A VERY APPROXIMATE THEORY FOR GAS TRANSPORT IN A POLYMER FOAM

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Date Published: December 1999

Prepared by the
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LOCKHEED MARTIN ENERGY RESEARCH CORP.
for the
U.S. DEPARTMENT OF ENERGY
under contract DE-AC05-96OR22464

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1. INTRODUCTION

The author is involved with a project that requires calculation of the flow of gas through thin sheets of a flexible polymer foam. Essentially, the foam is a collection of interconnected spherical holes in the polymer matrix. When the material is made, its porosity is in the range of 60–70%. Initially, the sheets are roughly a millimeter thick. In the application, the sheets are compressed between solid surfaces so that their thickness is reduced to approximately 50–75% of the original (thereby reducing the porosity to as low as 20%).

The project requires calculating gas transport in the longitudinal direction (in other words, parallel to the thin section of the sheets and perpendicular to the direction of compression). The transport calculations must be done in three different flow regimes. First, with gas pressures high enough so that the gas in the pores is in the continuum regime and thus the transport is governed by the usual equations for flow of a compressible gas in a porous medium. Second, with gas pressures low enough so that the flow is in the free molecular region. In the third regime, the foam is filled with a carrier gas (with pressure high enough to be in continuum) and the flow of interest is that of a small amount of an additional gas. In this third regime, the driving force is diffusion of the trace gas in the carrier.

The project allows for some limited experiments to measure the permeability of the foam. The objective of the portion of the project being discussed in the present document is to develop a very approximate, first order model that will allow us to use the results from permeability measurements to calculate flow in all three of the regimes. The theory needs to allow the following:

1. Given a measurement or measurements of flow through the foam, the model must allow calculations of transport in all three of the regimes—viscous, free molecular flow, and diffusive. It is expected that the measurements will be made in one regime only (most likely in free molecular flow) so that the theory needs to show how results from this one regime may be used in the others.
2. The model must include changes in the transport with changes in the compression of the foam.

It is, of course, desirable that the details of the transport be calculated with reasonable accuracy. However, a theory that provides results that are accurate within a factor of 2 would be useful.

2. THE SIMPLE CLUSTER OF TUBES APPROXIMATION

One of the earliest models of a porous medium is that of a bundle of tubes of uniform area. Bear¹ cites publications of this idea by Blake (1922), Kozeny (1927), and Fair and Hatch (1933). The reader will immediately object that a bundle of uniform tubes does not seem a very likely approximation to a collection of interconnected spherical cavities. The reason for using this bundle of tubes approximation is that the flow rates for a tube in laminar flow (the Poiseuille equation), free molecular flow (Knudsen's results), and one-dimensional diffusion can be written down in closed form. It is the author's hope that use of this model will allow results from permeability tests to provide parameters that can be used for calculating gas transport in all three of the regimes of interest.

The derivations that follow are the author's own. The author is sure that he is reinventing the wheel, but has found it necessary to derive the results from scratch in order to link the three different flow regimes.

The porous medium is simulated as a bundle of tubes of radius, r_t . In an area of height h and width w , there will be N_t of these tubes. The tubes are all of length $L/\sqrt{\hat{O}}$, where L is the length of the piece of porous material in the streamwise direction. The factor $\hat{O}$ is called the tortuosity factor and is the ratio of the square of the distance along the piece of porous medium in the streamwise direction to the length of the tubes ($\hat{O} \leq 1$ which implies that the tubes do not go straight through the block of porous material, but rather take a winding or "tortuous" path). Authors whose results are quoted by Bear suggest values of $\hat{O}$ in the range of 0.4-0.71 (Bear, p. 111) with a recommended value of 0.67 for isotropic unconsolidated media (Bear p. 112). There is a conflict between the notation for the tortuosity and the absolute temperature because both use an upper case letter "T." The author has written the tortuosity using a block font upper case Greek letter "tau" ($\hat{O}$) and the absolute temperature using an italic font upper case "T" (T). The author hopes that the difference in fonts plus the fact that, in the work he is documenting here, the absolute temperature usually appears as part of the product RT will minimize the ambiguity.

The first requirement for the equivalence of the bundle of tubes to the piece of porous material is that the volume of the tubes must equal the void volume in a block of foam of dimensions h by w by L . The equation for equality of void volumes is

$$N_t \delta r_t^2 \frac{L}{\sqrt{\hat{O}}} = n_0 h w L \quad (1)$$

where n_0 is the porosity of the foam as manufactured (i.e., uncompressed). This can be reduced to the following:

$$N_t \delta \frac{r_t^2}{\sqrt{\hat{O}}} = n_0 h w \quad (2)$$

At this point, there are two unknowns: N_t and r_t .

2.1 LAMINAR, VISCOUS FLOW

The author will need an expression for the drag of the gas flowing through the medium next. This

will give a second equation for the two unknowns. The author assumes that, in the continuum regimes the flow through the porous medium is governed by laminar, viscous flow. An additional approximation that will be made all through this document is that the flows are isothermal. For sheets as thin as those being modeled for this project with solid pieces bounding them, that approximation seems plausible. Using these assumptions and approximations, the laminar, viscous (Poiseuille) mass flow rate through a single tube is

$$\dot{m}_{tube} = - \frac{P}{RT} \frac{\partial r_t^4}{8\mu} \frac{\partial P}{\partial s} \quad (3)$$

or

$$\dot{m}_{tube} = - \frac{1}{2RT} \frac{\partial r_t^4}{8\mu} \frac{\partial P^2}{\partial s} \quad (4)$$

where μ is the laminar viscosity, R is the gas constant for this gas (i.e., the universal constant divided by the gas molecular weight), T is the absolute temperature, P is the absolute pressure, and ∂s is the distance along the flow direction (for the tortuous tube, $\partial s = L/\sqrt{\phi}$). The total mass flow rate through the bundle of tubes is the flow rate for each tube times the number of tubes, i.e.,

$$\dot{m}_{viscous} = - \frac{N_t}{2RT} \frac{\partial r_t^4}{8\mu} \frac{\partial P^2}{L} \sqrt{\phi} \quad (5)$$

The author wants to compare this result with the form for flow through a porous medium. For a compressible gas flowing through a porous medium of permeability k_0 (this is the material permeability, whose dimension is length squared), the mass flow rate is as follows (this is a well-known result that can be derived from an expression in Bird, Stewart, and Lightfoot², p. 150):

$$\dot{m}_{porous} = - \frac{k_0}{\mu} \frac{h w}{2RT} \frac{\partial P^2}{\partial x} \quad (6)$$

where ∂x is the distance along the length of the porous slab and $\partial x = L$. Equating the two expressions for total mass flow [Eqs. (5) and (6)] and canceling terms gives a second equation for relating the unknowns which is

$$N_t \partial r_t^4 \frac{\sqrt{\phi}}{8} = k_0 h w \quad (7)$$

One way to solve the two equations for two unknowns [Eqs. (2) and (7)] is to solve for the groups $N_t r_t^2$ and r_t^2 and then solve for N_t and r_t . After considerable algebraic manipulation, the results are

$$r_t = \sqrt{\frac{8k_0}{n_0 \hat{\mathbf{O}}}} \quad (8)$$

and

$$N_t = \frac{n_0^2 h w \hat{\mathbf{O}}^{3/2}}{8 \delta k_0} \quad (9)$$

In this model, the effective tube radius r_t is a function of material parameters and is therefore itself a material parameter. A valuable way to express the number of tubes is the number per unit area which is

$$\frac{N_t}{h w} = \frac{n_0^2 \hat{\mathbf{O}}^{3/2}}{8 \delta k_0} \quad (10)$$

This is also a material parameter.

