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Numerical Evaluation of an Improper Integral for Pressure Drop Calculation in Hollow Fiber Membrane

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The decrease in gas pressure within the bore of hollow fibers in membrane separation has received considerable interest. Typically, such complex problems are commonly addressed by the utilization of numerical methods. The pure numerical approaches are inadequate in providing a comprehensive understanding of the influence of physical features of fibers (such as length, inner diameter, and intrinsic gas permeance) and operating parameters (such as membrane pressure) on the pressure drop. Another approach is to present the pressure profile by an analytical expression. The integral equation derived from this approach requires a calculation of an improper integral. The improper integral is numerically estimated by a commercial mathematical package or by consulting tables from handbooks, which limit the application and is also implicit in nature. In this study, a simple technique is proposed so that the improper integral is easily and explicitly evaluated by any numerical integration scheme. The effect of fiber length, intrinsic gas permeance on the pressure profile at the permeate side of membrane are also discussed. The pressure profiles serve as a first indication for the design of hollow fiber membrane module.

1. Introduction

In the process of gas separation, membranes have been shown to play a significant part (Baker and Lokhandwala, 2008), and the majority of these membranes have a hollow fiber configuration (Bernardo et al., 2019). Self-support, high-pressure endurance, and extreme compactness are three distinguishing characteristics of hollow fibers (Ahmad et al., 2015), and it is commonly agreed that the commercial popularity can be directly attributed to the presence of these distinctive qualities (Bernardo and Clarizia, 2013).
The dimension of single hollow fiber has a significant impact on the degree to which hollow fiber module can be packed together (Wan et al., 2021). Utilizing smaller fibers helps to reduce the size of the membrane module. The Hagen-Poiseuille equation suggests that hollow fibers characterized by small size can lead to substantial pressure decreases within the lumen of the fibers. Because of this, the force which drive the gas permeation process through the fibers can become insignificant, with the degree of this lost being dependent on the reduction of the hollow fiber size. In order to make the most of the benefits offered by hollow fiber membranes in various applications, it is obvious that a reasonable compromise should be made about the conflict between the advantageous compactness and the disadvantageous pressure drop. Investigating the pressure drop that occurs within hollow fiber membranes is the initial step that must be taken in order to accomplish this goal.
There are numerous efforts on hollow fibers and the drop in gas pressure that the fibers cause. Thundyil and Koros (1997) propose a “succession of states” method to model the two dimensional mass transfer in a hollow fiber membrane. Coker et al. (1998) simulated a multicomponent gas separator using hollow-fiber membrane module. Lemanski et al. (1999) reported the effects of several fiber characteristics on the behavior of a hollow fiber gas separator. The main approach in those studies is developing numerical solutions to a set of equations.

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Although it was taken into account during computations, the influence that the pressure buildup had on the flow of gas through the membranes was frequently disregarded during discussion (Shao and Huang, 2006). Another promising approach is to conduct an analytical examination of this problem, in which the interaction mechanism can be explicitly disclosed.
In the work of Shao and Huang (2006), the gas pressure distribution in a hollow fiber is described by an improper integral equation, an assessment of the parameters pertaining to the gas pressure distribution was conducted. The improper integral can be converted to elliptic integral and the value can be obtained from the table in a manner that is analogous to the popular error function. It is also possible to determine the value by a trial and error technique by utilizing commercial software such as Mathcad. These techniques which require extensive mathematical knowledge or implicit in nature, limit the application in practice. In this study, a simple technique is proposed so that the improper integral is easily and explicitly evaluated by any numerical integration scheme.

2. Methodology

2.1 Analytical approach for pressure loss in hollow fibers

A schematic representation of a hollow fiber is shown in Figure 1. Both ends are attached to tube sheets, with the exception of one end, which is left exposed to serve as an outlet for the permeate that moves through the bore side of the fiber.

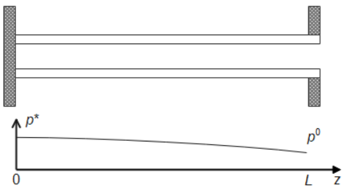

Figure 1: The schematic diagram of a single hollow fiber and the pressure profile in the permeate side

In the work of Shao and Huang (2006), an analytical approach was used to depict the gas pressure profiles in the bore of hollow fiber membranes. The authors proposed an equation to determine the gas pressure at any point on the membrane at the permeate side as Eq(1).

$$\int_{p}^{p^*} \frac{\sqrt{3}p\,dp}{\sqrt{3p_f\left(p^{*2}-p^2\right)-2\left(p^{*3}-p^3\right)}} = 8\sqrt{\frac{2RTD_oJ\mu}{D_i^4}}z \quad (1)$$

