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## ESTIMATION OF OVERALL SEPARATION FACTOR OF A GAS CENTRIFUGE FOR DIFFERENT MULTICOMPONENT MIXTURES BY SEPARATION THEORY FOR BINARY CASE

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### ABSTRACT

Many elements in nature have three or more isotopes. One of the important separation characteristics for a gas centrifuge for multicomponent isotope separation is the overall separation factor per unit molar weight difference,  $\gamma_0$ . It is desirable to estimate the value of  $\gamma_0$  for different process gases. A method of estimating  $\gamma_0$  is given in this paper. The concept of separative power of a gas centrifuge for a binary mixture is used. Finally, the parameters that influence the value of  $\gamma_0$  are shown and discussed.

*Key Words:* Gas centrifuge; Overall separation factor; Separative power

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## INTRODUCTION

The demand for stable isotopes has stimulated theoretical and experimental research on gas centrifuge processes. For gas centrifuge cascade analysis, it is necessary to know the separation characteristics of a single gas centrifuge. Many stable elements have three or more components, which necessitates that we consider the separation of multicomponent mixtures. One of the important separation characteristics of a gas centrifuge for separating multicomponent process gas is the separation factor. The separation factors of a gas centrifuge between the  $i$ th and the  $j$ th isotopes,  $\gamma_{ij}$ , can be expressed as  $\gamma_{ij} = \gamma_0^{M_j - M_i}$  (1), where  $\gamma_0$  is the overall separation factor for the unit molar weight mass difference.

De La Garza et al. (2,3) developed an R-matched cascade theory for multicomponent separation. The method was developed in a number of papers (4–7) for the gaseous diffusion process in which the separation factor is close to unity. Other papers (8–13) discussed the multicomponent separation cascade of stages with large separation factors and the separative power of a gas centrifuge for multicomponent separation.

In a previous paper (14), we discussed the parameters that influenced the overall separation factor per unit molar weight difference,  $\gamma_0$ . In that paper, we calculated  $\gamma_0$  by solving Onsager's pancake equation for the countercurrent flow field and the diffusion equation for some special examples. It was shown that the important parameters are  $\rho D$  and  $A^2$ .

The objective of the present paper is to find a method which may estimate the overall separation factor per unit molar weight difference,  $\gamma_0$ , for any process gas and explain the main parameters that influence  $\gamma_0$ . These parameters are found to be the feed flow rate, the product  $\rho D$ , and the speed parameter,  $A^2$ .

## THEORETICAL ANALYSIS

### Relation Between $\gamma_0$ and Feed Composition

The overall separation factor per unit molar weight difference,  $\gamma_0$ , is very important for gas centrifuges analysis, especially in separating multicomponent isotope mixtures. The question is whether  $\gamma_0$  depends on the composition in the feed flow. It is not easy to check it theoretically. Some calculations have been made and the results are shown for a gas centrifuge separating tungsten. For the process gas  $WF_6$ , the natural composition is listed in Table 1.

Several calculations have been made, and the results are given in Table 2. These results were obtained by changing the composition of  $C_{1F}$  to the composition of every other component. Say, if  $C_{1F}$  is 26.416% this means that the suppositional  $C_{1F}$  is 26.416 and  $C_{2F}$  is 0.14%. The other results in Table 2 are



# ESTIMATION OF OVERALL SEPARATION FACTOR

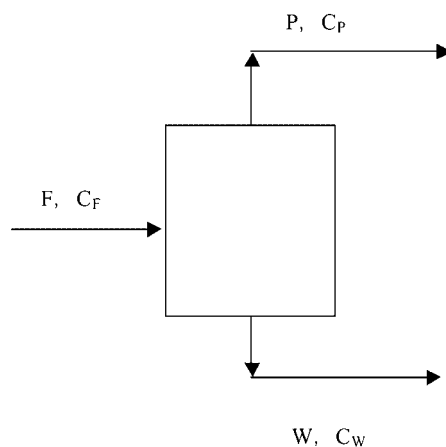
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**Table 1.** The Natural Composition of  $WF_6$  (%)