In addition to the full mass flow rate, the author needs an expression for the mass flux, which is the mass flow per unit area [the area is not the flow area (i.e., the area of the tubes) but rather the area of the porous material normal to the direction of the flow]. This is very simply the mass flow rate from Eq. (5) divided by the area hw as follows:

$$\left(\frac{\dot{m}}{\text{area}} \right)_{\text{viscous}} = - \frac{N_t}{h w} \frac{1}{2 R T} \frac{\delta r_t^4}{8 \mu} \frac{\ddot{a} P^2}{L} \sqrt{\hat{\mathbf{O}}} \quad (11)$$

The reader may note that the area hw shows up in the expression for N_t [Eq. (9)]. Therefore, the area hw will cancel out of the expression for mass flux, which is as expected (because one would not expect that a mass flux would be dependent on the flow area).

2.2 DIFFUSION

As was mentioned in the introduction, it is expected that some calculations of the diffusion of small pressures of gases in a high pressure of carrier gas will be needed. In ordinary diffusion, the mass flux is given by Fick's First Law and is the diffusivity of the trace gas in the carrier times the gradient of the density of the trace gas. The task of this section is to estimate how the presence of the porous medium will affect the transport of the trace gas. A very simple model for diffusion is to assume that the diffusion is one-dimensional along the length of the tube. If that is true, then the mass flow rate is the area available for flow (the number of tubes times the area of each individual tube) times the diffusivity of the trace gas in the carrier times the density gradient in the flow direction (i.e., the difference in density divided by the tube length, which is $L/\sqrt{\hat{\mathbf{O}}}$).

Therefore,

$$\dot{m}_{diffusion} = -N_t \delta r_t^2 D_i \ddot{a} \left(\frac{P_i}{R_i T} \right) \frac{\sqrt{\mathcal{O}}}{L} \quad (12)$$

or (for an isothermal system)

$$\dot{m}_{diffusion} = -N_t \delta r_t^2 \frac{D_i}{R_i T} \frac{\ddot{a} P_i}{L} \sqrt{\mathcal{O}} \quad (13)$$

where P_i is the partial pressure of trace gas i in the carrier, R_i is the gas constant of the trace gas (the universal gas constant divided by the molecular weight of gas i), and D_i is the diffusivity at small pressures of trace gas i in the carrier. For reference, it would be worth checking to see what the apparent diffusivity for the porous medium is. In other words, what is D_{eff} such that the mass flow is given by ordinary diffusion with that term for the diffusivity, i.e.,

$$\dot{m}_{diffusion} = -h w D_{eff} \frac{1}{R_i T} \frac{\ddot{a} P_i}{L} \quad (14)$$

If one equates the two expressions for diffusive mass flow [Eqs. (13) and (14)], substitutes for N_t and r_t , and cancels terms, the result is

$$D_{eff} = n_0 D_i \hat{\mathcal{O}} \quad (15)$$

The above equation is identical to that in Bear (ref. 1) on p. 112.

As before, the author would like an expression for mass flux, which is mass flow per unit area. From Eq. (13), this is

$$\left(\frac{\dot{m}}{area} \right)_{diffusion} = - \frac{N_t}{h w} \delta r_t^2 \frac{D_i}{R_i T} \frac{\ddot{a} P_i}{L} \sqrt{\mathcal{O}} \quad (16)$$

As was true for the mass flux for the laminar viscous flow, the area $h w$ will drop out of the mass flux because N_t is proportional to $h w$. The simplest expression for diffusive mass flux is Eq. (14) divided by $h w$, i.e.,

$$\left(\frac{\dot{m}}{area} \right)_{diffusion} = - D_{eff} \frac{1}{R_i T} \frac{\ddot{a} P_i}{L} = - n_0 D_i \hat{\mathcal{O}} \frac{1}{R_i T} \frac{\ddot{a} P_i}{L} \quad (17)$$

2.3 FREE MOLECULAR FLOW

As was stated in the introduction, it is expected that some calculations will have to be done in regions for which the pressure is so small that the flow is free molecular. From Roth³, p. 82, the conductance of a long tube of uniform, but arbitrary cross section and length $L/\sqrt{\bar{O}}$ in free molecular flow is as follows (with some changes in notation to match that author's):

$$C_{tube} = \frac{8}{3\sqrt{\bar{O}}} \sqrt{2RT} \frac{A_{tube}^2}{BL} \sqrt{\bar{O}} \quad (18)$$

where A_{tube} is the area of the tube normal to the flow direction and B is the wetted perimeter of the tube. The definition of conductance (units are volume divided by time) is that it is the factor such that the volumetric flow rate Q is proportional to the pressure difference divided by the average pressure, or

$$Q = -C \frac{\ddot{a}P}{\bar{P}} \quad (19)$$

Using this definition and multiplying by the average density, the mass flow rate (per tube) becomes

$$\dot{m}_{tube} = Q\bar{n} = Q \frac{P}{RT} = -C \frac{\ddot{a}P}{P} \frac{P}{RT} \quad (20)$$

(this is a generic mass flow rate that can be used for any kind of flow). Applying the free molecular conductance per tube [Eq. (18)] to this definition and multiplying by the number of tubes, the mass flow rate for a bundle of N_t tubes of arbitrary shape becomes

$$\dot{m}_{free} = -N_t \frac{8}{3\sqrt{\bar{O}}} \sqrt{2RT} \frac{A_{tube}^2}{BL} \sqrt{\bar{O}} \frac{\ddot{a}P}{RT} \quad (21)$$

or, for a round tube of radius r_t ,

$$\dot{m}_{free} = -N_t \frac{8}{3\sqrt{\bar{O}}} \sqrt{2RT} \frac{\bar{O}^2 r_t^4}{2\bar{O} r_t L} \sqrt{\bar{O}} \frac{\ddot{a}P}{RT} \quad (22)$$

Collecting and canceling terms, the mass flow rate becomes

$$\dot{m}_{free} = -N_t \frac{4}{3} \frac{\sqrt{2\bar{O}}}{\sqrt{RT}} \frac{r_t^3}{L} \sqrt{\bar{O}} \ddot{a}P \quad (23)$$

As before, the author wants a mass flux (flow rate per unit area). This is

$$\left(\frac{\dot{m}}{\text{area}} \right)_{\text{free}} = - \frac{N_t}{hw} \frac{4}{3} \frac{\sqrt{2\delta}}{\sqrt{RT}} \frac{r_i^3}{L} \sqrt{\hat{\Omega}} \Delta P \quad (24)$$

As was true for the mass flux for the laminar, viscous flow and diffusion, the area hw will drop out of the mass flux because N_t is proportional to hw .

