

## RULE OF THUMB FOR GAS PERMEATION SYSTEMS' CALCULATIONS

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### Abstract

In gas purification using polymeric membrane systems, different parameters affect on product specification. In these systems, pressure ratio, stage-cut, membrane selectivity and feed purity are important parameters which changing in these parameters results in a different product specification. Existence of a mathematical correlation between these parameters can be helpful and it gives a view that shows how can approach to products with desired specification. In present study, a correlation between effective parameters has been developed. This dimensionless mathematical model shows how product purity and recovery are influenced by membrane selectivity (DR; from 2 to 125) and feed purity in different stage-cut and a pressure ratio between 1/20 and 1/10.

**Keywords:** Gas Purification; Membrane Separation; Dimensionless Equation; Rule of Thumb.

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### 1. Introduction

Nowadays gas purification technology using membrane separation systems is known as a common separation process in the industry. Membrane systems selectively separate components in which the component with more selectivity passes through the membrane faster than other components. In this processes different parameters such as stage-cut, pressure ratio and feed purity affect the efficiency of the separation. Reference [1] discusses the impact of these parameters on separation efficiency. Due to high separation efficiency, lower capital and operating costs and other benefits such as compact units, many numbers of different membrane separation processes already have been studied and developed during recent decades. The processes such as N<sub>2</sub>-O<sub>2</sub> separation from air, H<sub>2</sub>-Hydrocarbon separation, N<sub>2</sub> and CO<sub>2</sub> separation from natural gas, H<sub>2</sub>S and water removal are common membrane processes which are used in industrial plants [2]. As reference [3] highlights, during the separation process of N<sub>2</sub> and O<sub>2</sub> from air, oxygen passes through the membrane faster than nitrogen because oxygen is more permeable (2<DR<20). Consequently, oxygen purity in permeate increases in comparison to the feed stream. In the H<sub>2</sub>-CH<sub>4</sub> separation process, polymeric membranes such as polyimide (DR=78,125,250) [4-5] membranes can be used to produce a high purity hydrogen stream. In this process permeate is enriched in hydrogen due to the higher selectivity of hydrogen. Reference [3] states that CO<sub>2</sub> can be removed as permeate from CO<sub>2</sub>-CH<sub>4</sub> streams using cellulose acetate (DR=15) or high performance membrane (DR=40). Also methane-permeable (DR=6) or nitrogen-permeable (DR=17) membranes can be used for separation N<sub>2</sub>-CH<sub>4</sub> streams [3]. Given that applications of membrane separation processes are various, the existence of a mathematic correlation that consists all these processes could be very helpful for studying the efficiency of these systems. In this present study, a new dimensionless model that can be widely utilized in different membrane processes has been developed.

## 2. Methodology

In the present research the required permeation data for membrane separation of a 2-component feed stream has been obtained using the previous method that had been discussed in reference [1] which was studied by our previous team (Mivechian *et al.*). Validation of this method was examined in reference [6]. In this paper, a new dimensionless model which can be correlated with the obtained permeation data has been introduced. In a 2-component system, we define DR as the permeability ratio of component i to j (i=component with higher permeability) and XR as purity ratio of i to j. The results show that if DR is constant, an increase or decrease in permeability of one component will not result in a change in the product purity. Similarly, changing pressure while the pressure ratio (PR) is constant makes no difference in purity of product. Based on the results, it has been observed that there is a relation between  $XR_{Feed}$ , DR and  $XR_{Product}$  (here, product refers to permeate). In other words, the results show that in specific PR and SC (stage-cut),  $XR_{Product}=f(XR_{Feed}, DR)$ . It has been seen that the permeation data is well correlated with Eq. 1.

$$XR_{Product} = A \cdot XR_{Feed}^n \cdot DR^m + B \cdot XR_{Feed}^k \cdot DR^t \quad \text{Eq. 1}$$

where A, B, n, m, k and t are constant parameters for each specific PR and SC.