	$C_{1F}$	$C_{2F}$	$C_{3F}$	$C_{4F}$	$C_{5F}$
Composition	0.14	26.416	14.409	30.618	28.417

**Table 2.**  $\gamma_0$  for Different Feed Composition

$C_{1F}$ (%)	$\gamma_0$ (Relative Value)
0.14	1.0000
26.416	1.0043
14.409	1.0035
30.618	1.0091
28.417	1.0098



**Figure 1.** A schematic of a separation unit.

obtained in a similar way. When  $C_{1F}$  equals 0.14% the feed flow has natural composition. In this case the value of  $\gamma_0$ , which is taken as 1.0000, is considered as the standard to compare with other values of  $\gamma_0$ .

As shown in Table 2 the difference among the five examples is small. In other words, the composition in feed flow has little influence on the overall



separation factor,  $\gamma_0$ , which suggests the idea that we may use binary separation system to calculate the overall separation factor,  $\gamma_0$ .

### Separative Power for Binary Case

A schematic of a separation unit is shown in Fig. 1 where  $F$ ,  $P$ , and  $W$  are the feed, heads, and tails flow rates, respectively, and  $C_F$ ,  $C_P$ , and  $C_W$  are the feed, heads, and tails composition, respectively.

The definitions of separation factors are as follows:

$$\alpha = \frac{C_P/(1 - C_P)}{C_F/(1 - C_F)} \quad (1)$$

$$\beta = \frac{C_F/(1 - C_F)}{C_W/(1 - C_W)} \quad (2)$$

$$\gamma = \alpha \cdot \beta = \frac{C_P/(1 - C_P)}{C_W/(1 - C_W)} \quad (3)$$

If the process gas is considered as a binary mixture and that the molar weight difference between two components is unity, the overall separation factor,  $\gamma$ , is just the overall separation factor for unit molar weight difference,  $\gamma_0$ . From the mass balance the following equation is obtained

$$C_F = \theta C_P + (1 - \theta)C_W \quad (4)$$

where  $\theta$  is the cut of the gas centrifuge,  $\theta = PV/F$ .

It is not difficult to obtain a relationship from the above expressions.

$$\theta = \frac{(\beta - 1)[1 + (\alpha - 1)C_F]}{\alpha\beta - 1} \quad (5)$$

Separative power of the gas centrifuge,  $\delta U$ , equals the increment of value through the gas centrifuge.

$$\begin{aligned} \delta U &= PV(C_P) + WV(C_W) - FV(C_F) \\ &= F[\theta V(C_P) + (1 - \theta)V(C_W) - V(C_F)] \end{aligned} \quad (6)$$

where  $V$  is the value function. For the binary separation case, the value function is defined as follows

$$V(C) = (2C - 1)\ln \frac{C}{1 - C}.$$



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Using Eq. (5) and the definition of the value function we obtain

$$\delta U = F \left[ \frac{(\alpha - 1)\beta \ln \beta - (\beta - 1)\ln \alpha}{\alpha\beta - 1} (1 - C_F) + \frac{(\beta - 1)\alpha \ln \alpha - (\alpha - 1)\ln \beta}{\alpha\beta - 1} C_F \right] \quad (7)$$

$\delta U$  is a function of  $F$ ,  $\alpha$ ,  $\beta$ , and  $C_F$ . In fact, there are five variables besides  $F$ , i.e.,  $\theta$ ,  $\gamma$ ,  $\alpha$ ,  $\beta$ , and  $C_F$ . However, two relations, i.e., Eqs. (3) and (4) exist, so only three of the five variables are independent. Then, we may say that  $\delta U$  is a function of  $F$ ,  $\theta$ ,  $\gamma$ , and  $C_F$ .

For some special cases  $\delta U$  is independent of  $C_F$ .