The author wants to reduce the free molecular flow mass flux equation by substituting for N_t and r_i to see what the result looks like. The result is

$$\left(\frac{\dot{m}}{\text{area}} \right)_{\text{free}} = - \frac{16}{3} \sqrt{\frac{k_0 n_0 \hat{\Omega}}{\delta RT}} \frac{\Delta P}{L} \quad (25)$$

As a footnote to this derivation, the author would like to mention the model of Satterfield and Sherwood.⁴ On pp. 16 and 17 of their book, they propose a model for "Knudsen diffusion," the term they use for what the author is calling "free molecular flow." Their model was developed for flow through catalyst beds, which are usually beds of particles of fairly uniform sizes and shapes. They postulate that the flow is through circular pores of constant diameter. The (average) pore size is calculated from the porosity, the density of the porous bed, and the ratio of surface area to mass. In order to account for the fact that the pores are not straight, nor are they of constant cross-sectional area or shape, the flow coefficient for the collection of pores is divided by a geometry factor $\hat{\Omega}$. The author has demonstrated that, if one calculates the surface area and porous material density from the porosity and the solid density (i.e., the density of the solid material making up the porous bed), the solid density cancels out and the mass flux from the model of Satterfield and Sherwood is identical to the author's mass flux for free molecular flow except that $\hat{\Omega}=1/\hat{\Omega}$. It should come as no surprise that the author's model and that of Satterfield and Sherwood give the same results except for the proportionality factor, because both are based on flow through an array of straight, round pores. Satterfield and Sherwood show values of $\hat{\Omega}$ derived from reductions of data on catalysts that range from 0.3 to 10. They comment that the wide variation in empirical values of $\hat{\Omega}$ is most likely due to the inability of the simple expression for average pore size to accurately describe the geometry. They point out that, in particular, when there is a large variation in true pore size, most of the flow is through the larger pores, whereas most of the surface area is due to the smaller pores.

3. EFFECTS OF COMPRESSION OF THE FOAM

As was stated in the introduction, a second major objective of this theory is to determine what happens to flow rates when the foam is compressed in the direction perpendicular to the flow. In other words, when the thin foam sheet becomes even thinner. The model for changing the flow parameters due to compression is particularly simple. The round tubes are flattened to ovals. The flow area changes while the perimeter, and therefore the surface area of the inside of the tube, remains the same. As a first-order approximation, the length of the tubes is left at $L/\sqrt{\hat{O}}$ with the tortuosity factor $\hat{O}$ unchanged.

3.1 LAMINAR, VISCOUS FLOW

For viscous flow, the flow rate through the tubes is governed by the usual transformations for noncircular tubes. This means the friction factor uses the hydraulic radius. Consider the flattened tube of length Δs and hydraulic radius r_h . From basic hydrodynamics (the Darcy formula for pressure drop with constant friction factor, the definition of hydraulic radius, and the friction factor for laminar viscous flow, should all be found in any decent reference on fluid dynamics)⁵ the pressure drop is as follows:

$$-\Delta P = \frac{1}{2} \tilde{n} v^2 f \frac{\Delta s}{2 r_h} \quad (26)$$

where f is the friction factor and v is the mass averaged velocity in the tube. The definition of the hydraulic radius is

$$r_h \equiv \frac{2A}{B} \quad (27)$$

where, as before, A is the flow area and B is the wetted perimeter of the tube. The laminar friction factor is as follows:

$$f = 64 \frac{\mu}{\tilde{n} v 2 r_h} \quad (28)$$

Substituting for the friction factor in the equation for pressure drop [Eq. (26)] and canceling terms leaves

$$-\Delta P = v \frac{8\mu \Delta s}{r_h^2} \quad (29)$$

Solving this equation for the velocity v and substituting into the definition of the mass flow rate (from the definition of hydraulic radius, the flow area equals half the hydraulic radius times the perimeter) gives the following form for the mass flow through a bundle of flattened tubes:

$$\begin{aligned}
\dot{m}_{\text{viscous flattened tube}} &= \tilde{n} v A = - \frac{P}{RT} \ddot{a} P \frac{r_h^2}{8\mu L} \sqrt{\overline{O}} N_t \frac{r_h}{2} B \\
&= - \frac{\ddot{a} P^2}{2RT} \frac{r_h^3 B}{16\mu L} \sqrt{\overline{O}} N_t
\end{aligned} \tag{30}$$

The perimeter of each individual tube is unchanged at $B=2\delta r_t$. Therefore,

$$\dot{m}_{\text{viscous flattened tube}} = - \frac{\ddot{a} P^2}{2RT} \frac{r_h^3 \delta r_t}{8\mu L} \sqrt{\overline{O}} N_t \tag{31}$$

As a check of the algebra, assume one has a circular tube such that $r_t=r_h$. Then the mass flow rate reduces to the following:

$$\dot{m} = - \frac{dP^2}{2RT} \frac{r_t^3 2\delta r_t}{16\mu L} \sqrt{\overline{O}} N_t = - \frac{dP^2}{2RT} \frac{\delta r_t^4}{8\mu L} \sqrt{\overline{O}} N_t \tag{32}$$

This is the same as Eq. (5), which gives mass flow rate in a bundle of round tubes.

The author has derived an expression for the mass flow rate for the bundle of ovals. Now, he needs to determine the mass flow rate as a function of the properties of the foam. Suppose the foam is compressed to a new porosity n_j . As has already been noted, the wetted perimeter B for each tube is unchanged and it is assumed that the length of the tubes is unchanged. Therefore, the flow area is directly proportional to the void volume. The author must now calculate the change in void volume. When the foam is compressed, the solid volume (i.e., the volume of the polymer in the foam) is unchanged. Therefore,

$$V_s = (1 - n_0) V_0 = (1 - n_1) V_1 \tag{33}$$

where V_s is the solid volume, V_0 is the initial volume of the foam (i.e., hwL) and V_1 is the volume after compression. For the foam before and after compression, the volume is the sum of the solid and void volumes. The void volumes are the total volumes times the porosities. Therefore, the void volume after compression may be expressed by either of the following:

$$V_{\text{void1}} = V_1 - V_s = V_1 - (1 - n_0) V_0 \tag{34}$$

and

$$V_{\text{void1}} = n_1 V_1 \tag{35}$$

Setting the two expressions equal leads to the following expression for V_1 :

$$V_1 = V_0 \frac{1-n_0}{1-n_1} \quad (36)$$

Multiplying both sides by n_1 to get void volume after compression gives

$$V_{\text{void}1} = V_0 n_1 \frac{1-n_0}{1-n_1} \quad (37)$$

The author has already noted that the assumptions made so far require that the flow area be proportional to the void volume. Therefore, the flow area becomes

$$A_1 = A_0 \frac{V_{\text{void}1}}{V_{\text{void}0}} = A_0 V_0 n_1 \frac{1-n_0}{1-n_1} \frac{1}{n_0 V_0} = A_0 \frac{n_1}{n_0} \frac{1-n_0}{1-n_1} \quad (38)$$

