-02	.56763E-02	.56393E-02	.56031E-02	.55120E-02	.54970E-02	
.3750	.59923E-02	.59471E-02	.59039E-02	.58626E-02	.58231E-02	.57214E-02	.57070E-02	
.4500	.61433E-02	.61031E-02	.60639E-02	.60266E-02	.59906E-02	.58906E-02	.59242E-02	
.5250	.64123E-02	.63745E-02	.63375E-02	.62960E-02	.62546E-02	.61614E-02	.61484E-02	
.6000	.66479E-02	.66206E-02	.65961E-02	.65509E-02	.64930E-02	.63921E-02	.63794E-02	
.6750	.68978E-02	.68732E-02	.68413E-02	.67935E-02	.67330E-02	.66259E-02	.66140E-02	
.7500	.71811E-02	.71491E-02	.71152E-02	.70704E-02	.70134E-02	.68934E-02	.68824E-02	
.8250	.74951E-02	.74561E-02	.74152E-02	.73634E-02	.72991E-02	.71730E-02	.71624E-02	
.9000	.78498E-02	.78026E-02	.77532E-02	.76991E-02	.76382E-02	.74897E-02	.74789E-02	
.9750	.82470E-02	.81926E-02	.81311E-02	.80627E-02	.79877E-02	.78333E-02	.78217E-02	
1.0500	.86841E-02	.86245E-02	.85582E-02	.84851E-02	.84048E-02	.82648E-02	.82520E-02	
1.1250	.91615E-02	.90971E-02	.90269E-02	.89508E-02	.88693E-02	.87494E-02	.87364E-02	
1.2000	.96737E-02	.96071E-02	.95296E-02	.94472E-02	.93593E-02	.92545E-02	.92424E-02	
1.2750	.99160E-02	.98492E-02	.97712E-02	.96826E-02	.95846E-02	.94695E-02	.94564E-02	
1.3500	.99160E-02	.98492E-02	.97712E-02	.96826E-02	.95846E-02	.94695E-02	.94564E-02	
1.4250	.99160E-02	.98492E-02	.97712E-02	.96826E-02	.95846E-02	.94695E-02	.94564E-02	
1.5000	.99160E-02	.98492E-02	.97712E-02	.96826E-02	.95846E-02	.94695E-02	.94564E-02	



OUTER STREAM MOLE FRACTIONS

RADII (FT)

Z (FT)	.1875	.2083	.2292	.2500	.2708	.2917	.3125	.3333
0.0000	.50000E-02	.50000E-02	.50000E-02	.50000E-02	.50000E-02	.50000E-02	.50000E-02	.50000E-02
.0750	.49851E-02	.49668E-02	.49485E-02	.49302E-02	.49119E-02	.48936E-02	.48753E-02	.48570E-02
.1500	.51154E-02	.51302E-02	.51450E-02	.51598E-02	.51746E-02	.51894E-02	.52042E-02	.52190E-02
.2250	.52972E-02	.53139E-02	.53306E-02	.53473E-02	.53640E-02	.53807E-02	.53974E-02	.54141E-02
.3000	.54972E-02	.55159E-02	.55346E-02	.55533E-02	.55720E-02	.55907E-02	.56094E-02	.56281E-02
.3750	.57070E-02	.57274E-02	.57478E-02	.57682E-02	.57886E-02	.58090E-02	.58294E-02	.58498E-02
.4500	.59262E-02	.59466E-02	.59670E-02	.59874E-02	.60078E-02	.60282E-02	.60486E-02	.60690E-02
.5250	.61454E-02	.61720E-02	.61986E-02	.62252E-02	.62518E-02	.62784E-02	.63050E-02	.63316E-02
.6000	.63795E-02	.64099E-02	.64403E-02	.64707E-02	.65011E-02	.65315E-02	.65619E-02	.65923E-02
.6750	.66190E-02	.66494E-02	.66798E-02	.67102E-02	.67406E-02	.67710E-02	.68014E-02	.68318E-02
.7500	.68639E-02	.68943E-02	.69247E-02	.69551E-02	.69855E-02	.70159E-02	.70463E-02	.70767E-02
.8250	.71174E-02	.71478E-02	.71782E-02	.72086E-02	.72390E-02	.72694E-02	.72998E-02	.73302E-02
.9000	.73789E-02	.74115E-02	.74441E-02	.74767E-02	.75093E-02	.75419E-02	.75745E-02	.76071E-02
.9750	.76487E-02	.76832E-02	.77177E-02	.77522E-02	.77867E-02	.78212E-02	.78557E-02	.78902E-02
1.0500	.79271E-02	.79637E-02	.80003E-02	.80369E-02	.80735E-02	.81101E-02	.81467E-02	.81833E-02
1.1250	.82147E-02	.82534E-02	.82921E-02	.83308E-02	.83695E-02	.84082E-02	.84469E-02	.84856E-02
1.2000	.85125E-02	.85534E-02	.85943E-02	.86352E-02	.86761E-02	.87170E-02	.87579E-02	.87988E-02
1.2750	.88226E-02	.88657E-02	.89088E-02	.89519E-02	.89950E-02	.90381E-02	.90812E-02	.91243E-02
1.3500	.91492E-02	.91944E-02	.92396E-02	.92848E-02	.93300E-02	.93752E-02	.94204E-02	.94656E-02
1.4250	.95034E-02	.95492E-02	.95950E-02	.96408E-02	.96866E-02	.97324E-02	.97782E-02	.98240E-02
1.5000	.99160E-02	.99521E-02	.10049E-01	.10121E-01	.10193E-01	.10265E-01	.10337E-01	.10409E-01

I. 2 ITERATIONS HAVE BEEN MADE



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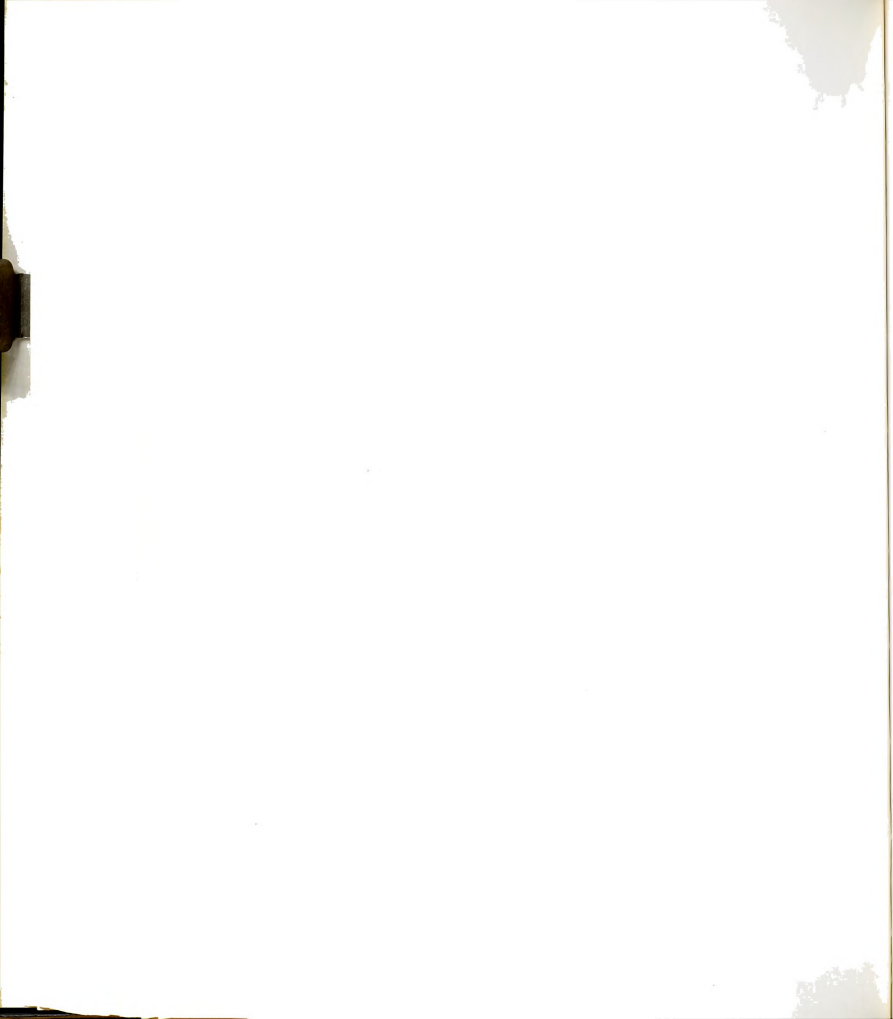
PROGRAM NCENTRI( INPUT, OUTPUT )
COMMON IW, IWPI, IWTO, IH, IHPI, DR1, DR2, DZ
COMMON PO, T, DP, WM1, WM2, OMEGA, A, VZMAXD, VZMAXU
COMMON YF, FSCFM, FRAC, FEED, PRICH, PLEAN
DIMENSION Y(21,15), P(15), R(15), VEL(15), Z(21)
DIMENSION B(15,33), C(315,33), COEFF(8)
DATA ( COEFF(I), I=1,8 ) / 1.0,4.0,2.0,4.0,2.125,3.375,3.375,
1 1.125 /
DATA MD, ND, NEQ, NEQD / 21, 15, 315, 33 /

C ..... THIS PROGRAM COMPUTES THE STEADY STATE MOLE FRACTION
C PROFILES IN THE COUNTERCURRENT RECTIFYING CENTRIFUGE .....
C
C READ 9001, ITER, IZOPT
C 9001 FORMAT( 215 )
C
C ..... CALL SUBROUTINE INITIAL TO INITIALIZE THE VARIABLES .....
C
CALL INITIAL( Y, P, R, Z, MD, ND, POWER )
DO 224 J = 1, IWTO
Y(1,J) = YF
224 Y(IHPI,J) = YF

C ..... CALL SUBROUTINE VELS TO COMPUTE THE VELOCITY AND PRESSURE
C PROFILES .....
C
CALL VELS( VEL, P, Y, R, MD, ND, POWER )

C ..... OUTPUT HEADING .....
C
PRINT 9000
9000 FORMAT( *1*, 48X, *GAS CENTRIFUGE ANALYSIS --- RECTIFYING*, //,
1 55X, *NUMERICAL SOLUTION TO PDEQ*, // )
C
C ..... OUTPUT CENTRIFUGE DIMENSIONS AND RPM .....
C

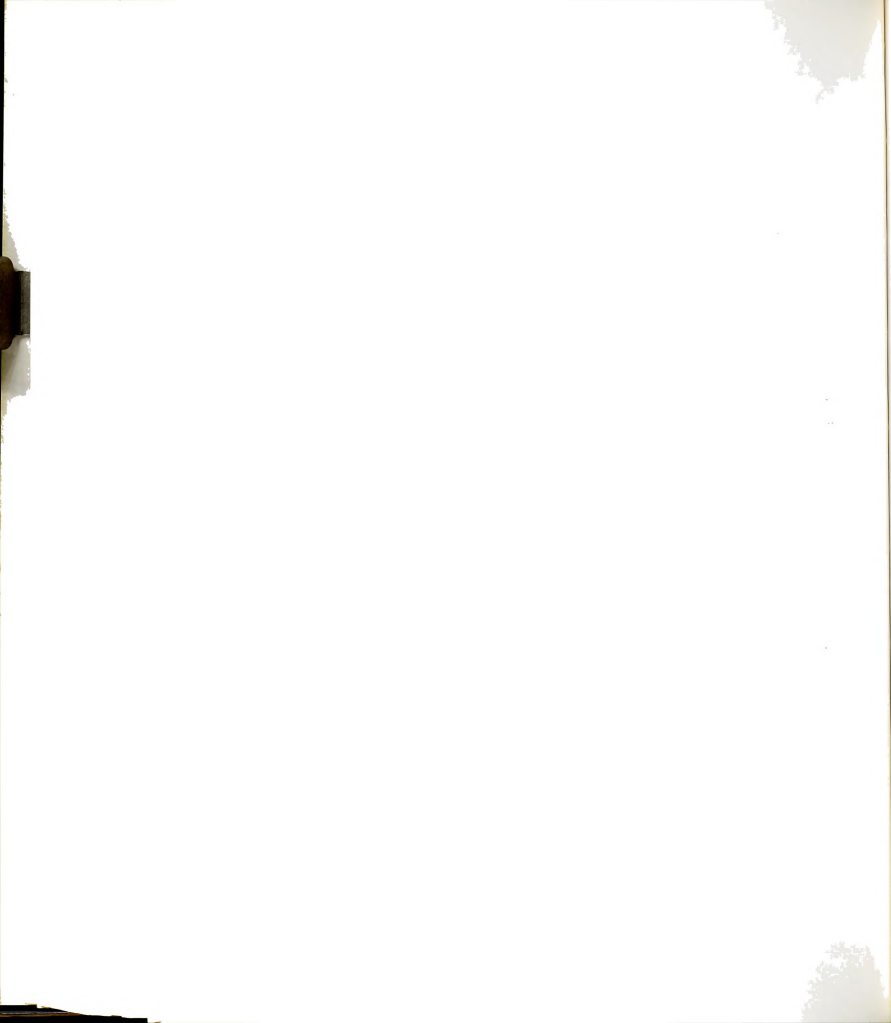
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RM = R(IWP1) * 12.0      $      RO = R(IWTWO) * 12.0
H = Z(IHP1) * 12.0
PRINT 9010, RO, H, OMEGA
9010 FORMAT( 20X, *A. CENTRIFUGE DIMENSIONS AND SPEED*, //, 30X, *1. R
      1 RADIUS(INCHES) ==, F10.3, /, 30X, *2. LENGTH(INCHES) ==, F10.2, /,
      2 30X, *3. REV PER MINUTE ==, F10.1, / )
C
C
C      ***** OUTPUT OPERATING CONDITIONS *****
PRINT 9020, T, PO, WM1, WM2, DP
9020 FORMAT( 20X, *8. OPERATING CONDITIONS*, //, 30X, *1. TEMPERATURE(
      1R) ==, F10.1, /, 30X, *2. AXIS PRESSURE(Psia) ==, F12.4, /, 30X,
      2 *3. HEAVY AND LIGHT SPECIE MOL WTS ==, 2F15.4, /, 30X, *4. DIFF
      3USIVITY TIMES PRESSURE(FIFT/SEC LBF/IN/IN) ==, E15.6, / )
C
C
C      ***** OUTPUT STREAM FLOWS *****
PRINT 9030, YF, FSCFM, FEED, FRAC, PRICH, PLEAN
9030 FORMAT( 20X, *C. STREAM FLOWS*, //, 30X, *1. FEED MOLE FRACTION(H
      1EAVY SPECIE) ==, E15.5, /, 30X, *2. FEED RATE IN SCFM AND LB MOLE
      2S/SEC ==, 2E15.5, * RESPECTIVELY*, /, 30X, *3. RICH STREAM/FEED
      3STREAM ==, F10.4, /, 30X, *4. RICH AND LEAN STREAM FLOWS(LB MOLES
      4/SEC) ==, 2E15.5, * RESPECTIVELY*, / )
C
C
C      ***** OUTPUT NUMERICAL PARAMETERS *****
D11 = DR1 * 12.0      $      D12 = DR2 * 12.0
DH = DZ * 12.0
PRINT 9040, RM, IM, D11, D12, IH, DH
9040 FORMAT( 20X, *D. NUMERICAL PARAMETERS*, //, 30X, *1. FLOW INTERSE
      1CTION(INCHES) ==, F10.4, /, 30X, *2. RADIAL INCREMENTS FOR THE IN
      2NER AND OUTER STREAMS ARE EQUAL AT*, IS, * EACH*, /, 30X, *3. DR
      3FOR THE INNER AND OUTER STREAMS RESPECTIVELY ==, 2F10.6, * INCHE
      4S*, /, 30X, *4. THE LENGTH IS DIVIDED INTO*, IS, * INCREMENTS*,
      5 /, 30X, *5. DL(INCHES) ==, F10.6, / )
C

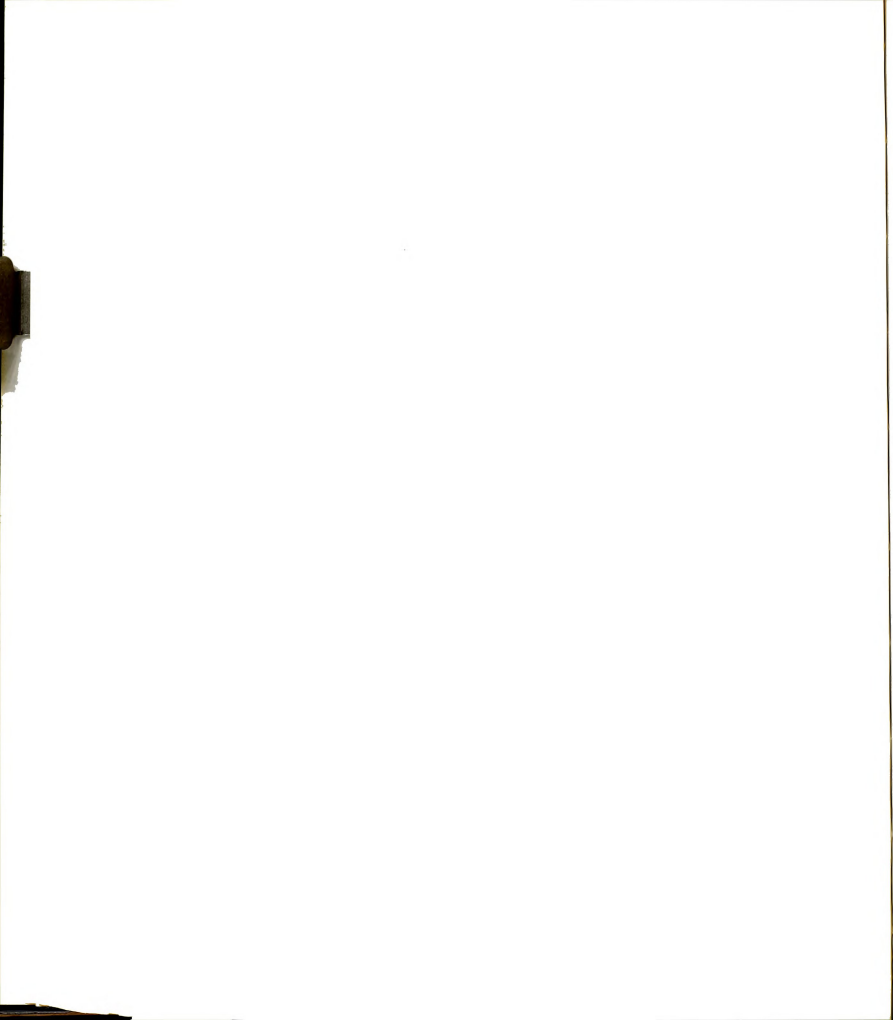
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C      ..... OUTPUT THE INITIAL PRESSURE AND VELOCITY DISTRIBUTIONS .....
C
9050 PRINT 9050
1, 43X, *RADIUS(INCHES)*, 6X, *PRESSURE(Psia)*, 4X, *VELOCITY(ft/SE
2C)*, / )
DO 9060 I = 1, IWTWO
RD = R(I) * 12.0
9060 PRINT 9070, RD, P(I), VEL(I)
9070 FORMAT( 38X, F15.3, F21.5, F20.6 )
PRINT 9080, VZMAXD, VZMAXU
9080 FORMAT( //, 25X, *THE MAXIMUM INNER AND OUTER VELOCITIES ARE*,
1 2E16.5, * FT/SEC RESPECTIVELY* )
C
C      ..... USING A SIMPLIFIED VERSION OF THE ANALYTICAL SOLUTION
C      THE MOLE FRACTIONS ARE ESTIMATED .....
C
S1 = 0.0 $ S2 = 0.0 $ S3 = 0.0
DO 222 I = 2, IWTWO
DUM = R(I) - R(I-1)
S1 = S1 + P(I) * VEL(I) * R(I) * DUM
S2 = S2 + S1 * R(I) * DUM
222 S3 = S3 + S1 * S1 / R(I) * DUM
S2 = - S2 * A / T * ( 1.0 - YF ) * 0.5855
S3 = S3 / DP * 0.5855 / T
S1 = DP * R(IWTWO) * R(IWTWO) / 2.0 * 0.5855 / T
DUM = PRICH / S2 + 1.0 $ S2 = S2 / ( S3 + S1 )
DO 223 I = 1, IHP1
S1 = EXP( S2 * DUM * Z(I) )
S1 = YF * DUM * S1 / ( 1.0 + (DUM-1.0) * S1 )
DO 223 J = 1, IWTWO
223 Y(I,J) = S1
C
C      ..... COMPUTE INNER AND OUTER FLOW RATES --- INTEGRATED .....
C
F1 = 0.0 $ F0 = 0.0

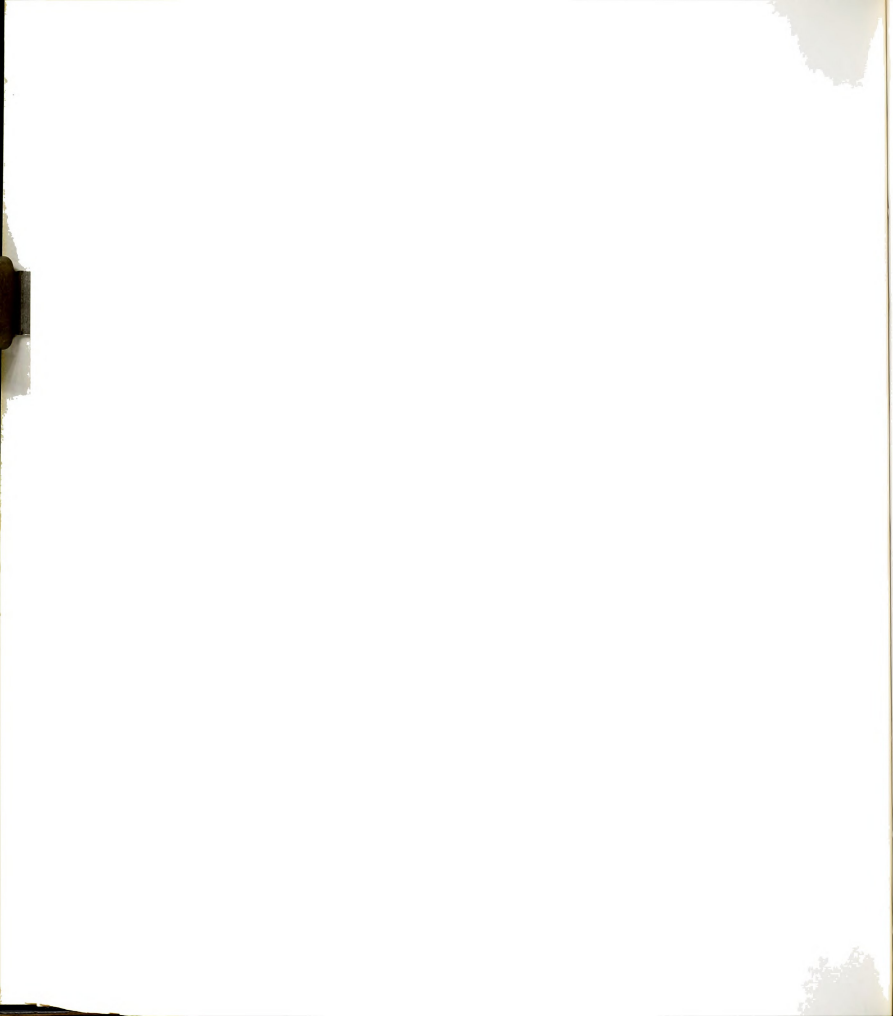
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DO 2000 J = 1, IWP1
  K = IW + J
  FI = P(J)*VEL(J)*R(J)*COEFF(J)
  FO = FO + P(K)*VEL(K)*R(K)*COEFF(J)
  RFI = -FI / PLEIN / T * 0.5859595173 * DR1 / 3.0
  RFO = FO / FEED / T * 0.5859595173 * DR2 / 3.0
  C
  C ..... APPLY A CORRECTION FOR THE DIFFERENT ERRORS .....
  C
  C
  C FO = ( -FI * DR1 + FO * FRAC * DR2 ) / DR2
  C ..... BEGIN SOLUTION BY SETTING CONSTANTS AND CLEARING C .....
  C
  C DO 9999 IT = 1, ITER
  C IMODE = 1 $ IEQ = 1 $ IA = 2*IWTWO*3 $ MEQ = IWTWO*IHPI
  C DO 2010 I = 1, MEQ
  C DO 2010 J = 1, IA
  C 2010 C(I,J) = 0.0
  C
  C ..... BEGIN WRITING THE EQUATIONS FOR EACH ROW .....
  C
  C DO 2020 I = 1, IHPI
  C DO 2030 II = 1, IWTWO
  C DO 2030 J = 1, IA
  C 2030 R(I,II,J) = 0.0
  C IF( I-2 ) 2040, 2050, 2040
  C 2050 IMODE = 2
  C 2040 CALL RDIFF( Y, R, B, C, IEQ, I, IA, MD, ND, NEG, NEQD )
  C CALL ZDIFF( FO, I, IA, Y, R, P, VEL, B, C, MD, ND, NEG, IEQ )
  C CALL DIAG56( IMODE, B, C, IWTWO, MEQ, IA, ND, NEG, NEQD )
  C 2020 IEQ = IEQ + IWTWO
  C
  C ..... SOLUTION COMPLETE GIVE ANSWERS TO Y .....
  C
  C IEQ = 0
  C DO 2060 I = 1, IHPI

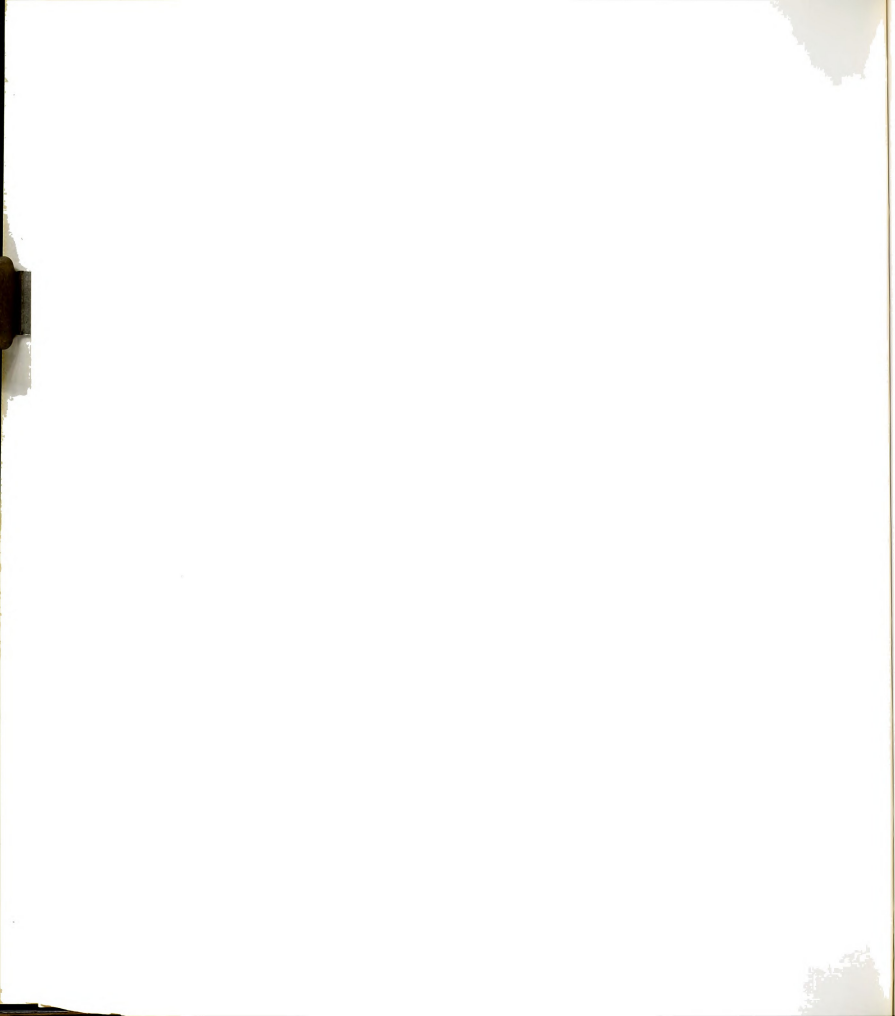
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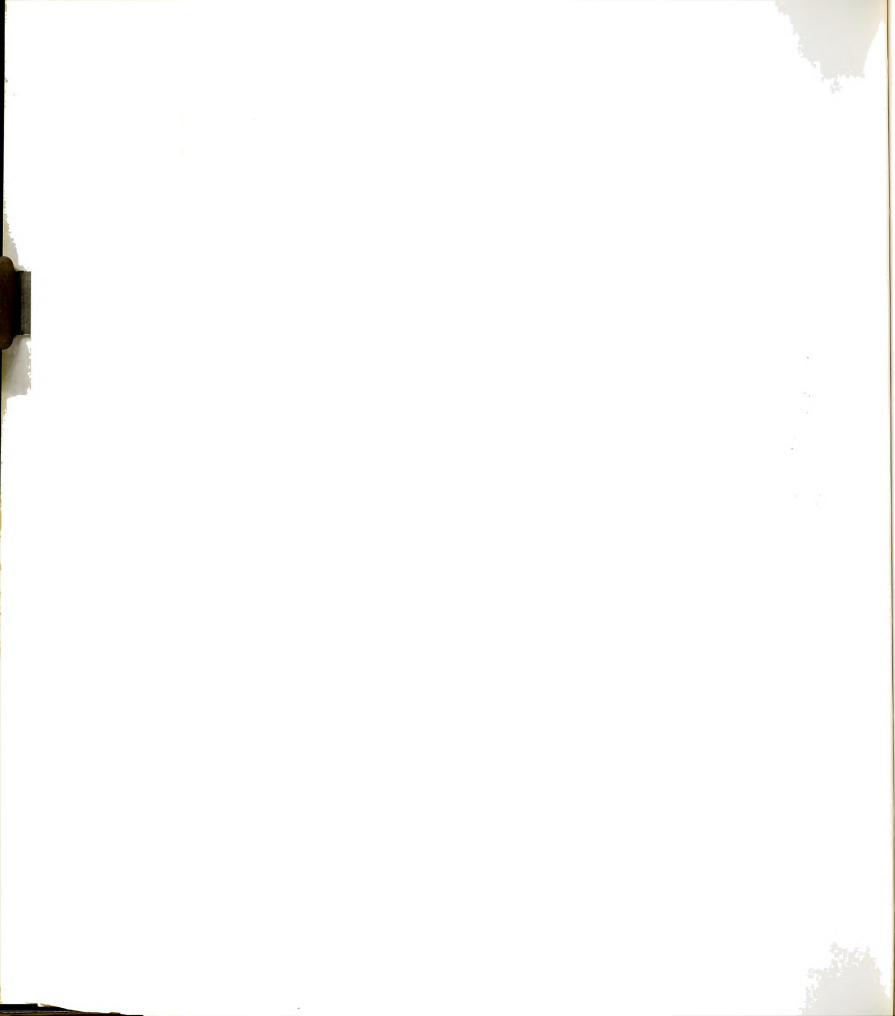


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DO 2060 J = 1, IWTWO
  IEQ = IEQ + 1
2060 Y(I,J) = C(IEQ,IA)
  YRO = Y(IHP1,1)
C
C ..... INTEGRATE TO FIND THE LEAN STREAM COMPOSITION .....
C
  YL = 0.0
  DO 2070 J = 1, IWP1
    DUM = P(J)*VEL(J)*R(J) $      DDUM = -DP * R(J) / DZ
    2070 YL = YL + (DUM*Y(1,J) + DDUM*( Y(2,J) - Y(1,J) ) ) * COEFF(J)
    YL = YL / FI
C
C ..... OUTPUT STREAM INTEGRATION ERROR .....
C
2520 PRINT 2820, RFI, RFO
2820 FORMAT( '1%, 20X, *F, THE RATIOS OF THE INTEGRATED TO ACTUAL FLOWS
1 OF THE INNER AND OUTER STREAMS ARE', /, 30X, 2F15.5 )
C
C ..... COMPUTE SEPARATIONS AND OUTPUT .....
C
  SL = YRO/(1.0-YRO) * (1.0-YL)/YL
  SF = YRO/(1.0-YRO) * (1.0-YF1)/YF
  YROYF = YRO/YF
  PRINT 2810, YF, YL, YRO, SL, SF, YROYL, YROYF
2810 FORMAT( '//, 20X, *G, RESULTS', /, 30X, *1. FEED, LEAN, AND RICH
1 STREAM MOLE FRACTIONS', /, 30X, 3E16.6, /, 30X, *2. SEPARATION FA
CTORS BASED ON THE LEAN AND FEED COMPOSITIONS', /, 30X, 2E16.6,
3 //, 20X, *3. RATIOS OF RICH TO LEAN AND RICH TO FEED MOLE FRACTI
ON', /, 30X, 2E16.6, /, 30X, *4. THE MOLE FRACTION PROFILES ARE
5 GIVEN ON THE NEXT TWO PAGES' )
  PRINT 7830
7830 FORMAT( '1%, //, 20X, *INNER STREAM MOLE FRACTIONS', /, )
  CALL CONCOUT( 2, R, Y, 0, 1, IWP1, IHP1, MD, ND )
  PRINT 7850
7850 FORMAT( '1%, //, 20X, *OUTER STREAM MOLE FRACTIONS', /, )

```





```

SUBROUTINE INITIAL( Y, P, R, Z, MD, ND, POWER )
COMMON IW, IWP1, IWTWO, IH, IHP1, DR1, DR2, DZ
COMMON PO, T, DP, WM1, WM2, OMEGA, A, VZMAXD, VZMAXU
COMMON YF, FSCFM, FRAC, FEED, PRICH, PLEAN
DIMENSION Y(MD,ND), P(ND), R(ND), Z(ND)

..... THIS SUBROUTINE READS IN OPERATING CONDITIONS AND
      INITIALIZES VARIABLES AND ARRAYS .....

..... INPUT DATA .....

READ 10, YF, WM1, WM2, T, PO, DP
10 FORMAT( 6F10.0 )
DP = DP / 929.0304 * 14.696
READ 15, RAD, RM, H, IW, IH, OMEGA
15 FORMAT( 3F10.0, 2I5, F10.0 )

..... COMPUTE INCREMENTS .....

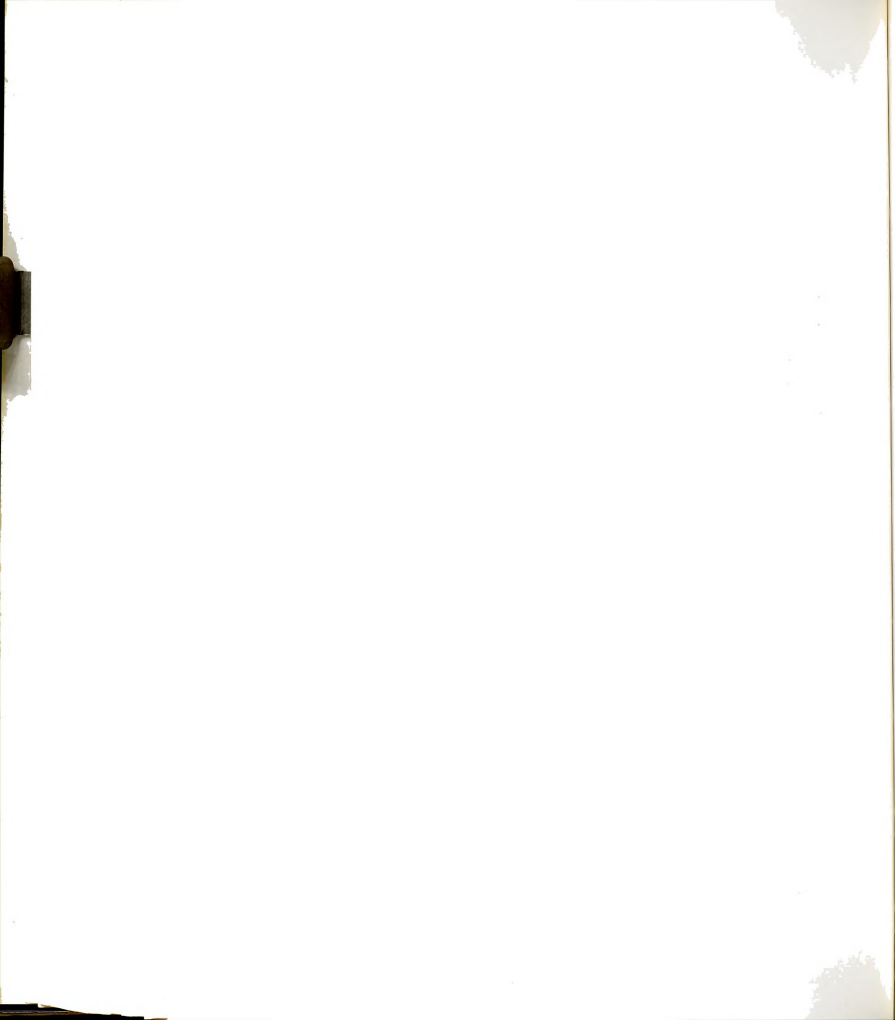
DR1 = RM / FLOAT( IW ) / 12.0
DR2 = ( RAD - RM ) / FLOAT( IW ) / 12.0
DZ = H / FLOAT( IH ) / 12.0
IWP1 = IW + 1
IHP1 = IH + 1
IWTWO = IWP1 + IW
R(1) = Z(1) = 0.0

..... COMPUTE INCREMENTAL HEIGHT AND RADIAL DISTANCES .....