A.  $C_F \ll 1$

For low composition  $C_F$ ,  $1 - C_F \approx 1$ .

$$\delta U_L = F \frac{(\alpha - 1)\beta \ln \beta - (\beta - 1)\ln \alpha}{\alpha\beta - 1} \quad (8)$$

or

$$\delta U_L = F \{ \ln[1 + \theta(\gamma - 1)] - \theta \ln \gamma \} \quad (9)$$

B.  $C_F \approx 1$

For high composition,  $1 - C_F$  is neglected.

$$\delta U_H = F \frac{(\beta - 1)\alpha \ln \alpha - (\alpha - 1)\ln \beta}{\alpha\beta - 1} \quad (10)$$

or

$$\delta U_H = F \{ \ln[1 + (1 - \theta)(\gamma - 1)] - (1 - \theta) \ln \gamma \} \quad (11)$$

C. Symmetric separation

In this case  $\alpha = \beta = \sqrt{\gamma}$ , and the separative power is

$$\delta U_S = F \frac{\sqrt{\gamma} - 1}{\sqrt{\gamma} + 1} \ln \sqrt{\gamma} \quad (12)$$

$\delta U_S$  is independent of  $\theta$ .

D.  $C_F = 0.5$

Let  $C_F = 0.5$ , a separative power called  $\delta U_M$  is obtained as:



$$\delta U_M = F \left[ (1 - \theta) \ln \gamma - \frac{\sqrt{(\gamma - 1)^2 (\theta - \frac{1}{2})^2 + \gamma - (\gamma - 1)(\theta - \frac{1}{2})} - 1}{\gamma - 1} \ln \gamma \right] \quad (13)$$

The dependence of separative power on  $C_F$  is shown in Fig. 2.

The curves in Fig. 2 show that the high composition approximation and symmetric separation overestimate the separative power, the low composition approximation underestimate the separative power, and the  $\delta U_M$ , i.e.,  $C_F = 0.5$  is a good one. The curves obtained in Fig. 2 are for the special case  $\gamma = 1.40$  and  $\theta = 0.45$ . For this example, the absolute value of the relative error of  $\delta U_M$  to  $\delta U$  for different  $C_F$  is less than 2%. The other three approximations have one sign error, i.e., the error is positive or negative for any  $C_F$ . For a very wide range of  $\gamma$  and  $\theta$ , the relative error of  $\delta U_M$  to  $\delta U$  for different  $C_F$  is small. For example, for  $\gamma_0 = 1.0 \sim 1.9$ ,  $\theta = 0.35 \sim 0.65$ , the absolute values of the relative error are less than 5%. It is possible to use  $\delta U_M$  to express the separative power without considering the feed composition.

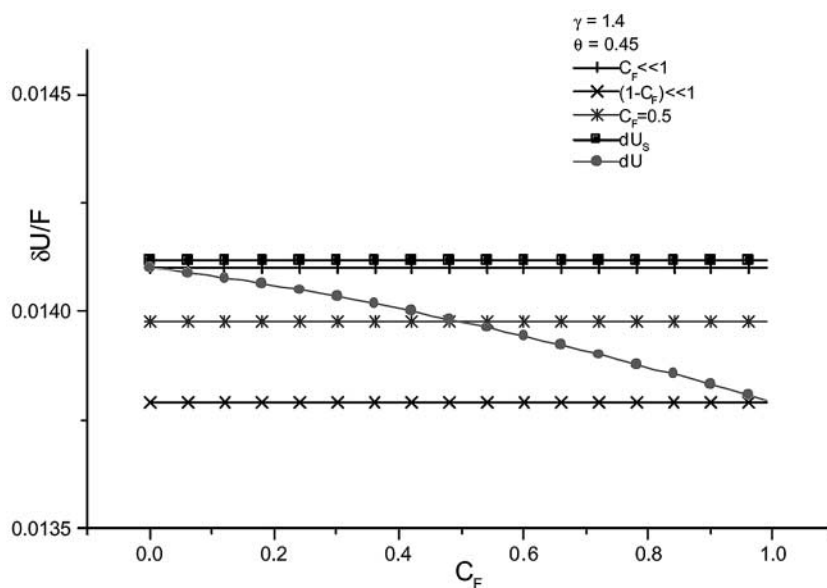


Figure 2. Dependence of separative power on  $C_F$ .