In which, p indicates the pressure in the bore side at location z, z the length coordinates along the membrane, D_i the inner diameter of the fiber, D_o the outer diameter of the fiber, J the intrinsic permeance of the membrane for the permeating gas, p_f the feed gas pressure, μ the viscosity of the permeate, R the universal gas constant, and T is the absolute temperature of the permeate.
If the physical characteristics (D_o, D_i, J, L) of the fibers are known and the operation parameters (p_f, p_0, T) are provided, the pressure profile can be determined as follows. First, the value of p^* at the potted wall can be estimated by solving the equation (1) at the open end of the fiber ($z = L$, $p = p_0$). From the obtained value of p^*, the local pressure at any point can be calculated by solving again the fundamental equation (1) for each value of z.The key for this approach is to exactly evaluate the improper integral in the left hand side of equation (1). The expression inside the integral is unbound when p approaches p^*. Because of the singularity of the integrand, the numerical method for direct estimation of the integral does not work well. This work proposes a simple approach for numerical calculation of the integral in the fundamental equation.

2.2 Numerical evaluation of the improper integral

As mentioned in the above section, the integral in the left hand side of Eq(1), which is singular at $p=p^*$, need to be evaluated.
Assign $x=p^*-p$, then $dx=-dp$. At $p=p^*$ then $x=0$ and at $p=p$ then $x=p^*-p$. The integral becomes Eq(2):

$$\int_{p^*-p}^{0} \frac{-\sqrt{3}\left(p^*-x\right)dx}{\sqrt{3p_f\left(p^{*2}-\left(p^*-x\right)^2\right)-2\left(p^{*3}-\left(p^*-x\right)^3\right)}} = \int_{0}^{p^*-p} \frac{\sqrt{3}\left(p^*-x\right)dx}{\sqrt{x}\sqrt{6p_fp^*-6p^{*2}-\left(3p_fx-6p^*x+2x^2\right)}} \quad (2)$$

Let define the new function $g(x)$ as in Eq(3)

$$g(x)=\begin{cases}\frac{\sqrt{3}(p^*-x)}{\sqrt{x}}\left(\frac{1}{\sqrt{6p_f p^*-6p^{*2}-(3p_f x-6p^*x+2x^2)}}-\frac{1}{\sqrt{6p_f p^*-6p^{*2}}}\right) & \text{when x>0}\\ 0 \quad \text{when x=0}\end{cases} \tag{3}$$

The continuity of the function $g(x)$ is investigated as in Eq(4):

$$\begin{aligned}&\lim_{x\to 0}\frac{\sqrt{3}(p^*-x)}{\sqrt{x}}\left(\frac{1}{\sqrt{6p_f p^*-6p^{*2}-(3p_f x-6p^*x+2x^2)}}-\frac{1}{\sqrt{6p_f p^*-6p^{*2}}}\right)\\ &=\lim_{x\to 0}\frac{\sqrt{3}(p^*-x)}{\sqrt{x}}\left(\frac{3p_f x-6p^*x+2x^2}{\sqrt{6p_f p^*-6p^{*2}-(3p_f x-6p^*x+2x^2)}\times\sqrt{6p_f p^*-6p^{*2}}}\right)=0\end{aligned} \tag{4}$$

Since the limit is exist, $g(x)$ is continuous and bounded at x=0. Because of the continuity, the integration of g(x) can be calculated with full confidence by any numerical method such as Simpson's rule (Chapra and Canale, 2009). In this study, Simson's 1/3 rule with 100 subintervals is employed for the evaluation of the integration $\int_0^{p^*-p} g(x)dx$. Then the integral I can be calculated as Eq(5) and Eq(6).

$$I=\int_0^{p^*-p} g(x)dx+\int_0^{p^*-p}\frac{\sqrt{3}(p^*-x)}{\sqrt{x}}\frac{1}{\sqrt{6p_f p^*-6p^{*2}}}dx \tag{5}$$

$$I=\int_0^{p^*-p} g(x)dx+\frac{\sqrt{2p^*(p^*-p)}}{\sqrt{(p_f-p^*)}}-\frac{\sqrt{2(p^*-p)^3}}{3\sqrt{(p_f p^*-p^{*2})}} \tag{6}$$

2.3 Estimating the potted-wall pressure p^*, and the pressure profile p across the length

The fundamental equation (1) is applied at $z=L$ for the estimation of p^* as in Eq(7)

$$I=\int_0^{p^*-p_0} g(x)dx+\frac{\sqrt{2p^*(p^*-p_0)}}{\sqrt{(p_f-p^*)}}-\frac{\sqrt{2(p^*-p_0)^3}}{3\sqrt{(p_f p^*-p^{*2})}}=\sqrt{\frac{2RTD_oJ\mu}{D_i^4}}L \tag{7}$$