DO 20 J = 2, IWTWO
  IF( J.GT. IHP1 ) GO TO 25
  R(J) = R(J-1) + DR1
  Z(J) = Z(J-1) + DR2
20 CONTINUE
DO 30 I = 2, IHP1
  Z(I) = Z(I-1) + DZ
30 CONTINUE

..... COMPUTE THE CONSTANT A .....

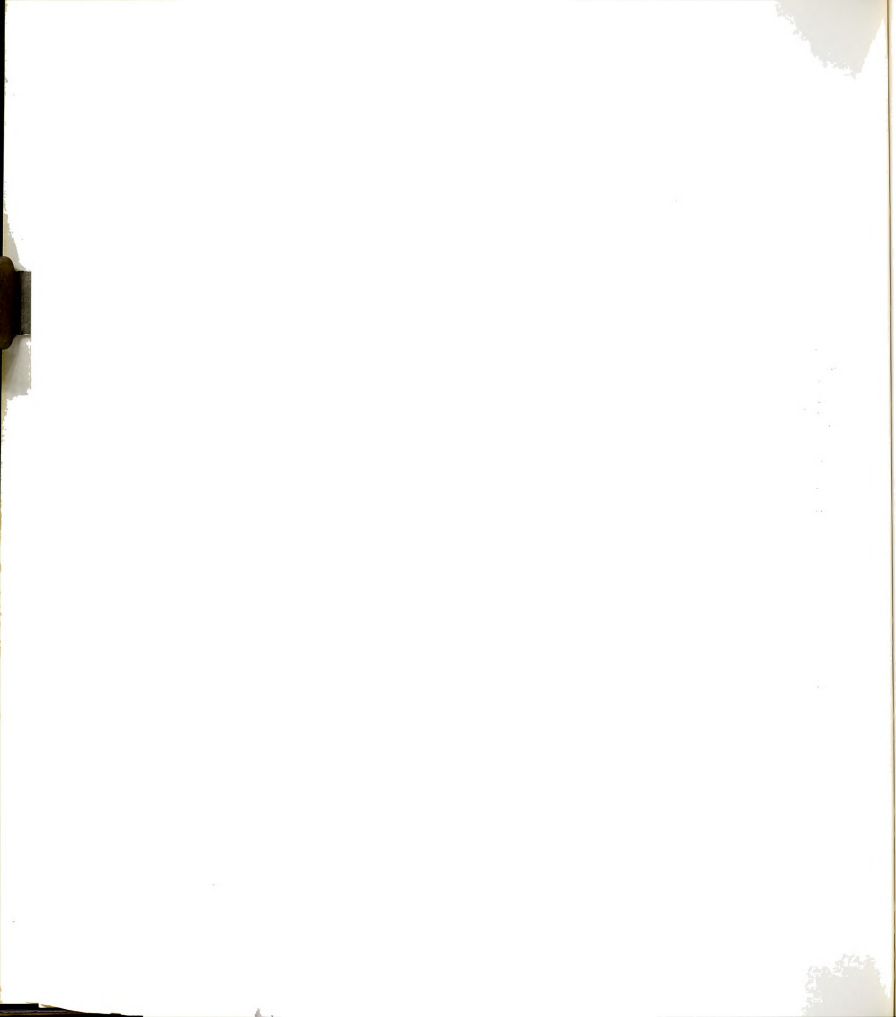
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C      A = OMEGA * OMEGA / T * 2.207381664E-07 * ( WM1 - WM2 )
C
C      ..... INPUT FEED RATE AND FRACTION TAKEN IN RICH STREAM .....
C
C      ..... POWER IS THE PARAMETER WHICH DETERMINES THE TYPE OF FLOW ----
C      POWER = 1 = LAMINAR FLOW, POWER = 0 = PLUG FLOW .....
C
C      READ 10, FSCFM, FRAC, POWER
C      FEED = FSCFM / 21539.19488
C      PRICH = FEED * FRAC * 5      PLEAN = FEED - PRICH
C      RETURN
C      END

```



```

SUBROUTINE VEL( P, Y, R, MD, ND, POWER )
COMMON IW, IWP1, IWTWO, IH, IHP1, DR1, DR2, DZ
COMMON PO, T, DP, WM1, WM2, OMEGA, A, VZMAXD, VZMAXU
COMMON YF, FSCFM, FPAC, FEED, PRICH, PLEAN
DIMENSION VEL(ND), P(ND), Y(ND,ND), R(ND)

..... THIS SUBROUTINE COMPUTES THE VELOCITY PROFILES FOR THE
TWO STREAMS .....

..... COMPUTE THE AVERAGE MOL WT OF THE INNER STREAM .....

I = 1 $ C1 = 0.0
DO 10 J = 2, IWP1
  C1 = C1 + Y(I,J-1)*R(J-1) + Y(I,J)*R(J)
10 C1 = C1 * DR1 / R(IWP1) / R(IHP1)
  C1 = WM1*C1 + WM2 * ( 1.0-C1 )

..... COMPUTE THE MAXIMUM INNER VEL AND THE VEL PROFILE .....

A1 = A/( WM1-WM2 ) $ RR = R(IWP1) * R(IHP1)
DUM1 = C1 * A1 * RR / 2.0 GO TO 5
IF( POWER .EQ. 1 ) GO TO 5

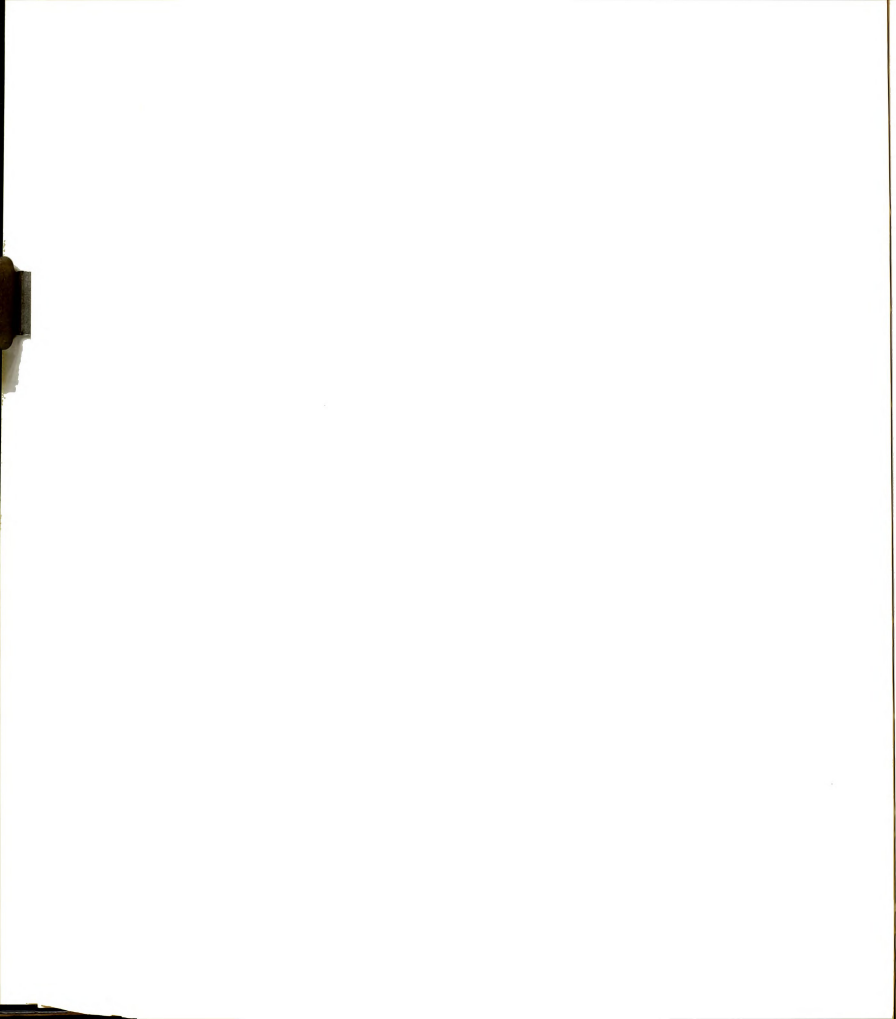
..... THE INNER STREAM IS FLOWING IN PLUG FLOW .....

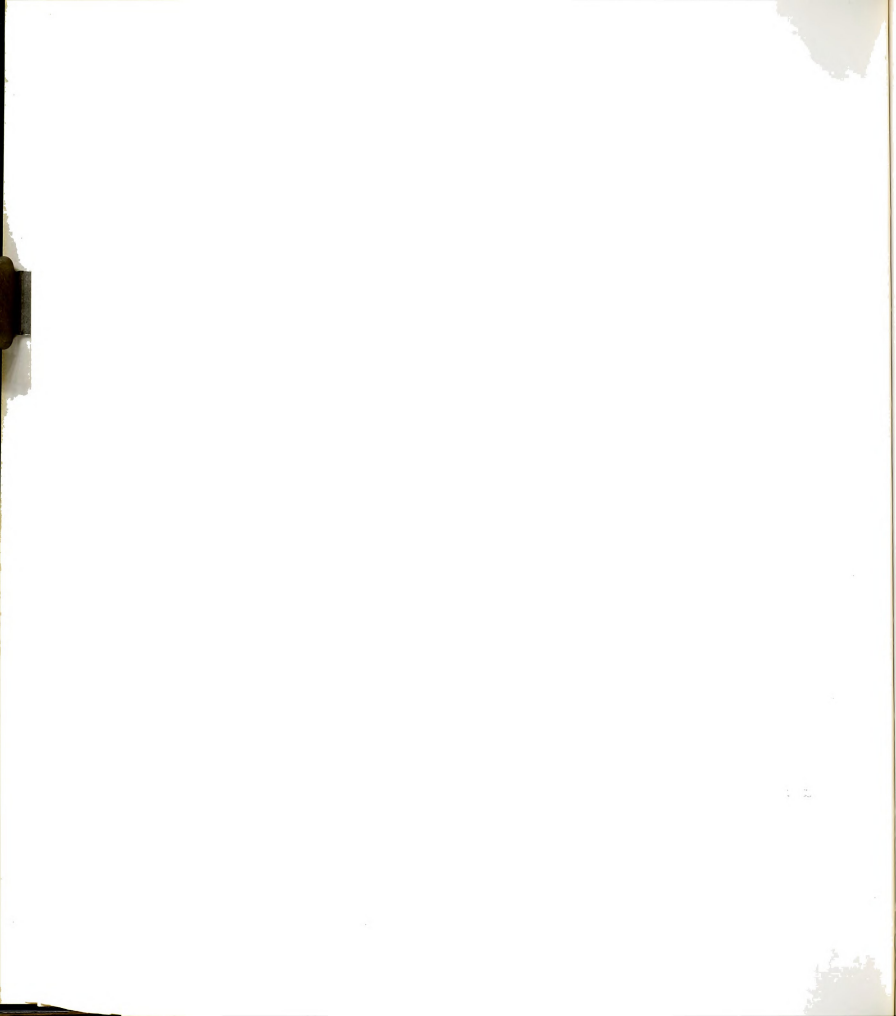
DUM = PO / C1 / A1 * ( EXP( DUM1 ) - 1.0 )
VZMAXD = - PLEAN * T / DUM * 1.706602539
DO 6 J = 1, IWP1
  P(J) = PO * EXP( C1 * A1 * R(J) * R(J) / 2.0 )
6 VEL(J) = VZMAXD
  VEL(IWP1) = 0.0 $ GO TO 7

..... LAMINAR PROFILE .....

5 DUM = PO / C1 / A1 * ( ( EXP(DUM1) - 1.0 ) / DUM1 - 1.0 )
VZMAXD = -PLEAN * T / DUM * 1.706602539

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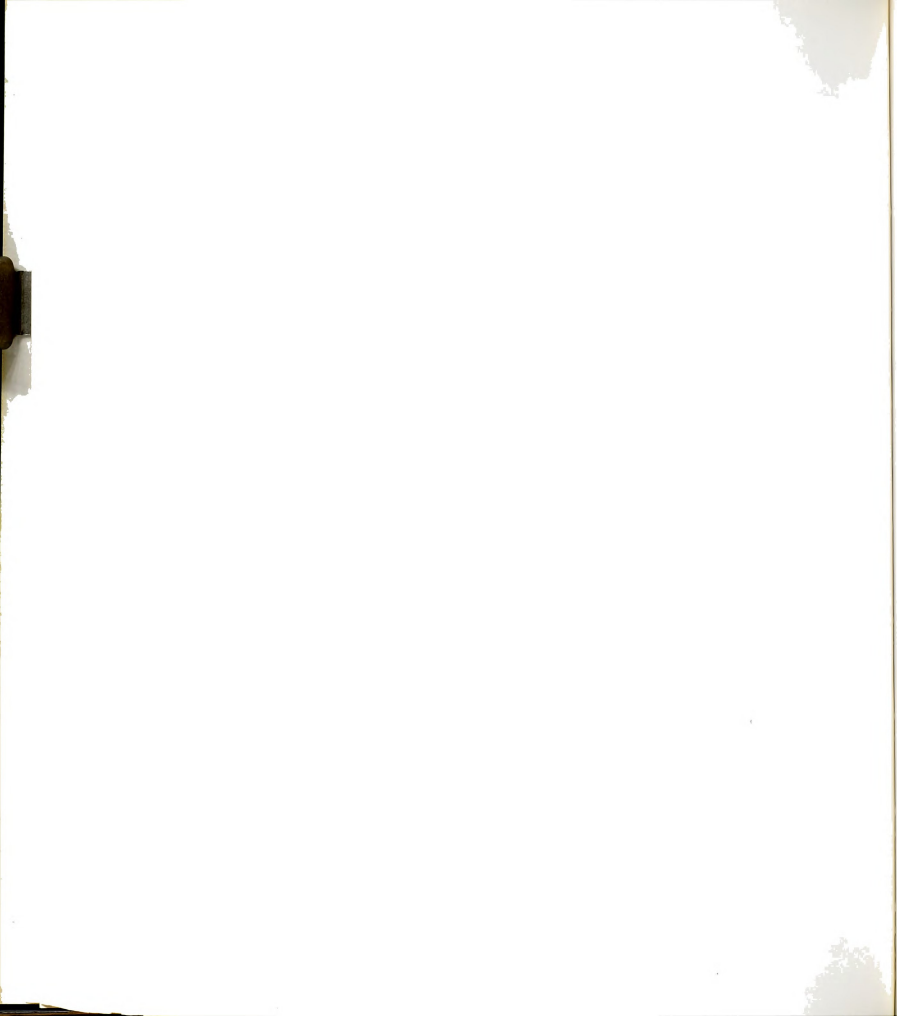




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S = ( S + E1*(RK*RK-1.0) + (E2-E1)/DUM2 ) / A1 / C2
VZMAXU = FEED / CC / S $ E1 = VZMAXU / C
DO 40 J = K, IWTWO
P(J) = PK * EXP( C2 * A1 * R(J) * R(J) / 2.0 )
40 VEL(J) = E1 * ( 1.0 - R(J)*R(J)/RRR + RT * ALOG( R(J)/R(IWTWO)))
RETURN
END

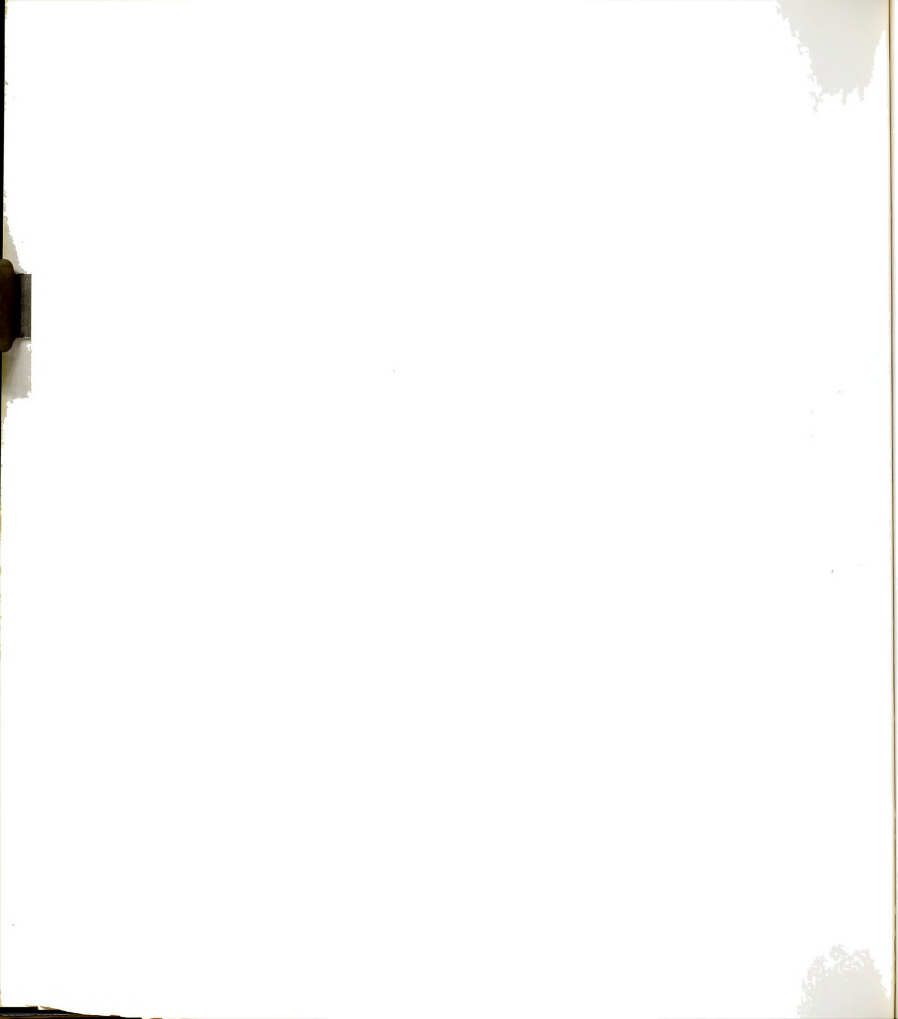
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```

C
C
C
C
SUBROUTINE SURVEL( B, A, S )
..... THIS SUBROUTINE IS USED TO COMPUTE THE SERIES NEEDED
        FOR THE CALCULATION OF THE OUTER VELOCITY .....
K = 1 $ N = 1 $ S = 0.0
AS = BS = 1.0 $ BS = BS * B $ K = K * N
10 AS = AS * A $
DS = ( AS - BS ) / FLOAT( N * K ) $ S = DS + S
IF( ABS( DS / S ) .LT. 1.0E-07 ) RETURN
N = N + 1 $ GO TO 10
END

```



```

SUBROUTINE ROIFF( Y,R,B,C,IEQ,IR,IA,MD,ND,NEQ,NEQD )
COMMON IY, IH1, IY2, IH, IH1, DR1, DR2, DZ
COMMON PO, T, DP, WM1, WM2, OMEGA, A, VZMAXD, VZMAXU
COMMON YF, FSCFM, FRAC, FEED, PRICH, PLEAN
DIMENSION Y(HD,ND), R(ND), B(ND,NEQD), C(NEQ,NEQD)
DIMENSION CC(4,8), CO(5,6)
DATA ITIME/ 1 /

```

```

C ..... THIS SUBROUTINE WRITES THE R DIRECTION FINITE DIFFERENCE
C EQUATIONS .....
C

```

```

IF( ITIME .GT. 1 ) GO TO 1000
ITIME = 2

```

```

C ..... DUE TO THE CHANGING INCREMENT SIZE AT THE INTERSECTION
C SPECIAL DIFFERENCE COEFFICIENTS MUST BE GENERATED .....
C

```

```

CC(1,5) = -2.0*DR1 $ CC(2,5) = -DR1 $ CC(3,5) = DR1
CC(4,5) = DR1+DR2 $ CALL SPECIAL( CO, CC, 4, 1 )
CC(1,5) = -2.0*DR1 $ CC(2,5) = -DR1 $ CC(3,5) = DR2
CC(4,5) = 2.0*DR2 $ CALL SPECIAL( CO, CC, 4, 3 )
CC(1,5) = -DR1-DR2 $ CC(2,5) = -DR2 $ CC(3,5) = DR2
CC(4,5) = 2.0*DR2 $ CALL SPECIAL( CO, CC, 4, 5 )
DR1 = 1.0/DR1/DR1 $ DR2 = 1.0/DR2/DR2
1000 IF( IR .EQ. IH1 ) GO TO 200

```

```

C ..... NO FLUX THROUGH THE AXIS .....
C

```

```

C(IEQ,1) = -415.0/72.0*DR1 - 2.0*A*( 1.0-Y(IR,1) )
C(IEQ,2) = 8.0*DR1 $ C(IEQ,3) = -3.0*DR1
C(IEQ,4) = 8.0/9.0*DR1 $ C(IEQ,5) = -DR1/8.0

```

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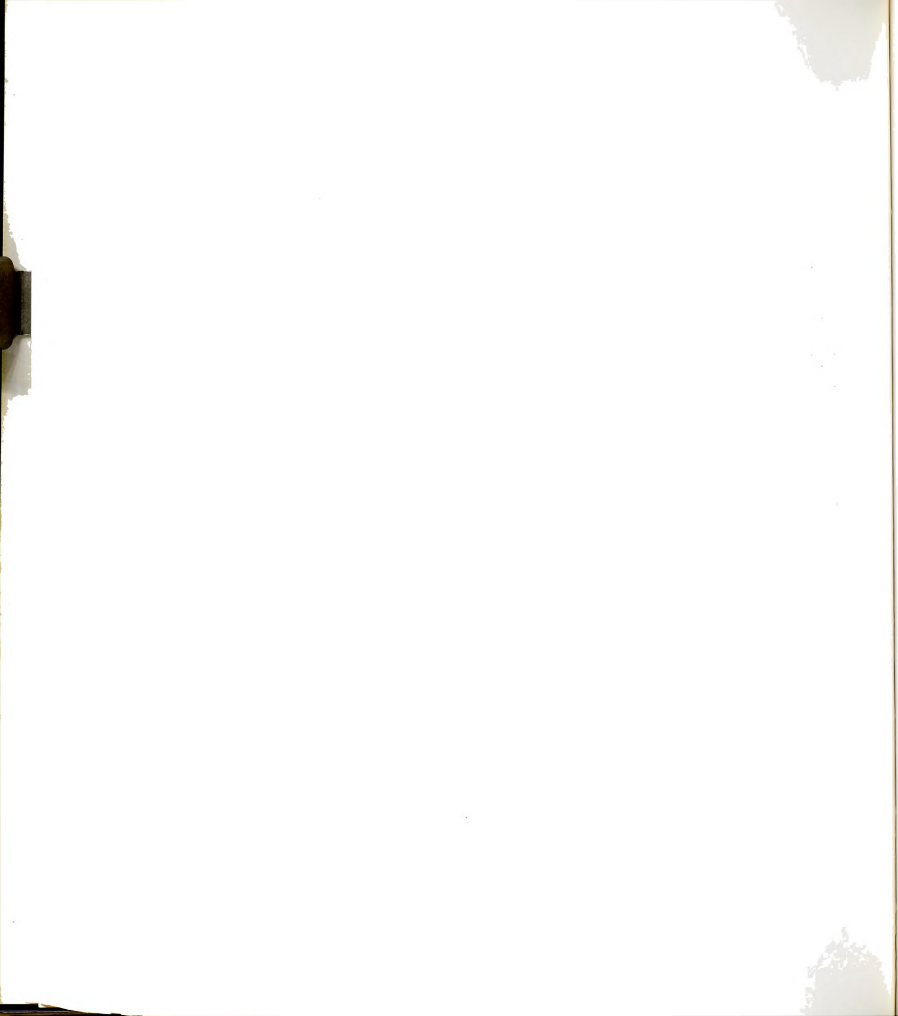
C ..... SECOND POINT IN FROM THE AXIS .....
C

```

```

JJ = IEQ + 1 $ K = IW - 1
DUM = ( 1.0/R(2) - A*R(2)*( 1.0-2.0*Y(IR,2) ) ) / DR1

```



```

C(J,J,1) = -1.25*DRDR1 - 13.0/12.0*DUM - 2.0*A*( 1.0-Y(IR,2) )
C(J,J,2) = -DRDR1/3.0+2.0*DUM $ C(J,J,3) = 7.0/6.0*DRDR1-DUM
C(J,J,4) = -DRDR1/2.0*DUM/3.0 $ C(J,J,5) = DRDR1/12.0-DUM/20.0
B(2,1) = 10.0/12.0*DRDR1 - 0.2*DUM

..... INTERIOR POINTS (INNER FLOW) OVER TO 1 POINT BEFORE THE
INTERSECTION .....

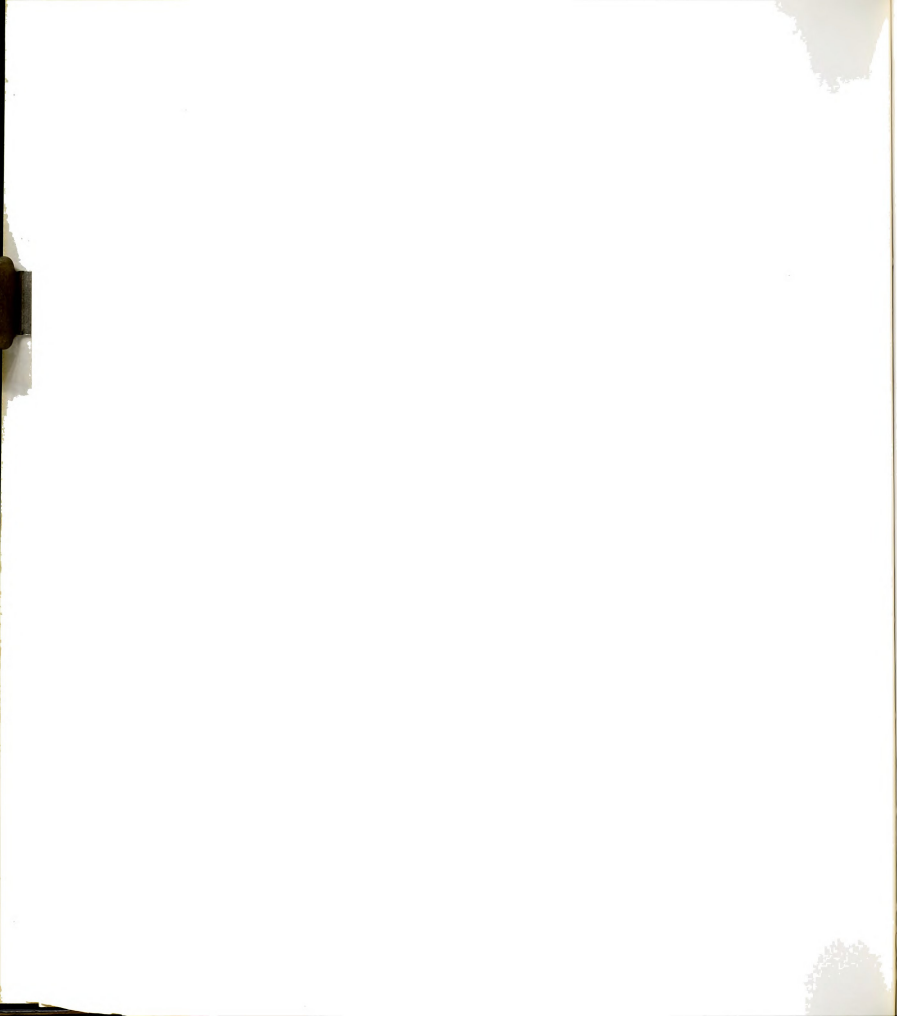
DO 110 J = 3, K
DUM = ( 1.0/R(J) - A * R(J) * ( 1.0-2.0*Y(IR,J) ) ) / DR1
JJ = IEQ+J-1 $ C(J,J,2) = (4.0*DRDR1+2.0*DUM)/3.0
C(J,J,1) = -2.5*DRDR1 - 2.0*A*( 1.0-Y(IR,J) )
C(J,J,3) = -DRDR1*DUM/12.0 $ B(J,1) = (4.0*DRDR1-2.0*DUM)/3.0
110 B(J,2) = ( -DRDR1 + DUM ) / 12.0

..... DUE TO UNEQUAL INCREMENT SIZES AT THE FLOW INTERSECTION
SPECIAL FINITE DIFFERENCE EQUATIONS ARE USED .....

ISTOP = IWPI+1 $ ISTART = IW $ K = 1 $ M = 2
IF( IR .EQ. 1 ) ISTOP = IW
GO TO 210
200 ISTART = IW+2 $ ISTOP = ISTART $ K = 5 $ M = 6
210 DO 230 J = ISTART, ISTOP
DUM = 1.0/R(J) - A * R(J) * ( 1.0-2.0*Y(IR,J) )
JJ = IEQ+J-1 $ B(J,2) = CO(1,K)*DUM + CO(1,M)
C(J,J,1) = CO(5,K)*DUM + CO(5,M) - 2.0*A*( 1.0-Y(IR,J) )
B(J,1) = CO(2,K)*DUM + CO(2,M) $ C(J,J,2) = CO(3,K)*DUM + CO(3,M)
C(J,J,3) = CO(4,K)*DUM + CO(4,M) $ K = M + 1
230 M = K + 1
IF( IR .EQ. 1 ) RETURN

C ..... INTERIOR POINTS (OUTER FLOW) OVER TO 1 POINT BEFORE THE
C INTERSECTION .....
C
C K = IWPI + 2 $ M = IWTWO - 2
DO 240 J = K, M

```



```

DUM = ( 1.0/R(J) - A*(J) * ( 1.0-2.0*Y(IR,J) ) ) / DR2
JJ = IEQ+J-1 $ C(JJ,2) = ( 4.0*DRDR2+2.0*DUM ) / 3.0
C(JJ,1) = -2.5*DRDR2 - 2.0*A*( 1.0-Y(IR,J) )
C(JJ,3) = -(DRDR2+DUM)/12.0 $ B(J,1) = ( 4.0*DRDR2-2.0*DUM ) / 3.0
240 B(J,2) = ( -DRDR2 + DUM ) / 12.0

```

C
C
C

..... ONE POINT IN FROM THE WALL

```

J = IWTWO-1 $ JJ = IEQ+J-1
DUM = ( 1.0/R(J) - A*(J) * ( 1.0-2.0*Y(IR,J) ) ) / DR2
C(JJ,1) = -1.25*DRDR2 + 13.0/12.0*DUM - 2.0*A*( 1.0-Y(IR,J) )
C(JJ,2) = DRDR2/1.2+0.2*DUM $ R(J,1) = -DRDR2/3.0-2.0*DUM
B(J,2) = 7.0/6.0*DRDR2+DUM $ B(J,3) = -DRDR2/2.0-DUM/3.0
B(J,4) = DRDR2/12.0 + DUM/20.0

```

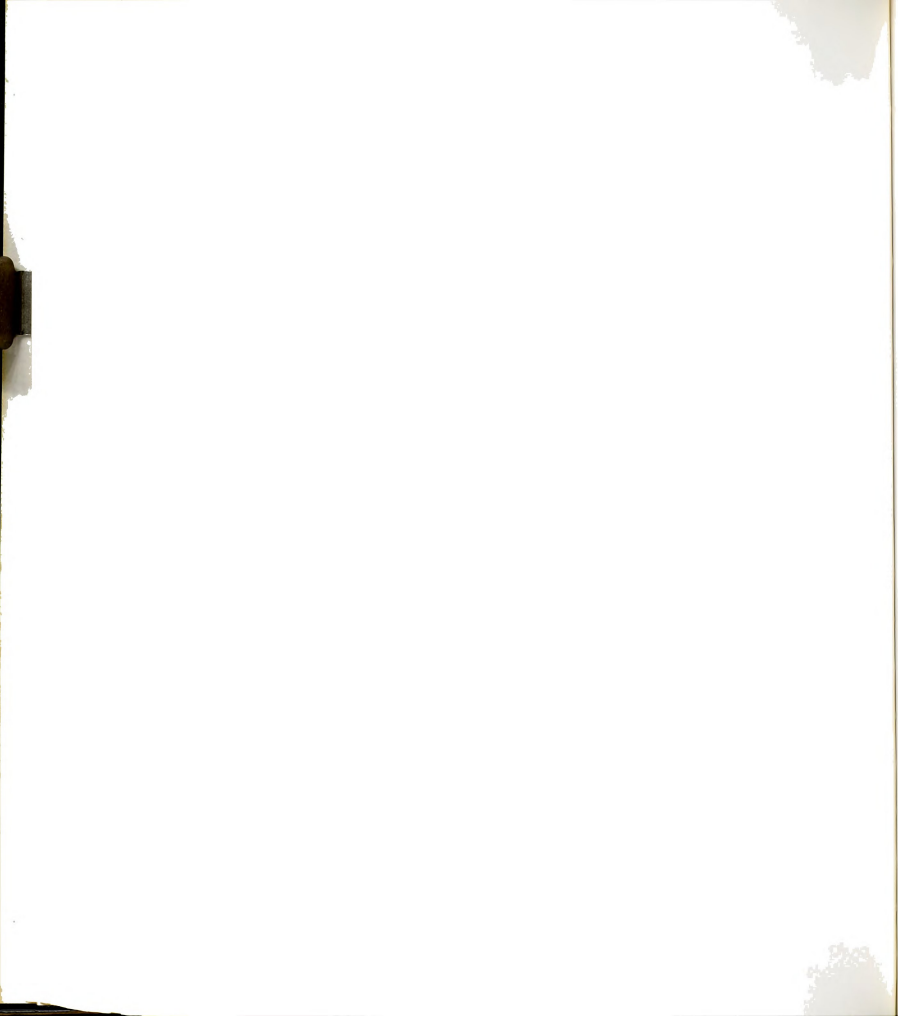
C
C
C

..... NO FLUX THROUGH THE WALL

```

J = IWTWO $ JJ = IEQ+J-1
DUM = 1.0/R(J) - A * R(J) * ( 1.0-2.0*Y(IR,J) )
C(JJ,1) = ( -415.0/72.0+25.0/6.0*DRDR2*A*(J) * ( 1.0-Y(IR,J) ) ) *
1 DRDR2 - 2.0*A*( 1.0-Y(IR,J) ) + DUM*A*(J) * ( 1.0-Y(IR,J) )
B(J,1) = 8.0*DRDR2 $ B(J,2) = -3.0*DRDR2
B(J,3) = 8.0/9.0*DRDR2 $ R(J,4) = -DRDR2/8.0
RETURN
END