In this study, these constants were found for different SC and a PR of  $1/20 < PR < 1/10$ . When the  $XR_{Product}$  is calculated the purity of component i in product ( $X_{Product}$ ) can be determined as follow:

$$X_{Product} = \frac{XR_{Product}}{XR_{Product} + 1} \quad \text{Eq. 2}$$

Also, the purity of i in feed stream ( $X_{Feed}$ ) is:

$$X_{Feed} = \frac{XR_{Feed}}{XR_{Feed} + 1} \quad \text{Eq. 3}$$

Now recovery of component i (RE) can be calculated using Eq. 4.

$$RE = \frac{X_{Product} \cdot SC}{X_{Feed}} \quad \text{Eq. 4}$$

## 3. Results and discussion

Considering Eq. 1 has 6 different constants, 6 different conditions have been used in order to find these constants for each specified SC and PR. If we define  $g(X_{Feed}, DR)=f(XR_{Feed}, DR)$ , 6 conditions of  $g(0.1,2)$ ,  $g(0.1,30)$ ,  $g(0.3,2)$ ,  $g(0.3,30)$ ,  $g(0.5,2)$  and  $g(0.5,30)$  are used to determine the constants of Eq.1 for  $DR=2$  to  $DR=30$ . To calculate the constants for  $DR=30$  to 125, another 6 conditions of  $g(0.1,30)$ ,  $g(0.1,125)$ ,  $g(0.3,30)$ ,  $g(0.3,125)$ ,  $g(0.5,30)$  and  $g(0.5,125)$  were taken. By solving system of equations, the constants of Eq. 1 have been obtained and are shown in Table 1 and Table 2. The calculations were based on a reasonable PR of 1/20 to 1/10. It should be noted that  $XR_{Product}$  is related to PR and consequently, it affects on values of the constants. But the gas permeation data for each PR between 1/20 and 1/10 clearly showed negligible difference in product purity. Therefore, in the present study the effect of changing the PR between 1/20 and 1/10 has been ignored.

If membrane calculations based on the presented method of reference [1] is called the accurate method and calculations in the present study using Eq. 1 is called estimation method; we define deviation as Eq. 5 to examine validation of Eq. 1.

$$\text{Deviation} = X_{Acc} - X_{Est} \quad \text{Eq. 5}$$

where  $X_{Est}$  and  $X_{Acc}$  are calculated purity of component i in product based on estimated and accurate methods, respectively.

Deviation values for different DR,  $X_{Feed}$  and SC parameters are given in Table 3 to Table 14. As these tables show, the estimation method for  $30 < DR < 125$  gives clearly better results (absolute value of deviation is small) in comparison to  $2 < DR < 30$ .

Table 1 Constants of Eq. 1 for  $2 < DR < 30$  ( $1/20 < PR < 1/10$ )

	SC=0.3	SC=0.4	SC=0.5	SC=0.6	SC=0.7	SC=0.8
A	1.60264	1.43158	1.39829	1.36744	1.30931	1.2255
B	0.006991	0.004223	0.004574	0.007531	0.013616	0.020874
n	1.01273	1.01759	1.02078	1.02162	1.01996	1.01599
m	0.04206	0.179707	0.142814	0.088716	0.047857	0.021275
k	1.85381	2.48229	3.05516	2.96215	2.64957	2.47241
t	2.23634	2.31238	2.14628	1.72981	1.24824	0.828196

Table 2 Constants of Eq. 1 for  $30 < DR < 125$  ( $1/20 < PR < 1/10$ )

	SC=0.3	SC=0.4	SC=0.5	SC=0.6	SC=0.7	SC=0.8
A	13.7247	8.18319	4.37761	2.69525	1.90458	1.46449
B	0.003356	0.038598	0.265299	1.21342	0.567006	0.20185
n	1.54579	1.47344	1.30585	1.18408	1.10871	1.05927
m	-0.01514	0.006984	0.001288	0.000154	1.08E-05	2.81E-07
k	3.21795	5.45762	7.09122	6.28384	5.51893	4.93023
t	1.98482	1.44473	0.841709	0.12499	0.009869	0.000333

Table 3 Deviation values for stage-cut of 0.8 and  $2 < DR < 30$  (Refer to Table 1,  $1/20 < PR < 1/10$ )

	SC=0.1	SC=0.3	SC=0.5	SC=0.7	SC=0.9
DR=2	0%	0%	0%	-1%	-3%
DR=9	0%	2%	4%	5%	0%
DR=16	0%	1%	2%	4%	0%
DR=23	0%	0%	1%	3%	0%
DR=30	0%	0%	0%	2%	0%

Table 4 Deviation values for stage-cut of 0.8 and  $30 < DR < 125$  (Refer to Table 2,  $1/20 < PR < 1/10$ )