From Eqs. (27) and (38) (noting that $A_0 = \delta r_t^2$), the author gets the following relationship for the hydraulic radius after compression:

$$r_h = \frac{2A_1}{B} = 2 \frac{\delta r_t^2}{2 \delta r_t} \frac{n_1}{n_0} \frac{1-n_0}{1-n_1} = \frac{n_1}{n_0} \frac{1-n_0}{1-n_1} r_t \quad (39)$$

Therefore, the mass flow rate for laminar, viscous flow after compression is as follows:

$$\begin{aligned} \dot{m}_{\text{viscous } n=n_1} &= -\frac{\ddot{a} P^2}{2RT} \frac{2 \delta r_t^4}{16\mu L} \sqrt{\overline{O}} N_t \left[\frac{n_1}{n_0} \frac{1-n_0}{1-n_1} \right]^4 \\ &= -\frac{\ddot{a} P^2}{2RT} \frac{\delta r_t^4}{8\mu L} \sqrt{\overline{O}} N_t \left[\frac{n_1}{n_0} \frac{1-n_0}{1-n_1} \right]^4 \end{aligned} \quad (40)$$

The reader may remember that the terms r_t and N_t are both functions of the porosity and permeability of the uncompressed material.

As before, the author wants a mass flux. This time, things will be a bit more complex. The area he wants is that of the compressed foam. The area on which N_t is based is that of the uncompressed foam. Because w and L are unchanged, the ratio of areas before and after compression is the same as the ratio of volumes before and after compression. Therefore,

$$\text{area}_1 = \text{area}_0 \frac{V_1}{V_0} = hw \frac{1-n_0}{1-n_1} \quad (41)$$

The expression for mass flux becomes

$$\left. \frac{\dot{m}}{area} \right)_{viscous n=n_1} = - \frac{\ddot{a} P^2}{2RT} \frac{\delta r_t^4}{8\mu L} \sqrt{\mathcal{O}} N_t \left[\frac{n_1}{n_0} \frac{1-n_0}{1-n_1} \right]^4 \left[\frac{1-n_0}{1-n_1} \right] \quad (42)$$

or

$$\left. \frac{\dot{m}}{area} \right)_{viscous n=n_1} = - \frac{\ddot{a} P^2}{2RT} \frac{\delta r_t^4}{8\mu L} \sqrt{\mathcal{O}} \frac{N_t}{hw} \left[\frac{n_1}{n_0} \right]^4 \left[\frac{1-n_0}{1-n_1} \right]^3 \quad (43)$$

For convenience, the author wants to calculate an effective permeability for compressed material called k_l . This factor makes the compressed viscous mass flux equal to a porous medium flux with $k=k_l$, i.e.,

$$\left. \frac{\dot{m}}{area} \right)_{k=k_1} = - \frac{k_1}{\mu} \frac{1}{2RT} \frac{\ddot{a} P^2}{\ddot{a} x} \quad (44)$$

Substituting the expressions for r_t and N_t into the equation for viscous compressed flux [Eq. (43)], the flux is

$$\left. \frac{\dot{m}}{area} \right)_{viscous n=n_1} = - \frac{\ddot{a} P^2}{2RT} \frac{k_0}{\mu L} \left[\frac{n_1}{n_0} \right]^4 \left[\frac{1-n_0}{1-n_1} \right]^3 \quad (45)$$

Equating the two different expressions for viscous mass flux and canceling terms, the result for k_l is

$$k_1 = k_0 \left[\frac{n_1}{n_0} \right]^4 \left[\frac{1-n_0}{1-n_1} \right]^3 \quad (46)$$

3.2 DIFFUSION

As before, the diffusive mass flow is the flow area times the density gradient times the diffusivity. Using the changed flow area for compressed foam, the mass flow becomes

$$\dot{m}_{diffusion n=n_1} = - N_t \delta r_t^2 \frac{n_1}{n_0} \frac{1-n_0}{1-n_1} \frac{D_i}{R_i T} \frac{\ddot{a} P_i}{L} \sqrt{\mathcal{O}} \quad (47)$$

The author wants to calculate a mass flux. As before, he used the ratio of flow areas [Eq. (41)] to get the following:

$$\left. \frac{\dot{m}}{area} \right)_{diffusion n=n_1} = -N_t \delta r_t^2 \frac{n_1}{n_0} \frac{1-n_0}{1-n_1} \frac{D_i}{R_i T} \frac{\ddot{a}P_i}{L} \sqrt{\hat{\mathbf{O}}} / \left[h w \frac{1-n_0}{1-n_1} \right] \quad (48)$$

or with further cancellation and reduction

$$\left. \frac{\dot{m}}{area} \right)_{diffusion n=n_1} = -\frac{N_t}{h w} \delta r_t^2 \frac{n_1}{n_0} \frac{D_i}{R_i T} \frac{\ddot{a}P_i}{L} \sqrt{\hat{\mathbf{O}}} \quad (49)$$

If he substitutes for N_t and r_t and simplifies, the result is

$$\left. \frac{\dot{m}}{area} \right)_{diffusion n=n_1} = -n_1 \frac{D_i}{R_i T} \frac{\ddot{a}P_i}{L} \hat{\mathbf{O}} \quad (50)$$

From this, the effective diffusivity is

$$D_{eff n=n_1} = n_1 D_i \hat{\mathbf{O}} \quad (51)$$

which can be compared to Eq. (15). As one can see, this simple model says that the effective diffusivity is the molecular diffusivity times the porosity times the tortuosity (remember that $\hat{\mathbf{O}} \leq 1$) for any porosity. If, as the author is assuming, $\hat{\mathbf{O}}$ is unchanged by compression, then the fractional change in effective diffusivity is the same as the fractional change in porosity.

3.3 FREE MOLECULAR FLOW

The equation for conductance of a long tube in free molecular flow already has the tube area and perimeter [see Eq. (18) or (21)]. If the author substitutes the expression for the flow area in compressed foam [Eq. (38)] into the equation for mass flow for a tube of arbitrary shape [Eq. (21)], he gets the following:

$$\dot{m}_{free n=n_1} = -N_t \frac{8}{3\sqrt{\delta}} \sqrt{\frac{2}{RT}} \frac{\ddot{a}P}{L} \sqrt{\hat{\mathbf{O}}} \delta^2 r_t^4 \left[\frac{n_1}{n_0} \frac{1-n_0}{1-n_1} \right]^2 \frac{1}{2\delta r_t} \quad (52)$$

Further cancellation of terms and reduction leads to

$$\dot{m}_{free n=n_1} = -N_t \frac{4}{3} \sqrt{\frac{2\delta}{RT}} \frac{r_t^3}{L} \sqrt{\hat{\mathbf{O}}} \ddot{a}P \left[\frac{n_1}{n_0} \frac{1-n_0}{1-n_1} \right]^2 \quad (53)$$

As before, the author wants a mass flux. Dividing for the true area, he gets

$$\left. \frac{\dot{m}}{area} \right)_{free=n_1} = -N_t \frac{4}{3} \sqrt{\frac{2\delta}{RT}} \frac{r_t^3}{L} \sqrt{\tilde{O}} \ddot{a}P \left[\frac{n_1}{n_0} \frac{1-n_0}{1-n_1} \right]^2 \left[h w \frac{1-n_0}{1-n_1} \right] \quad (54)$$