```

```

SUBROUTINE SPECIAL( FIN, C, N, NC )
DIMENSION C(4,8), FIN(5,6)

..... THIS SUBROUTINE COMPUTES FINITE DIFFERENCE FORMULAS .....

..... BEGIN BY WRITING THE COEFFICIENTS FOR THE TAYLOR SERIES .....

      N = N + N      $      NPI = N + 1      $      K = N - 1
DO 10 I = 1, N      $
NF = 1 + I          $      DX = C(I,5)      $      DUM = 1.0
DO 20 J = 1, N
NF = NF * J          $      DUM = DUM * DX
20 C(I,J) = DUM / FLOAT(NF)

..... AUGMENT WITH THE IDENTITY .....

DO 30 J = NPI, M
30 C(I,J) = 0.0
10 C(I,N+1) = 1.0

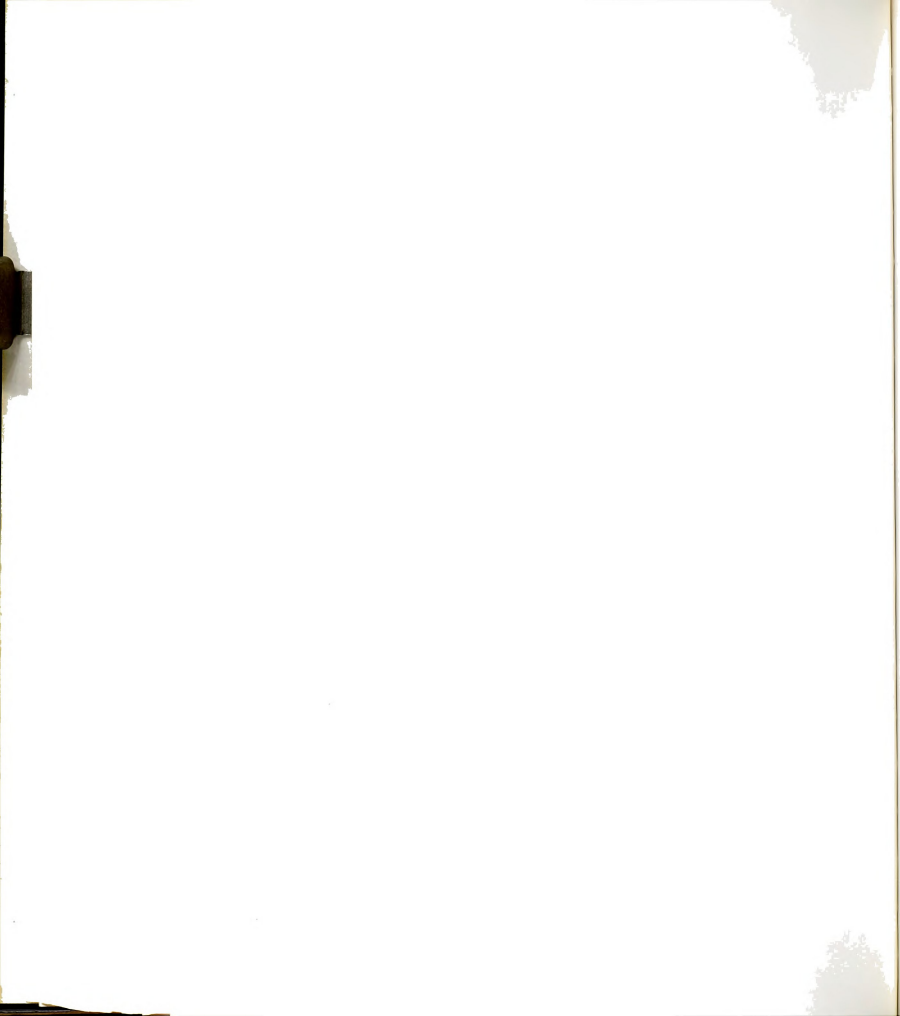
..... FINDING THE INVERSE ----- FIRST UPPER TRIANGULATE .....

DO 40 I = 1, K
L = I + 1
DO 40 J = L, N
DUM = C(J,I) / C(I,I)
DO 40 MM = L, M
40 C(J,MM) = C(J,MM) - DUM * C(I,MM)

..... BACK SUBSTITUTE TO FIND THE INVERSE .....

DO 50 I = 1, N
NPI = N + 1      $      C(N,NPI) = C(N,NPI) / C(N,N)
DO 50 J = 1, K
L = N - J      $      LPI = L + 1      $      SUM = C(L,NPI)
DO 60 MM = LPI, N

```



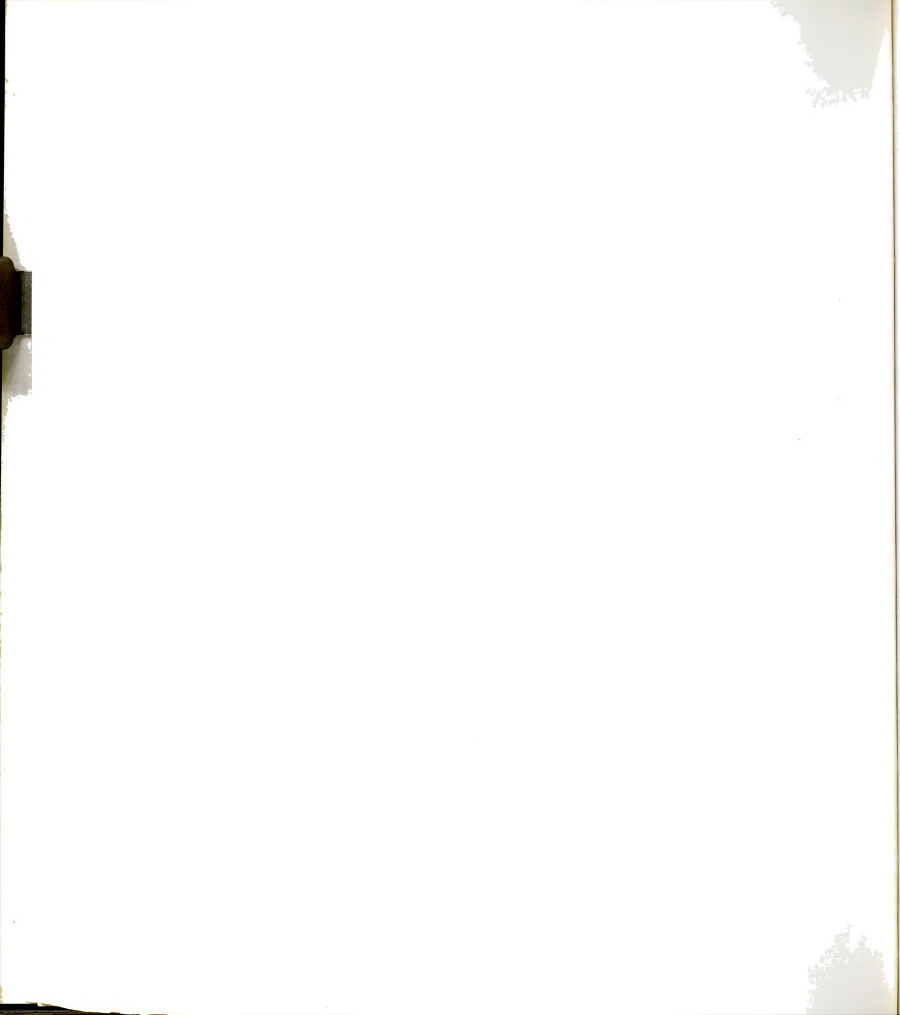
```

60 SUM = SUM - C(L,MM) * C(MM,NPI)
50 C(L,NPI) = SUM / C(L,L)

C
C
C
C
..... GIVE THE FIRST AND SECOND DERIVATIVES TO FIN --- THE CENTRAL
POINT IS IN THE LAST ROW .....

DO 70 I = 1, 2
K = 0 $ DUM = 0.0 $ NCC = NC - 1 + I
DO 80 J = NPI, M
K = K + 1 $ DUM = DUM - C(I,J)
80 FIN(K,NCC) = C(I,J)
70 FIN(K+1,NCC) = DUM
RETURN
END

```



```

SUBROUTINE ZOIFF( SO,I,IA,Y,R,P,VEL,B,C,MD,ND,NEQ,NEQD, IEQ, )
COMMON IW, IWTWO, IH, IHPI, DRI, DR2, DZ
COMMON PO, I, DP, WM1, WM2, OMEGA, A, VZMAXD, VZMAXU
COMMON YF, FSCFM, FRAC, FEED, PRICH, PLEAN
DIMENSION Y(MD,ND),R(ND),P(ND),VEL(ND),B(ND,NEQD),C(NEQ,NEQD)
DIMENSION D(20), CO(8)
DATA ( CO(I),I=1,8 ) / 1.0,4.0,2.0,4.0,2.125,3.375,3.375,1.125 /

..... THIS SUBROUTINE WRITES THE Z DIRECTION FINITE DIFF EOS .....
IF( I .GT. 1 ) GO TO 100

..... INITIALIZE SOME CONSTANTS .....

DO 10 J = 1, IWTWO
10 D(J) = - P(J) * VEL(J) / DP / DZ
DZDZ = 1.0/DZ/DZ $ M = IWTWO + 1
MM = M + IWTWO $ N = M - 1 $ NN = N + N

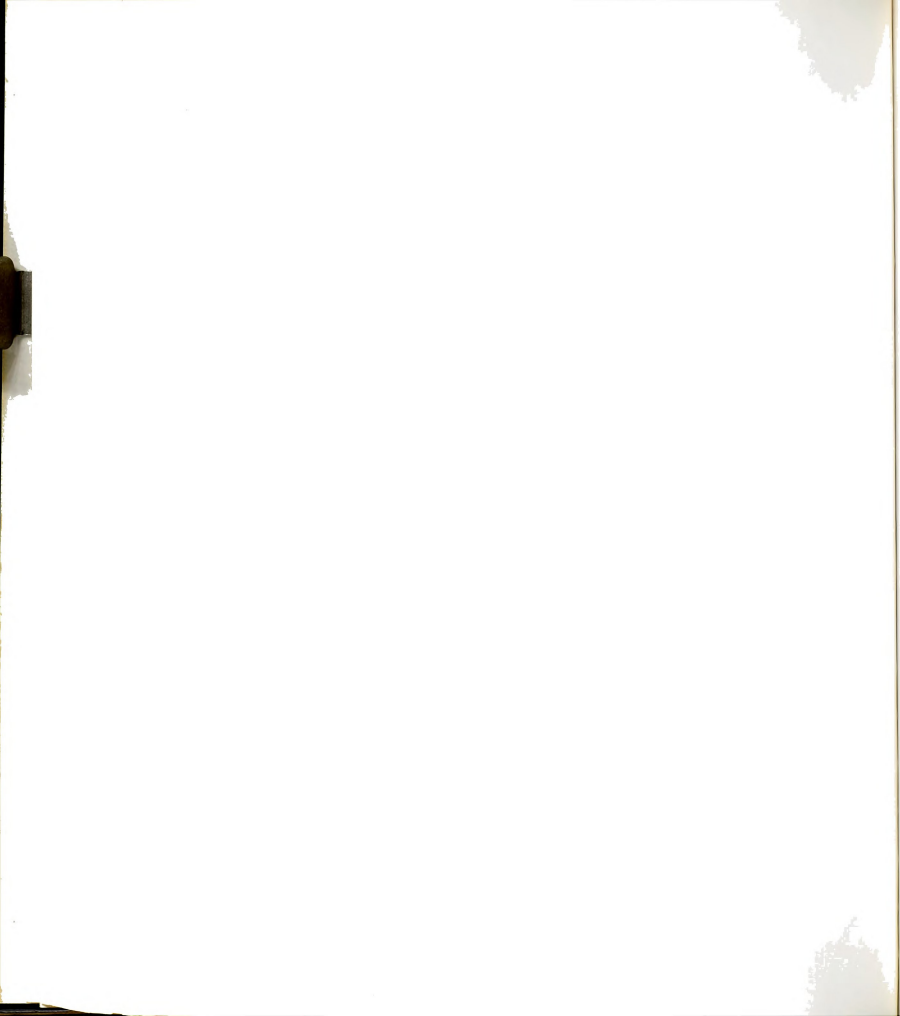
..... SPECIAL EQUATIONS ALONG THE TOP .....

DO 20 J = 1, IW
JJ = IEQ+J-1 $ C(JJ,1) = C(JJ,1) + DZDZ - 1.5*D(J)
C(JJ,M) = -2.0 * DZDZ + 2.0 * D(J)
20 C(JJ,MM) = DZDZ - D(J)/2.0
DO 25 J = IWPI, IWTWO
JJ = IEQ + J - 1 $ C(JJ,1) = 1.0
25 C(JJ,IA) = YF
RETURN
100 IF( I .GT. 2 ) GO TO 200

..... SPECIAL EQUATIONS FOR THE SECOND ROW FROM THE TOP .....

DO 30 J = 1, IWTWO
JJ = IEQ+J-1 $ C(JJ,MM) = -D(J)/6.0
C(JJ,1) = C(JJ,1) - 2.0*DZDZ - D(J)/2.0

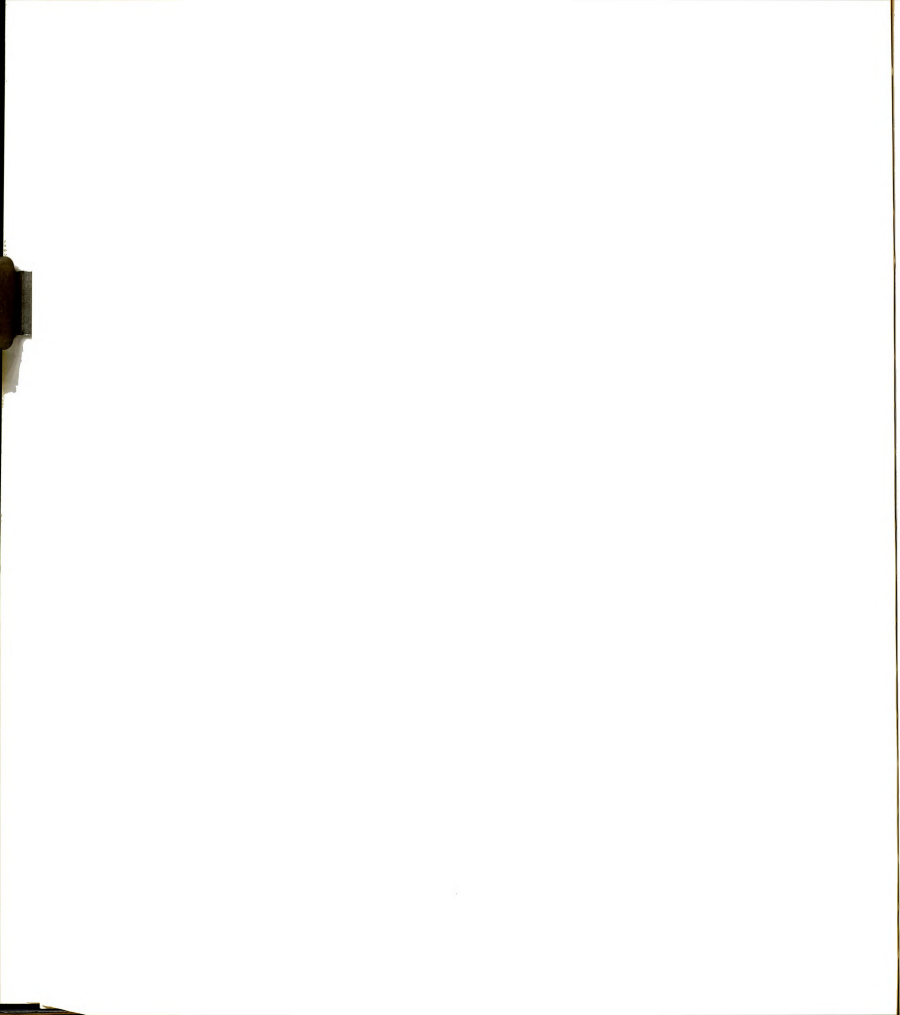
```



```

C(JJ,M) = DZDZ + D(J)
30 B(J,N) = DZDZ - D(J)/3.0
RETURN
200 IF( I .GE. IH ) GO TO 300
C
C ..... EQUATIONS FOR ALL INTERIOR POINTS .....
C
DO 40 J = 1, IWTWO
JJ = IEQ+J-1 $ C(JJ,1) = C(JJ,1) - 2.5*DZDZ
C(JJ,M) = (4.0*DZDZ+2.0*D(J))/3.0
C(JJ,MM) = -(DZDZ+D(J))/12.0 $ B(J,N) = (4.0*DZDZ-2.0*D(J))/3.0
40 B(J,NN) = (-DZDZ+D(J))/12.0
RETURN
300 IF( I .EQ. IH1 ) GO TO 400
C
C ..... SPECIAL EQUATIONS FOR ONE ROW BEFORE THE BOTTOM .....
C
DO 50 J = 1, IWTWO
JJ = IEQ + J - 1 $ B(J,NN) = D(J)/6.0
C(JJ,1) = C(JJ,1)-2.0*DZDZ+D(J)/2.0 $ B(J,N) = DZDZ-D(J)
50 C(JJ,M) = DZDZ + D(J) / 3.0
RETURN
C
C ..... SPECIAL EQUATIONS FOR THE BOTTOM .....
C
400 K = IWP1 + 1
DO 60 J = K, IWTWO
JJ = IEQ + J - 1
C(JJ,1) = C(JJ,1)+DZDZ+1.5*D(J) $ B(J,N) = -2.0*DZDZ-2.0*D(J)
60 B(J,NN) = DZDZ + D(J)/2.0
K = IW - 1
C
C ..... ALL FLOWS UP IN THE INNER STREAM ARE EQUAL AT THE BASE .....
C
DO 65 J = 1, K
JJ = IEQ + J - 1 $ C(JJ,1) = 1.0

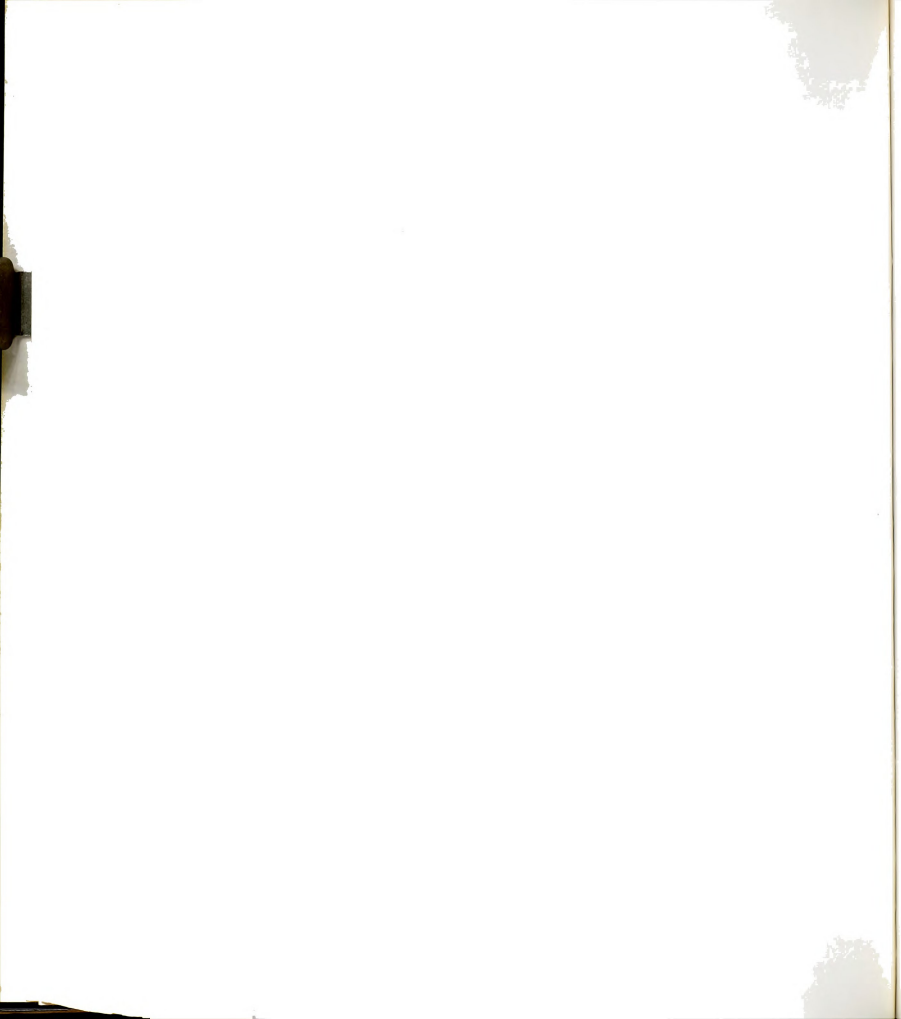
```

```

65 C(JJ,2) = -1.0
   JJ = IEQ + IWPI - 1
   C(JJ,1) = 1.0
   JJ = IEQ + IW - 1
DO 70 J = IWPI, INTWO
   II = J - IW
   $ LL = N - II
   $ KK = NN - II
   $ DDUM = P(J) * VEL(J) * R(J)
   $ DDUM = -DP * R(J) / DZ
   C(JJ,II+1) = (DDUM+1.5*DDUM)*CO(II)
   $ B(IW,LL) = -2.0*DDUM*CO(II)
70 B(IW,KK) = DDUM / 2.0 * CO(II)
   RETURN
END

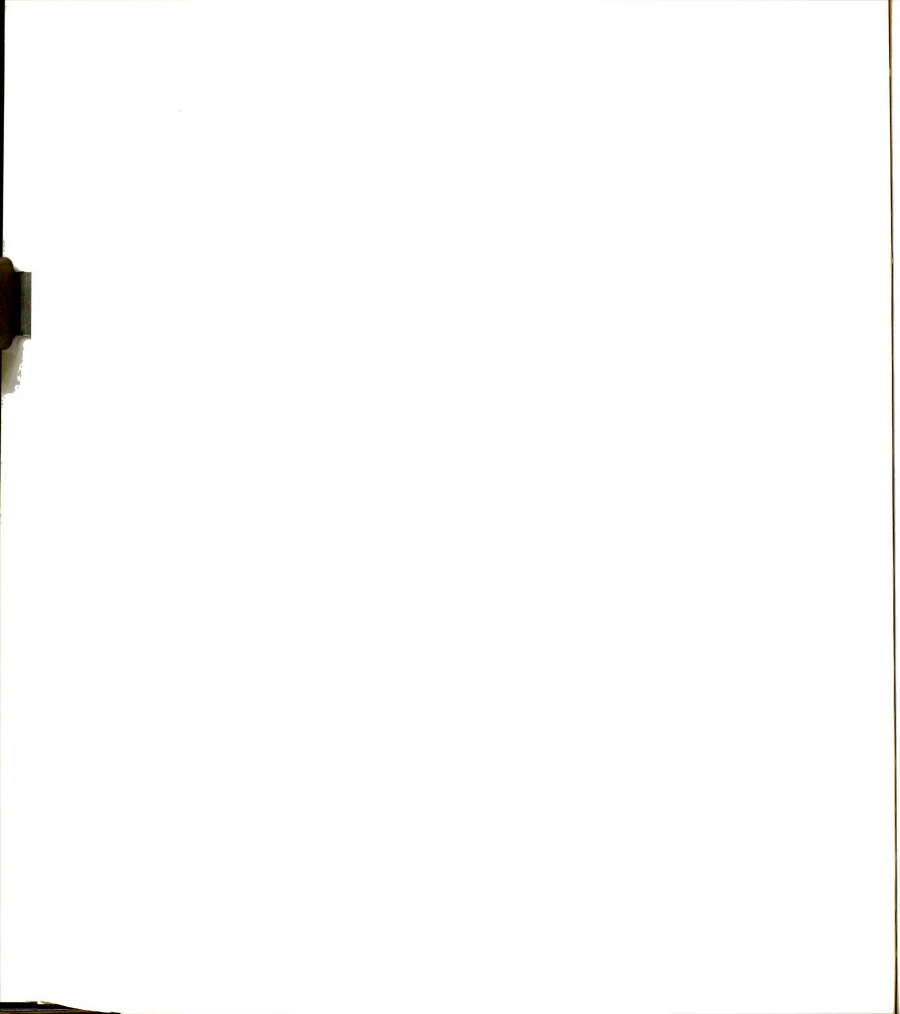
```



```

C C SUBROUTINE DIAG567( MODE, B, C, IC, IER, IE, ND, NEQ, NEQD )
C C DIMENSION B(4200)
C C DOUBLE PRECISION BD
C C DIMENSION B(ND,NEQD), C(NEQ,NEQD)
C C
C C ..... THIS SUBROUTINE COMPUTES THE SOLUTION TO A SET OF
C C SIMULTANEOUS EQUATIONS RESULTING FROM THE FINITE
C C DIFFERENCE APPROXIMATION OF A TWO DIMENSIONAL PARTIAL
C C DIFFERENTIAL EQUATION .....
C C
C C ..... THE EQUATIONS ARE RECEIVED IN SETS RESULTING FROM
C C THE FINITE DIFFERENCE APPROXIMATIONS FOR A COMPLETE ROW
C C OR COLUMN OF THE GRID .....
C C
C C GO TO( 10, 20 ), NODE
C C
C C ..... START COUNTER AND CALCULATE ARRAY SIZE .....
C C
10 NEQ = 0
   IC = 1
   K = 1
   SUM = 1.0E-10
   IMID = FLOAT(M) / 2.0
   ITIS = 0
C C
C C ..... ARRANGE B IN THE RIGHT ORDER .....
C C
20 DO 30 I = 1, IC
   DO 30 J = 1, IMID
      L = K-J-1
      X = B(I,J)
      B(I,L) = B(I,L)
      IF( ITIS .EQ. 0 ) GO TO 150
C C
C C ..... THE LAST EQUATION OF THE PRECEDING SET OF EQUATIONS HAD A
C C VERY SMALL NUMBER LEFT ON THE DIAGONAL AFTER UPPER
C C TRIANGULATION HAD BEEN COMPLETED .....
C C
C C ..... SWITCH WITH THE NEXT EQUATION .....

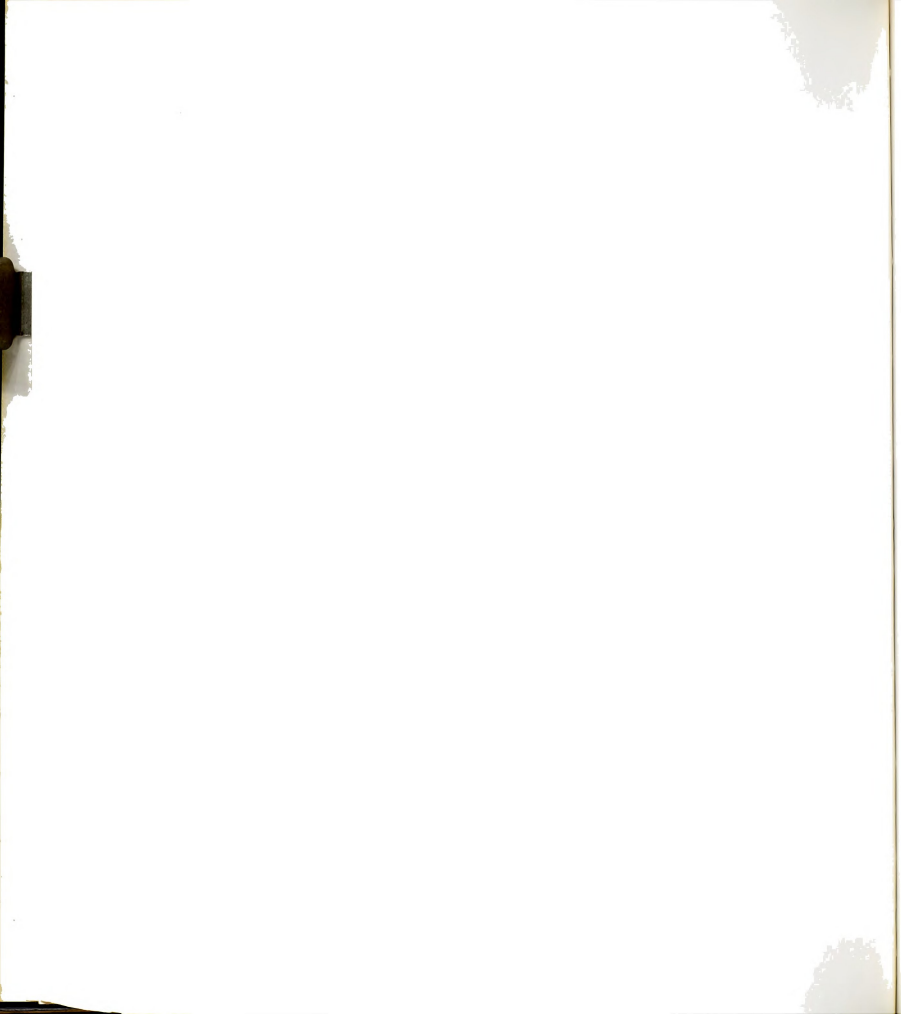
```



```

C      CALL SWITCH( B, C, MEQ, I, M, K, IE, ND, NEQ, NEQD, BD )
C
C      ..... REUPPER TRIANGULATE THE EQUATION .....
C
C      CALL UPPER7( C, K, M, MEQ, IE, NEQ, NEQD, BD )
C
C      ..... IF ANOTHER VERY SMALL NUMBER IS ENCOUNTERED ON THE DIAGONAL
C      CALCULATIONS ARE TERMINATED .....
C
C      IF( ABS(C(MEQ,1))/SUM*FLOAT(MEQ) .GT. 1.0E-07 ) GO TO 96
C      PRINT 110 $ STOP
C      110 $ SUM = SUM + ABS( C(MEQ,1) )
C      96 ITIS = 0 $
C      ..... BEGIN UPPER-TRIANGULATING .....
C
C      150 DO 40 I = 1, IC
C      MEQ = MEQ + 1 $ ICHECK = 0
C      DO 45 J = 1, M
C      45 BD(J) = DBLE( B(I,J) )
C      200 CALL UPPER7( C, K, M, MEQ, IE, NEQ, NEQD, BD )
C
C      ..... CHECK FOR A VERY SMALL NUMBER LEFT ON THE DIAGONAL .....
C      IF( ABS(C(MEQ,1))/SUM*FLOAT(MEQ) .GT. 1.0E-07 ) GO TO 55
C
C      ..... A VERY SMALL NUMBER WAS LEFT ON THE DIAGONAL .....
C
C      ..... IF A POW SWITCHING OPERATION HAS ALREADY BEEN PERFORMED ON
C      THIS EQUATION --- CALCULATIONS ARE TERMINATED .....
C
C      ..... IF THIS IS THE LAST EQUATION OF THE LAST SET ---
C      CALCULATIONS ARE TERMINATED .....
C
C      ..... IF THIS IS THE LAST EQUATION OF THIS SET THE ROW SWITCHING
C      WILL BE PERFORMED AFTER A NEW SET IS RECEIVED .....

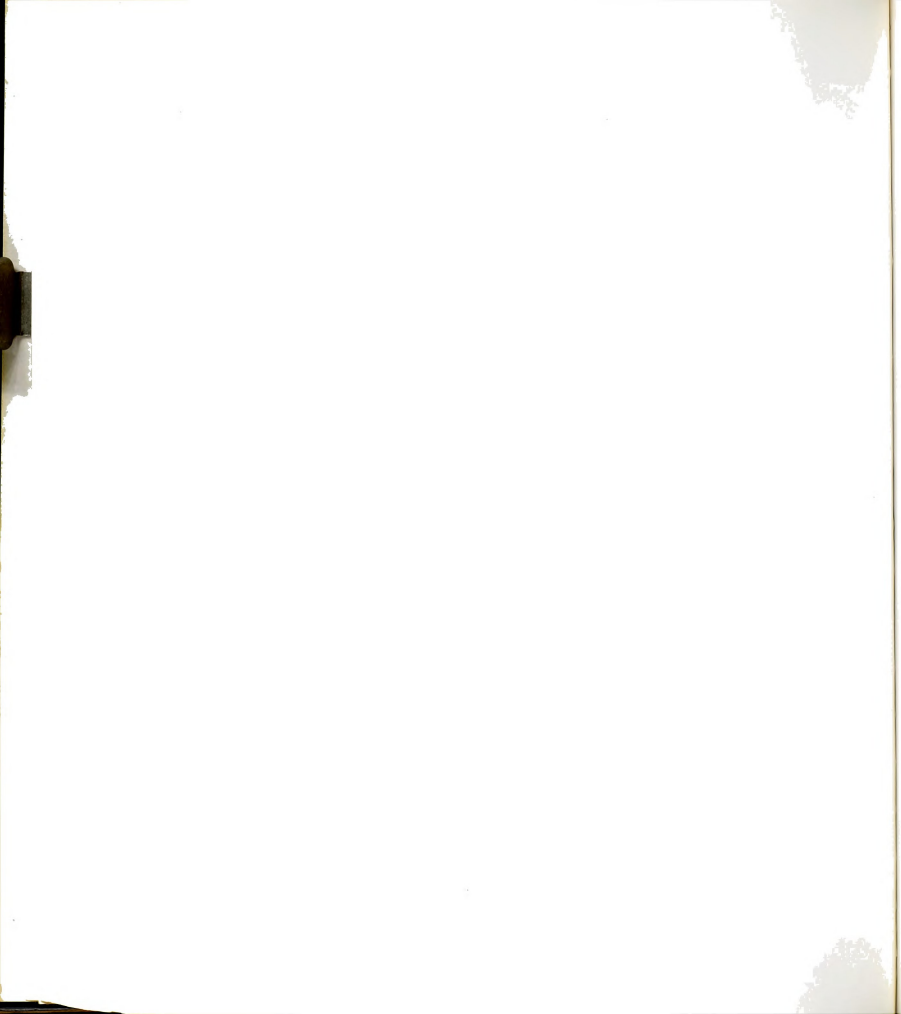
```



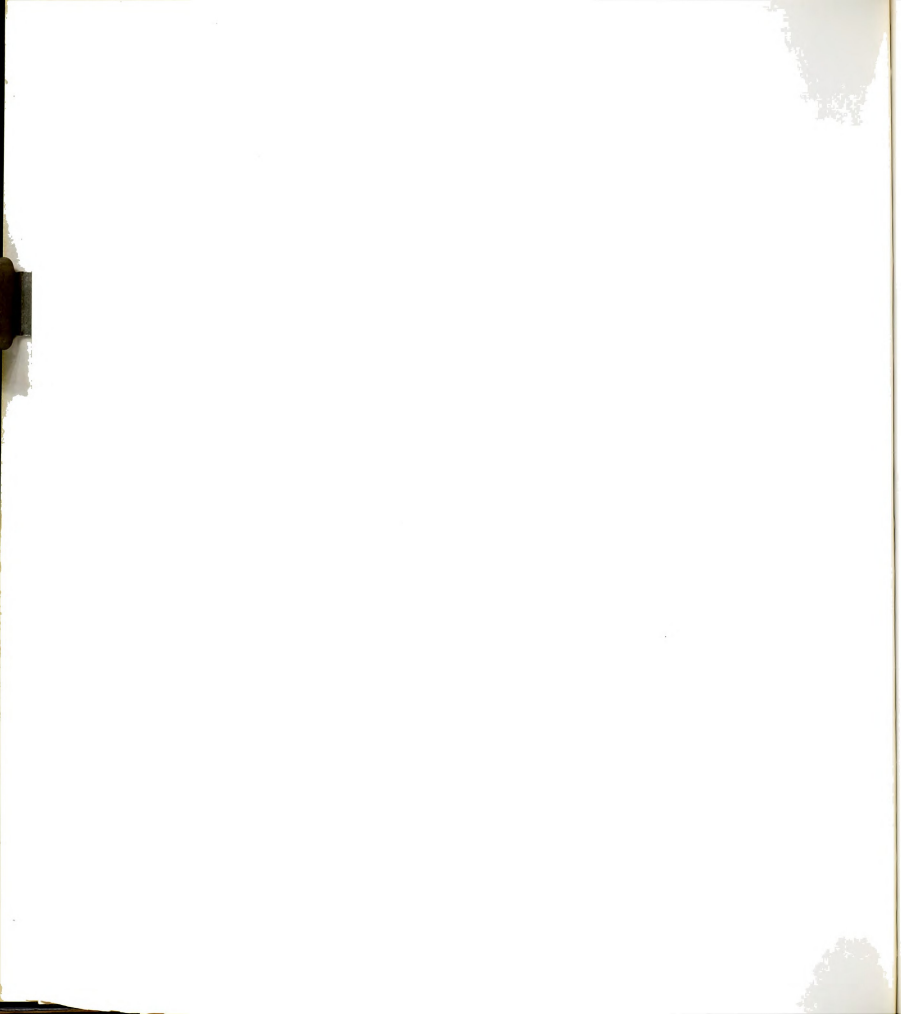
```

C      IF( ICHECK .GT. 0 )      GO TO 95
ICHECK = 1
IF( I .NE. IC )      GO TO 100
IF( MEQ .LT. IEQ )      GO TO 105
95 PRINT 110
110 FORMAT( 20X, *A VERY SMALL NUMBER WAS LEFT ON THE DIAGONAL WITH N
10WAY OF REMOVING IT --- CALCULATIONS ARE TERMINATED* )
105 I1IS = 1 $      GO TO 40
100 IP = I + 1
C      ..... SWITCH WITH THE NEXT EQUATION .....
C      CALL SWITCH( B, C, MEQ, IP, N, K, IE, ND, NEQ, NEQD, BD )
GO TO 200
55 SUM = SUM + ABS( C(MEQ,I) )
40 CONTINUE
C      ..... CHECK TO SEE IF ALL THE EQS HAVE BEEN UPPER-TRIANGULATED ....
C      IF( MEQ .LT. IEQ )      RETURN
C      ..... BEGIN BACK SUBSTITUTING .....
C      C(IEQ,IE) = C(IEQ,IE) / C(IEQ,I)
KK = K - 1
DO 70 I = 1, KK
L = IEQ - I $      X = C(L,IE)
DO 75 J = 1, I
75 X = X - C(L,J+1) * C(L+J,IE)
70 C(L,IE) = X / C(L,I)      RETURN
N = IEQ - 1
DO 80 I = K, N
L = IEQ - I $      X = C(L,IE)
DO 90 J = 1, KK