### Estimation of the Overall Separation Factor, $\gamma_0$

According to Cohen's theory (15) for binary gas centrifuge separation, the maximum theoretical separative power of a gas centrifuge,  $\delta U_{\max, \text{theor}}$  is equal to

$$\delta U_{\max, \text{theor}} = \frac{\pi}{2} \rho D \left( \frac{\Delta M \Omega^2 r_a^2}{2RT_0} \right)^2 Z_H \quad (14)$$

where  $\rho$  is the density of process gas,  $D$  is the diffusion coefficient of process gas,  $\Omega$  is the angular velocity of the gas centrifuge,  $r_a$  is the radius of the cylinder,  $Z_H$  is the length of the cylinder,  $T_0$  is the temperature, and  $R$  is the universal gas constant.

Suppose  $\Delta M = 1$ , then we have:

$$\delta U_{\max} = \frac{\pi}{2} \rho D \left( \frac{A^2}{M} \right)^2 Z_H \quad (15)$$

Here  $A^2 \equiv M \Omega^2 r_a^2 / 2RT$ ,  $M$  is the molar weight of the process gas.

The actual separative power of a gas centrifuge,  $\delta U_R$  is less than  $\delta U_{\max}$ , and it is a product of  $\delta U_{\max}$  and separation efficiency,  $E$ .

$$\delta U_R = E \delta U_{\max} \quad (16)$$

$E$  may be expressed in terms of four efficiency factors (16).

$$E = E_C E_I E_F E_E \quad (17)$$

where  $E_C$  is the circulation efficiency,  $E_I$  is the ideality efficiency,  $E_F$  is the flow pattern efficiency, and  $E_E$  is the experimental efficiency. The circulation efficiency for a countercurrent gas centrifuge is given by

$$E_C = \frac{m^2}{(1 + m^2)}$$

where  $m$  is a number which is proportional to the circulation rate. It is reasonable to take  $m = 4$  which gives  $E_C = 0.94$ . The ideality efficiency,  $E_I$ , depends on the distribution of the circulation rate along the rotating axes. If the circulation rate is constant along the axes, maximum value of  $E_I$  is 0.8145. Of course, when the distribution of circulation rate is close to an optimal one  $E_I$  can approach unity. The flow pattern efficiency depends on the value of the speed parameter  $A^2$ . For modern gas centrifuge  $A^2$  is very high for uranium isotope separation, but sometimes it is not very high for non-uranium isotope separation, especially for light and middle weight isotopes. Figure 3 shows a dependence of  $E_F$  on  $A^2$  which is obtained following Ref. (17).





The maximum  $E_F$  exists near  $A^2 = 6.0$ . As to the experimental efficiency,  $E_E$ , many factors may affect it. When no reference data are present, let  $E_E = 1.00$ .

Now we may estimate the value of  $\gamma_0$ . First the necessary data are needed, such as  $\rho D$  of the process gas, the molar weight of the process gas, the peripheral velocity of the cylinder,  $V = \Omega r_a$ , etc. Then, the expected separation power of the gas centrifuge is obtained from  $\delta U_R$ . Choosing one of the separation power expressions  $\delta U_L$ ,  $\delta U_H$ ,  $\delta U_S$ , or  $\delta U_M$ , say  $\delta U_M$ , and taking  $\delta U_M = \delta U_R$ , finally the overall separation factor per unit molar weight difference,  $\gamma_0$ , is obtained by Eq. (13).