Further cancellation leads to

$$\left. \frac{\dot{m}}{area} \right)_{free=n_1} = -\frac{N_t}{h w} \frac{4}{3} \sqrt{\frac{2\delta}{RT}} \frac{r_t^3}{L} \sqrt{\tilde{O}} \ddot{a}P \left[\frac{n_1}{n_0} \right]^2 \frac{1-n_0}{1-n_1} \quad (55)$$

As before, the author wants to reduce the compressed free molecular flow mass flux equation by substituting for N_t and r_t to see what a mass flux based on material and gas properties looks like. The result is

$$\left. \frac{\dot{m}}{area} \right)_{free=n_1} = -\frac{16}{3} \sqrt{\frac{k_0 n_0 \tilde{O}}{\delta RT}} \frac{\ddot{a}P}{L} \left[\frac{n_1}{n_0} \right]^2 \frac{1-n_0}{1-n_1} \quad (56)$$

In an earlier section, the author derived Eq. (46), which gives an effective compressed material permeability k_l . This factor makes the compressed viscous mass flux equal to a porous medium flux with $k=k_l$. The author now wishes to find an effective free molecular permeability $k_{l\,free}$. He defines $k_{l\,free}$ as the factor such that the free molecular mass flux for a material with $k=k_{l\,free}$ and $n=n_1$ is as follows:

$$\left. \frac{\dot{m}}{area} \right)_{free=n_1} = -\frac{16}{3} \sqrt{\frac{k_{l\,free} n_1 \tilde{O}}{\delta RT}} \frac{\ddot{a}P}{L} \quad (57)$$

The analogy between Eq. (25) for uncompressed material and Eq. (57) for compressed material should be obvious. Setting this expression equal to that for mass flux for compressed free molecular flow [Eq. (56)] and solving for $k_{l\,free}$, the result is

$$k_{l\,free} = k_0 \left[\frac{n_1}{n_0} \right]^3 \left[\frac{1-n_0}{1-n_1} \right]^2 \quad (58)$$

If one compares this to Eq. (46), the expression for the effective compressed material permeability for laminar, viscous porous medium flow k_l , it is obvious that the expressions are different. The powers for both the ratio of porosity and the ratio of 1-porosity are different. The laminar, viscous mass flux responds to changes in compression more strongly than the mass flux in free molecular flow. Therefore, the laminar, viscous effective permeability responds to changes in compression more strongly than the effective permeability in free molecular flow.

4. COMBINING CONTINUUM AND FREE MOLECULAR FLOWS

In the project for which this work is being done, the permeability measurements will almost all be done with compressed foam. The author wants to be able to infer the material properties for the uncompressed foam from these measurements. A complication is that it may not be clear whether a measurement is being done in the viscous regime, free molecular flow, or some combination of the two. The author needs to determine the characteristics of the flow in the combined regime.

A rather simple approach to calculating flow when one is dealing with a combination of viscous and free molecular flow (or when one does not have a good idea which region one is in) is to combine the mass flow rates from viscous and free molecular flow (this approach, although rather simplified, is common in the literature as shown by Brunner and Batzer).⁶ The combined mass flux can be found from the equation for viscous flow in a compressed foam, Eq. (45), plus that for free molecular flow, Eq. (56), and is as follows:

$$\left(\frac{\dot{m}}{area} \right)_{viscous + free n=n_1} = - \frac{\ddot{a}P^2}{2RT} \frac{k_0}{\mu L} \left[\frac{n_1}{n_0} \right]^4 \left[\frac{1-n_0}{1-n_1} \right]^3 - \frac{16}{3} \sqrt{\frac{k_0 n_0}{\delta RT}} \frac{\sqrt{\Theta}}{L} \left[\frac{n_1}{n_0} \right]^2 \frac{1-n_0}{1-n_1} \quad (59)$$

There is a variation of this form the author prefers that comes about from making the substitution $\ddot{a}P^2 = 2P\ddot{a}P$ into the portion for the viscous mass flux. The reason for doing this is that the entire equation then becomes proportional to $\ddot{a}P/L$ and the behavior of the viscous portion with changes in pressure becomes obvious. This alternate form is

$$\left(\frac{\dot{m}}{area} \right)_{viscous + free n=n_1} = - \frac{\ddot{a}P}{L} \left\{ \frac{P}{RT} \frac{k_0}{\mu} \left[\frac{n_1}{n_0} \right]^4 \left[\frac{1-n_0}{1-n_1} \right]^3 + \frac{16}{3} \sqrt{\frac{k_0 n_0}{\delta RT}} \sqrt{\Theta} \left[\frac{n_1}{n_0} \right]^2 \frac{1-n_0}{1-n_1} \right\} \quad (60)$$

As one can see from study of this equation, as pressure becomes small, the viscous portion of the mass flux becomes small and eventually the flow is all in the free molecular regime. On the other hand, for pressure large enough, the viscous term will dominate and the flow will almost all be contributed by the viscous flux.

The author would like to mention another source that uses the concept of a simple combination of the laminar, viscous flux with that from free molecular flow. Hoglund, Shacter, and von Halle⁷ go through a derivation of the free molecular flow through a tube that is the same as the author's. They then comment that there should be an additional contribution from viscous flow and account for the geometric effects by having separate correction factors for each term. The form from Hoglund, Shacter, and von Halle (Eq. 47) is as follows:

$$N = \frac{a}{\sqrt{M}} \ddot{a}P + \frac{b}{\mu} \ddot{a}P^2 \quad (61)$$

where N is the molar flux of gas and a and b are constants that account for geometric factors. Clearly the first term is the free molecular flow while the second is the viscous contribution. If the terms are divided in the equation for mass flux [Eq. (60)] by molecular weight (to convert to molar flux), expressions for a and b can be derived. Hoglund, Shacter, and von Halle comment that it should be possible to determine the magnitudes of the geometric factors by making measurements at different pressures. If this same idea is followed and enough measurements obtained, then one should also be able to estimate the geometric factors for viscous and free molecular flow. A caveat is that the measurements will need to be done with pressures both low enough to be fully in free molecular flow and high enough to be fully in the continuum.

5. INFERRING PERMEABILITY FROM COMPRESSED FOAM EXPERIMENTS

Presumably all the parameters in Eq. (60) are known except the uncompressed permeability k_0 (provided that one has an estimate of $\hat{\mathbf{O}}$). Then, Eq. (60) is a quadratic equation that can be used to infer k_0 . As an alternative, if one does not have an estimate of $\hat{\mathbf{O}}$, one can use the combination of a measurement made at a pressure high enough to be in the continuum range and another at a pressure low enough to be in the free molecular range to infer values of k_0 and the product $k_0\hat{\mathbf{O}}$. If one has a series of measurements ranging from the continuum regime through the free molecular regime, one may be lucky enough to find that a single value of k_0 and a single value of the product $k_0\hat{\mathbf{O}}$ will match the data. If the measurements are only in the continuum regime, then one can not infer a value of $\hat{\mathbf{O}}$. On the other hand, if the measurements are only in the free molecular regime, then one can not separate k_0 from the product $k_0\hat{\mathbf{O}}$.