```

```
90 X = X - C(L,J+1) * C(L+J,IE)
80 C(L,IE) = X / C(L,1)
  RETURN
  END
```



```

SUBROUTINE SWITCH7( B, C, MEQ, I, M, K, IE, ND, NEQ, NEQD, BD )
DIMENSION BD(200)
DOUBLE PRECISION BD
DIMENSION B(ND,NEQD), C(NEQ,NEQD)

..... THIS SUBROUTINE SWITCHES AN EQ WITH THE ONE AHEAD OF IT .....

MM = M - 1
DO 10 J = 1, MM
  BD(J) = ONLY B(I,J)
  10 B(I,J) = 0.0
  BD(1) = 0.0D+00
  C(MEQ,1) = B(I,M)
  MK = K - 1
  DO 115 J = 1, MK
    L = J + 1
    X = C(MEQ,L)
    C(MK,J) = X
    115 C(MK,J) = X
    X = C(MEQ,IE)
    C(MK,IE) = X
  RETURN
END

```

```

SUBROUTINE SWITCH7( B, C, MEQ, I, M, K, IE, ND, NEQ, NEG, BD )
DIMENSION BD(200)
DOUBLE PRECISION BD
DIMENSION B(ND,NEQ), C(NEQ,NEQ)

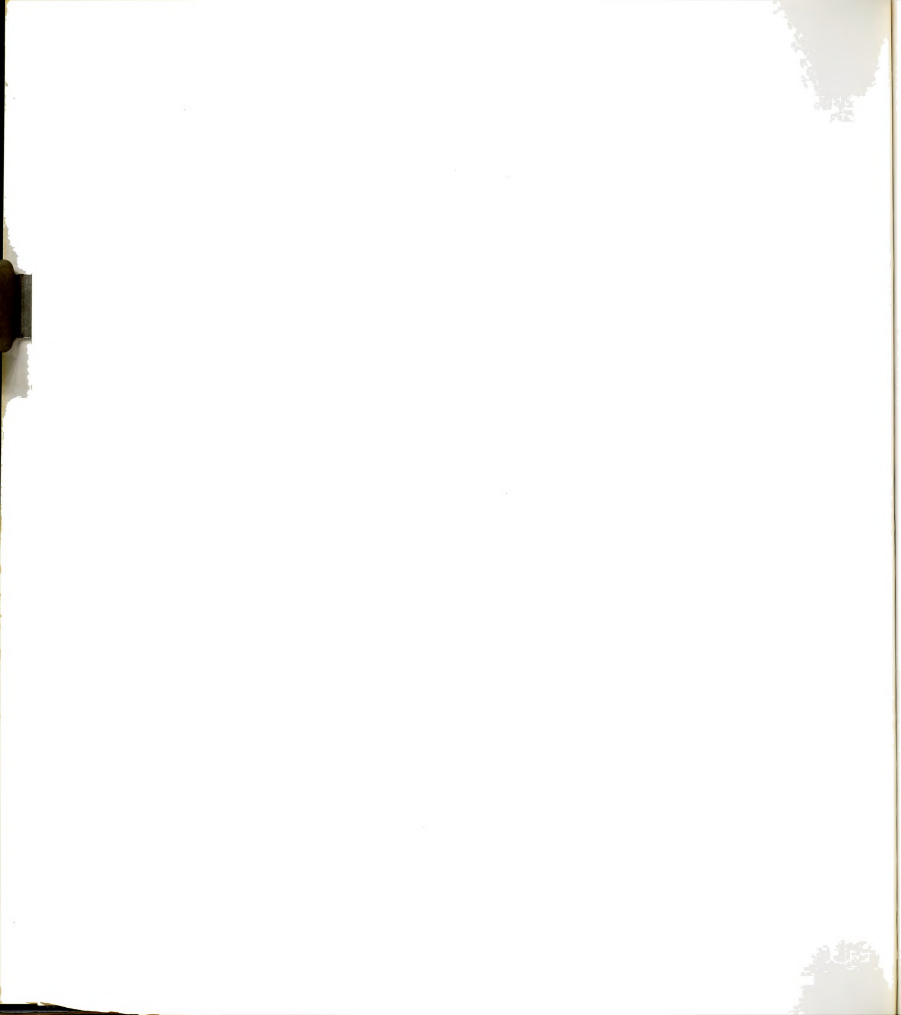
```

..... THIS SUBROUTINE SWITCHES AN EQ WITH THE ONE AHEAD OF IT

```

MM = M - 1
DO 10 J = 1, MM
  BD(0,J) = C(0,J)
  DO 11 I = 0, C
    BD(I,J) = 0.0
    BD(1) = 0.0D+00
    C(MEQ,1) = B(I,K)
    KK = K - 1
    DO 115 J = 1, KK
      L = J + 1
      X = C(MEQ,L)
      115 C(MK,J) = X
      X = C(MEQ,IE)
      C(MK,IE) = X
    RETURN
  END

```



```

SUBROUTINE UPPER7( C, K, M, MEQ, IE, NEQ, NEQD, BD )
  DIMENSION BD(200)
  DOUBLE PRECISION SD, XD, DUM
  DIMENSION C(NEQ,NEQD)

```

C
C
C
C

```

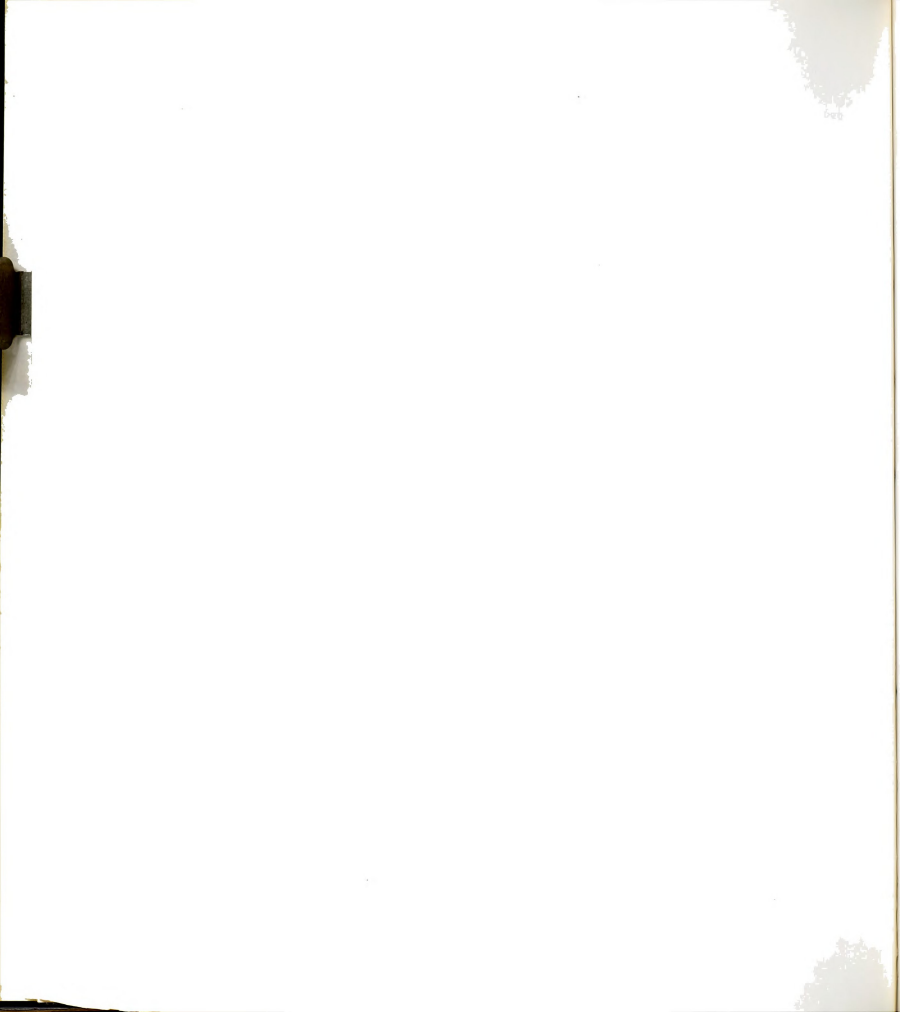
..... THIS SUBROUTINE UPPER TRIANGULATES A ROW OF THE COEFFICIENT
        MATRIX .....

```

```

  LL = MEQ - K + 1
  DUM = DBLE( C(MEQ,IE) )
  DO 50 J = 1, M
    IF( BD(J) ) 10, 50, 10
    L = LL + J
    XD = - BD(J) / DBLE( C(L,1) ) $ MM = 0 X = SNGL( XD )
    DO 60 N = 2, K
      NN = J + N - 1
      IF( NN .GT. M ) GO TO 65
      BD(NN) = BD(NN) + XD * DBLE( C(L,N) )
      GO TO 60
    65 MM = MM + 1
      C(MEQ,MM) = C(MEQ,MM) + X * C(L,N)
    60 CONTINUE
      DUM = DUM + XD * DBLE( C(L,IE) )
    50 CONTINUE
      C(MEQ,IE) = SNGL( DUM )
      RETURN
      END

```



```

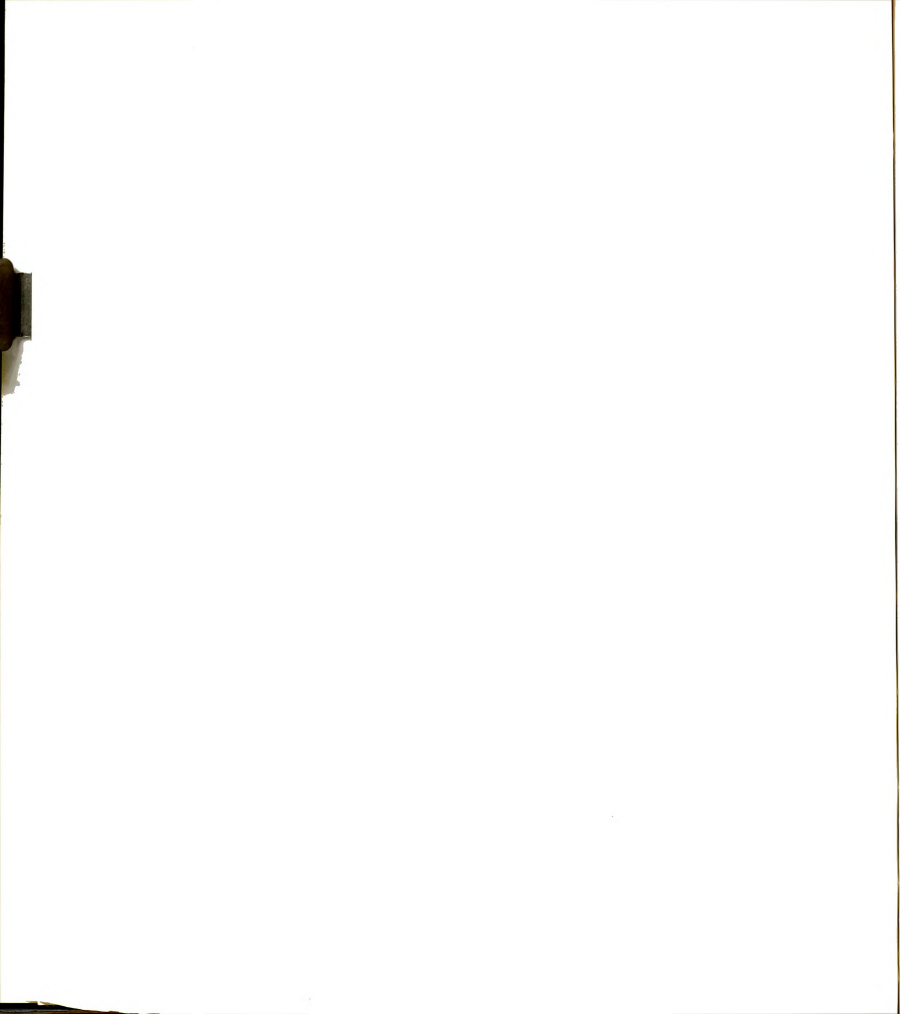
SUBROUTINE CONCOU( Z, R, Y, NOPT, ISTART, ISTOP, IHPl, MD, ND )
DIMENSION Z(MD), R(ND), Y(MD*ND), DOT1(10), DOT2(10)
DATA ( DOT1(I), I = 1,10 ) / 10*6H..... /
DATA ( DOT2(I), I = 1,10 ) / 10*6H..... /

..... THIS SUBROUTINE IS USED TO OUTPUT ARRAYS .....

IF( NOPT.EQ. 1 ) GO TO 10
K = ISTOP GO TO 15
10 K = ISTART
15 PRINT 25, ( R(I), I = ISTART, ISTOP )
25 FORMAT( /, 68X, *RADII(FT)*, //, 12X, 10( F10.4, 2X ) )
PRINT 30, ( DOT1(I), DOT2(I), I = 1, K )
30 FORMAT( /, 5X, *Z(FT)*, 2X, 20A6 )
PRINT 35
35 FORMAT( 12X, *.* )
DO 40 I = 1, IHPl
40 PRINT 45, Z(I), ( Y(I,J), J = ISTART, ISTOP )
45 FORMAT( 1X, F9.4, 2X, *.*, 10E12.5 )
PRINT 50
50 FORMAT( /// )
RETURN
END

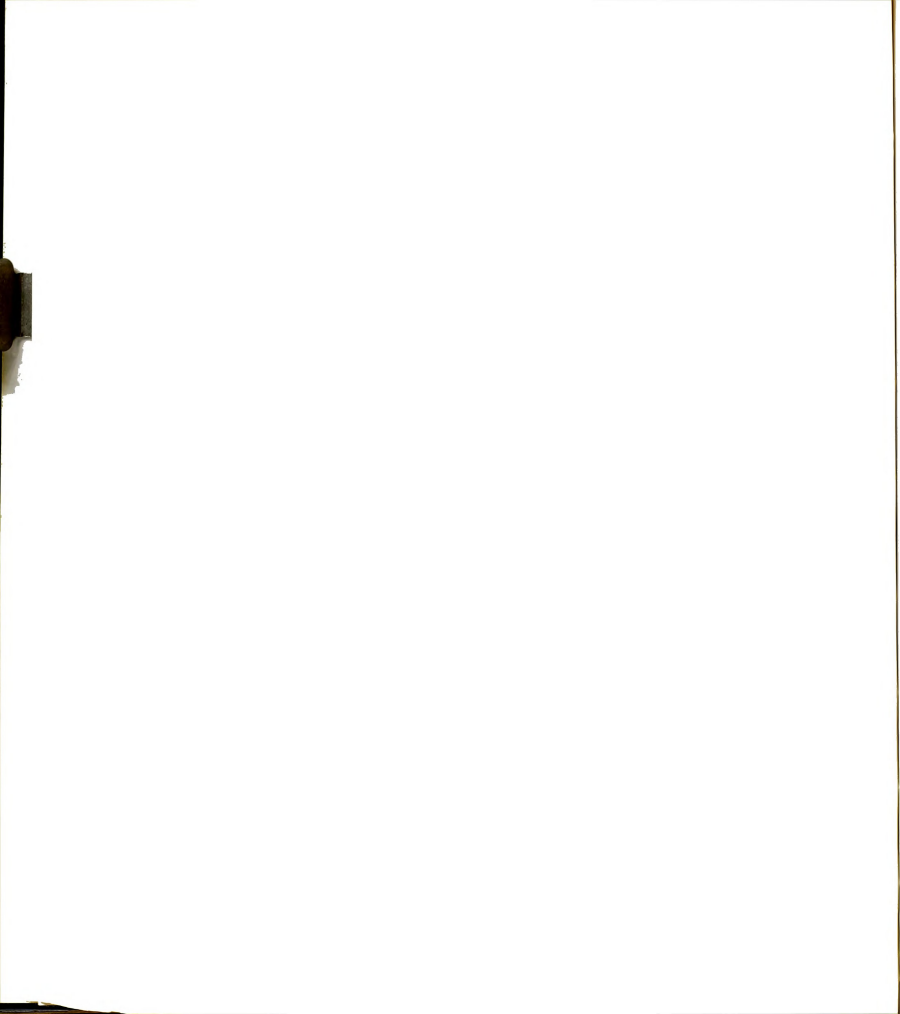
```

C
C
C



APPENDIX E

FORTRAN PROGRAM USED TO EVALUATE THE
APPROXIMATE ANALYTICAL SOLUTION OF
THE COUNTERCURRENT CENTRIFUGE



APPENDIX E

FORTRAN PROGRAM USED TO EVALUATE THE APPROXIMATE ANALYTICAL SOLUTION OF THE COUNTERCURRENT CENTRIFUGE

As established in Section V-B, the equation of continuity for Species 1 in the countercurrent centrifuge is

$$\frac{1}{r} \frac{\partial}{\partial r} [Ar^2 y(1-y) - r \frac{\partial y}{\partial r}] + \frac{Pv(r)}{D_{12} P} \frac{\partial y}{\partial z} - \frac{\partial y^2}{\partial z^2} = 0,$$

where $v(r)$ is the axial velocity profile assumed to be only a function of r .

In Chapter V-C-2 the solution was found to be

$$\tanh(uwL) = \frac{(y_p - y_f) w}{y_p - 2y_p y_f + y_f + (y_p - y_f) q},$$

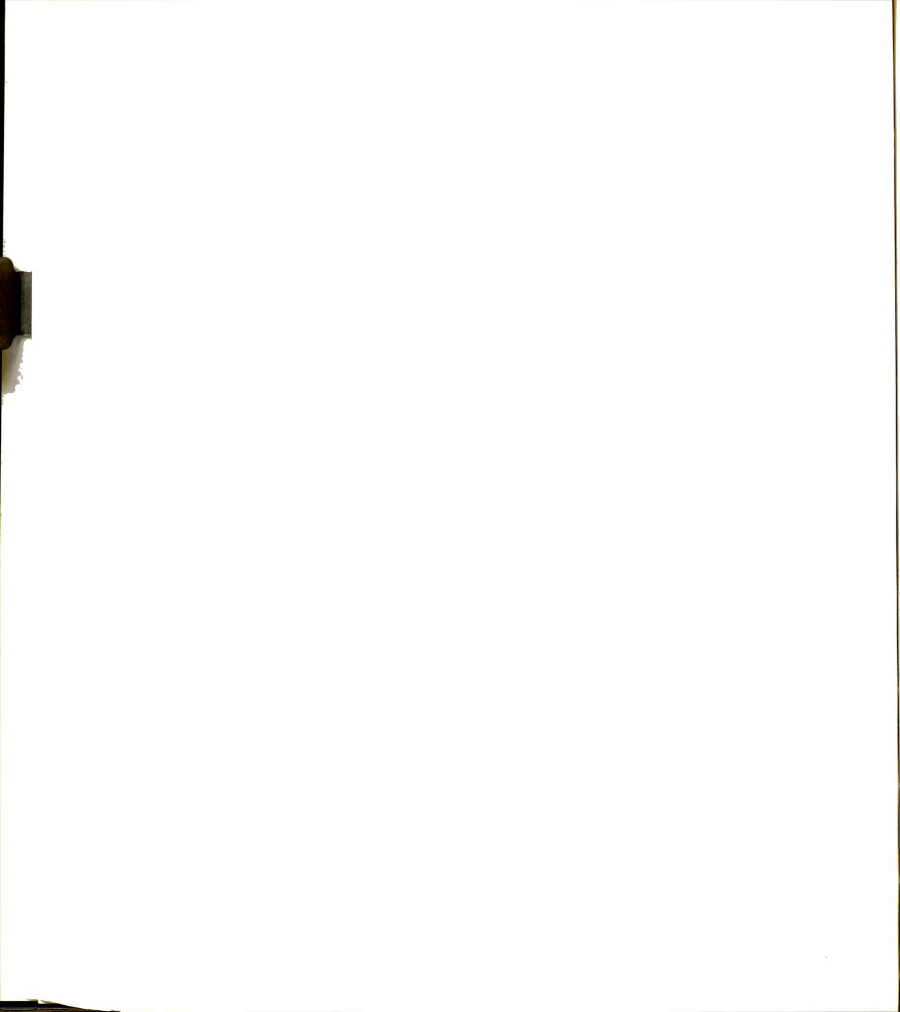
where $q = Q/C_1$,

$$w = [1 - 2q(1 - 2y_p) + q^2]^{1/2},$$

$$u = C_1/C_5/2 = C_1/(C_2 + C_3)/2,$$

$$C_1 = \frac{2\pi A}{RT} \int_0^R w \, r \, dr \int_0^r P \, v(r) \, r \, dr,$$

$$C_2 = \frac{2\pi}{RT} \frac{PD_{12} R_w^2}{2},$$



$$c_3 = \frac{2\pi}{RT} \frac{1}{PD_{12}} \int_0^{R_w} \frac{dr}{r} \left[\int_0^r P v(r) r dr \right]^2 ,$$

$$Q = \frac{2\pi}{RT} \int_0^{R_w} P v(r) r dr ,$$

y_f = the feed composition ($z = 0$), and

y_p = the product composition at the other end ($z = L$).

To evaluate the integrals and then solve the nonlinear equation to get the product composition a general FORTRAN program, CENTRI, was written. The program is general in the sense that it can be used to analyze virtually any binary gas separation in any type of countercurrent centrifuge with any internal flow arrangement. Table E-1 contains a list of the operating parameters required by program CENTRI. Since the program can handle such things as the presence of a center pipe (laminar angular velocity gradient); velocity profiles ranging between, and including, plug type and laminar velocity profiles; and the possibility of both the inner and outer streams being annular and located near the wall, all integrations are carried out numerically using the trapezoidal rule with 1000 radial increments. Techniques used to establish the magnitudes of the velocity profiles are as described in Chapter V-B.

With reference to Table E-1, the following calculations are undertaken when computing the separations in either a rectifying, stripping, or stripping-rectifying centrifuge. Table E-2 contains a description of the subroutines needed by CENTRI.

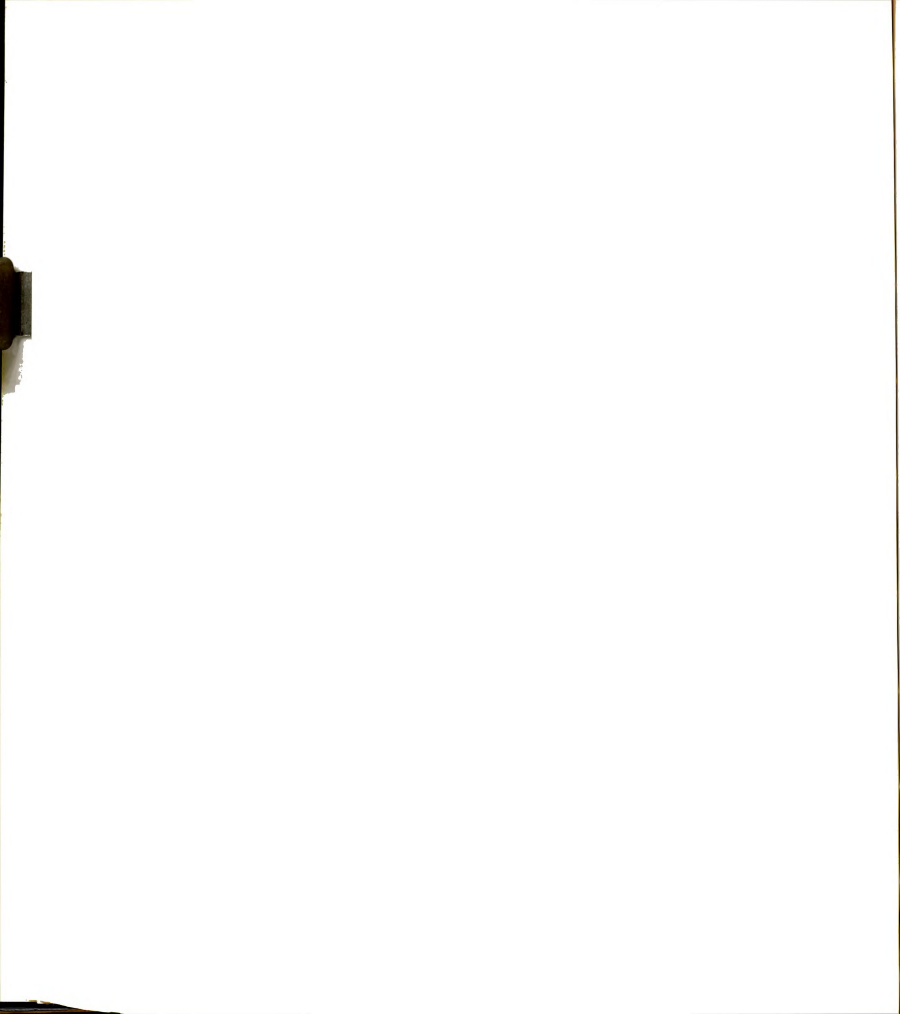


TABLE E-1.--Operating Parameters Required by Program CENTRI.

Parameter	Units	Description
WM1	lb _m /lb-mole	Molecular weight of the heavy species
WM2	lb _m /lb-mole	Molecular weight of the light species
P0	lb _f /in ²	Absolute axis pressure
T	°R	Absolute operating temperature
DP	lb _m /ft/sec	Diffusivity times the mass density at the operating temperature
VIS	lb _m /ft/sec	Gas viscosity

(This completes the first data card.) FORMAT (6F10.0)

YF	None	Feed gas mole fraction
SCFMD	scfm	Inner stream flow rate
SCFMU	scfm	Outer stream flow rate
OMEGA	RPM	Centrifuge rotational speed
VPOWER	None	VPOWER can range between 0 (plug type flow) and 1 (laminar type flow)

(This completes the second data card.) FORMAT (6F10.0)

RIS	inches	If RIS = 0, then no center pipe is assumed. If RIS is not zero then RIS is taken as the center pipe radius
RI	inches	The innermost position of the inner stream (does not have to coincide with the axis or center pipe radius)
RM	inches	Flow intersection between the inner and outer streams
RW	inches	Centrifuge radius
H	inches	Centrifuge length

(This completes the third data card.) FORMAT (6I10.0)

NOPT	None	If NOPT = 0, then the flow intersection is left as read in. If NOPT = 1 and laminar flow is specified the flow intersection is adjusted so that the inner and outer streams have equal shear rates at the intersection.
IDIV	None	Must be 1 or greater. It allows the separations at various axial positions to be computed, i.e., dh = H/IDIV.
ITOPT	None	If ITOPT = 0, then a negative height, H, causes calculations for for a stripping centrifuge to be performed, a positive height defines a rectifying centrifuge. If ITOPT = 1, a stripping-rectifying centrifuge is assumed with the stripping section data read first.
LOPT	None	May be used only if ITOPT = 0. If LOPT = 0, then the flows given are used. If LOPT = 1, then the ratio of the inner to the outer stream is maintained, but their magnitudes are adjusted to give the maximum separation.

(This completes the fourth and final data card.) FORMAT (4I5)

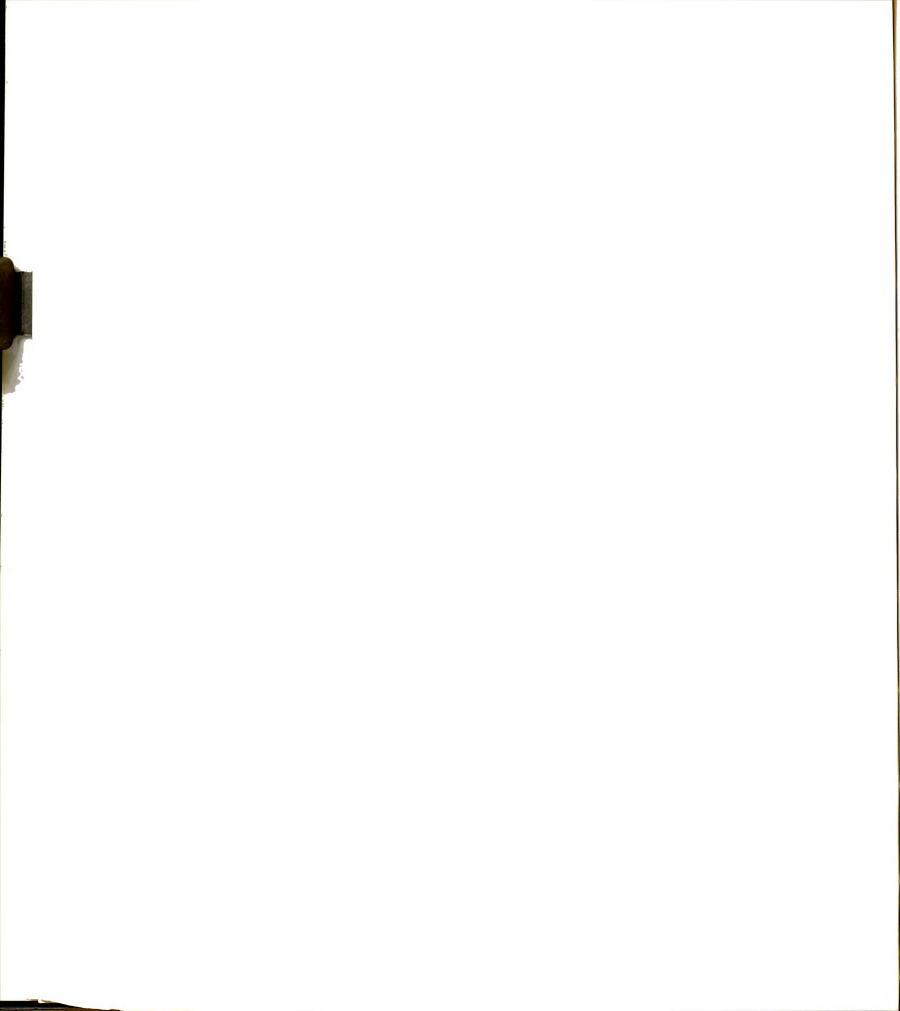


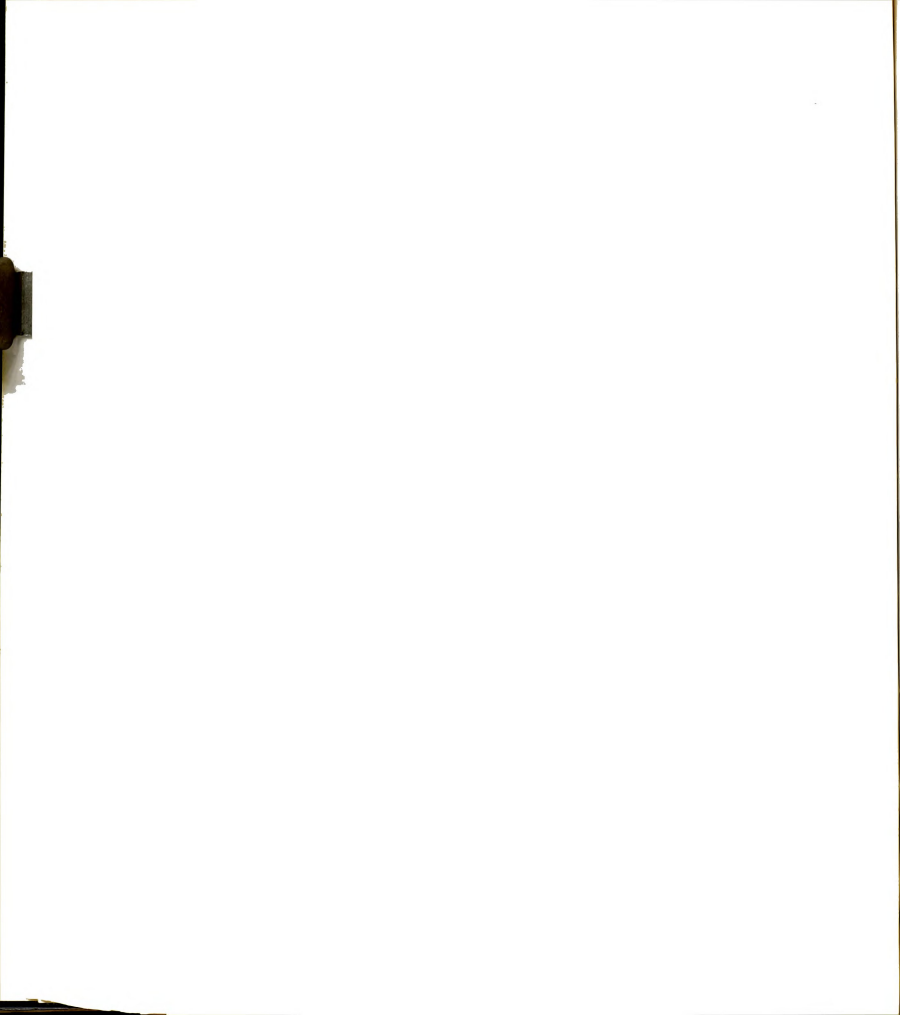
TABLE E-2.--Subprograms Associated With Program CENTRI.

Subprogram	Duties
PRESSU	Computes the average pressure of the inner and outer streams.
MAXVEL	Computes the maximum velocity of the inner and the outer streams.
TWO	Used to compute the separations when the centrifuge contains both stripping and rectifying sections.
CONVERG	A scientific subroutine used to find a root of a non-linear equation after the root has been bracketed.
SWITCH	Used by CONVERG to update the closeness of the bracket.
CHECK	Used by CONVERG to speed convergence when the guesses bracketing the root are far apart.
FASTC	A short version of CONVERG used by TWO to converge on the composition at the feed locations.

1. Rectifying centrifuge: This is the most easily handled case. After computing the constants in the above analytical solution, for any height, the true value of y_p is bracketed by guessing values of y_f and 1.0. Using these guesses, subroutine CONVERG quickly converges to the true value of y_p . Having computed the value of y_p , the lean stream composition is computed using the expression

$$y_1 = \frac{SCFMU \cdot (YF - YP) + SCFMD \cdot YP}{SCFMD}$$

2. Stripping centrifuge: In this type of centrifuge the feed enters as the inner stream. A portion of the leaving inner stream is removed as the lean product stream with the remainder recycled as the



entering outer stream. The leaving outer stream is the rich product stream.

By guessing a value of the lean stream composition, y_1 , the rich stream composition can be computed by mass balance.

$$y_r = \frac{SCFMD*(YF - YL) + SCFMU*YL}{SCFMU}$$

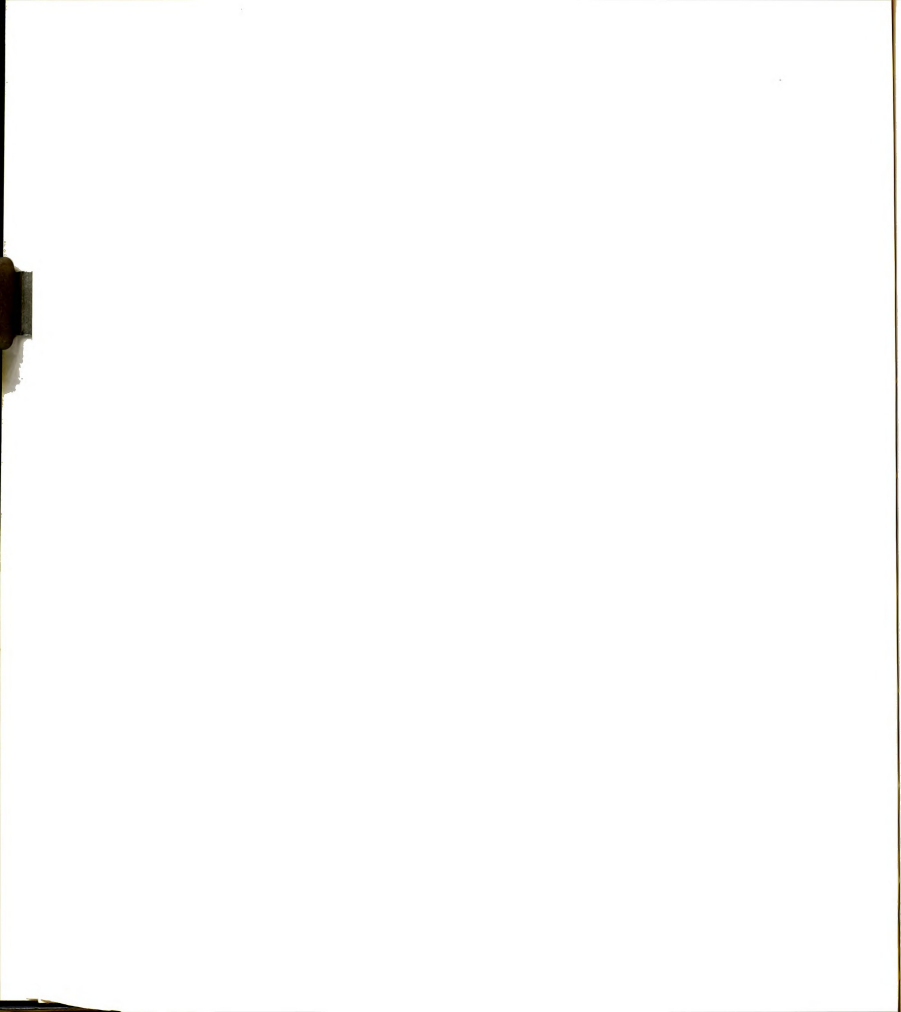
This value, however, must also agree with that calculated by the analytical (approximate) solution based on the guessed lean product stream composition. Using 0.0 and y_f as guesses to bracket the true lean stream composition, subroutine CONVERG is used to converge to the true value of y_1 .