As an example, suppose that the peripheral velocity of the gas centrifuge cylinder,  $V = 500$  m/sec, the feed flow rate  $F = 6$  g/hr,  $\theta = 0.45$ ,  $\rho D = 3.098 \times 10^{-5}$  kg/m/sec, the process gas is Xe, its average molar weight  $M = 131.29$ . Finally,  $\gamma_0 = 2.18$ .

When we change the value of  $\theta$  and keep the other parameters unchanged, we obtain the dependence of  $\gamma_0$  on the cut,  $\theta$  which is shown in Fig. 4. The curve is similar to Fig. 2 in paper (13).

Figure 5 shows the dependence of  $\gamma_0$  on the feed flow rate with the other parameters unchanged.

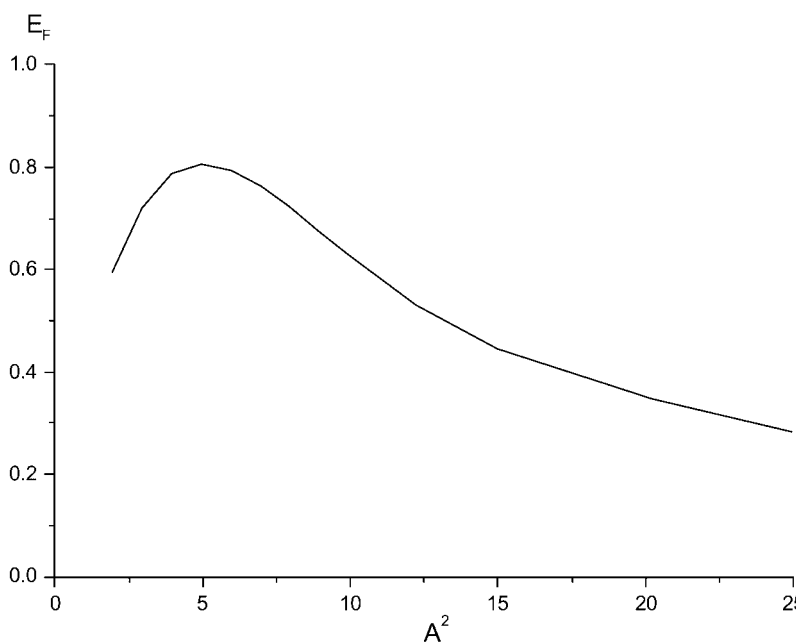


Figure 3. Dependence of  $E_F$  on  $A^2$ .



The results of the example are compared with that obtained by solving a set of diffusion equations in a multicomponent mixtures in a gas centrifuge (14). The values and curve trends are agreed very well.

### DISCUSSION AND CONCLUSIONS

Using the concept of separative power of binary case the estimation of the overall separation factor per unit molar weight difference,  $\gamma_0$ , is possible. From Eqs. (13) and (15)  $\gamma_0$  is a function of the following parameters: the cut  $\theta$ , the feed flow rate  $F$ , parameter  $\rho D$ , and speed parameter  $A^2$ . We will discuss the influence of the parameters below.

A. The dependence of  $\gamma_0$  on  $\theta$  is shown in Fig. 4. The relationship between  $\gamma_0$  and  $F$  is shown in Fig. 5. These two figures are obtained with the other data fixed.

B. Influence of  $A^2$ .

Suppose the following parameters are fixed:

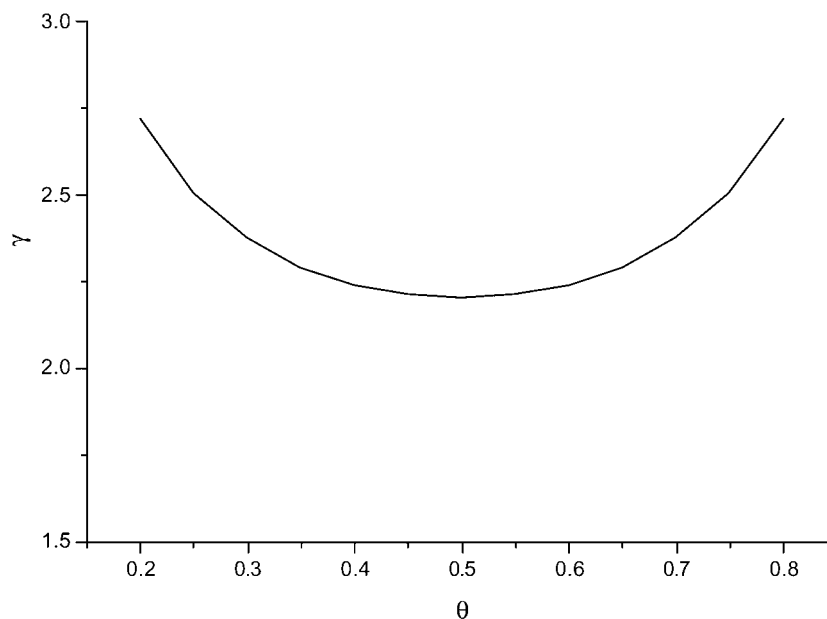


Figure 4. Dependence of  $\gamma_0$  on  $\theta$ .



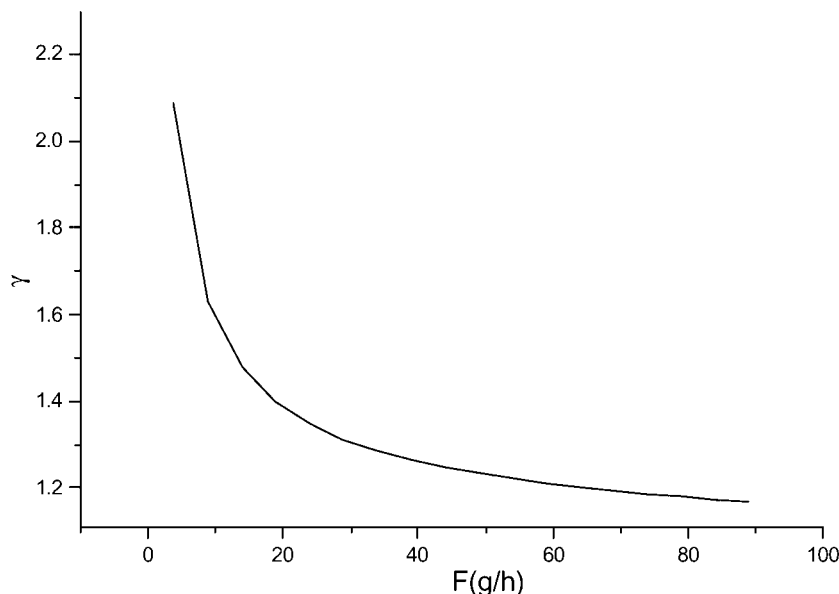


Figure 5. Dependence of  $\gamma_0$  on the feed flow rate,  $F$ .

$V = \Omega r_a = 500$  m/sec,  $\theta = 0.45$ ,  $\rho D = 3 \times 10^{-5}$  kg/m/sec,  $F = 50$  g/hr. We obtained the dependence of  $\gamma_0$  on  $A^2$  as shown in Fig. 6.

If the feed flow rate is changed from 50 to 6 g/hr, then Fig. 7 is obtained. The difference between Figs. 6 and 7 is the feed flow rate. The larger the rate, the lower is the separation factor. Both the curves have a maximum near  $A^2 = 6.0$ . The results are similar to that in paper (14). The reason why the curve has its maximum at this value is because flow pattern efficiency has a maximum near  $A^2 = 6.0$  (see Fig. 3).

#### C. Influence of $\rho D$ .

Taking  $V = \Omega r_a = 500$  m/sec,  $\theta = 0.45$ ,  $A^2 = 18.0$ , and  $F = 50$  g/hr, the dependence of  $\gamma_0$  on  $\rho D$  is calculated and shown in Fig. 8. Using  $F = 6$  instead of 50 g/hr and  $A^2 = 6.0$  instead of 18.0, the curve  $\gamma_0 \sim \rho D$  is shown in Fig. 9.