In this equation, the only unknown variable is p^*. This equation can be obtained by numerical method for non-linear equation. This work used a bisection method (Chapra and Canale, 2009) for finding the root p^* of Eq(7). The starting bracketing interval for the bisection method is $[p_0,p_f]$ because the value p^* must fall within this range. After the calculation of the pressure p^* has been completed, the pressure p at any position z along the fibers can be obtained by solving Eq(8)for each value of z within the range between 0 and L:

$$I=\int_0^{p^*-p} g(x)dx+\frac{\sqrt{2p^*(p^*-p)}}{\sqrt{(p_f-p^*)}}-\frac{\sqrt{2(p^*-p)^3}}{3\sqrt{(p_f p^*-p^{*2})}}=\sqrt{\frac{2RTD_oJ\mu}{D_i^4}}z \tag{8}$$

Bisection methods were also employed to find the root of Eq(8).

3. Results and Discussion

3.1 Gas pressure profiles of the permeate side in hollow fibers

As mentioned above, the pressure profiles in the permeate side of hollow fibers membrane can be numerically calculated from Eq. (7) and Eq. (8). The gas pressure distribution in the permeate side of several hollow fibers with various lengths (20, 40, and 60 cm) are presented in Figure 2. The values of the necessary parameters are provided as follows: feeding side pressure, P_f=200 kPa; open end pressure at permeate side, P_o=100 kPa; intrinsic permeance, 3.0 × 10−9 mol/(m^2.s.Pa); temperature, 308 K; viscosity, 1.766 × 10^{-5} Pa.s; outer diameter of the fiber, D_o=0.0025 m; inner diameter of the fiber, D_i=0.002 m. The calculated results at two different length (L=0.2 m and L=0.4 m) are also compare to the results obtained by MathCad software which was reported in Shao and Huang (2006).

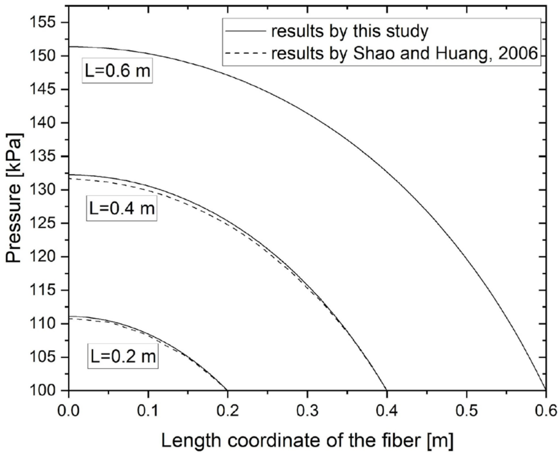

Figure 2: The pressure profile in permeate side of fibers with different lengths

From the figure, it can be obtained that the difference between the highest pressure and the lowest pressure in the permeate side is significant. The relative difference can be as high as 50 % when the fiber length is 0.6 m, and the sharpest pressure change appear at the open end of the fibers. Due to the significance of the variation, the pressure profile should be incorporated into calculations of membrane modules rather than the constant pressure assumption.

3.2 Effect of fiber length on the gas pressure drop

In order to study the effect of fiber length on the gas pressure drop in the permeate side, the pressure profiles of different fiber length (from 0.2 m to 2 m with the step size of 0.2 m) are calculated. The values of other parameters are the same as the ones in section 3.1. The relation between the gas pressure drop and the fiber length are shown in Figure 3.

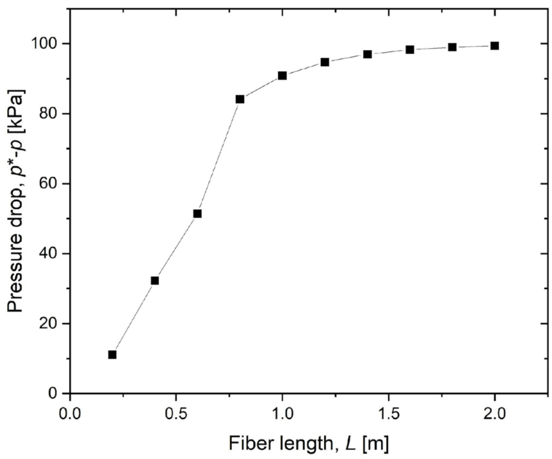

Figure 3: The relation between the gas pressure drop and the fiber length

From the figure, it can be obtained that with an increase of fiber length, the pressure drop increases sharply at the initial. Then, when the fiber length is higher than 1.0 m, the pressure drop just slightly increases and then reaches a plateau. Because of this, in order to keep a high driving force throughout the length of the membrane, it is recommended that the length of the fiber does not exceed 80 cm (when 3.0×10^{-9} mol/(m^2.s.Pa) is the permeance of the fiber).