3. Stripping-rectifying centrifuge: After computing the constants in the analytical (approximate) solution for both the stripping and the rectifying sections the following is the flow of calculations used to arrive at a solution:

A. Bracket the true inner stream composition just past the feed position by guessing; $y_f/10$ and $(y_f + 9)/10$.

B. This represents the composition of the feed stream to the stripping section. Using the ideas in "2" above, the composition of the lean product stream leaving the stripper and the composition of the outer stream passing the feed position can be computed.

C. The composition of the outer stream passing the feed position represents the feed to the rectifying section. Using the ideas in "1" above, the rich product stream composition



leaving the rectifier and the composition of the inner stream just before the addition of the feed can be computed.

D. A mass balance is then written about the feed position. This is done by finding the composition after the mixing of the inner stream leaving the rectifier and the incoming feed occurs. If this composition, which is the stripper feed composition, matches the assumed value of this composition, calculations are complete. Otherwise, subroutine FASTC is used to provide a better approximation of the composition of the stripper feed and calculations are returned to step "B" above.

While program CENTRI was used to provide many of the results embodied in the preceding work, a further example of its applicability is included here. Beams (4) published experimental results which were obtained when separating UF_6 (235 and 238 isotopes) in a countercurrent rectifying centrifuge. The following are the operating conditions which were included with the experimental results:

$$\text{MW}_1 = 352$$

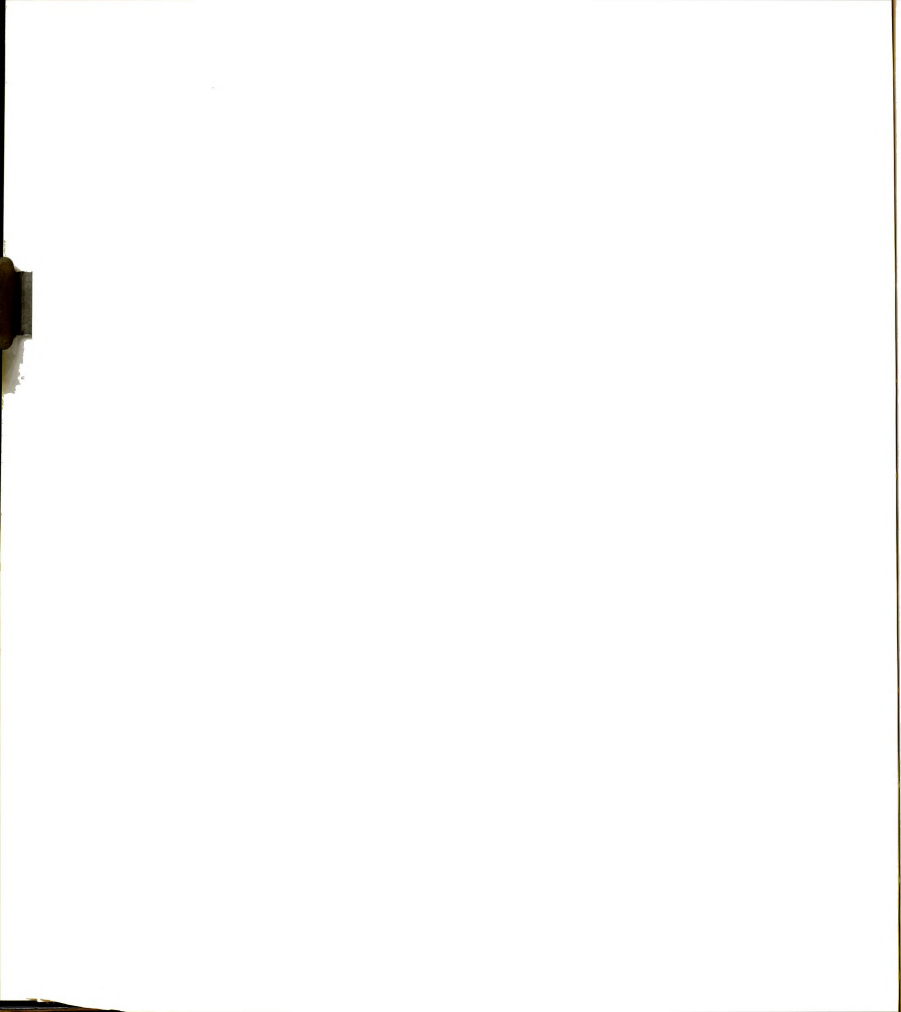
$$\text{MW}_2 = 349$$

$$\text{Temperature} = 626.4^\circ\text{R}$$

Axis pressure: a value was not given, but was assumed to be 0.1 psia. As shown in Chapter V-D-3, the actual pressure does not affect the separation.

$$\text{Feed composition, } y_f = 0.9928 \text{ (U}_{238}\text{)}$$

$$D_{12}^0 = 1.744 \times 10^{-5} \text{ lb}_m/\text{ft}/\text{sec} \text{ (computed from Beam's results)}$$



Centrifuge radius = 3.673 inches

Inner flow radius = 1.912 inches

Centrifuge length = 136 inches

Due to the length of his centrifuge it was assumed that laminar flow would best approximate the velocity profiles in his centrifuge.

Furthermore, the flow intersection was adjusted so that the shear rates of the inner and outer streams were equal at the flow intersection. Table E-3 contains the feed and product stream flow rates for his various experimental runs along with the separations he observed and computed theoretically. Also included in Table E-3 are the theoretical separations and the ratio of the feed rate to the optimum feed rate computed by CENTRI. As can be seen in Table E-3, the agreement between the experimental results and those computed by CENTRI are rather good.

While a complete listing and description of all the parameters computed and printed by CENTRI will not be given here in the text, a sample output follows. The sample output is for the separation of the gas pair $\text{SO}_2\text{-N}_2$ in a countercurrent rectifying centrifuge which fully illustrates and defines all parameters computed. Output for a stripping centrifuge is identical and that for a stripper-rectifier combination consists of two pages detailing the parameters for each section.

Following the sample output is a complete listing of CENTRI and its associated subroutines. Included in the program and subprogram

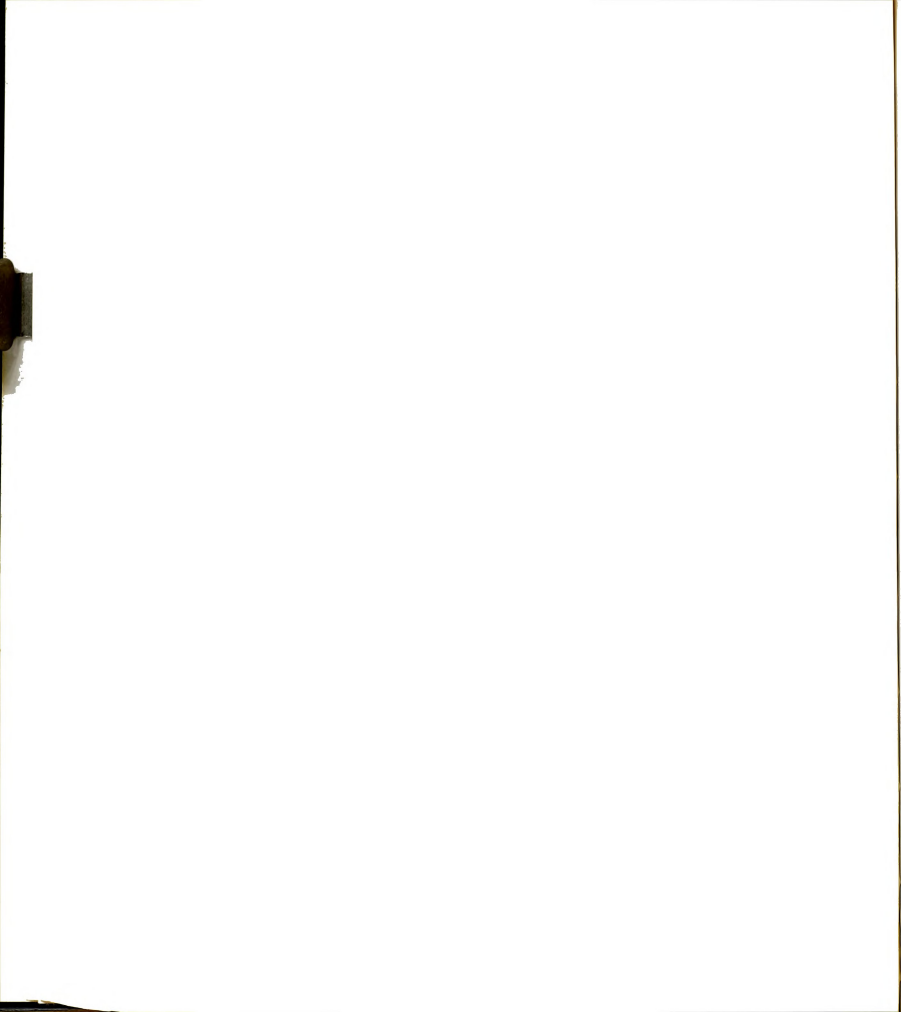
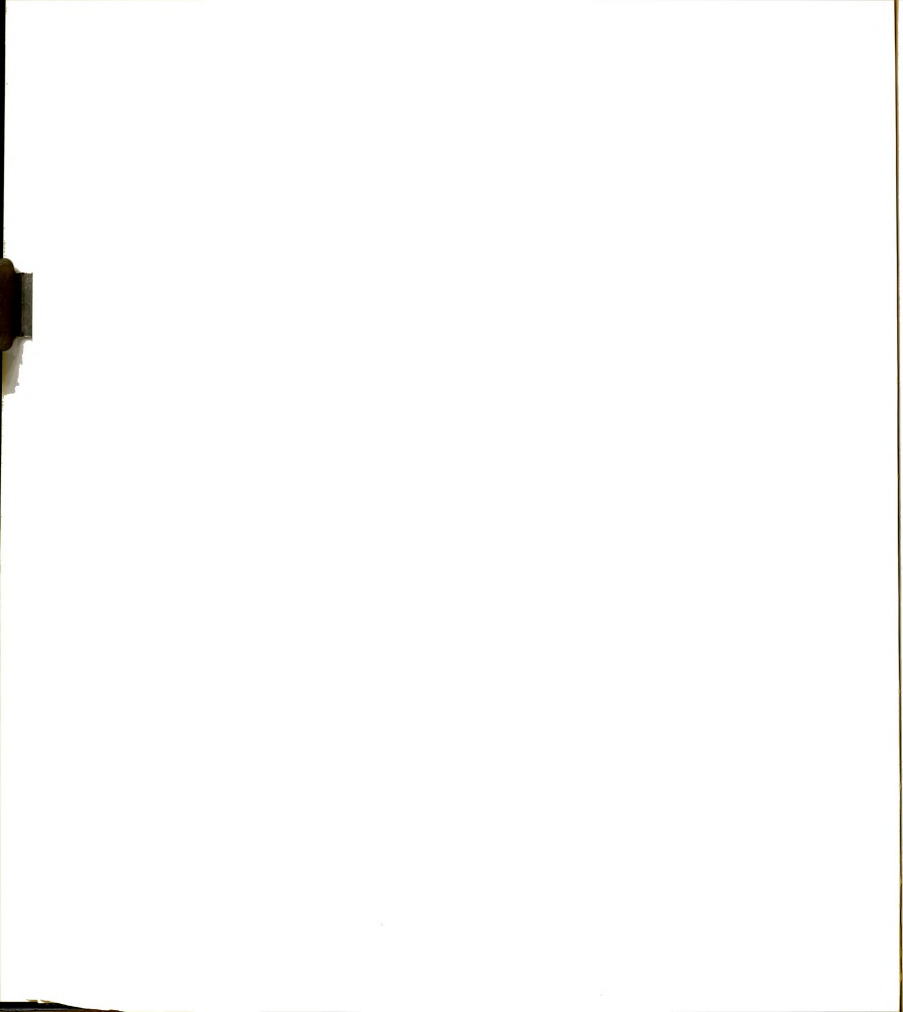


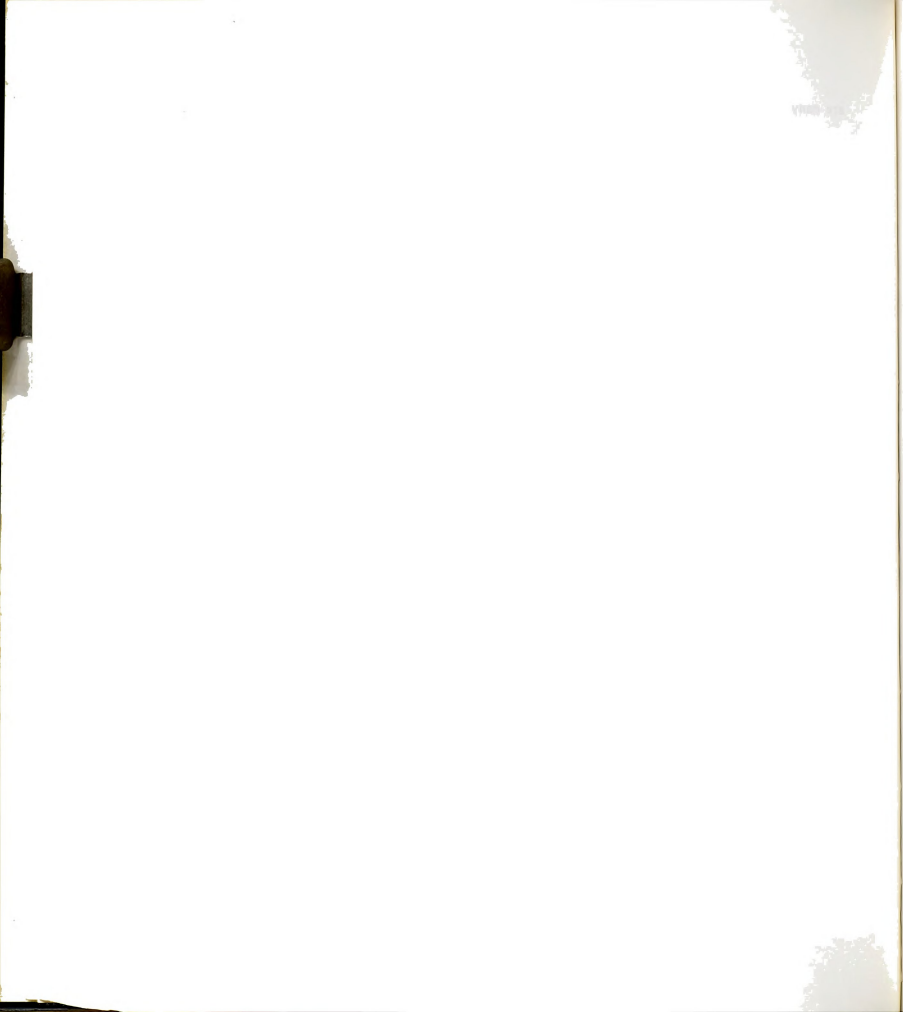
TABLE E-3.--A Comparison of Experimental Separations Observed by Beams (4) and Those Computed by CENTRI for the Enrichment of Uranium.

Feed Rate (mg/sec)	Rich Stream (mg/sec)	Separations for U ²³⁵			
		Beam's Results		Results Computed	
		Separation Factor	Experimental	Separation Factor	Feed/ Optimum Feed
36.4	2.87	1.177	1.042	1.095	1.386
38.0	2.80	1.182	1.118	1.103	1.456
62.1	2.55	1.181	1.115	1.166	2.468
41.1	3.45	1.165	1.105	1.088	1.556
43.0	3.46	1.164	1.131	1.093	1.634
42.7	3.34	1.167	1.117	1.096	1.627
41.4	3.35	1.165	1.124	1.092	1.573
45.7	3.35	1.169	1.125	1.068	1.642
44.4	4.59	1.135	1.113	1.103	1.752
61.8	4.32	1.147	1.112	1.096	1.643
41.5	2.67	1.190	1.132	1.105	2.376
43.0	1.98	1.218	1.146	1.119	1.606
56.3	3.41	1.165	1.119	1.165	1.699
41.5	6.01	1.100	1.093	1.045	1.462



are many comment cards which reiterate details given here and some cases describe in more detail certain aspects.

The program was executed on a CDC 6500 digital computer requiring 2 seconds of central processor time for the solution of a rectifying or a stripping centrifuge.



GAS CENTRIFUGE ANALYSIS
--- COUNTERCURRENT OPERATION --- RECTIFYING CENTRIFUGE

A. OPERATING CONDITIONS

1. TEMPERATURE = 530.00 R
2. AXIS PRESSURE = 14.7000 PSIA
3. PRESSURE AT FLOW INTERFACE = 15.9622 PSIA
4. AVERAGE PRESSURE OF CENTER FLOW = 15.3224 PSIA
5. WALL PRESSURE = 19.0804 PSIA
6. AVERAGE PRESSURE OF OUTER FLOW = 17.4750 PSIA
7. INNER RADIUS = 0.000 INCHES
8. CENTRIFUGE RADIUS = 4.000 INCHES
9. CENTRIFUGE RPM = 20000.0 OR PERIPHERAL SPEED = 698.132 FT/SEC
10. AVERAGE RPM = 20000.0

B. GAS PROPERTIES

1. HEAVY SPECIE MOL WT = 64.0000
2. LIGHT SPECIE MOL WT = 28.0000
3. HEAVY SPECIE MOLE FRACTION IN THE FEED = .5000E-02
4. FEED GAS MOLECULAR WT = 28.1800
5. DIFFUSIVITY TIMES DENSITY AT THE ABOVE TEMPERATURE = .10553E-04 LBM/FT/SEC
6. VISCOSITY AT THE ABOVE TEMPERATURE = .11693E-04 LBM/FT/SEC

C. GAS FLOW RATE --- $V_{MAX} * ((LAMINAR(H)) * 1.0000)$

1. INNER STREAM FLOW RATE = .2000E-01 SCFM -OR- .92854E-06 LB MOLES/SEC
2. OUTER STREAM FLOW RATE = .2000E-01 SCFM -OR- .92854E-06 LB MOLES/SEC
3. INNER FLOW / OUTER FLOW = 1.00000
4. INNER FLOW RADIUS = 0.000 INCHES --- WITH R(INNER)/R(WALL) = 0.00000
5. FLOW INTERSECTION = 2.25 INCHES --- WITH R(INTERSECT)/R(WALL) = .56200
6. INNER STREAM MAX VEL = -.00625 AND OUTER STREAM MAX VEL = .00192 FT/SEC
7. POWER REQUIRED TO ROTATE THE GAS WITH THE ABOVE FLOW PATTERN = .20026E+00 WATTS
8. POWER LOST BY RADIAL SHEARING = 0. WATTS/FT

D. CALCULATION PARAMETERS

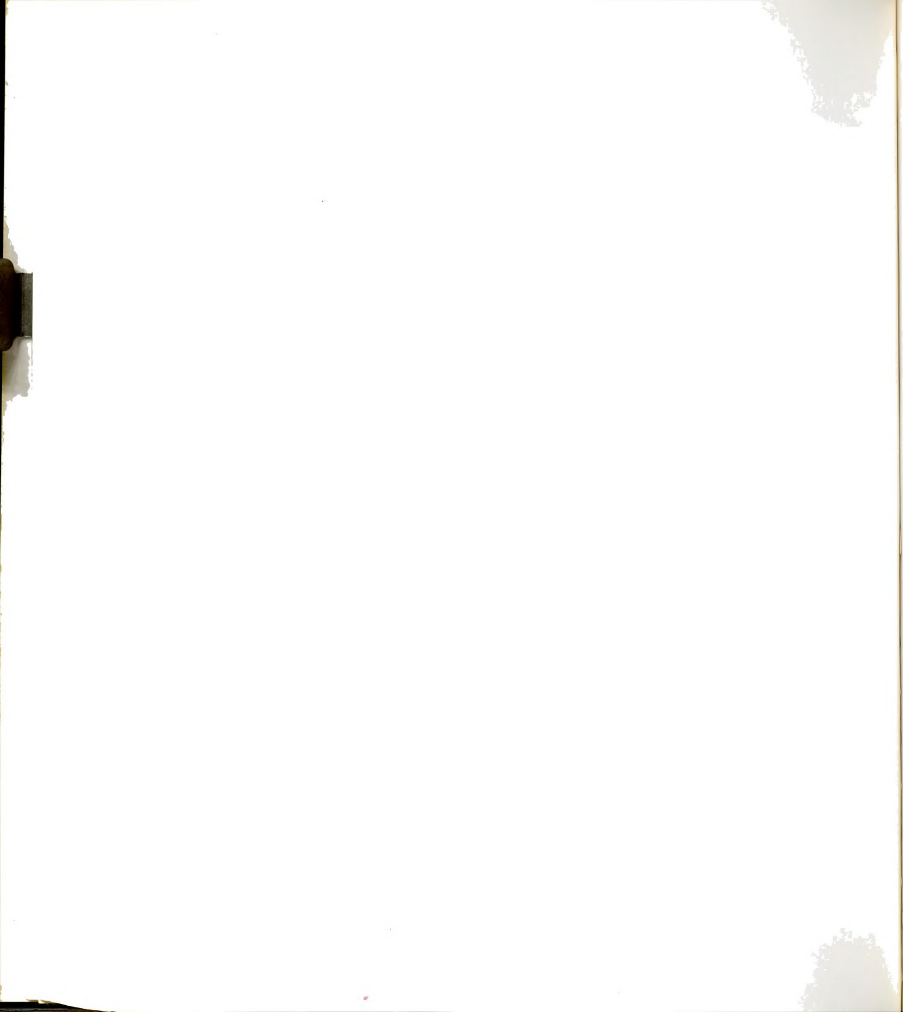
1. C1 = .164466E-06 LB MOLES/SEC, C2 = .130720E-06 LB MOLES FT/SEC
2. C3 = .262141E-06 LB MOLES FT/SEC, C5 = .392861E-06 LB MOLES FT/SEC
3. C1/C5/2.0 = .289318E+00 /FT, (FLOWU-FLOWD)/C1 = 0.
4. HOLDUP = C6 = .103158E-02 LB MOLES/FT
5. SEPARATIVE POWER = .172128E-07 LB MOLES/FT/SEC
6. TOTAL FLOW / OPTIMUM FLOW = .141611E+01

E. SEPARATIONS AT VARIOUS LENGTHS --- WHERE YF = THE FEED COMPOSITION,
YP = THE PRODUCT STREAM COMPOSITION, AND YW = WASTE STREAM COMPOSITION OF THE HEAVY SPECIE

Z (INCHES)	YP/YF	YP/YW	SEP FAC(F)	SEP FAC(W)	STAGES	EFFICIENCY
0.00	1.0000000	1.0000000	1.0000000	1.0000000	.00000	0.
18.00	1.8656234	1.8656234	1.8737741	1.8737741	2.20452	0.

F. SIMPLE AND NO PRODUCTION CENTRIFUGE CHARACTERISTICS

1. SIMPLE SEPARATION FACTOR = 1.3954120 AND Y/YF = 1.3926586
2. NO PROD SEPARATION FACTOR = 1.8737741 AND Y/YF = 1.8656234
(COMPUTED WITH THE R(INTERSECT) USED ABOVE)



```

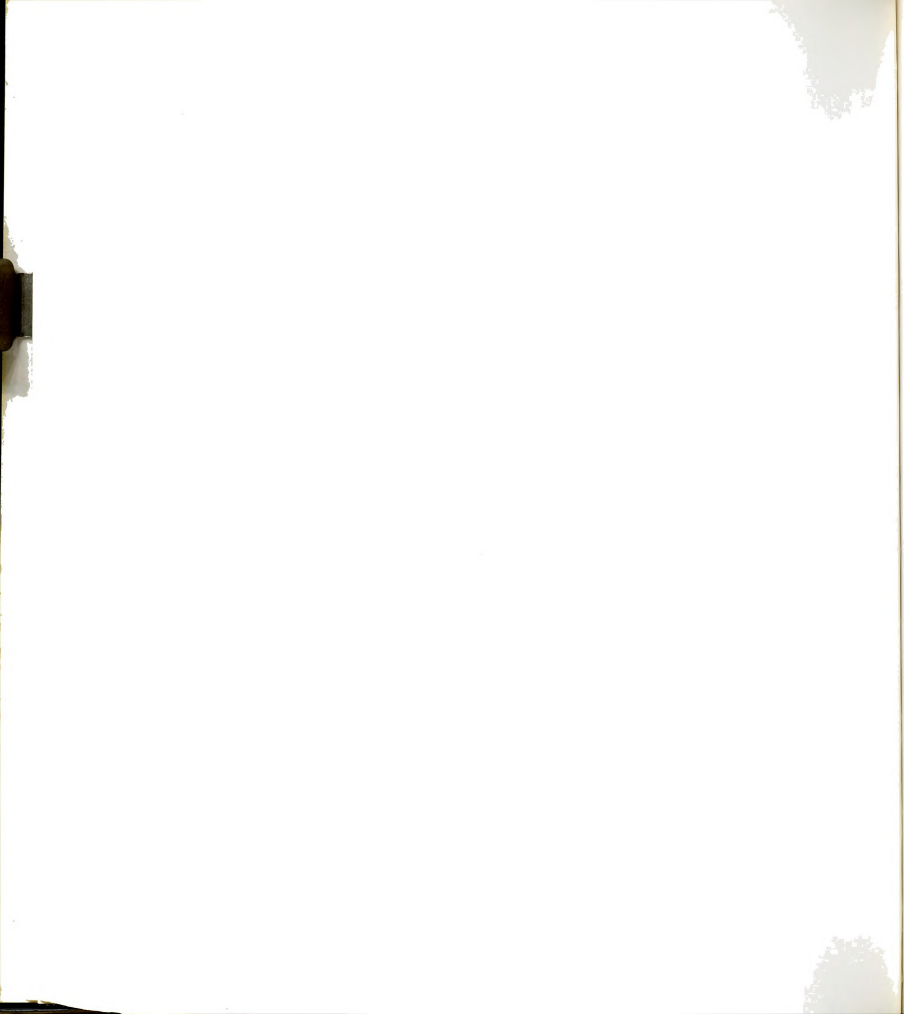
PROGRAM CENTRI( INPUT, OUTPUT )
DIMENSION RAD(1001), PWR(1001)
DIMENSION YOYF(10), PRESS(1001), RADPSEC(1001)
DATA P, PIE, GC / 10.7229, 3.14159, 32.174 /
DATA NP, NPI / 1000, 1001 /
DATA ITWO/ 0 /

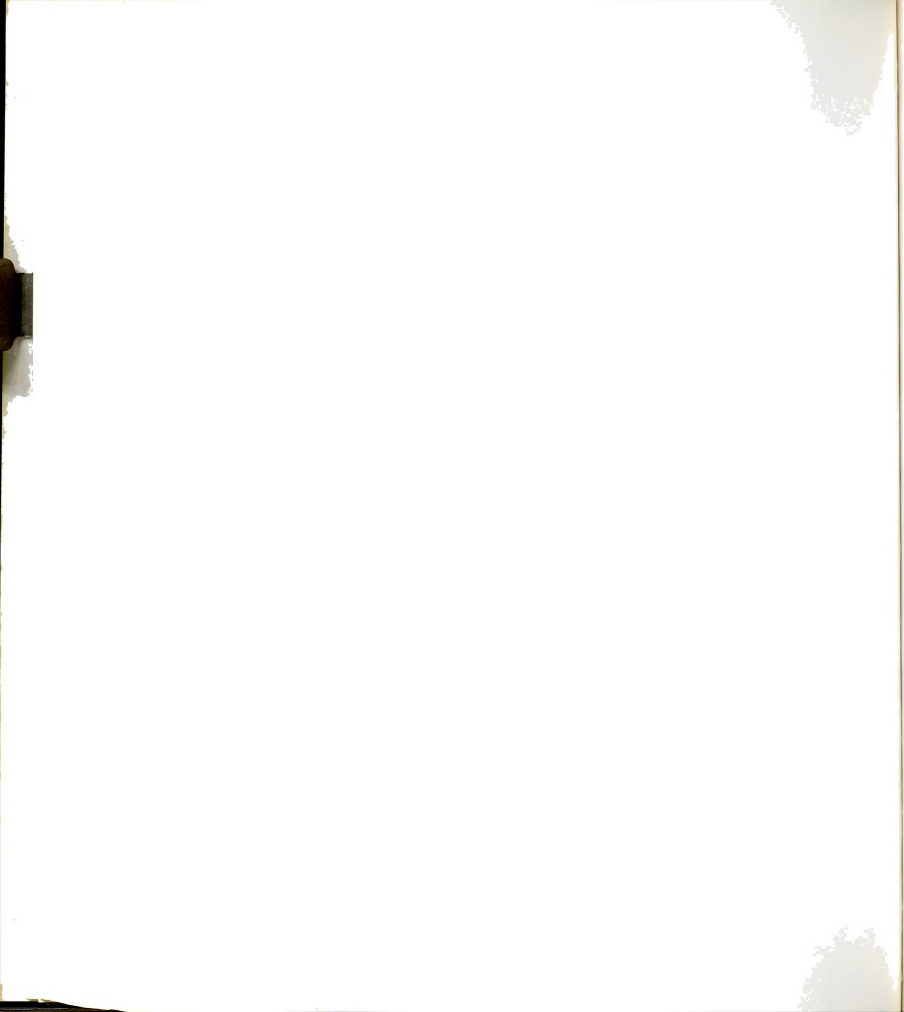
..... THIS PROGRAM USES THE SIMPLIFIED SOLUTION (ANALYTICAL) TO
        COMPUTE THE SEPARATIONS IN THE COUNTERCURRENT CENTRIFUGE.
        THE PROGRAM CAN HANDLE PROBLEMS INVOLVING STRIPPING,
        RECTIFYING OR COMBINATION STRIPPING-RECTIFYING CENTRIFUGES.
        THE FOLLOWING OPTIONS ARE AVAILABLE ---
        ITOPT = 0 RECTIFYING IF H IS + AND STRIPPING IF
                   H IS -
        LOPT MAY BE USED ONLY IF ITOPT IS 0
                   = 0 USES THE FLOWS GIVEN
                   = 1 THE FLOW ARE MULTIPLIED BY THE PROPER
                       FACTOR SO THAT THE OPTIMUM SEPARATION IS
                           FOUND
        ITOPT = 1 STRIPPING AND RECTIFYING CENTRIFUGE
        NOPT = 0 THE PROGRAM USES THE FLOW INTERSECTION
                   GIVEN
                   = 1 ( VPOWER MUST BE 1.0 ) THE FLOW
                       INTERSECTION IS ADJUSTED SO THAT THE SHEAR
                       FORCES AT THE INTERSECTION ARE CONTINUOUS
                       FOR LAMINAR VELOCITY PROFILES
        IDIV = HAS MEANING ONLY IF ITOPT = 0
               THE NUMBER OF DIVISIONS THE GIVEN LENGTH
               WILL BE DIVIDED INTO .....

        ..... INPUT DATA AND PARAMETERS .....

9000 READ 10, WM1, WM2, PO, I, DP, VIS
10 FORMAT( 6F10.0 )
IF( WM1 .LT. 0.0 ) STOP

```

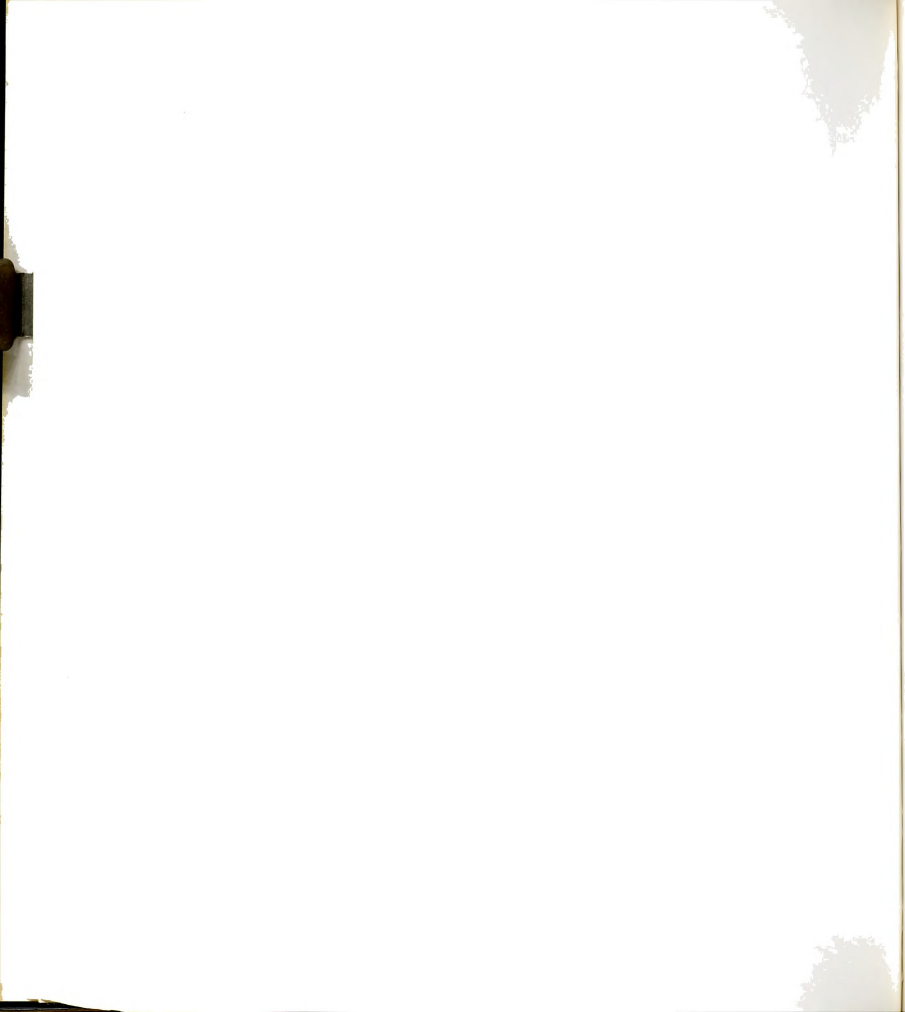





```

C
C
C
DR = DR / 12.0      $      HF = H / 12.0
..... COMPUTE THE INCREMENTAL RADII .....
RAD(I) = RISF
DO 100 I = 2, NP
  RAD(I) = RAD(I-1) + DR      $      PRESS(I) = 1.0
  RAD(NP1) = RWF
  RADPSEC(I) = 0.0
  X = FLOAT(NP) * (RM-RISF)/(RWF-RISF) + 1.0      $      RM = RAD(MM)
  MM = INT( X + 0.5 )
..... COMPUTE DIMENSIONLESS PRESSURES AND RAD/SEC .....
IF( RISF .EQ. 0.0 )      GO TO 17
..... IF THERE IS A CENTER PIPE .....
RK = RISF / RWF      $      PHI = RWF / ( RK*RK - 1.0 )
B = A * 2.0 * PHI * PHI
DO 18 J = 2, NP1
  RADPSEC(J) = PHI * ( RK*RK*RWF/RAD(J)/RAD(J) - 1.0/RWF )
  C = 0.5 * RK*RK*RISF*RISF * ( 1.0/RISF/RISF - 1.0/RAD(J)/RAD(J) )
  1      + 2.0*RK*RK * ALOG( RISF/RAD(J) ) +
  2      0.5/RWF/RWF * ( RAD(J)*RAD(J) - RISF*RISF )
  18 PRESS(J) = EXP( C * B )
  GO TO 19
..... IF THERE IS NOT A CENTER PIPE .....
C
C
C
17 DO 16 I = 2, NP1
  RADPSEC(I) = 1.0
  16 PRESS(I) = EXP( A * RAD(I)*RAD(I) )
  19 X = FLOAT(NP) * ( RIF-RISF ) / ( RWF-RISF ) + 1.0
  NN = INT( X + 0.5 )
  X = FLOAT(NP) * (RM-RISF) / (RWF-RISF) + 1.0