Figures 8 and 9 show that the higher the value of  $\rho D$ , the larger is the separation factor,  $\gamma_0$ . This is because the separative power is proportional to  $\rho D$ . The conclusions are:

- A. For estimation of the overall separation factor per unit molar weight difference,  $\gamma_0$ , it is possible to use the concept of separative power for binary mixture.



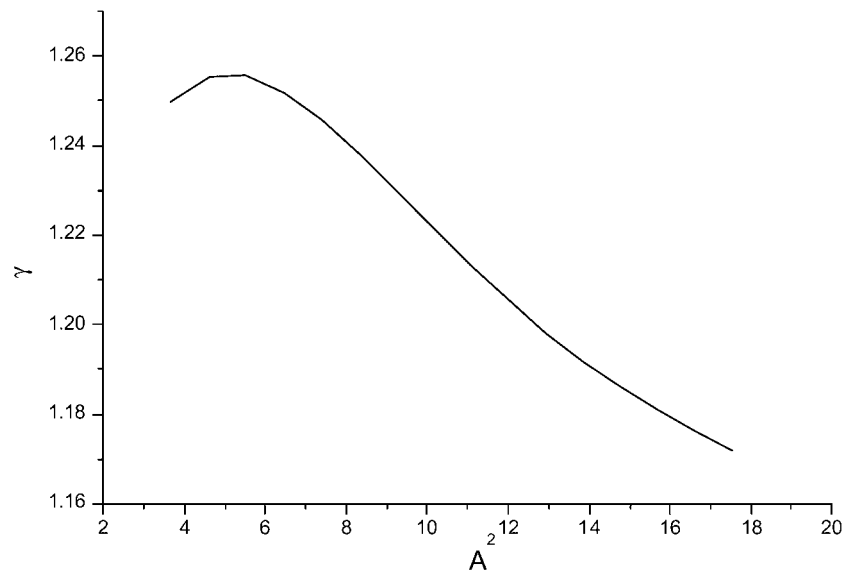


Figure 6. Dependence of  $\gamma_0$  on  $A^2$ .

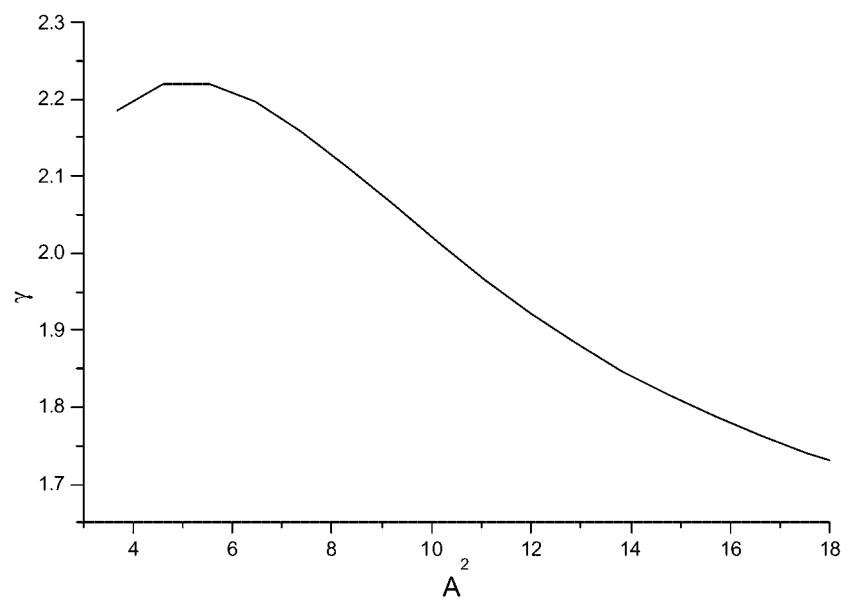


Figure 7. Dependence of  $\gamma_0$  on  $A^2$ .