	SC=0.1	SC=0.3	SC=0.5	SC=0.7	SC=0.9
DR=30	0%	0%	0%	-7%	-1%
DR=50	0%	0%	0%	-7%	-1%
DR=70	0%	0%	0%	-7%	0%
DR=90	0%	0%	0%	-7%	0%
DR=110	0%	0%	0%	-7%	0%

Table 5 Deviation values for stage-cut of 0.7 and  $2 < DR < 30$  (Refer to Table 1,  $1/20 < PR < 1/10$ )

	SC=0.1	SC=0.3	SC=0.5	SC=0.7	SC=0.9
DR=2	0%	0%	0%	-1%	-3%
DR=9	1%	4%	7%	5%	-1%
DR=16	0%	2%	5%	4%	-1%
DR=23	0%	1%	3%	3%	-1%
DR=30	0%	0%	0%	2%	0%

Table 6 Deviation values for stage-cut of 0.7 and  $30 < DR < 125$  (Refer to Table 2,  $1/20 < PR < 1/10$ )

	SC=0.1	SC=0.3	SC=0.5	SC=0.7	SC=0.9
DR=30	0%	0%	0%	-4%	-1%
DR=50	0%	0%	0%	-2%	0%
DR=70	0%	0%	0%	-2%	0%
DR=90	0%	0%	0%	-1%	0%
DR=110	0%	0%	0%	-1%	0%

Table 7 Deviation values for stage-cut of 0.6 and  $2 < DR < 30$  (Refer to Table 1,  $1/20 < PR < 1/10$ )

	SC=0.1	SC=0.3	SC=0.5	SC=0.7	SC=0.9
DR=2	0%	0%	0%	-1%	-3%
DR=9	2%	7%	10%	2%	-2%
DR=16	1%	5%	7%	1%	-1%
DR=23	0%	3%	3%	0%	-1%
DR=30	0%	0%	0%	-1%	-1%

Table 8 Deviation values for stage-cut of 0.6 and  $30 < DR < 125$  (Refer to Table 2,  $1/20 < PR < 1/10$ )

	SC=0.1	SC=0.3	SC=0.5	SC=0.7	SC=0.9
DR=30	0%	0%	0%	-3%	-1%
DR=50	0%	0%	0%	-2%	0%
DR=70	0%	0%	0%	-1%	0%
DR=90	0%	0%	0%	-1%	0%
DR=110	0%	0%	0%	-1%	0%

Table 9 Deviation values for stage-cut of 0.5 and  $2 < DR < 30$  (Refer to Table 1,  $1/20 < PR < 1/10$ )

	SC=0.1	SC=0.3	SC=0.5	SC=0.7	SC=0.9
DR=2	0%	0%	0%	-1%	-3%
DR=9	3%	10%	10%	1%	-2%
DR=16	2%	8%	7%	-1%	-1%
DR=23	1%	4%	3%	-2%	-1%
DR=30	0%	0%	0%	-2%	-1%

Table 10 Deviation values for stage-cut of 0.5 and  $30 < DR < 125$  (Refer to Table 2,  $1/20 < PR < 1/10$ )

	SC=0.1	SC=0.3	SC=0.5	SC=0.7	SC=0.9
DR=30	0%	0%	0%	-3%	-1%
DR=50	0%	0%	0%	-2%	0%
DR=70	0%	0%	0%	-1%	0%
DR=90	0%	0%	0%	-1%	0%
DR=110	0%	0%	0%	-1%	0%

Table 11 Deviation values for stage-cut of 0.4 and  $2 < DR < 30$  (Refer to Table 1,  $1/20 < PR < 1/10$ )

	SC=0.1	SC=0.3	SC=0.5	SC=0.7	SC=0.9
DR=2	0%	0%	0%	0%	-1%
DR=9	4%	12%	10%	2%	-1%
DR=16	3%	11%	6%	0%	-1%
DR=23	2%	6%	2%	-1%	-1%
DR=30	0%	0%	0%	-1%	0%

Table 12 Deviation values for stage-cut of 0.4 and  $30 < DR < 125$  (Refer to Table 2,  $1/20 < PR < 1/10$ )

	SC=0.1	SC=0.3	SC=0.5	SC=0.7	SC=0.9
DR=30	0%	0%	0%	-2%	-1%
DR=50	0%	1%	0%	-1%	0%
DR=70	0%	1%	0%	-1%	0%
DR=90	0%	1%	0%	-1%	0%
DR=110	0%	0%	0%	-1%	0%