```





```

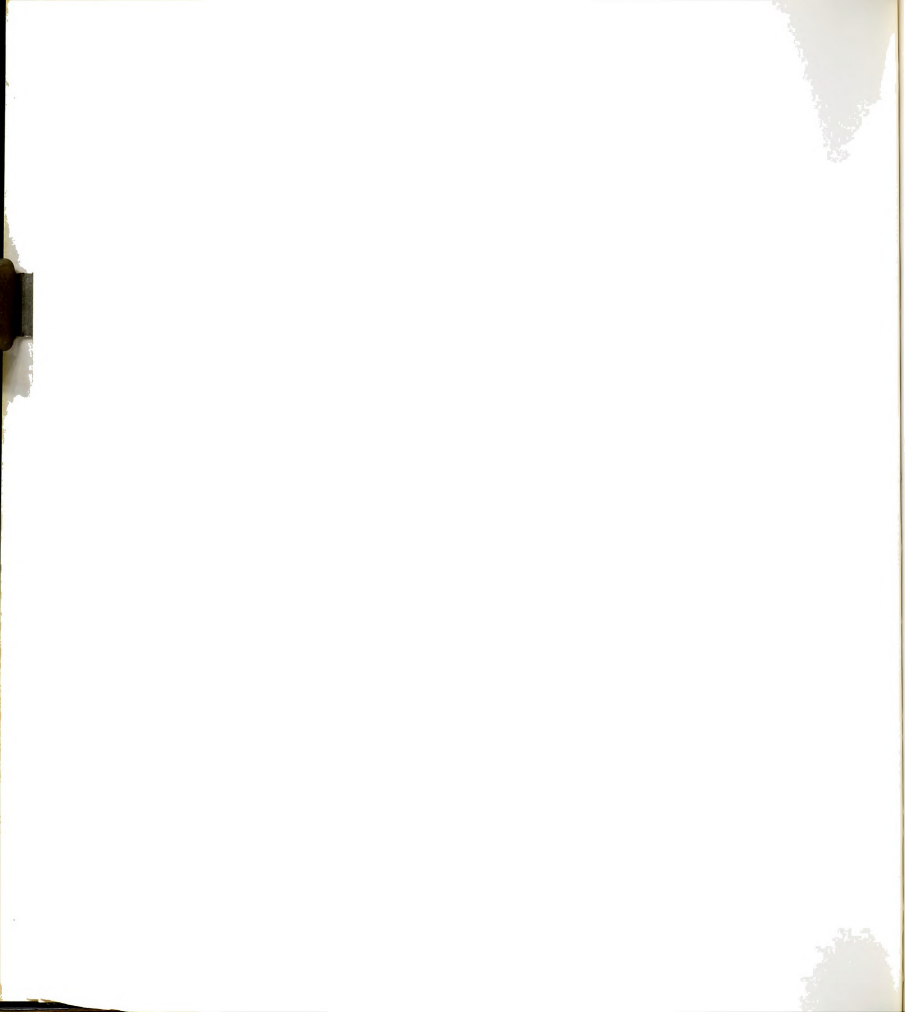
CALL CONVERG( RM, ZERO, RMG, IND, 1 )
X = FLOAT(NP) * (RM-RISF)/(RWF-RISF) + 1.0
MM = INT( X + 0.5 ) $ RM = RAD(MM)
X = FLOAT( MM - MMS )
IF( ABS( X ) .LT. 4.0 ) GO TO 5110
IF( IND ) 21, 22, 23
21 PRINT 24 $ STOP
24 FORMAT( 25X, *DID NOT BRACKET RM* )

C
C
C
C
C ..... COMPUTE THE MAXIMUM VELOCITIES IF THE BEST RM WAS NOT
C REQUESTED .....
C
5110 MM = INT( FLOAT( MM+MMS ) / 2.0 )
RM = RAD(MM)
20 CALL MAXVEL( RTOPO,RAD,PRESS,NP1,NN,MM,FLOWD,VD,VPOWER )
CALL MAXVEL( RTOPO,RAD,PRESS,NP1,MM,NP1,FLOWU,VU,VPOWER )

C
C
C ..... COMPUTE THE FOLLOWING PRESSURES --- AVERAGE PRESSURE
C OF THE CENTER STREAM, PRESSURE AT THE INTERSECTION OF
C THE FLOW STREAMS, AVERAGE PRESSURE OF THE OUTER STREAM,
C AND THE WALL PRESSURE .....
C
22 CALL PRESSU( RAD, PRESS, NP1, NN, MM, PINT, PAVD )
CALL PRESSU( RAD, PRESS, NP1, MM, NP1, PWALL, PAVU )
PINT = PINT * P0 $ PAVD = PAVD * P0
PWALL = PWALL * P0 $ PAVU = PAVU * P0

C
C
C ..... COMPUTE THE FUNCTION VELOCITY TIMES PRESSURE AT THE
C VARIOUS RADII AND USE THE TRAPAZOIDAL RULE TO COMPUTE THE
C THE KINETIC REQUIRED TO ROTATE THE GAS WITH THE
C GIVEN FLOW PATTERN .....
C
ENERGY = 0.0 $ PWR(1) = 0.0
RK = RIF / RM $ B = RM * RM
IF( RIF .EQ. 0.0 ) RK = 1.0E-99
D = ( 1.0-RK*PK ) / ALOG(1.0/RK) $ C = D / 2.0

```

```

C = 1.0 - C * ( 1.0-ALOG(C) )
DO 150 I = 2, MM
  IF( RAD(I) .LT. RIF ) GO TO 201
  DUM = RAD(I) * RAD(I)
  XX = ( 1.0 - DUM/B + D*ALOG( RAD(I)/RM ) ) / C
  IF( XX .NE. 0.0 ) XX = XX ** VPOWER
  PWR(I) = -VD * XX * PRESS(I) * RAD(I)
GO TO 150

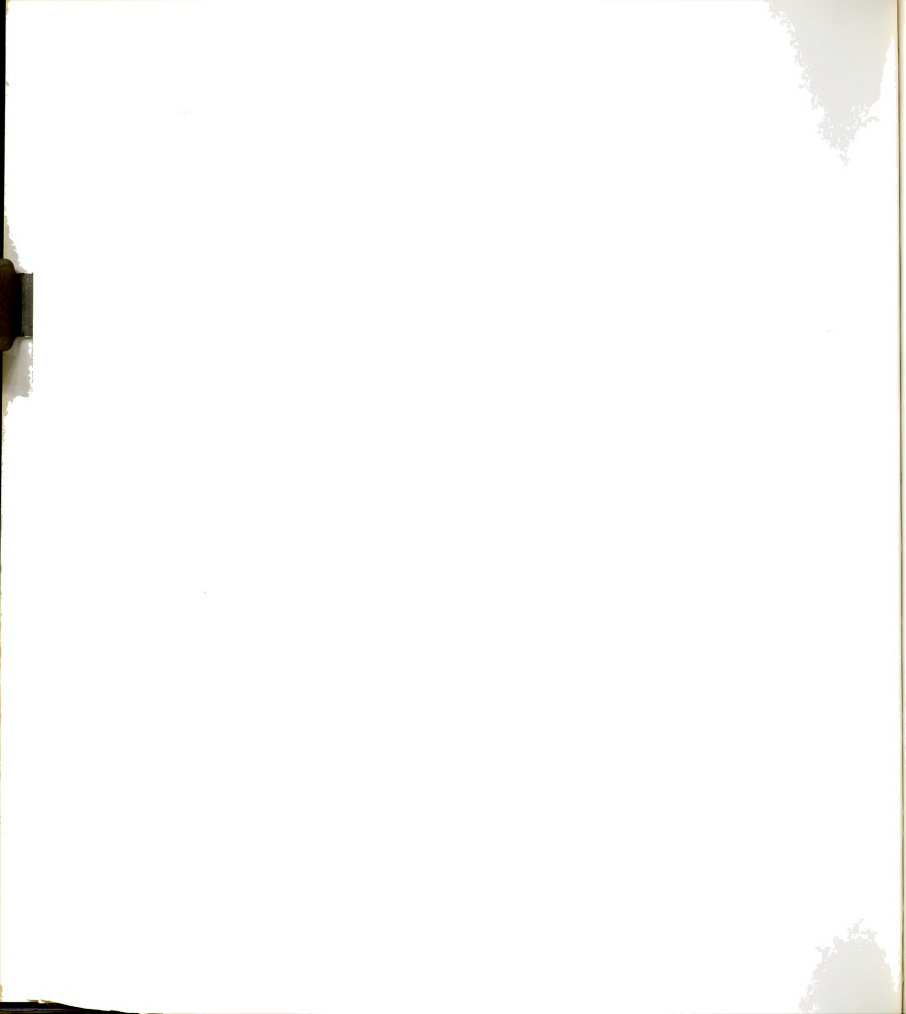
201 PWR(I) = 0.0
150 ENERGY = ENERGY - PWR(I) * RAD(I)*RAD(I) * RADPSEC(I)*RADPSEC(I)
RK = RM/RWF $ B = RWF*RWF $ K = MM + 1
D = ( 1.0-RK*RK ) / ALOG(1.0/RK) $ C = D / 2.0
C = 1.0 - C * ( 1.0-ALOG(C) )
DO 250 J = K, NP1
  DUM = RAD(J) * RAD(J)
  XX = ( 1.0 - DUM/B + D*ALOG( RAD(J)/RWF ) ) / C
  IF( XX .NE. 0.0 ) XX = XX ** VPOWER
  PWR(J) = VU * XX * PRESS(J) * RAD(J)
250 ENERGY = ENERGY + PWR(J) * RAD(J)*RAD(J) * RADPSEC(J)*RADPSEC(J)

C ..... COMPLETE THE CALCULATIONS FOR THE KINETIC ENERGY/SEC
C ( FT-LBF )/SEC AND CONVERT TO WATTS .....
C
C ENERGY = ENERGY * DR / R10P0 / GC * RADPS * RADPS * WM
C ENERGY = ENERGY / 778.0 * 0.293 * 3600.0

C ..... COMPUTE ENERGY/FT/SEC USED BY SHEARING WITH THE CENTER
C PIPE --- THEN CONVERT TO WATTS/FT .....
C
C RK = R1SF/RWF $ RK = RK*RK / ( 1.0-RK*RK )
C ENPFT = 4.0*PIE * VIS * RADPS * RWF*RWF*RK * RADPS / GC
C ENPFT = ENPFT / 778.0 * 0.293 * 3600.0

C ..... COMPUTE THE INTEGRAL --- VEL * PRESS * RAD .....
C
C SUM = 0.0 $ X = PWR(I)

```



```

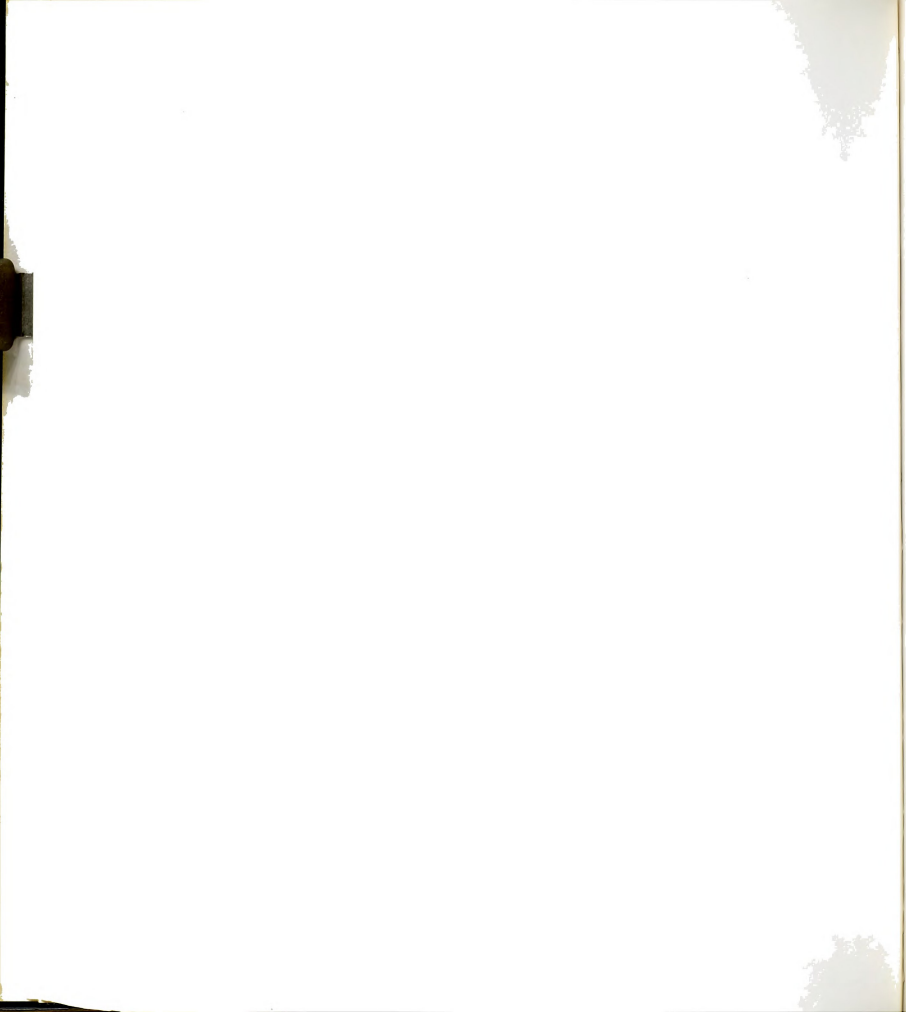
DO 300 I = 2, NP1 $
XX = X $
D = XX + X $
300 SUM = D + SUM
PWR(NP1) = SUM

C
C
C
..... COMPUTE THE INTEGRALS ---- PWR * RAD AND PWR*PWR/RAD .....
SUM = 0.0 $ DUM = 0.0
XS = 0.0 $ XD = 0.0
DO 350 I = 2, NP1 $
XSD = XD $ XD = PWR(I)*PWR(I)
XSS = RADPSEC(I)*RADPSEC(I)*PWR(I)*RAD(I) $ XD = XD/RAD(I)
SUM = SUM + XSS + XS
DUM = DUM + XSD + XD
350 SUM = SUM * DR*DR/4.0 $ DUM = DUM * DR*DR*DR/8.0

C
C
C
..... COMPUTE THE EQUATION PARAMETERS .....
P = FLOWU - FLOWD
C1 = 2.0/RTOPO*( WM2-WM1 ) * RADPS*RADPS / GC/R/T*SUM / 144.0
C2 = PIE / R / T * DP * ( RWF*RWF - RISF*RISF ) $ C5 = C2+C3
C3 = 2.0 / RTOPO / DP * P0 * DUM $ C = P / C1
B = C1 / C5 / 2.0 $ GO TO 8000
IF( IGOBACK .EQ. 0 ) $ C6 = 0.0
OPT = 1.0 / SQRT( C2/C3 )

C
C
C
..... CHECK IF THE OPTIMUM FLOW PROBLEM IS TO BE WORKED .....
IF( LOPT .EQ. 0 ) GO TO 351
SCFMD = SCFMD/OPT $ SCFMD = SCFMD/OPT
FLOWD = FLOWD/OPT $ FLOWD = FLOWD/OPT
LOPT = 0 $ GO TO 20
351 SUM = 0.0 $ XR = 0.0
DO 701 I = 2, NP1 $
XX = X $ XRR = XR

```



```

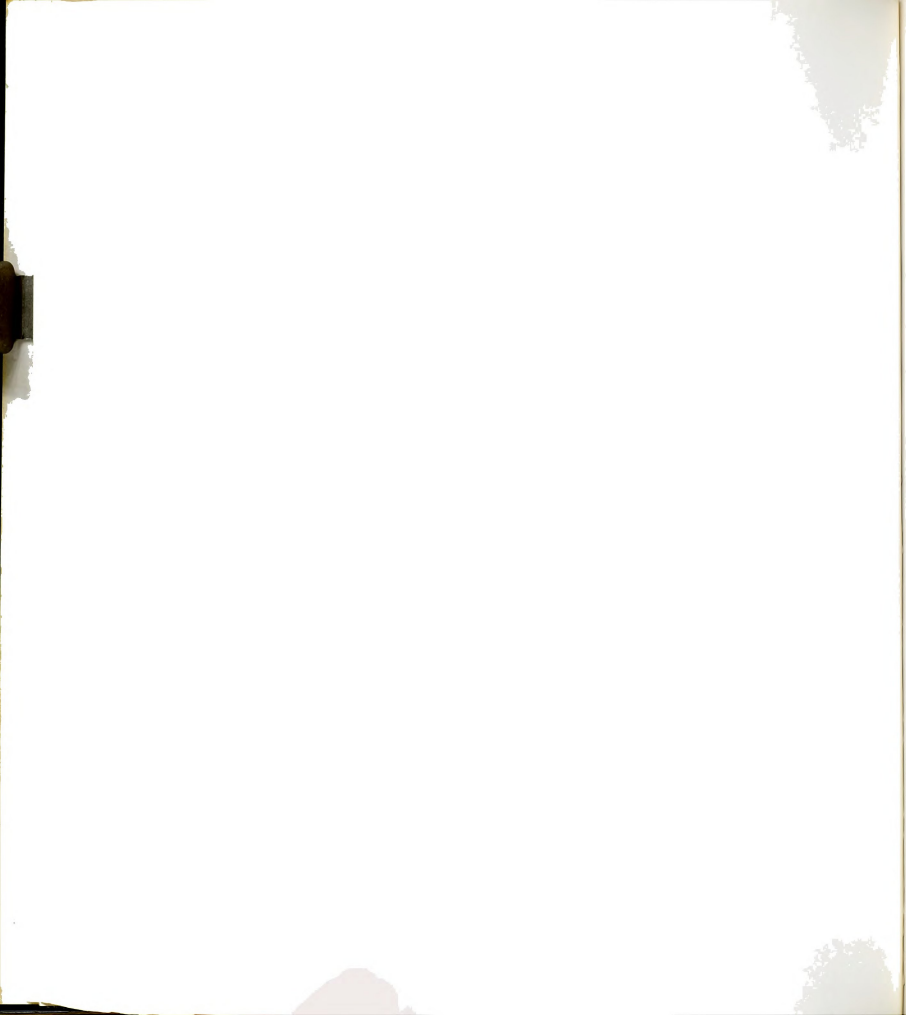
X = PRESS(I) * RAD(I)      $      XR = X * RADPSEC(I)
C6 = C6 + X + XX
701 SUM = SUM + XR + XRR
SPEEDA = OMEGA * SUM / C6
C6 = C6 / RTOPO * DR
SEPPOW = C1 * C1 / C5 / 4.0

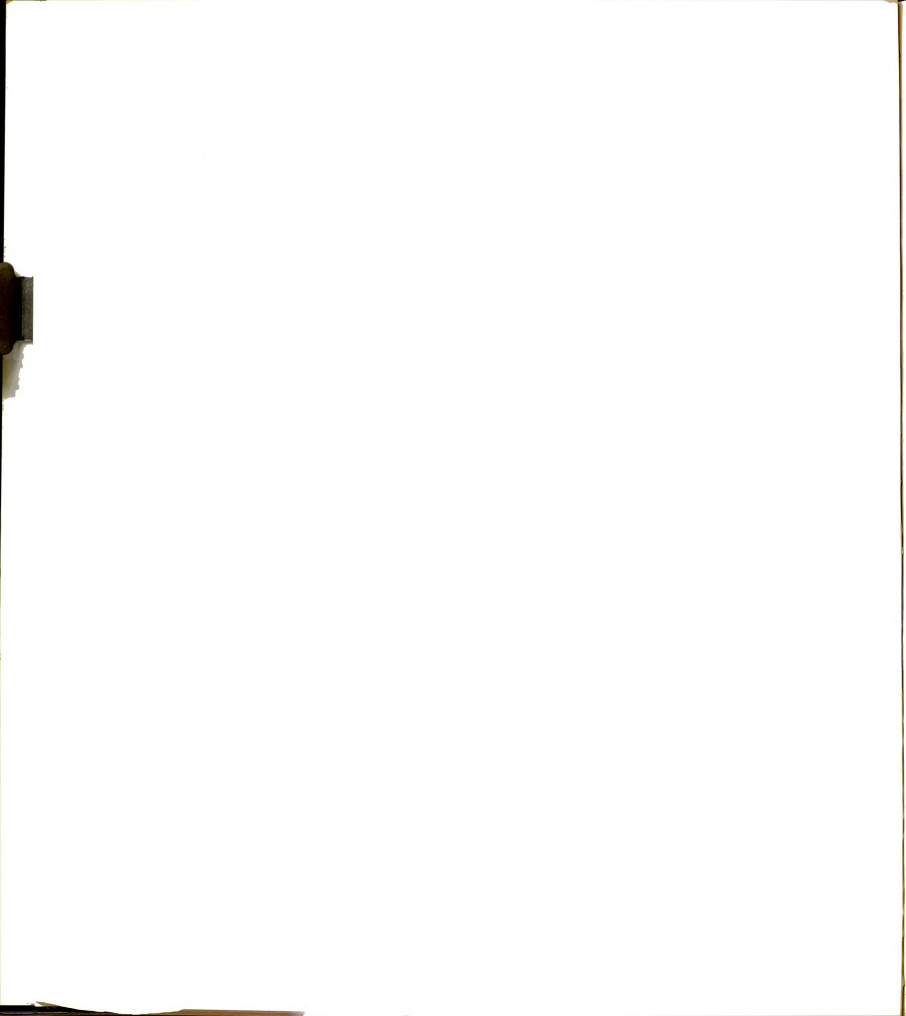
C      ..... SIMPLE CENTRIFUGE SEPARATION FACTOR .....
C
C      SEPFAC = ALOG( PRESS(NP1) ) / WM
C      SEPFAC = EXP( ( WM1-WM2 ) * SEPFAC )
C      DY = SEPFAC * YF / (1.0-YF)      $      DY = DY / (1.0+DY) - YF
C      IF( ITOPT .EQ. 1 )      GO TO 1011

C      ..... AT VARIOUS LENGTHS SOLVE FOR Y/YF .....
C
C      DH = HF / FLOAT( IDIV )      $      Z = DH
C      YOYF(1) = 1.0
C      K = IDIV + 1
C      DO 550 I = 2, K
C      IF( DH .GT. 0.0 )      GO TO 551

C      ..... STRIPPING CENTRIFUGE --- SOLVE BY BRACKETING THE LEAN
C      COMPOSITION .....
C
C      Y = YF      $      YG = 0.0      $      IND = 1
552 DELTA = SQRT( 1.0 + 2.0*C*( 1.0-2.0*Y ) + C*C )
DUM = EXP( B * DELTA * Z )      $      D = 1.0 / DUM
TANH = ( DUM-D ) / ( DUM+D ) / DELTA
YR = Y * ( 1.0 - TANH*(1.0-C) ) / ( TANH*(1.0-2.0*Y+C) + 1.0 )
ZERO = FLOWD*YF - FLOWU*YR + P*Y
CALL CONVERG( Y, ZERO, YG, IND, 0 )
IF( IND ) 553, 554, 552
553 PRINT 556      $      STOP
556 FORMAT( *I*, 20X, *DID NOT BRACKET THE EXIT MOLE FRACTION* )
554 Y = YR      $      GO TO 560

```





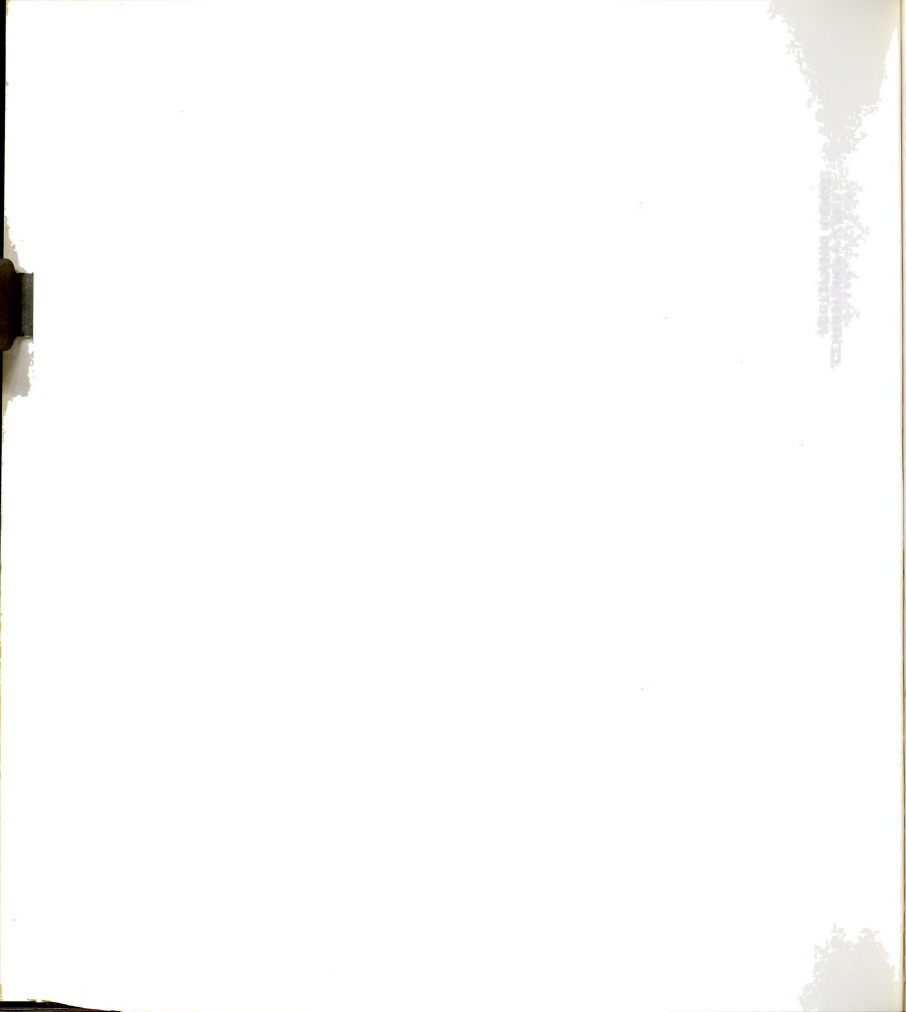
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1      YB, YT, YF, YR
1012 FORMAT( /, 20X, *E. STRIPPING ---- RECTIFYING CENTRIFUGE*, //,
1 25X, *1. STRIPPING LENGTH =*, F10.2, * INCHES, RECTIFYING LENGT
2H =*, F10.2, * INCHES*, /, 25X, *2. FEED RATE =*, E15.5, * SCFM
3 -OR-*, E15.5, * LB MOLES/SEC*, /, 25X, *3. LEAN STREAM RATE =
4*, E15.5, * SCFM -OR-*, E15.5, * LB MOLES/SEC*, /, 25X, *4. RI
5CH STREAM RATE =*, E15.5, * SCFM -OR-*, E15.5, * LB MOLES/SEC
6*, /, 25X, *5. RICH / FEED =*, F15.5, /, 25X, *6. Y(LEAN) =*,
7 E14.5, * AND Y(RICH) =*, E14.5, /, 25X, *7. STRIPPER FE
8ED, Y =*, E14.5, * AND RECTIFIER FEED, Y =*, E14.5 )
YF = YFSIO

C      ..... BEGIN OUTPUT .....
C
C      ..... HEADING .....
C
1091 PRINT 1000
1000 FORMAT( *1*, /, 56X, *GAS CENTRIFUGE ANALYSIS* )
IF( ITOPT.EQ. 0 .AND. H.GT. 0.0 ) PRINT 1096 RECTIFYIN
1096 FORMAT( 52X, *---- COUNTERCURRENT OPERATION ----
1G CENTRIFUGE* )
IF( ITOPT.EQ. 0 .AND. H.LT. 0.0 ) PRINT 1099 STRIPPING
1099 FORMAT( 52X, *---- COUNTERCURRENT OPERATION ----
1 CENTRIFUGE* )
IF( ITOPT.EQ. 1 .AND. ITWO.EQ. 0 ) PRINT 1097 STRIPPING
1097 FORMAT( 52X, *---- COUNTERCURRENT OPERATION ----
1 SECTION*, / )
IF( ITWO.EQ. 1 ) PRINT 1098 RECTIFYIN
1098 FORMAT( 52X, *---- COUNTERCURRENT OPERATION ----
1G SECTION*, / )

C      ..... OPERATING CONDITIONS .....
C
C PRINT 1100, T, PO, PINT, PAVD, PWALL, PAVU, RIS, RW, OMEGA, SPEED
1100 FORMAT( 20X, *A. OPERATING CONDITIONS*, //, 25X, *1. TEMPERATURE
1=*, F10.2, * R*, /, 25X, *2. AXIS PRESSURE =*, F10.4, * PSIA*, /,

```



```

2 25X, *3. PRESSURE AT FLOW INTERFACE =*, F10.4, * PSIA*, /, 25X,
3 *4. AVERAGE PRESSURE OF CENTER FLOW =*, F10.4, * PSIA*, /, 25X,
4 *5. WALL PRESSURE =*, F10.4, * PSIA*, /, 25X, *6. AVERAGE PRESSU
5 RE OF OUTER FLOW =*, F10.4, * PSIA*, /, 25X, *7. INNER RADIUS =*
6, F10.3, * INCHES*, /, 25X, *8. CENTRIFUGE RADIUS =*, F10.3, PE
7 * INCHES*, /, 25X, *9. CENTRIFUGE RPM =*, F10.1, 5X, * OR
8 RPHICAL SPEED =*, F10.3, * FI/SEC* )
PRINT 1111, SPEEDA
1111 FORMAT( 25X, *10. AVERAGE RPM =*, F10.1 )

C
C ***** CONVERT BACK TO DIFFUSIVITY TIMES DENSITY AND OUTPUT
C GAS PROPERTIES *****
C
DP = DP / T / R * WM
PRINT 1200, WM1, WM2, YF, WM, DP, VIS
1200 FORMAT( /, 20X, *8. GAS PROPERTIES*, /, 25X, *1. HEAVY SPECIE M
10L WT =*, F10.4, /, 25X, *2. LIGHT SPECIE MOL WT =*, F10.4, /,
2 25X, *3. HEAVY SPECIE MOLE FRACTION IN THE FEED =*, E13.4, /,
3 25X, *4. FEED GAS MOLECULAR WT =*, F10.4, /, 25X, *5. DIFFUSIVIT
4 Y TIMES DENSITY AT THE ABOVE TEMPERATURE =*, E13.5, * LBM/FT/SEC*
5 /, 25X, *6. VISCOSITY AT THE ABOVE TEMPERATURE =*, E13.5,
6 * LBM/FT/SEC* )

C
C ***** COMPUTE FLOW RATIO AND FLOW INTERSECTION TO WALL RADIUS
C AND OUTPUT GAS FLOW RATE *****
C
RATIO = FLOWD/FLOWU $ DUM = RM / RWF
RM = RM * 12.0 $ VD = - VD
PRINT 1299, VPORER
1299 FORMAT( /, 20X, *C. GAS FLOW RATE --- VMAX*, 1H*,*((LAMINAR(R))*)
1 , 2H*, F6.4, * )
PRINT 1300, SCFMD, FLOWD, SCFMDU, FLOWU, RATIO
1300 FORMAT( /, 25X,
1 *1. INNER STREAM FLOW RATE =*, E15.4, * SCFM*, 5X, *-OR-*, E15.5
2 , * LB MOLES/SEC*, /, 25X, *2. OUTER STREAM FLOW RATE =*, E15.4,
3 * SCFM*, 5X, *-OR-*, E15.5, * LB MOLES/SEC*, /, 25X, *3. INNER F

```



```

4LOW / OUTER FLOW =*, F12.5 )
IF( NOPT .NE. 1 )
PRINT 1605
1605 FORMAT( /, 30X, *--- THE INTERSECTION OF THE STREAMS WAS ADJUSTED
1 TO BALANCE SHEAR FORCES ---*, / )
2005 Z = R1 / RW
PRINT 1601, R1, Z
1601 FORMAT( 25X, *, INNER FLOW RADIUS =*, F6.3, * INCHES --- WI
1H R(INNER)/R(WALL) =*, F10.5 )
PRINT 1600, RM, DUM, VD, VU, ENERGY, ENPFT
1600 FORMAT( 25X, *, FLOW INTERSECTION =*, F6.2, * INCHES --- WIT
1H R(INTERSECT)/R(WALL) =*, F10.5, /, 25X, *, INNER STREAM MAX VE
2L =*, F9.5, * AND OUTER STREAM MAX VEL =*, F9.5, * FT/SEC*, /,
3 25X, *, POWER REQUIRED TO ROTATE THE GAS WITH THE ABOVE FLOW PATI
4ERN =*, E15.5, * WATTS*, /, 25X, *, POWER LOST BY RADIAL SHEARIN
5G =*, E15.5, * KALIS/FT* )
C
C
C ..... OUTPUT CALCULATION PARAMETERS .....
PRINT 2500, C1, C2, C3, C5, B, C, C6, SEPOW, OPT
2500 FORMAT( /, 20X, *, D. CALCULATION PARAMETERS*, /, 25X, *, C1 =*
1 ,E15.6, * LB MOLES/SEC, C2 =*, E15.6, * LB MOLES FT/SEC*, /,
2 25X, *, C3 =*, E15.6, * LB MOLES FT/SEC, C5 =*, E15.6, * LB
3 MOLES FT/SEC*, /, 25X, *, C1/C5/2.0 =*, E15.6, */FT, (FLOW-FLWD/
4)/C1 =*, E15.6, /, 25X, *, HOLDUP = C6 =*, E15.6, * LB MOLES/
5FT*, /, 25X, *, SEPARATIVE POWER =*, E15.6, * LB MOLES/FT/SEC*,
6 /, 25X, *, TOTAL FLOW / OPTIMUM FLOW =*, E15.6 )
IF( ITOPT .EQ. 0 ) GO TO 2001
IF( ITWO .EQ. 1 ) GO TO 1013
ITWO = 1
GO TO 9001
1013 DH = 0.0 $ K = 1 $ Z = HSTO + H
ENERGY = ENERGY + ESTO $ FLOWU = FEED $ FLOWD = FEED-P
YOYF(1) = YT/YF $ YFL = 1.0-YF $ YPH = YT
YPL = 1.0 - YT $ YWH = YB $ YWL = 1.0 - YB
C
C ..... OUTPUT SEPARATIONS AT VARIOUS LENGTHS .....

```



```

C 2001 PRINT 2000
2000 FORMAT( /, 20X, *E. SEPARATIONS AT VARIOUS LENGTHS --- WHERE YF
1= THE FEED COMPOSITION,*,/, 27X, *YP = THE PRODUCT STREAM COMPOS
2ITION, AND YW = WASTE STREAM COMPOSITION OF THE HEAVY SPECIE*,
3 //, 25X, *Z(INCHES)*, 6X, *YP/YF*, 8X, *YP/YW*, 4X, *SEP FAC(F)*,
4 6X, *SEP FAC(W)*, 6X, *STAGES*, 6X, *EFFICIENCY*, / )
IF( ITOPT .EQ. 1 ) GO TO 2003
IF( DH .GE. 0.0 ) GO TO 561
DUM = -DH $ DUM = P $ FLOWD = - DUM
FLOWU = FLOWD $ DH = DH * 12.0
561 Z = 0.0
2003 DO 2100 I = 1, K
IF( ITOPT .EQ. 1 ) GO TO 2004
C ..... COMPUTE ALL MOLE FRACTIONS .....
C
C YFL = 1.0-YF $ YPH = YOYF(I)*YF $ YPL = 1.0-YPH
C YWH = ( YF*FLOWU-P*YPH )/FLOWD $ YWL = 1.0-YWH
C
C ..... COMPUTE THE ENTROPY LOST UNMIXING THE GASES .....
C
2004 EPP = T * R * 144.0 / 778.0 * 0.293 * 3600.0
EPP = EPP * ( P * ( YPH*ALOG( YPH ) + YPL*ALOG( YPL ) )
1 + FLOWD * ( YWH*ALOG( YWH ) + YWL*ALOG( YWL ) )
2 - FLOWU * ( YF*ALOG( YF ) + YFL*ALOG( YFL ) ) )
EPP = EPP / ENERGY
C
C ..... COMPUTE THE SEPARATION FACTORS WITH RESPECT TO THE
C PRODUCT AND WASTE STREAMS .....
C
ALPHAF = YPH/YPL * YFL/YF
ALPHAW = YPH/YPL * YWL/YWH
STAGES = (YPH-YWH)/DY $ YOYW = YPH / YWH
IF( YOYF(I) .EQ. 1.0 ) EPP = 0.0
PRINT 2200, Z, YOYF(I), YOYW, ALPHAF, ALPHAW, STAGES, EPP

```




```

2200 FORMAT( 21X, F10.2, F16.7, F13.7, F12.7, 5X, F11.7, F12.5, E16.5)
2100 Z = Z + DH
C
C ..... COMPUTE THE SEPARATION FACTOR IF THERE IS NO PRODUCTION .....
C
SCFMD = SCFMD $ NOPT = 0 $ IGOBACK = 0
IF( IIOPT .EQ. 1 ) H = Z
ITWO = 0 $ IIOPT = 0 $ GO TO 90
C
C ..... COMPUTE SEPARATION ABILITIES OF THE SIMPLE AND NO
C PRODUCTION CENTRIFUGES .....
C
8000 YSOYF = DY / YF + 1.0
DUM = EXP( B * HF )
IF( HF .LT. 0.0 ) DUM = 1.0 / DUM
DUR = ( DUM - 1.0 / DUM ) / ( 1.0 + DUM )
YNOYF = ( 1.0 + DUM ) / ( 1.0 - DUM + 2.0 * DUM * YF )
DUM = YNOYF * ( 1.0 - YF ) / ( 1.0 - YNOYF * YF )
PRINT 2300, SEPFAC, YSOYF, DUM, YNOYF
2300 FORMAT( /, 20X, *F, SIMPLE AND NO PRODUCTION CENTRIFUGE CHARACTE
1RISTICS*//, 25X, *1. SIMPLE SEPARATION FACTOR =*, F12.7, * AND
2 Y/YF =*, F12.7 /, 25X, *2. NO PROD SEPARATION FACTOR =*, F11.
37, * AND Y/YF =*, F12.7 /, 30X, *( COMPUTED WITH THE RINTERS
4ECT) USED ABOVE ) * )
GO TO 9000
END

```



```

C
C
C
C
SUBROUTINE PRESSU( R, P, NP1, N, M, PI, PA )
  DIMENSION R(NP1), P(NP1)

  ..... THIS SUBROUTINE COMPUTES THE AVERAGE PRESSURE OF EITHER
           THE INNER OR OUTER STREAM .....