6. CONCLUSIONS

At least in principle, the author has developed a method for calculating mass flows and fluxes in a foam for laminar, viscous flow, diffusion, and free molecular flow. The model allows for extrapolation of permeability measurements made in the continuum range to flows in the free molecular range and vice versa. The model allows for changes in the flow characteristics with changes in the level of compression in the foam. Thus, the author has achieved the objectives specified in the introduction. By adopting the principle of combining the viscous and free molecular mass fluxes, he has gone a step further and developed an expression for flow at pressures where both mechanisms are important.

Among many objections the reader may have to this model, one in particular is that a bundle of tubes of constant cross section seems a poor representation of a lattice composed of linked spherical pores. The hope for this model is that the geometry factors will tend to operate in the same fashion for all three flow regimes, that is, that the additional flow resistance (or more exactly the fractional increase in flow resistance) due to the actual geometry will tend to be of the same magnitude for all three regimes. As already noted, in principle one should be able to infer the permeability and the tortuosity from suitable measurements and thereby be able to calculate the viscous and free molecular flows. As for diffusion, the simple approximation that was rederived [see Eq. (51)] and that exists in Bear¹ is that the effective diffusivity is the gas diffusivity times the product of the porosity and the tortuosity (the latter two terms represent the effect of the porous medium). That result is common enough in the literature so that hopefully the simplified diffusion model will be sufficient.

On pp. 179-180, Bear¹ discusses results from a model by Blick (1966). Blick simulates the porous medium as a bundle of tubes with orifices located at spacings of approximately one tube diameter. This is a somewhat more plausible model for the array of spherical pores than a bundle of tubes of uniform diameter. To use Blick's model, some guesses about the ratio of the diameters of the orifices to the diameter of the tube would have to be made to model the drag of the orifices. At the moment, the author does not see that there would be any benefit in using that model.

REFERENCES

1. Jacob Bear, *Dynamics of Fluids in Porous Media*, Dover Publications, Inc., New York, 1972.
2. R. B. Bird, W. E. Stewart, and J. N. Lightfoot, *Transport Phenomena*, John Wiley and Sons, New York, 1960.
3. A. Roth, *Vacuum Technology*, North-Holland, New York, 1976.
4. C. N. Satterfield, and T. K. Sherwood, *The Role of Diffusion in Catalysis*, Addison-Wesley, New York, 1963.
5. R. V. Giles, *Schaum's Outline Series Theory and Problems of Fluid Mechanics and Hydraulics*, 2nd edition, McGraw-Hill, New York, 1962.
6. W. F. Brunner, jr., and T. H. Batzer, *Practical Vacuum Techniques*, Reinhold Publishing Corp., New York, 1965.
7. R. L. Hoglund, J. Shacter, and E. von Halle, "Diffusion Separation Methods," in Kirk-Othmer: *Encyclopedia of Chemical Technology*, Vol. 7, 3rd Ed., John Wiley and Sons, 1979.

APPENDIX A: INFERRING MATERIAL PERMEABILITY OR EFFECTIVE DIFFUSIVITY FROM CHEMICAL PERMEABILITY

In the chemical literature, measured permeabilities are given in units of $\text{cc}_{\text{stp}}\text{-cm/s-cm}^2\text{-cm Hg}$. The author refers to the permeability in those units as "chemical permeability" and gives it the symbol $\tilde{A}$ following the example of J. H. Leckey in one of his reports. The chemical permeability is not just a property of the porous material (and its compression), but also includes properties of the gas as well as experimental conditions such as pressure and temperature. In this appendix (Appendix A), the author will go through the exercise of inferring the material permeability from the measured chemical permeability and the properties of the gas.

The first thing the author wants to do is a units conversion. He will convert $\tilde{A}$ in its customary units ($\text{cc}_{\text{stp}}\text{-cm/s-cm}^2\text{-cm Hg}$) to an SI equivalent $\tilde{A}_{\text{SI}}$ whose units are $\text{kg-m/s-m}^2\text{-Pa}$. The units conversion is as follows:

$$\begin{aligned}\tilde{A}_{\text{SI}} (\text{kg-m/s-m}^2\text{-Pa}) &= \tilde{A} (\text{cc}_{\text{stp}}\text{-cm/s-cm}^2\text{-cm Hg}) \times 10^{-6} (\text{m}^3_{\text{STP}}/\text{cc}_{\text{stp}}) \times 10^{-2} (\text{m/cm}) / [10^{-4} (\text{m}^2/\text{cm}^2) \\ &\quad \times 76.0 (\text{cm Hg/atm}) / [1.01325 \times 10^5 (\text{Pa/atm})] / [2.2414 \times 10^{-2} (\text{m}^3_{\text{STP}}/\text{mol})] \\ &\quad \times M (\text{kg/mol}) \\ &= \tilde{A} (\text{cc}_{\text{stp}}\text{-cm/s-cm}^2\text{-cm Hg}) M (\text{kg/mol}) \\ &\quad \times 3.346 \times 10^{-6} (\text{mol-m/s-m}^2\text{-Pa})/(\text{cc}_{\text{stp}}\text{-cm/s-cm}^2\text{-cm Hg})\end{aligned}$$

Now the author will work out how to infer the material permeability k from $\tilde{A}$. The definition of $\tilde{A}$ comes from the following mass balance:

$$\frac{\dot{m}}{A} = -\tilde{A} \frac{\ddot{a}P}{L} \quad (\text{A.1})$$

where all the terms have consistent units. If all the other terms have SI units (i.e., mass in kg, pressure in Pa, and length in m), then $\tilde{A}$ is replaced by $\tilde{A}_{\text{SI}}$ (note that the units of $\tilde{A}_{\text{SI}}$ are seconds). First, the permeability for laminar, viscous (continuum) flow needs to be worked out. The mass flux for the porous medium is Eq. (6) slightly rearranged and is as follows:

$$\left(\frac{\dot{m}}{A} \right)_{\text{Darcy}} = \frac{k}{\mu} \frac{\bar{P}}{RT} \frac{\ddot{a}P}{L} \quad (\text{A.2})$$

Material permeability is given the symbol k and the author neglects to specify whether the value is for the compressed or uncompressed material. If the two mass fluxes are equated, one arrives at the following:

$$\tilde{A}_{\text{SI}} \frac{\ddot{a}P}{L} = \tilde{A} M \times 3.346 \times 10^{-6} \frac{\ddot{a}P}{L} = \frac{k}{\mu} \frac{\bar{P}}{RT} \frac{\ddot{a}P}{L} \quad (\text{A.3})$$

Canceling terms and substituting for the gas constant (i.e., universal gas constant = 8.3143 J/mol divided by molecular weight in kg/mol), the following equivalent between chemical permeability and material permeability (k has units of m^2) assuming continuum flow is found:

$$k = \tilde{A}\mu \frac{T}{\bar{P}} \times 2.782 \times 10^{-5} \quad (\text{A.4})$$

For this equation to be valid, the pressure in the permeability experiment must be high enough that the flow through the pores of the porous material is in the continuum regime. Remember that $\tilde{A}$ has its customary units ($\text{cc}_{\text{stp}}\text{-cm/s-cm}^2\text{-cm Hg}$) and all the other terms in the above equation have SI units. Note that, in this appendix, the absolute temperature T does not always appear as part of the product RT . Therefore, the reader must be careful to distinguish between the temperature (whose symbol is the italic upper case " T ") and the tortuosity (whose symbol is a block upper case " τ ", $\hat{\mathbf{O}}$).