Table 13 Deviation values for stage-cut of 0.3 and  $2 < DR < 30$  (Refer to Table 1,  $1/20 < PR < 1/10$ )

	SC=0.1	SC=0.3	SC=0.5	SC=0.7	SC=0.9
DR=2	0%	0%	0%	0%	0%
DR=9	10%	18%	12%	4%	0%
DR=16	10%	15%	7%	1%	0%
DR=23	7%	8%	3%	0%	0%
DR=30	1%	2%	0%	-1%	0%

Table 14 Deviation values for stage-cut of 0.3 and  $30 < DR < 125$  (Refer to Table 2,  $1/20 < PR < 1/10$ )

	SC=0.1	SC=0.3	SC=0.5	SC=0.7	SC=0.9
DR=30	1%	2%	0%	-1%	0%
DR=50	2%	5%	1%	-1%	0%
DR=70	2%	5%	1%	-1%	0%
DR=90	2%	5%	1%	0%	0%
DR=110	1%	4%	0%	0%	0%

The results for SC=0.8 are shown on Table 3 and Table 4. These tables state the deviation values for different data points were small. Deviation values for stage-cut of 0.7 are shown in Table 5 and Table 6. As seen, these tables indicate acceptable deviation for different data; but table 6 shows better convergence. For SC=0.6, the deviation values are given in Table 7 and Table 8. According to these tables, when  $30 < DR < 125$ , the deviation is adequately close to zero in all the data points; but as it could be seen for  $2 < DR < 30$ , the deviation around data point of  $g(0.5,9)$  is near 10%. However, in other data points, Table 7 shows acceptable deviation values for  $2 < DR < 30$ . The results for SC=0.5 are presented in Table 9 and Table 10. As these tables show, when  $30 < DR < 125$  the deviation is negligible once more. For  $2 < DR < 30$ , the deviation values are within an acceptable range for most of the time. However, these values around points of  $g(0.3,9)$  and  $g(0.5,9)$  are near 10%. Table 11 and Table 12 show results for SC=0.4. As it could be seen, acceptable results are obtained for a DR between 30 and 125 and once again the deviation is small. Also, for  $2 < DR < 30$ , there is small deviation unless the points are around  $g(0.3,9)$ ,  $g(0.5,9)$  and  $g(0.3,16)$ . Deviation values for stage-cut of 0.3 are given in Table 13 and Table 14. As Table 14, for  $30 < DR < 125$ , the results are well-converged and consequently the deviation values are acceptable in any points. But, for  $30 < DR < 125$  and around points of  $g(0.1,9)$ ,  $g(0.3,9)$ ,  $g(0.5,9)$ ,  $g(0.1,16)$  and  $g(0.3,16)$ , the deviation is significant. Therefore, the main conclusion regarding the different stage-cuts is that if the DR is between 30 and 125 results are well-converged and the deviation values satisfactorily are near zero but for  $2 < DR < 30$ , in some points these values are significant and must be noted.

#### 4. Conclusion

A dimensionless model has been discussed in this paper which can be utilized to predict purity and the recovery of products between the parameter of  $1/20 < PR < 1/10$  and  $2 < DR < 125$ . To achieve better results, the constants of these equations have been obtained for each DR range of  $2 < DR < 30$  and  $30 < DR < 125$  separately. The results show that if DR is between 30 and 125 the deviation values are negligible; but for  $2 < DR < 30$ , in some cases these values are significant and this must be noted. The presented model is able to be used for several industrial membrane separation processes. Such membrane separation systems include  $N_2$ - $O_2$  separation system (Air separation,  $2 < DR < 20$ ), hydrogen separation from hydrogen-methane streams ( $30 < DR < 125$ ) or  $CO_2$ - $CH_4$  and  $N_2$ - $CH_4$  separation processes can be mentioned.

#### Symbols

<i>I</i>	Component with higher permeability	<i>RE</i>	Recovery of component <i>i</i> in permeate stream
<i>J</i>	Component with lower permeability	<i>SC</i>	Stage-cut (flow rate ratio of permeate to feed)
<i>DR</i>	Permeability ratio of component <i>i</i> to <i>j</i> (selectivity)	<i>X</i>	Mole fraction (purity) of component <i>i</i>
<i>PR</i>	Pressure ratio of permeate to feed	<i>XR</i>	Mole fraction ratio of <i>i</i> to <i>j</i> (in 2-component systems)

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