  DR = R(2) - R(1)
  PI = P(M)
  L = N + 1
  SUM = 0.0
  S = P(N)*R(N)
  DO 30 J = L, M
    XX = X
    X = P(J) * R(J)
    SUM = SUM + XX + X
  30 SUM = ( SUM*DR/2.0 ) / ( ( R(M)*R(M)-R(N)*R(N) )/2.0 )
  PA = SUM
  RETURN
END

```



```

SUBROUTINE MAXVEL( RTOPO,R,P,NPI,N,M,FLOW,V,VPOWER )
DIMENSION R(NPI), P(NPI)

..... THIS SUBROUTINE COMPUTES THE MAXIMUM VELOCITY IN EITHER
          THE INNER OR OUTER STREAM .....

..... IF VPOWER IS 1.0 THEN HAVE LAMINAR FLOW .....

DR = R(2) - R(1)
L = N ^ 1
X = 0.0
RK = R(1) / R(M)
D = ( 1.0 - P*RK ) / ALOG( 1.0/RK )
C = 1.0 - C * ( 1.0 - ALOG( C ) )
DO 30 I = L, M
  Y = X
  XX = ( 1.0 - R(I)*R(I)/Z + D*ALOG( R(I)/R(M) ) ) / C
  IF( XX .NE. 0.0 )
    Z = R(I) * P(I) * XX
    SUM = SUM + X ^ Y
  V = FLOW * RTOPO / DR * C / SUM
RETURN
END

```

C
C
C
C
C

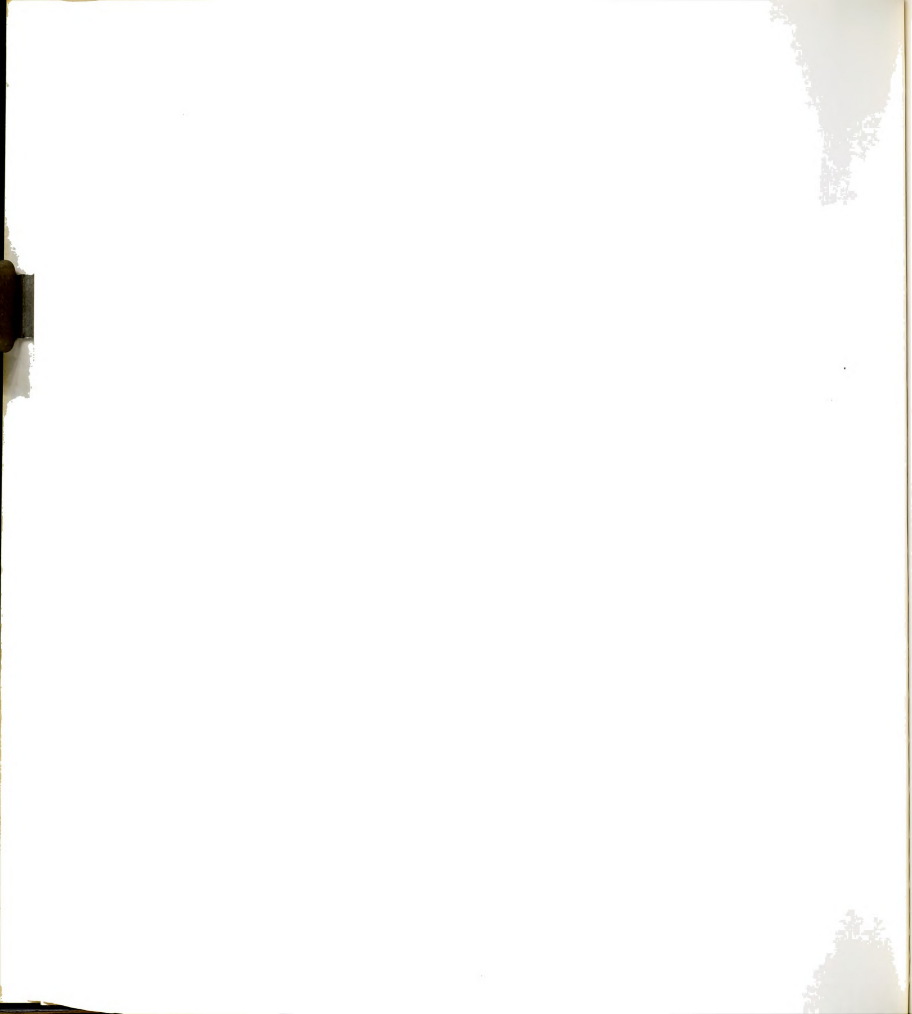


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SUBROUTINE TWO( B, C, HF, YF, YB, YT, FLOWD, FLOWU, P, YR )
DATA N/ 0 /
..... THIS SUBROUTINE IS USED WHEN BOTH A STRIPPING AND A
RECTIFYING CENTRIFUGE ARE USED .....
IF( N .GT. 0 ) GO TO 10
..... INITIALIZE PARAMETERS FOR THE STRIPPING SECTION AND RETURN
FOR THE PARAMETERS DEFINING THE RECTIFYING SECTION .....
      BS = B $ CB = C $ HFB = HF
      FLOWDB = FLOWD $ FLOWUB = FLOWU
      PB = P $ N = 1 $ KND = 1
      YFC = YF/10.0 $ YFCG = 0.1*YF*0.9 $
RETURN
..... THE SOLUTION IS FOUND BY BRACKETING THE COMPOSITION AT THE
FEED POSITION. FOR EACH GUESS OF THE COMPOSITION AT THIS
POSITION THE CALCULATIONS ARE PERFORMED FOR THE STRIPPING
AND RECTIFYING SECTIONS. A MATERIAL BALANCE IS THEN
WRITTEN CHECKING TO SEE IF THE COMPOSITION COMPUTED AT THE
FEED POSITION AGREES WITH THE GUESSED VALUE. IF NOT
REPEAT WITH A BETTER GUESS .....
..... WITH A GIVEN COMPOSITION AT THE FEED POSITION COMPUTE THE
COMPOSITIONS LEAVING THE STRIPPING SECTION .....
10 YB = 0.0 $ YBG = YFC $ IND = 1
40 DELTA = SQRT( 1.0 + 2.0*CB*( 1.0-2.0*YB ) + CB*CB )
A = EXP( BR*DELTA*HFB ) $ AI = 1.0 / A
TD = ( A-AI ) / ( A+AI ) / DELTA
Y = YB * ( 1.0-TD*(1.0-CB) ) / ( TD*(1.0-2.0*YB+CB) + 1.0 )
ZERO = FLOWD*YFC - FLOWUB*Y + PB*YB
CALL CONVERG( YB, ZERO, YBG, IND, 0 )

```



```

SUBROUTINE CONVERG( X, ZERO, XGUESS, INDEX, NOPT )
C
C ..... THIS CONVERGING SUBROUTINE REQUIRES THAT THE ZERO POINT
C OF THE FUNCTION BE BRACKETED --- ONCE THIS IS ACCOMPLISHED
C THEN A POLYNOMIAL OF DEGREE TWO IS USED TO
C INTERPOLATE TO THE ZERO POINT --- IF THIS CAN NOT BE
C DONE THEN A LINEAR INTERPOLATION IS USED --- IF THE ZERO
C IS INCREASING IN MAGNITUDE THEN THE NEW GUESS AT THE
C ARGUMENT IS SIMPLY 1/4 TH THE SEPARATION FROM THE
C SINGLY REPRESENTED SIDE .....
C
DATA CLIMIT/ 1.0E-11 /
XKEEP = X $ ZERO = ZERO
IF( ZERO ) 240, 10, 240
C
C ..... CHECK TO SEE WHICH MODE CONVERG IS IN .....
C INDEX = 1 --- CONVERG IS BEING INITIALIZED
C INDEX = 123456 --- TEST TO SEE IF THE ZERO IS BRACKETED
C INDEX = 654321 --- CONVERGING ON THE ZERO VALUE
C INDEX = ANYTHING ELSE TERMINATES THE PROGRAM .....
C
240 IF( INDEX - 654321 ) 1, 2, 60
1 IF( INDEX - 123456 ) 3, 4, 60
3 IF( INDEX - 1 ) 60, 5, 60
C
C ..... INITIALIZING MODE .....
C
5 ITER = 1 $ XZERO = ZERO
IF( NOPT .EQ. 1 ) PRINT 100, ITER, X, ZERO
100 FORMAT( //, 54X, *CONVERGING SUBROUTINE OUTPUT*, //, 43X,
1 *ITERATION*, 9X, *VARIABLE*, 14X, *ZERO*, //, 43X, 16, 3X,
2 2E20.8 )
INDEX = 123456
CALL SWITCH( XFOS, ZEROPOS, XNEG, ZERONEG, XKEEP, ZERO )
X = XGUESS $ KOPT = 1 $ GO TO 50
C

```



```

C      ..... MODE TO CHECK IF THE ZERO IS BRACKETED .....
C
4 IF( NOPT .EQ. 1 ) PRINT 110, ITER, X, ZERO
110 FORMAT( 4X, I6, 3X, 2E20.8 )
IF( ZERO / XZERO .GT. 0.0 ) GO TO 45
XDIV = 10.0
DIVISOR = XDIV
INDEX = 654321
CALL CHECK( ISIT, XS, XPOS, ZEROPOS, XNEG, ZERONEG, XKEEP, ZERO )
IF( ISIT ) 223, 224, 223
223 CALL SWITCH( XPOS, ZEROPOS, XNEG, ZERONEG, XKEEP, ZERO )
X = XS
GO TO 50
224 KOPT = 0
CALL SWITCH( XPOS, ZEROPOS, XNEG, ZERONEG, XKEEP, ZERO )
BX = ( ZEROPOS + ZERONEG ) / DIVISOR
GO TO 322
C      ..... CONVERGING MODE .....
C
2 IF( NOPT .EQ. 1 ) PRINT 110, ITER, X, ZERO
CALL CHECK( ISIT, XS, XPOS, ZEROPOS, XNEG, ZERONEG, XKEEP, ZERO )
IF( ISIT .EQ. 0 ) GO TO 220
CALL SWITCH( XPOS, ZEROPOS, XNEG, ZERONEG, XKEEP, ZERO )
X = XS
GO TO 50
C      ..... TO GET A NOTION AS TO HOW WELL THE FUNCTION IS BEING
C      REPRESENTED INTERPOLATE TO THE SUM OF THE NEW ZERO AND
C      AN OLD ZERO OF OPPOSITE SIGN DIVIDED BY A NUMBER LARGER
C      THAN 10 --- THIS ALSO KEEPS THE BRACKET WIDTH DECREASING .
C
220 IF( KOPT .EQ. 1 ) GO TO 801
A = BX / ZERO
IF( A .GT. 0.1 .AND. A .LT. 10.0 ) DIVISOR = DIVISOR * XDIV
IF( A .GT. 0.5 .AND. A .LT. 2.0 ) DIVISOR = DIVISOR * XDIV
GO TO 802
801 KOPT = 0
802 IF( ZERO ) 800, 10, 810

```



```

800 BX = ( ZERO + ZEROPOS ) / DIVISOR
FIRSTP = ( ZERO - ZEROPOS ) / ( X - XPOS )
IF( ZERO .GT. ZERONEG ) GO TO 850
KOPI = 1
XDUM = X/4.0 + XPOS * 3.0/4.0
CALL SWITCH( XPOS, ZEROPOS, XNEG, ZERONEG, XKEEP, ZEROT )
X = XDUM
GO TO 320

810 BX = ( ZERO + ZERONEG ) / DIVISOR
FIRSTP = ( ZERO - ZERONEG ) / ( X - XNEG )
IF( ZEROPOS .GT. ZERO ) GO TO 850
KOPI = 1
XDUM = X/4.0 + XNEG * 3.0/4.0
CALL SWITCH( XPOS, ZEROPOS, XNEG, ZERONEG, XKEEP, ZEROT )
X = XDUM
GO TO 320

C ..... ESTABLISH THE FIRST AND SECOND DERIVATIVES .....
C
C 850 A = XNEG-X $ B = XPOS-X $ DET = B*A-A*B*B
C
C ..... IF THE DETERMINANT IS ZERO REVERT TO LINEAR INTERPOLATION ..
C
IF( DET .EQ. 0.0 ) GO TO 840
FIRST = ( (ZEROPOS-ZERO)*A - (ZERONEG-ZERO)*B ) / DET
SECOND = ( B*(ZERONEG-ZERO) - A*(ZEROPOS-ZERO) ) / DET
IF( ABS(FIRST) .GT. 10.0*ABS(FIRSTP) ) GO TO 840

C ..... COMPUTE THE NEW X ES .....
C
C
A = FIRST*FIRST + 4.0*SECOND*( BX-ZERO )
IF( A .LE. 0.0 .OR. SECOND .EQ. 0.0 ) GO TO 840
IF( ABS( FIRST*FIRST/A-1.0 ) .LE. 1.0E-05 ) GO TO 840
X1 = X + ( -FIRST - SORT(A) ) / SECOND / 2.0
X2 = X + ( -FIRST + SORT(A) ) / SECOND / 2.0
CALL SWITCH( XPOS, ZEROPOS, XNEG, ZERONEG, XKEEP, ZEROT )

C ..... CHECK TO SEE IF EITHER ONE OF THE X ES LIE IN THE RANGE .....
C
C
A = ( ABS(XPOS-X1) + ABS(XNEG-X1) ) / ABS( XPOS-XNEG )

```




```

IF( ABS( A-1.0 ) -1.0E-07 ) 920, 920, 910
920 X = X1 $ GO TO 320
910 A = ( ABS(XPOS-X2) + ABS(XNEG-X2) ) / ABS( XPOS-XNEG )
IF( ABS( A-1.0 ) -1.0E-07 ) 930, 930, 322
930 X = X2 $ GO TO 320

C ..... LINEAR INTERPOLATION EQUATION .....
C
C
840 CALL SWITCH( XPOS, ZEROPOS, XNEG, ZERONEG, XKEEP, ZERO1 )
322 X = ( RX - ZERONEG ) / ( ZEROPOS - ZERONEG )
X = XNEG * ( 1.0 - X ) + XPOS * X

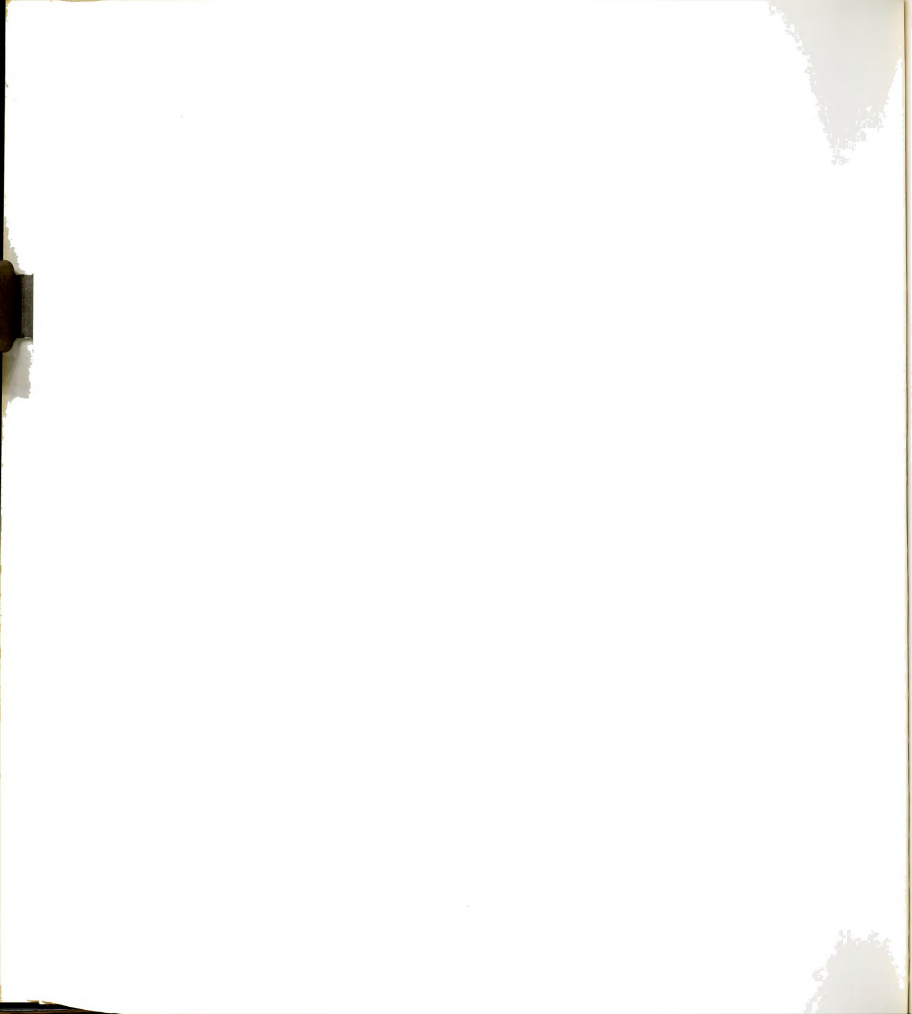
C ..... THE TEST OF CONVERGENCE IS PRINCIPALLY MADE ON THE BASIS OF
C DEGREE OF CHANGE OF THE VALUE OF X .....
C
320 IF( X ) 300, 310, 300
310 TESTX = ABS( XKEEP - X ) $ GO TO 40
300 TESTX = ABS( ( XKEEP - X ) / X )
40 IF( TESTX - CLIMIT ) 10, 10, 50
50 ITER = ITER + 1 $ RETURN

C ..... OUTPUT IF INDEX IS NOT INITIALIZED PROPERLY .....
C
60 PRINT 61 $ STOP
61 FORMAT( '1*, /', 5X, 'THE VALUE OF INDEX WAS EITHER NOT INITIA
LIZED WITH 1 OR, WAS ALTERED DURING THE CONVERGENCES ---- CALCULA
TIONS ARE TERMINATED' )

C ..... DID NOT BRACKET THE ZERO .....
C
45 INDEX = - 1000 $ RETURN

C ..... CONVERGENCE .....
C
10 IF( NOPT.EQ. 1 ) PRINT 11, X
11 FORMAT( 36X, 'CONVERGED VALUE =', E18.8, // )

```



INDEX = 0 \$ RETURN
END



```

C
C
C
C
SUBROUTINE SWITCH( XPOS, ZEROPOS, XNEG, ZERONEG, X, ZERO )
..... THIS SUBROUTINE SIMPLY UPDATES THE CLOSENESS TO THE
ZERO POINT .....
      IF( ZERO ) 1, 2, 3
1 XNEG = X      ZERONEG = ZERO
  RETURN
3 XPOS = X      ZEROPOS = ZERO
2 RETURN
  END

```



SUBROUTINE CHECK(ISIT,X,XPOS,ZEROPOS,XNEG,ZERONEG,XKEEP,ZEROT)

..... THIS SUBROUTINE USES A GEOMETRIC MEAN TO REDUCE THE
RATIO OF THE XES THAT BRACKET THE ZERO POINT TO LESS
THAN FIVE AND GREATER THAN 0.2

```

IF( ZEROT ) 30, 5, 40
30 A = XKEEP $ B = XPOS $ C = ZEROT $ D = ZEROPOS
GO TO 50
40 A = XNEG $ B = XKEEP $ C = ZERONEG $ D = ZEROT
50 IF( B ) 1, 2, 1
2 IF( A ) 4, 5, 6
4 IF( A + 10.0 ) 7, 5, 5 $ GO TO 20
7 X = - SQRT( - A ) $
6 IF( A - 10.0 ) 5, 5, 8 $ GO TO 20
8 X = SQRT( A ) $
1 IF( A ) 10, 11, 10
11 IF( B ) 12, 5, 13
12 IF( B + 10.0 ) 14, 5, 5 $ GO TO 20
14 X = - SQRT( - B ) $
13 IF( B - 10.0 ) 5, 5, 15 $ GO TO 20
15 X = SQRT( B ) $
10 X = A / B
IF( X ) 16, 5, 17
17 IF( X .LT. 5.0 .AND. X .GT. 0.2 ) GO TO 5
X = SQRT( A * B )
IF( B .LT. 0.0 ) X = - X
GO TO 20
16 X = 0.0
20 XNEG = A $ XPOS = B $ ZERONEG = C $ ZEROPOS = D
ISIT = 1 $ RETURN
5 ISIT = 0 $
END

```



```

C
C
C
C
C
C
SUBROUTINE FASTC( X, Z, XG, IND )
..... THIS SUBROUTINE IS USED TO FIND THE VALUE OF X THAT WILL
MAKE Z GO TO ZERO ----- THE SUBROUTINE REQUIRES THAT
THE X TO MAKE Z GO TO ZERO IS BRACKETED .....

      IF( Z ) 5, 100, 5
      5 IF( IND-2 ) 10, 20, 30
      10 IND = 2 $ ZK = Z
      GO TO 30
      20 IF( Z/ZK .LT. 0.0 ) GO TO 40
      IND = -1 $
      40 IND = 3
      30 IF( Z ) 50, 100, 60
      50 ZN = Z $ XN = X
      GO TO 70
      60 ZP = Z $ XP = X
      70 IF( IND .GT. 2 ) GO TO 80
      X = XG $
      80 DUM = ( ZP + ZN ) / 50.0
      X = ( XP-XN ) / ( ZP-ZN ) * ( DUM-ZN ) $ XK = X
      DUM = ABS( X-XK )
      IF( ABS( DUM/X ) .GT. 1.0E-07 ) RETURN
      100 IND = 9 $
      END

```



APPENDIX F

DESCRIPTION OF EXPERIMENTAL EQUIPMENT AND ANALYSIS OF ITS PERFORMANCE



APPENDIX F

DESCRIPTION OF EXPERIMENTAL EQUIPMENT AND ANALYSIS OF ITS PERFORMANCE

As part of an overall analysis of gas centrifugation it was deemed necessary that an experimental program to be undertaken paralleling an extensive theoretical analysis. It was hoped, with the aid of the experimental device, that assumptions regarding internal flow profiles could be evaluated as part of an overall comparison between experimental and calculated results.

A. Background

German isotope separation efforts in the early 1940s were concentrated on short bowl centrifuges ($L/D \sim 5$) operating in a vacuum to reduce friction and hence power requirements. The short bowls were able to operate at higher rotational speeds (larger pressure diffusion) without crossing the first whirling speed (Chapter IV). The German centrifuge developments were demonstrated in both Russia and the United States (University of Virginia) by Zippe (7). Publication of current work and, to a large degree, past work, which detailed the design aspects of the gas centrifuge are classified due to its potential use in the enrichment of Uranium. However, unclassified publications of Zippe's demonstration devices at the University of



Virginia are available. These publications served as a basis for the construction of an experimental centrifuge.

The centrifuges built and operated by Zippe were small in size (up to 4 inches in diameter and up to 20 inches in length) with very small (milligrams/sec) feed rates. It was realized that for the concept of gas centrifugation to be extended into the realm of such things as flue gas desulfurization that feed rates would have to be increased significantly and consequently also the size of the centrifuges used by Zippe. Nevertheless, Zippe's work represented the best available information to be used as an experimental guide.

B. Centrifuge Design

Figure F-1 contains a schematic diagram illustrating the principles of Zippe's design. It should be noted immediately that the design contains a stationary center pipe which is subject to the results presented in Chapter II-E.

Feed gas flows into the center of the rotating bowl (A) through one of the concentric center pipes. The feed gas is accelerated to spin with the bowl by the momentum of the surrounding gas which obtains its energy by shearing with the centrifuge wall. Drag on the stationary pitot tube (O) located at the top of the bowl tends to move the gas inward toward the axis, while the rotating disk (N) at the bottom of the bowl tends to move the gas near the axis, slowed due to shear with the stationary center pipe, outward to the wall. The effect is to create a countercurrent flow with an outer gas stream



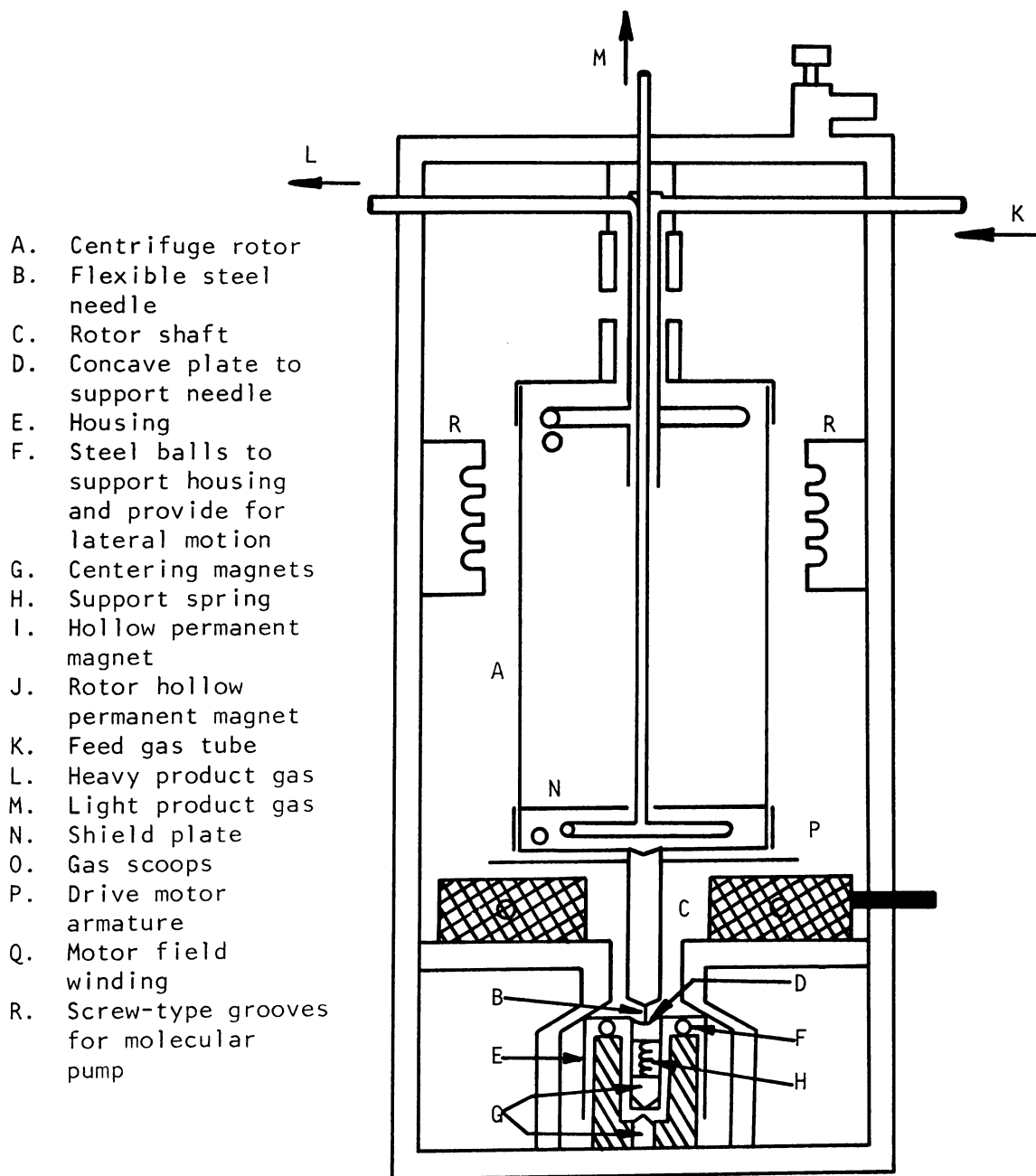


Figure F-1.--A Schematic of the Zippe Gas Centrifuge.



moving up along the periphery to the top pitot tube (O) where it is directed downward in the inner stream.

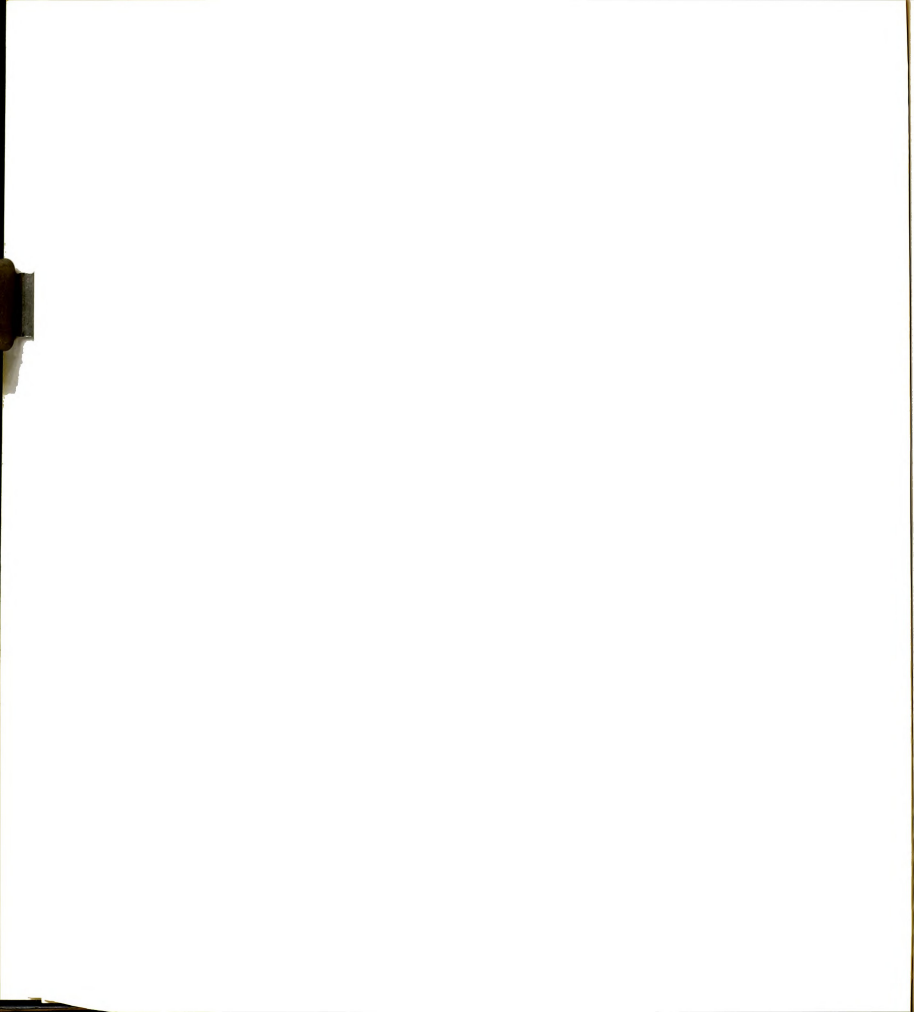
The top pitot tube (O) also serves to extract a portion of outer stream (L) which is richer in heavier species. On the other hand, the stationary pitot tube (O) at the bottom shielded by the rotating baffle (N) extracts a portion of the inner stream (M) which is leaner in the heavier species.

The entire bowl spins in a vacuum chamber with the vacuum being produced (after start up) by a molecular pump (R). Support for the bowl is concentrated on a needle bearing running in damped bearing housing (D). Vertical alignment of the rotating cylinder is maintained by a magnetic bearing (I, J) at the top. Other bearing components shown are used to further keep the centrifuge centered and reduce vibrational problems.

To eliminate the need for any mechanical connections the armature (P, a disk) of the induction drive motor is attached directly to the centrifuge bottom end cap. The field windings (Q) for the induction motor are attached to the vacuum housing directly under the armature.

C. Modifications Made in Zippe's Design

When Zippe's centrifuge design was scaled up to a centrifuge design having a length of 40 inches and a diameter of 8 inches, several modifications of his basic design were necessary. Figure F-2 contains a schematic diagram of the modified form of the Zippe gas centrifuge which was constructed. The device, made of high tensile



- A. Centrifuge rotor
8" x 40" x 1/4" wall
- B. Bottom shaft
- C. Bottom bearing assembly
- D. Top bearing assembly and
center pipe support
assembly
- E. Bottom center pipe
support assembly
- F. Feed gas tube
(middle pipe)
- G. Rich gas tube
(outer pipe)
- H. Lean gas tube
(inner tube)
- I. Pitot tubes
- J. Shield plate
- K. Small drive shaft
- L. Drive motor
(series wound)
- M. Frame assembly

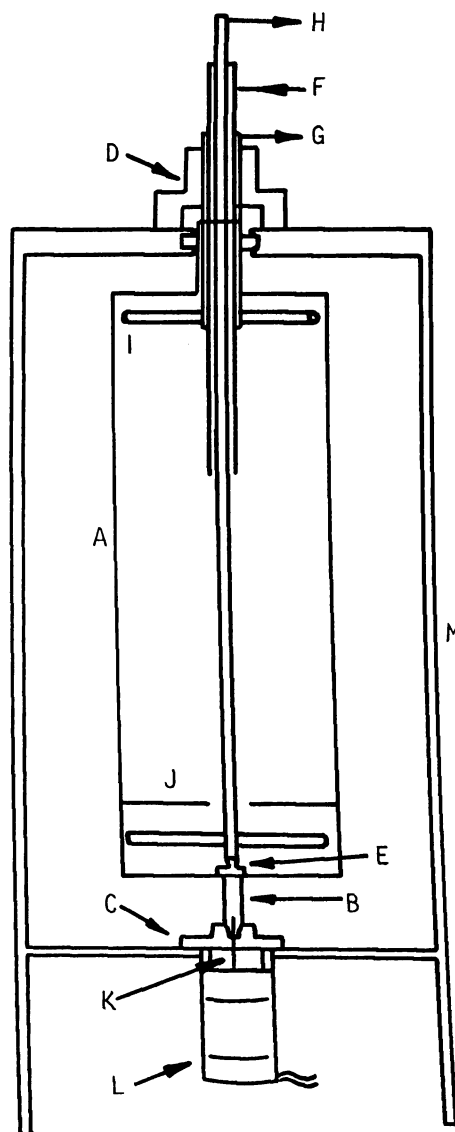


Figure F-2.--Schematic of the Experimental Centrifuge.



strength aluminum alloy, is 8 inches in diameter (outer) with a 1/4-inch wall and 40 inches long. The basic modifications that were made are as follows:

1. Centrifuge Housing

Zippe's centrifuge ran in a sealed housing which was evacuated to provide less windage losses (lower power requirements) and to provide pressures low enough so that the UF_6 was not only gasified for feed stock, but remained so at the centrifuge wall. The molecular pump that he used provided extra vacuum along the lower part of the centrifuge further reducing windage losses.