Next, the permeability for free molecular flow is worked out. The mass flux for free molecular flow is Eq. (25) with the subscript "0" dropped from k_0 and n_0 . If the two mass fluxes are equated the following is arrived at:

$$\tilde{A}M \times 3.346 \times 10^{-6} \frac{\ddot{a}P}{L} = \frac{16}{3} \sqrt{\frac{k_{\text{free}} n \hat{\mathbf{O}}}{\delta RT}} \frac{\ddot{a}P}{L} \quad (\text{A.5})$$

Canceling terms, and substituting as before, the following equivalent between chemical permeability and material permeability assuming free molecular flow is gotten:

$$k_{\text{free}} = \tilde{A}^2 \frac{TM}{n \hat{\mathbf{O}}} \times 1.0283 \times 10^{-11} \quad (\text{A.6})$$

For this equation to be valid, the pressure in the permeability experiment must be low enough that the flow through the pores of the porous material is in the free molecular regime. The reader should remember that, if the theory presented in the present report is correct, then the value of k measured in either the continuum regime or that of free molecular flow should be the same.

Last, the effective diffusivity for diffusion is worked out. The mass flux for diffusion is Eq. (17). If the two mass fluxes are equated, then:

$$\tilde{A}M_i \times 3.346 \times 10^{-6} \frac{\ddot{a}P}{L} = D_{\text{eff}} \frac{1}{R_i T} \frac{\ddot{a}P}{L} \quad (\text{A.7})$$

where M_i is the molecular weight of the trace gas "i." Canceling terms, and substituting as before, the following equivalent between chemical permeability and effective diffusivity assuming diffusion driven flow is gotten:

$$D_{\text{eff}} = \tilde{A}T \times 2.782 \times 10^{-5} \quad (\text{A.8})$$

Note that, although the author expects k and k_{free} to be (more or less) material properties (with corrections as necessary for compression) and therefore to be approximately the same for most gases and temperatures, he does not expect such an invariance for D_{eff} . Instead, he would expect D_{eff} to be dependent on the gases involved

and on the temperature as well, of course, as on the porous material and its compression. The author might expect, however, that the ratio of D_{eff} to the diffusivity of the trace gas in the stagnant carrier to be a property of the material and the degree of compression.

APPENDIX B: SOME CLOSED-FORM SOLUTIONS FOR FLOW IN A POROUS MEDIUM

For permeability measurements, it can be convenient to have experiments under conditions for which a closed-form solution is known. In this appendix, a number of such solutions are presented.

B. 1 CLOSED FORM SOLUTIONS FOR LAMINAR, VISCOUS (DARCY) FLOW

B. 1. 1 Laminar, Viscous (Darcy) Flow on a Hemishell

One potential configuration for a permeability experiment is a hemispherical sheet of porous material between two concentric solid hemispherical pieces of slightly different radii (the difference in radii becomes the compressed thickness of the porous sheet). The author will now outline a solution for the laminar, viscous compressible Darcy flow in a hemishell.

According to *Transport Phenomena* by Bird, Stewart, and Lightfoot (ref. 3), p. 150, the velocity equation for compressible Darcy flow is as follows:

$$v = -\frac{k}{\mu} \frac{dP}{dx} \quad (\text{B.1})$$

where v is the velocity, P is the pressure, and x is a direction measured parallel to the flow. The author defines $\tilde{E}$ as the angle measured from the pole. The equation for the mass flow becomes

$$\tilde{n} v = \frac{\dot{m}}{\text{area}} = -\tilde{n} \frac{k}{\mu} \frac{dP}{dx} \quad (\text{B.2})$$

The author assumes cylindrical symmetry. He also assumes that boundary layer effects in the gap are small compared to the resistance caused by the foam and that therefore the flow field can be accurately enough approximated as uniform across the gap. With these assumptions, the problem becomes one-dimensional with the independent variable being the angle $\tilde{E}$ or the distance x , the two being equivalent. The ideal gas equation of state for an isothermal system is

$$\frac{P}{\tilde{n}} = RT \quad (\text{B.3})$$

The equation for the flow area as a function of angle is

$$A = 2\tilde{\delta} r h \sin \tilde{E} \quad (\text{B.4})$$

where r is the inner radius of the hemishell and h is the height of the gap measured radially from the center (therefore the outer radius is $r+h$). The expression for area is an approximation assuming $r \gg h$. The steady state continuity condition is that the mass flow rate is constant at all angles. Therefore, the steady state

equation for the pressure field is

$$\dot{m} = -\frac{k}{\mu} \frac{1}{RT} P \frac{dP}{dx} 2\delta r h \sin \tilde{E} \quad (\text{B.5})$$

The distance for the differential x is

$$x = r \tilde{E} \quad (\text{B.6})$$

Therefore, the differential equation is

$$\dot{m} = -\frac{k}{\mu} \frac{1}{RT} \frac{P}{r} \frac{dP}{d\tilde{E}} 2\delta r h \sin \tilde{E} \quad (\text{B.7})$$

After canceling the r , rearranging terms, and solving the differential equation, the author gets

$$\frac{1}{2} P^2 = -\frac{\dot{m} \mu RT}{2\delta k h} \ln\left[\tan \frac{\tilde{E}}{2}\right] + C \quad (\text{B.8})$$

where C is an integration constant. The boundary condition is that pressure is P_b at the outer boundary $\tilde{E}_b$. This may or may not be at the equator ($\tilde{E} = \delta/2$). Evaluating the boundary condition gets

$$P_b^2 = -\frac{\dot{m} \mu RT}{2\delta k h} \ln\left[\tan \frac{\tilde{E}_b}{2}\right] + C \quad (\text{B.9})$$

and therefore,

$$P^2 = P_b^2 - \frac{\dot{m} \mu RT}{\delta k h} \left\{ \ln\left[\tan \frac{\tilde{E}}{2}\right] - \ln\left[\tan \frac{\tilde{E}_b}{2}\right] \right\} \quad (\text{B.10})$$

The equation for velocity comes from a solution to Eq. B. (1). The answer is

$$v = \frac{1}{r} \frac{1}{P} \frac{\dot{m} RT}{2\delta h} \frac{1}{2} \frac{1}{\sin \tilde{E}} \quad (\text{B.11})$$

One may note that the pressure and therefore also the velocity are singular at $\tilde{E} = 0$ because the log of $\tan(0)$ is infinite.