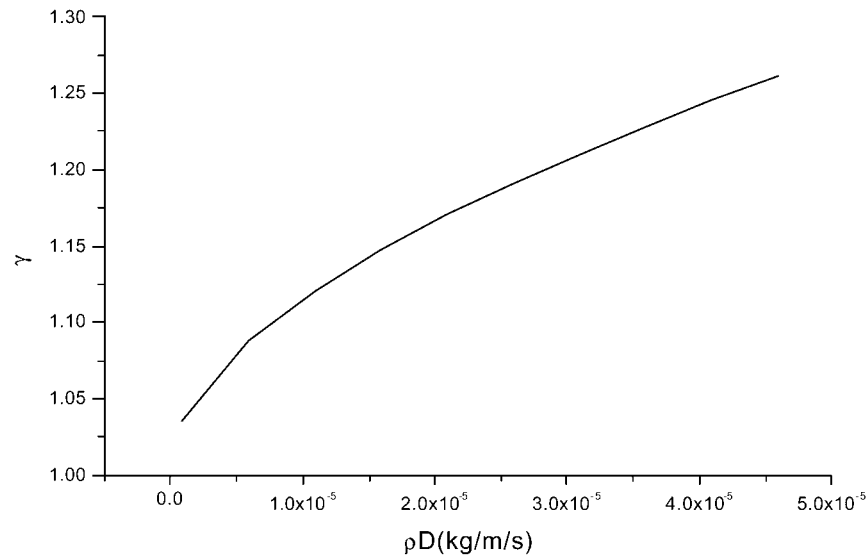


Figure 8. Dependence of  $\gamma_0$  on  $\rho D$ .

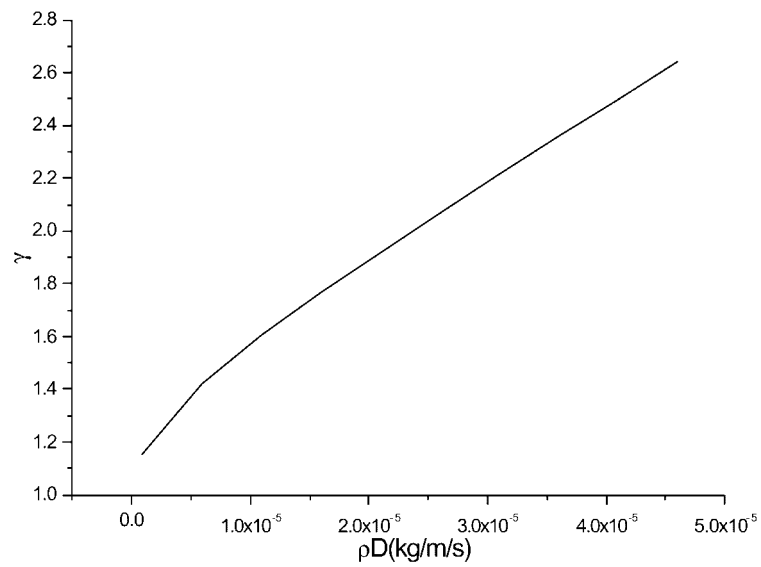


Figure 9.  $\gamma_0 \sim \rho D$ .



- B. The feed composition has little influence on separative power. It is better to take  $C_F = 0.5$  and use  $\delta U_M$  as the separative power when we estimate  $\gamma_0$ .
- C.  $\gamma_0$  is a function of  $\theta$ ,  $F$ ,  $\rho D$ , and  $A^2$ . In the range of  $\theta$  between 0.2 and 0.8,  $\gamma_0$  changes a little with the minimum about  $\theta = 0.5$ . When  $F$  increases,  $\gamma_0$  decreases, and  $\gamma_0$  increases with  $\rho D$ .  $\gamma_0$  has a maximum near  $A^2 = 6.0$ .

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