Operating the centrifuge under a vacuum, however, is not compatible with the separation of ordinary gas mixtures. That is, in the case of the desulfurization of flue gas, a further increase in the already tremendous volumes of gas that must be processed by pressure reduction plus the energy required to do so, would immediately prohibit use of the gas centrifuge. The centrifuge itself could be run under a vacuum, leaving the inside at atmospheric pressure; however, the problems associated with fabricating seals capable of withstanding the high rotational speeds, yet not adding a significant additional power requirement, seemed insurmountable. Thus, it was decided to operate the centrifuge both internally and externally at atmospheric pressure.

The support frame (M), constructed in place of the vacuum housing, allowed complete accessibility to the centrifuge by the surrounding air. However, even though the centrifuge was operated

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under conditions where windage losses were high, the air movement around it was sufficient to prevent any detectable temperature rise.

2. Drive Motor

In Zippe's design the centrifuge was driven by a "pancake" type induction motor powered by a variable frequency power supply. The armature of the motor was a disk attached to the base of the centrifuge with the field windings mounted directly under it. By the nature of its design (giving large magnetic flux losses, long magnet paths, and large air gaps), this type of motor is much more inefficient than a conventional induction motor. Hence, while such a motor was designed and built, it could not be made to operate the centrifuge at the desired speeds without drawing excessive current and causing heating problems.

To avoid these problems, but have an electric driver which did not require special gears and/or belts and pulleys, a series wound motor was decided upon. The motor was rated at 3 horsepower and was able to run the centrifuge at 10,000 RPM at 190 volts drawing approximate 7.25 amps (~ 1380 watts). The efficiency under these conditions as given by the manufacturer is 71% implying nearly 980 watts of power that were required to drive the centrifuge at this speed.

3. Bottom Bearing and Drive Assembly

Zippe's centrifuge design made use of a needle bearing to represent an almost frictionless point of contact. However, while testing the "pancake" type motor, as a driver, it was found that

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such a bearing was unacceptable for the centrifuge design used in this work. Due to the weight (~ 40 lbs) of the centrifuge the bearing wore excessively, becoming a significant source of drag. To alleviate this situation an assembly (C) was used which housed a pair of ball bearings which could not only support the end thrust due to the weight of the centrifuge, but could be operated at high rotational speeds.

Like Zippe's design this bottom bearing assembly was not rigidly attached to the frame. It was mounted on rubber grommets which allowed small vertical and horizontal motions due to vibrations.

The inside of the bottom shaft of the centrifuge and the drive motor shaft was bored and made to receive a 1/8-inch drive shaft (K) connecting the centrifuge and the drive motor. Universal type joints were used to connect the drive shaft to the centrifuge shaft and to the motor shaft. This allowed motions of the centrifuge and the drive motor due to vibrations to be isolated from each other since they were not rigidly connected.

4. Top Bearing Assembly

The magnetic bearing used in Zippe's design was sufficient to retain the centrifuge in a vertical position and served to eliminate energy losses. Such a bearing, however, simply could not be made strong enough (magnetically) to safely control the larger centrifuge used in this work.

To give the necessary control, a ball bearing assembly (D) was used which gave the necessary support plus allowed for small horizontal and vertical motions of the centrifuge. The assembly also acted as a seal to prevent gas from entering or being lost from the centrifuge.

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5. Center Pipe Support

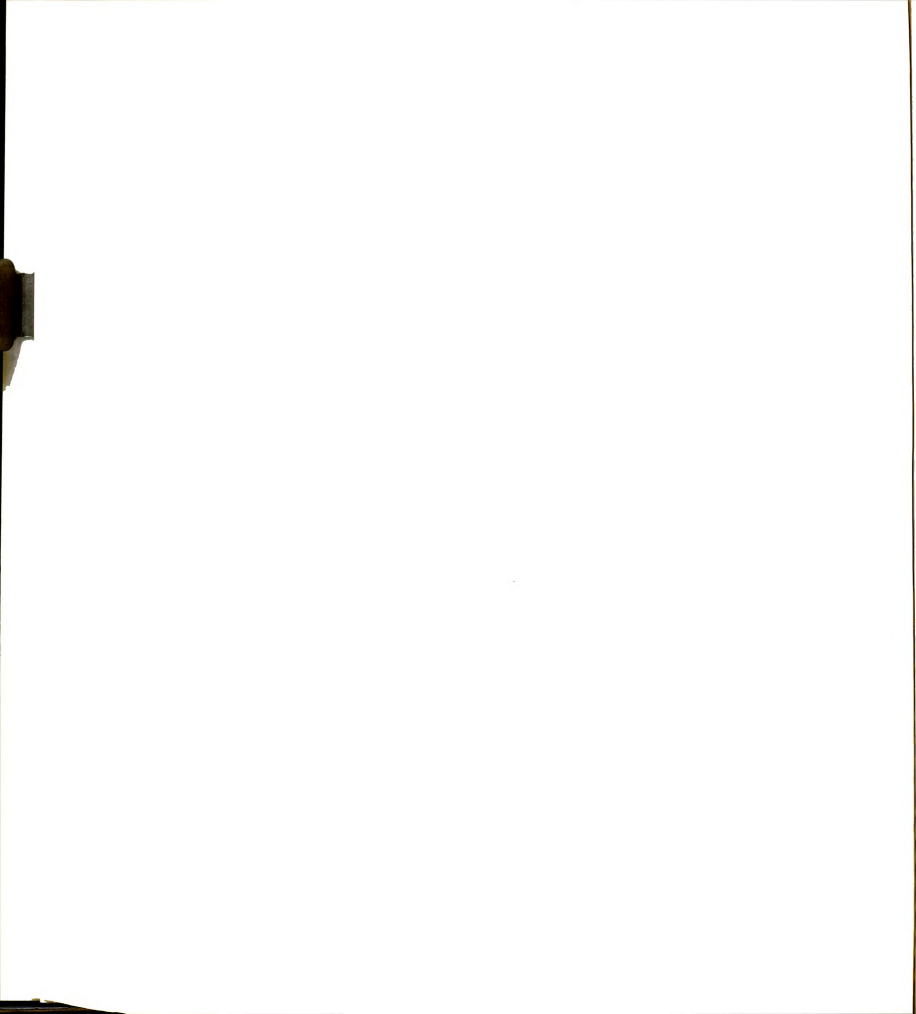
Even though the concentric pipes leaving the top of the centrifuge were secured in place, centrifuge vibrations caused the pipe to vibrate to the point of concern. This situation was easily corrected by extending a very small shaft (1/8" x 1") from the end of pipe. The bottom of the shaft was then held in the center of the centrifuge by a small ball bearing set in the bottom end cap.

Other than using $\text{SO}_2\text{-N}_2$ as the gas pair instead of gasified UF_6 , the above are the only modifications made to Zippe's design. Furthermore, these modifications are, except for the stabilizing ball bearing used at the end of the center pipe, external modifications. The only internals of the centrifuge, other than the center pipe, are the pitot tubes and they were constructed similar to those used by Zippe.

Figure F-3 contains a photograph of the experimental centrifuge illustrating the center pipe with pitot tubes, centrifuge bowl, the support frame with the drive motor attached in its normal position and the gas metering (control) panel.

D. Experimental Apparatus

Figure F-4 contains a flow chart of the experimental apparatus. Feed gas was prepared in quantity by mixing SO_2 and N_2 in a pressurized cylinder. The feed gas was then analyzed with an infrared spectrophotometer which had been calibrated for SO_2 concentrations ranging between 500 and 4000 ppm. The feed gas, after passing through a rotameter, goes directly to the centrifuge. Lean and rich product streams



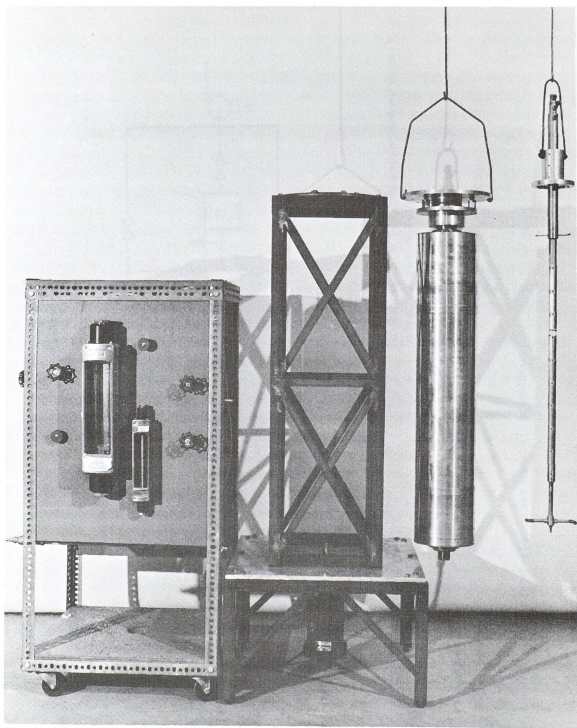
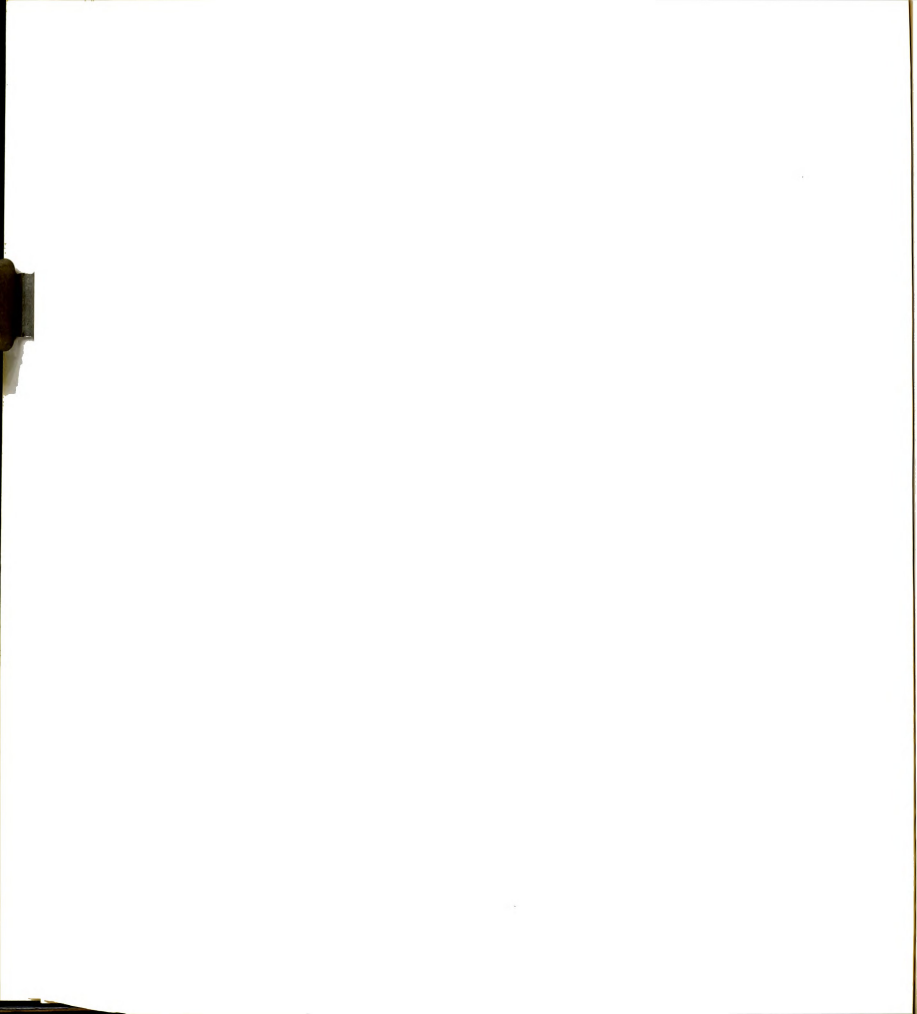


Figure F-3.--Experimental Centrifuge and Auxiliaries.



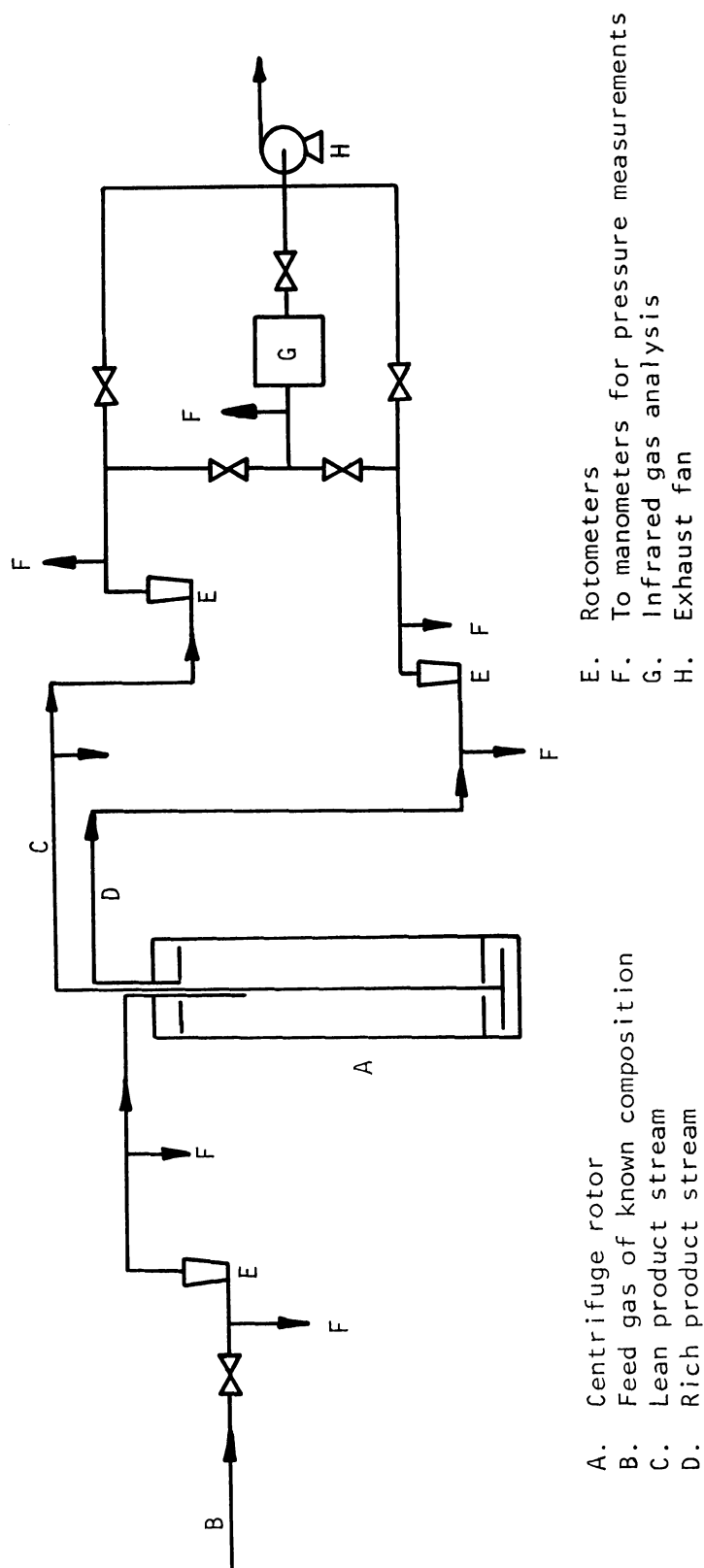


Figure F-4.--Flow Chart of the Experimental Apparatus.



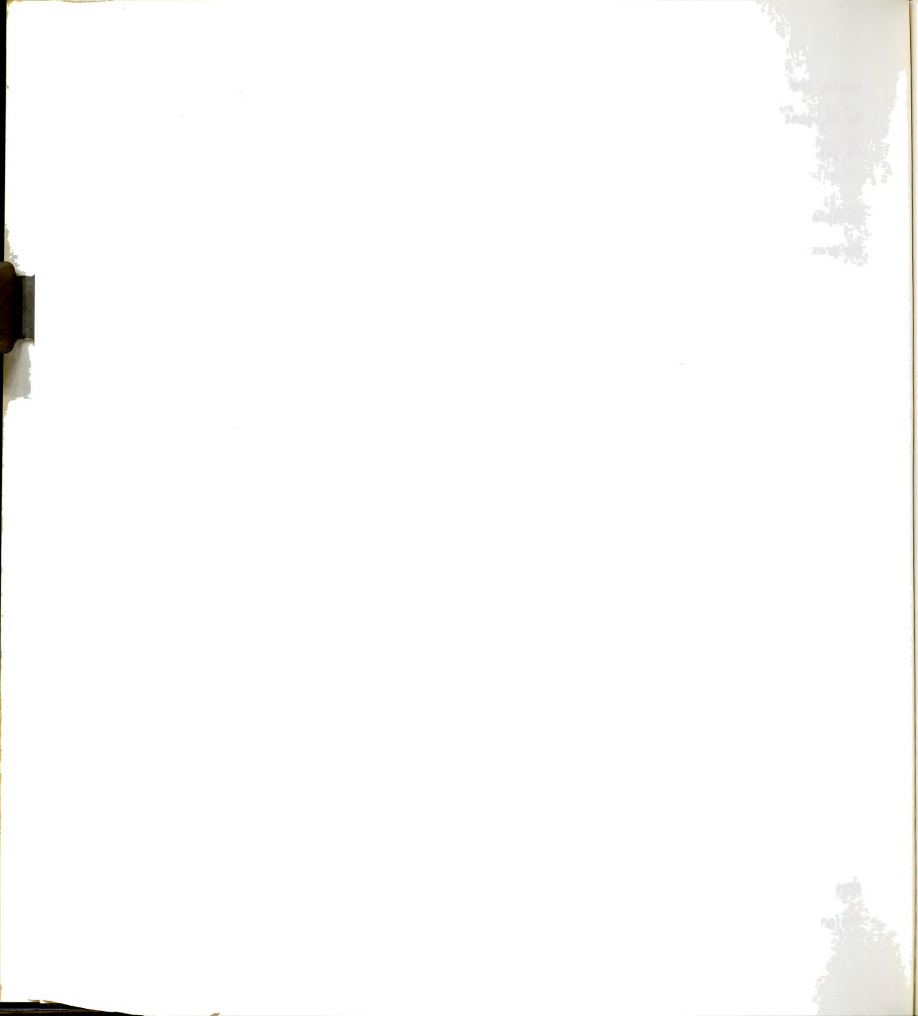
leaving the centrifuge pass through rotameters and are then analyzed for SO_2 content by the infrared spectrophotometer. After being analyzed the gas exits the system via an exhaust fan.

Needle valves were used throughout the system to direct and throttle the flow. With the aid of the calibrated rotameters and the pressure measurements, the mass balance was easily closed to within a few percent of the feed flow rate. The centrifuge speed was measured by a calibrated strobe light.

E. Experimental Runs

Due to limitations in the design of the centrifuge (top seal) all experiments were run at atmospheric pressure. Likewise, with no provisions for temperature control, the experiments were performed at room temperature, $\sim 70^\circ\text{F}$. The maximum centrifuge rotational speed that could be obtained was 12000 RPM with most experimental runs performed at 10000 RPM.

Several experimental runs were made varying the feed rate from 1/10 to 5 scfm all yielding no measurable separation. In all cases care was made to insure that the mass balance was satisfied. Confronted with the situation of not seeing any measurable separation, the experimental procedure was gone over many times to insure that poor experimental technique was not a factor. Having been satisfied that the experimental procedure was correct, several few slight internal modifications of the centrifuge were made. This modifications included: polishing the inner surface of the centrifuge, making the center pipe as streamlined as possible, and changing the size and design of the pitot tubes. After each modification the experimental



runs were repeated, but still no measurable separation could be realized. At this point in time the theoretical analysis was nearing completion, giving results which warranted termination of the experimental program.

F. Conclusions

The Zippe type centrifuge is both a rectifying and a stripping centrifuge. That is, the section above the feed enriches the heavy species while that below the feed enriches the lighter species. Using the computer program described in Appendix E, the following comparison was made between the observed and calculated separations seen by Zippe and those observed and calculated for this work:

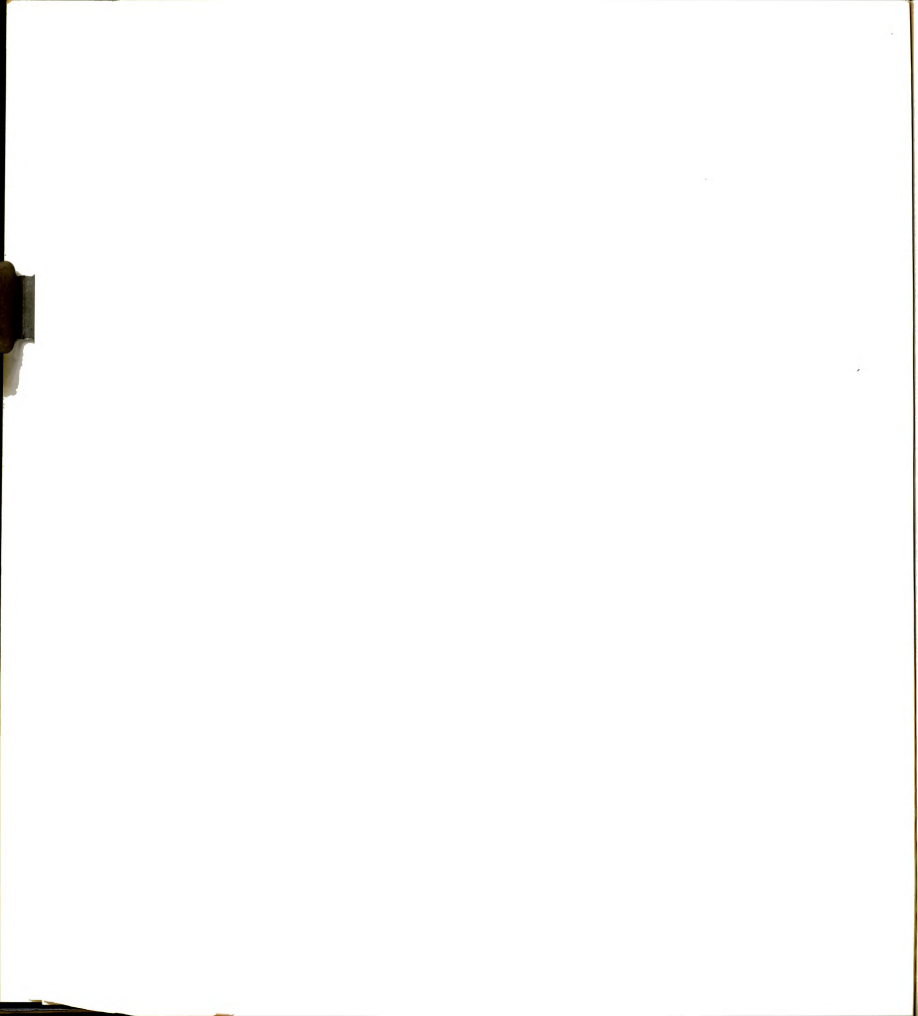
	<u>Zippe (7)</u>	<u>Modified Design</u>
Gas pair	UF ₆ (235, 238)	SO ₂ -N ₂
Temperature (°C)	~ 80	~ 25
Axis pressure (mm Hg)	~ .1	~ 760
Feed concentration (mole fraction)	.9928 [UF ₆ (238)]	.002 (SO ₂)
Centrifuge diameter (inches)	2.92	7.5
Centrifuge length (inches) (for axial flow)	12	34
Rotational speed (RPM)	90,000	11,000
Inner peripheral velocity (ft/sec)	1146	360
Length/diameter	4.1	4.5
Feed rate (scfm)	.00034 (2.55 mg/sec)	.1
Feed inlet	midpoint	midpoint



	<u>Observed</u>	<u>Calculated</u>	<u>Observed</u>	<u>Calculated</u>
Rich/lean	1	1	1	1
Separation factor,				
$\alpha = \frac{y_r}{1-y_r} \cdot \frac{1-y_1}{y_1}$	1.216	1.243	(no mea- surable)	1.045
Rich stream concentration (mole fraction)	--	.9936 [UF ₆ (238)]	--	.002044 (SO ₂)
Lean stream concentration (mole fraction)	--	.9920 [UF ₆ (238)]	--	.001956 (SO ₂)
Power to the centrifuge driver (watts)	6.25	--	--	1650
Power estimated to rotate the gas	--	.92	--	1.66
Efficiency (%)	--	14.7	--	.1

Analysis of Zippe's work indicated that the feed rate was 35.6% as large as the outer stream. This factor was used in the calculation for the SO₂-N₂ separation present above.

While a feed rate of 0.1 scfm was the lowest used experimentally (limited by equipment design and flows need for gas analysis), calculations show that a feed rate of .0075 scfm (feed = 35.6% of the outer stream) gives a maximum separation factor of 1.283. Or, the lowest feed rate in the experiments was approximately 13.3 times too large. It should be pointed out that if the experiments had been carried out in a centrifuge identical in size to Zippe's rotating at 90000 RPM at a temperature of 25°C, the optimum feed rate would be .0028 scfm giving a separation factor of 11.5 for SO₂ in N₂ (2000 ppm SO₂).



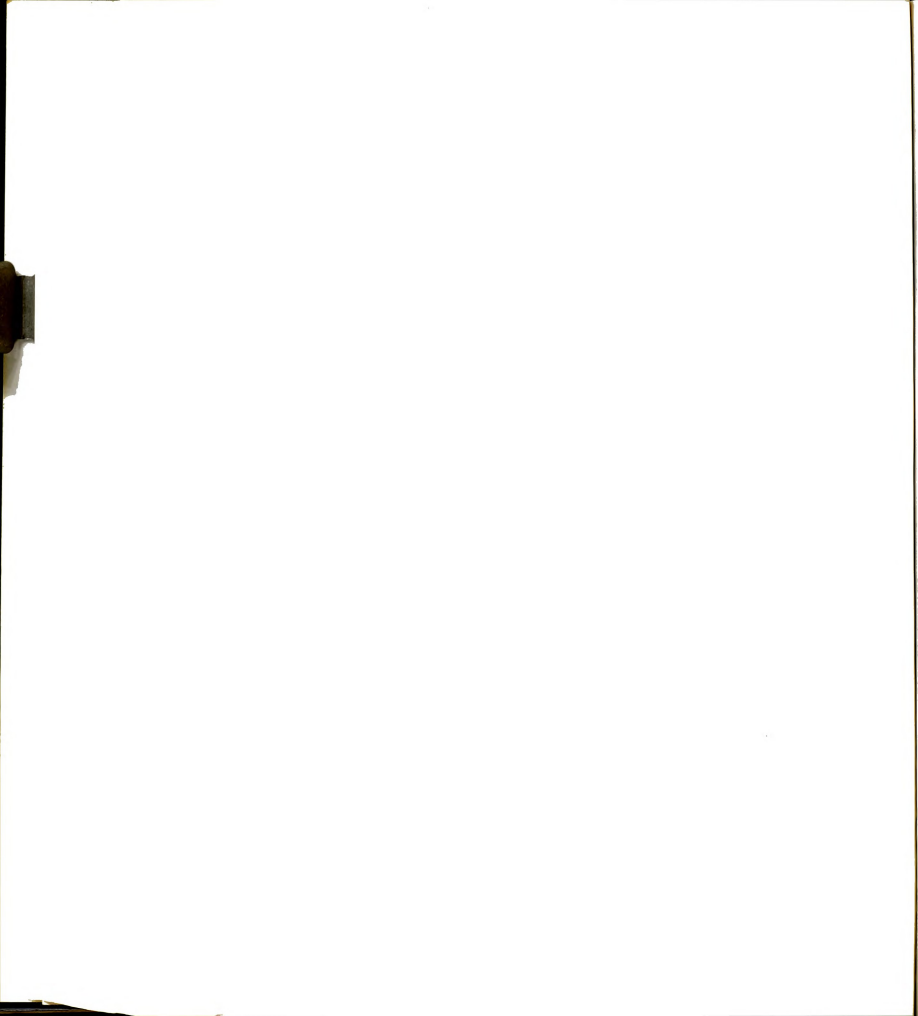
With the above points in mind, coupled with the overall analysis presented in this work, the following conclusions regarding the experimental work were drawn:

1. While a separation is predicted at a feed rate of 0.1 scfm, the concentration difference between the rich and the lean streams is only 88 ppm SO_2 (44 ppm when compared to the feed). With a feed composition of 2000 ppm SO_2 the rich and lean streams would have had to have been at least 150 ppm different than the feed for a crude quantitative analysis by the infrared spectrophotometer used.

2. The centrifuge and its auxiliaries were designed for feed rates higher than 0.1 scfm. For operation at feed rates 10 or more times smaller complete redesigning of the equipment would have been required.

3. At the very low axis pressures used by Zippe ($\sim .1$ mm Hg) as was shown in Chapter II the transition speed (point at which turbulence would be promoted by the stationary center pipe) is estimated to be well above the rotational speed of 90000 RPM used by Zippe. For a mixture of SO_2 - N_2 at atmospheric pressure, however, the transition speed is estimated to be ~ 2800 RPM. Hence, even though a small separation was predicted in the experimental equipment, uncontrollable turbulence would have undoubtedly erased it.

Also, at the low pressures used by Zippe, the axial flow caused by drag on the top pitot tubes was very small and the internal circulation rate was near the optimum. Zippe used several pitot tube designs, finally deciding on the ones which gave him the best separation at what he described as "very low feed rates." Although he did

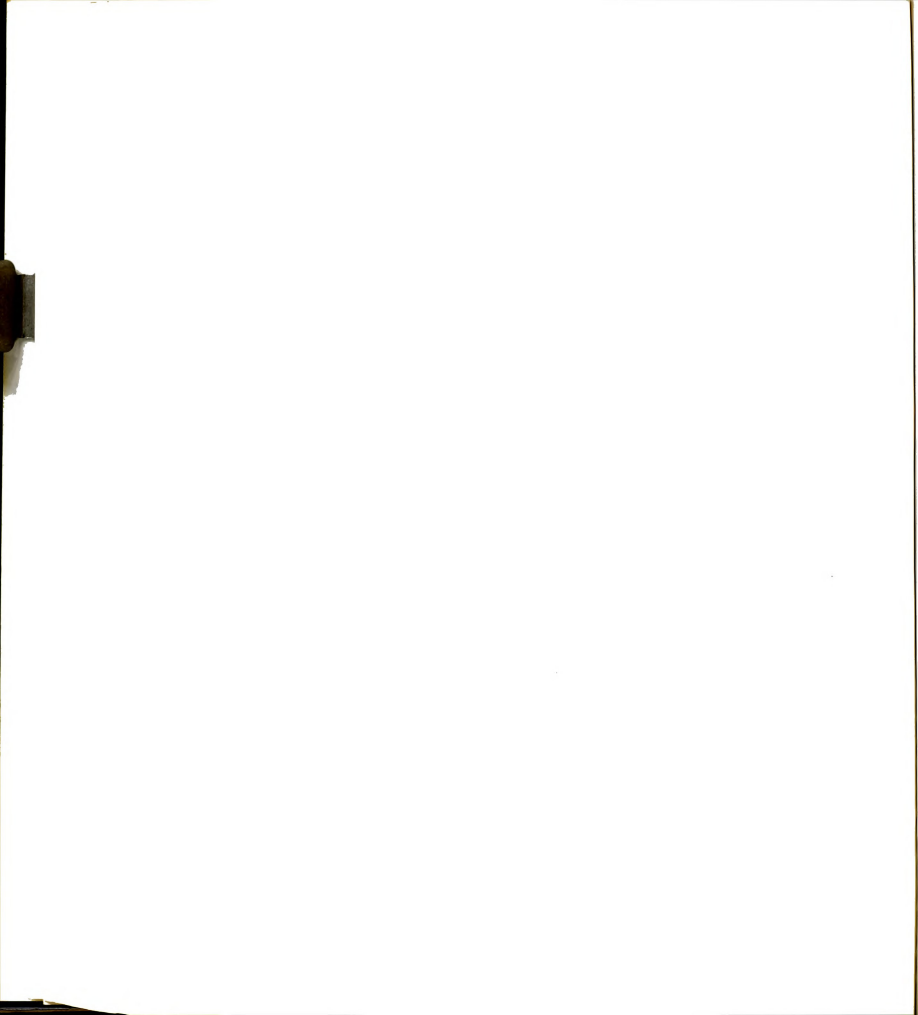


not mention it, in lieu of the material in this work, what he actually was doing was finding the tube arrangement which gave him optimum internal flow at nearly total reflux ("very low feed rates").

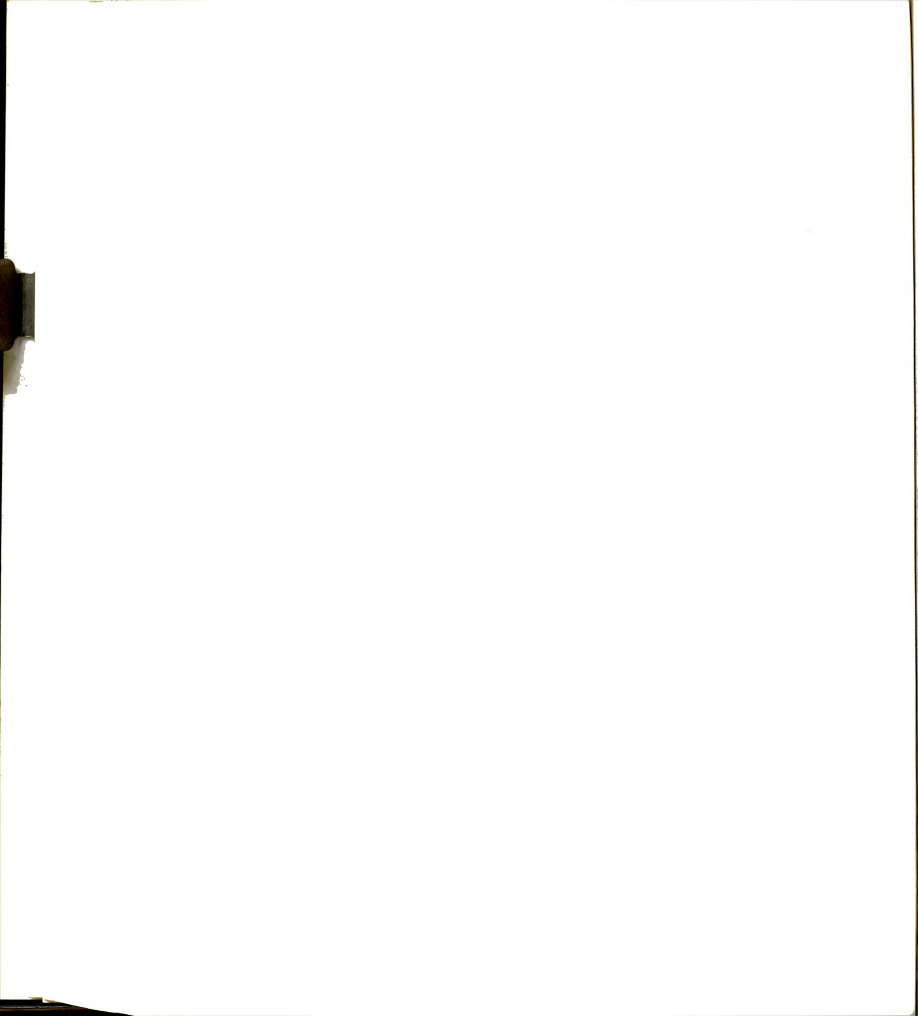
It was originally hoped (before the theoretical analysis) that the flow rates allowable in the centrifuge design used for this work would be sufficient large (~ 5 scfm) so that the effects of uncertainties in the pitot tube design would be insignificant. That is, it was hoped that the increase in internal flow created by the increased drag (higher pressure) on the pitot tubes would be comparable to the increase in allowable flow rates. However, as was shown above, the optimum feed rate was only .0075 scfm or an increase of 22 times over those in Zippe's centrifuge. Hence, the design of the pitot tubes for the current centrifuge design and operating conditions take on tremendous importance. However, the development of sufficient theory to be able to design pitot tubes giving the small flows required was considered beyond the scope of this work (not meaning to imply that such a feat is even possible).

4. Even if the experimental centrifuge could have been made to operate ideally at atmospheric pressure and at a feed rate of 0.0075 scfm, this very small feed rate puts the Zippe type centrifuge completely out of the range of applicability for the separation of SO_2 from flue gas.

It was felt that these four conclusions more than constituted sufficient reason to abandon the current experimental program involving the Zippe type centrifuge. That is, while it was shown that results



presented by Zippe were predictable based on the analysis in this work, attempting to scale-up his centrifuge design and operate it at atmospheric pressure presented unsurmountable problems fundamental to the basic design. Furthermore, even if these problems could be solved, the very small optimum feed rates and low separation factors expected are completely inconsistent with application of the Zippe type centrifuge to the removal of SO_2 from coal fired power plant stack gas.









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