3.3 Effect of gas permeance on the pressure profiles

The pressure profiles in the permeate side with five different gas permeance (from $1 \cdot 10^{-9}$ to $5 \cdot 10^{-9}$ mol/(m^2.s.Pa)) are presented in Figure 4. The values of other required parameters are provided as follows: feeding side pressure, P_f=200 kPa; open end pressure at permeate side, P_o=100 kPa; temperature, 308 K;

viscosity, 1.766 · 10^{-5} Pa.s; outer diameter of the fiber, D_o=0.0025 m; inner diameter of the fiber, D_i=0.002 m, fiber length, L=0.6 m.

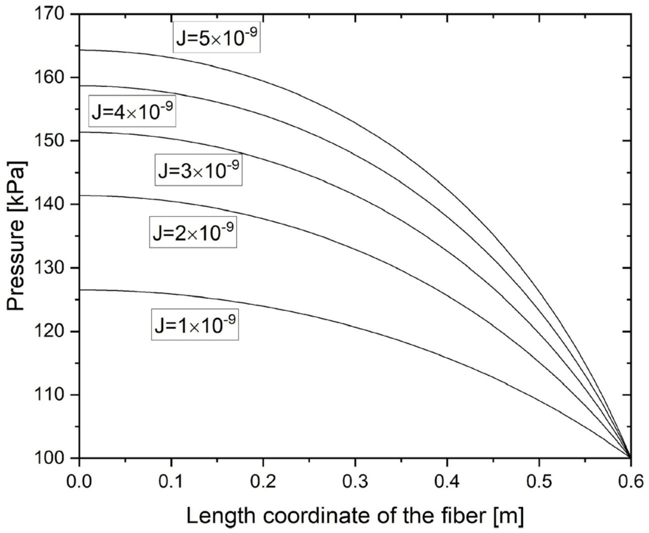

Figure 4: Change in pressure profile in the permeate side of fibers with gas permeance

From the figure, it can be obtained that when the permeance of the gas increases, the pressure gradient in the permeate side also increases. In order to check the dependence of the pressure drop (p^*-p_0) in the permeate side upon the gas permeance J, their relation is presented in Figure 5.

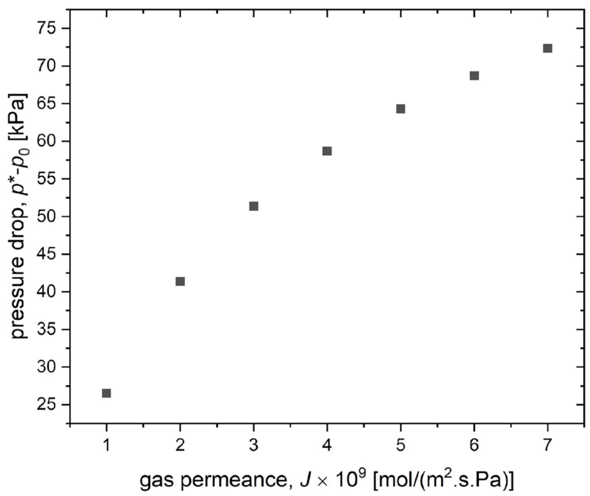

Figure 5: The relation between pressure drop and gas permeance

From the figure, the power-law correlation is suggested to present the relation between the pressure drop and the gas permeance as follows:

$$\Delta p = p^* - p_0 = AJ^m \quad (9)$$

A regression analysis was conducted to confirm the correlation. After linearization and linear fitting, the correlation equation was obtained as:

$$\Delta p = 1.979 \times 10^9 J^{0.514} \quad (9)$$

The correlation coefficient R^2 which is 0.9869 shows the good fitting of the proposed equation. The exponent which is around 0.5 also well agrees with the exponent of *J* in the equation (7).

4. Conclusions

In this study, the pressure profiles in permeate side of a hollow fiber membrane is obtained from an analytical model by a new method. A simple treatment of the improper integral is proposed so that the model can be confidently solved by any numerical integration. The effects of fiber length and permeance on the pressure drop were also investigated. From the results, the pressure drop was found to depend on the square of the gas permeance. The pressure gradient was found to be significant when the fiber length is shorter than 1 m. The pressure profiles serve as a first indication for the design of hollow fiber membrane module.

Nomenclature

z – membrane length coordinate, m
p – pressure of the permeate at location z, Pa
p_f – feed gas pressure, Pa
p* – pressure at sealed wall, Pa
D_i – inner diameter of the fiber, m
D_o – outer diameter of the fiber, m
J – intrinsic permeance, mol/(m^2.s.Pa)
μ – viscosity of the permeate, Pa s
R – universal gas constant,
T –absolute temperature of the permeate, K
x – variable
R^2 – correlation coefficient

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