If the author has a pressure P_{pole} measured at the pole and lets the half angle of the area subtended by the pressure tap be $\tilde{E}_{pole}$, then the relationship between the mass flow rate, the material and gas parameters, and the permeability is

$$P_{pole}^2 = P_b^2 - \frac{\dot{m} \mu R T}{\delta k h} \left\{ \ln \left[\tan \frac{\dot{E}_{pole}}{2} \right] - \ln \left[\tan \frac{\dot{E}_b}{2} \right] \right\} \quad (\text{B.12})$$

Given pressures at the pole and exits and also material and gas parameters, one can solve Eq. B.(12) for the mass rate. Alternatively, if one has all the information except the permeability, one may solve Eq. B.(12) for the permeability. As was noted earlier, this form does not work for $\dot{E}_{pole} = 0$ because the log of the tangent is singular at a zero angle.

B. 1. 2 Laminar, Viscous (Darcy) Flow on a Disk

Another simple configuration for permeability measurements is a flat disk of porous material between two solid flat disks. Now the author will solve for the steady state laminar, viscous compressible Darcy flow for a disk.

The equations for velocity, mass flux, and state for compressible Darcy flow for an ideal gas are B.(1), B.(2), and B.(3). For a disk, the flow area is a function of radius x (which is also the direction of flow) and is

$$A = 2\delta x h \quad (\text{B.13})$$

Combining Eqs. B.(1), B.(2), and B.(13), the resulting mass flow equation is as follows:

$$\dot{m} (= \text{constant}) = -\tilde{n} \frac{k}{\mu} \frac{dP}{dx} 2\delta x h \quad (\text{B.14})$$

Applying the ideal gas equation of state, the mass flow equation becomes

$$\dot{m} = -\frac{P}{RT} \frac{k}{\mu} \frac{dP}{dx} 2\delta x h \quad (\text{B.15})$$

If the author assumes isothermal conditions (i.e., T is not dependent on x), integrates Eq.B.(15) for pressure squared as a function of x , and applies the boundary condition that $P=P_{in}$ at $x=x_{in}$, the result is

$$P^2 = P_{in}^2 - \frac{\dot{m}}{\delta h} R T \frac{\mu}{k} \ln \left(\frac{x}{x_{in}} \right) \quad (\text{B.16})$$

If the author applies the outlet conditions (i.e., $P=P_{out}$ at $x=x_{out}$), he gets the following equation for the total pressure drop as a function of mass rate and other terms:

$$P_{in}^2 - P_{out}^2 = \frac{\dot{m}}{\delta h} RT \frac{\mu}{k} \ln \left(\frac{x_{out}}{x_{in}} \right) \quad (\text{B.17})$$

An alternate form for this equation is

$$\begin{aligned} (P_{in} - P_{out}) 2\bar{P} &= (P_{in} - P_{out})(P_{in} + P_{out}) \\ &= \frac{\dot{m}}{\delta h} RT \frac{\mu}{k} \ln \left(\frac{x_{out}}{x_{in}} \right) \end{aligned} \quad (\text{B.18})$$

Applying the ideal gas equation of state, another form is

$$(P_{in} - P_{out}) 2\bar{n} = \frac{\dot{m}}{\delta h} \frac{\mu}{k} \ln \left(\frac{x_{out}}{x_{in}} \right) \quad (\text{B.19})$$

where $\bar{n}$ is the average of the densities in the inlet and outlet. As before, one may solve Eq. B.(18) for mass rate or for permeability as needed.

B. 2 CLOSED FORM SOLUTIONS FOR FREE MOLECULAR FLOW

B. 2. 1 Free Molecular Flow on a Hemishell

The major difference between free molecular flow and continuum flow in the compressible Darcy equation is that the mass flux is proportional to the pressure gradient, but not to the pressure gradient times the pressure (or alternately to the gradient of pressure squared—the two are mathematically equivalent). For an isothermal system, the equation for the mass flux is as follows:

$$\frac{\dot{m}}{A} = \frac{D_{keff}}{RT} \frac{dP}{dx} \quad (\text{B.20})$$

where D_{keff} is a mass transfer coefficient for free molecular flow with the dimensions of a diffusivity. By comparison with Eq. (57), it is clear that D_{keff} is given by the following:

$$D_{keff} = \frac{16}{3} \sqrt{\frac{k_{1free} n_1 \hat{O} RT}{\delta}} \quad (\text{B.21})$$

where $k_{l\ free}$ is an effective permeability for compressed material in free molecular flow. The relationship between the uncompressed material permeability and the permeability of compressed material in free molecular flow was given in Eq. (58) of the main section of the present report. According to the theory from the main part of the present report, the permeability for compressed material in free molecular flow is the same as that in laminar, viscous compressible Darcy flow.

The flow area and the relationship between the distance x and the angle $\tilde{E}$ are given in Eqs. B.(4) and B.(6), respectively. The differential equation for pressure field becomes

$$\dot{m} = \frac{D_{keff}}{RT} \frac{dP}{r d\tilde{E}} 2\delta r h \sin \tilde{E} \quad (\text{B.22})$$

The solution to this is

$$P = - \frac{\dot{m} RT}{2\delta D_{keff} h} \ln \left[\tan \frac{\tilde{E}}{2} \right] + C \quad (\text{B.23})$$

Applying the boundary pressure condition at the boundary angle as before, the solution becomes

$$P = P_b - \frac{\dot{m} RT}{2\delta D_{keff} h} \left\{ \ln \left[\tan \frac{\tilde{E}}{2} \right] - \ln \left[\tan \frac{\tilde{E}_b}{2} \right] \right\} \quad (\text{B.24})$$

Applying the conditions at the pressure tap at the pole, one gets

$$P_{pole} = P_b - \frac{\dot{m} RT}{2\delta D_{keff} h} \left\{ \ln \left[\tan \frac{\tilde{E}_{pole}}{2} \right] - \ln \left[\tan \frac{\tilde{E}_b}{2} \right] \right\} \quad (\text{B.25})$$

As has been the case for earlier solutions in this appendix, one can use Eq. B.(25) to calculate mass rate or D_{keff} . Using Eq. B.(21), one can calculate $k_{l\ free}$ from D_{keff} .

B. 2. 2 Free Molecular Flow on a Disk

By analogy with the subsections on Darcy flow on a disk and free molecular flow on a hemishell, the author can derive the following differential equation for pressure:

$$\dot{m} = \frac{D_{keff}}{RT} \frac{dP}{dx} 2\delta x h \quad (\text{B.26})$$

Applying the boundary conditions at the inner and outer boundaries of the disk as before, he can derive the following equation for free molecular flow in a disk:

$$\dot{m} \ln \frac{r_{in}}{r_{out}} = \frac{2\delta h}{RT} D_{keff} (P_{in} - P_{out}) \quad (\text{B.27})$$

As has been the case for earlier solutions in this appendix, one can use Eq. B.(27) to calculate mass rate or D_{keff} . Using Eq. B.(21), one can calculate k_{lfree} from D_{keff} .

B. 3 CLOSED FORM SOLUTIONS FOR DIFFUSIVE FLOW

The solutions for diffusion driven flow in a hemishell and a disk are identical to those for free molecular flow except that one must substitute $n_1 D \hat{O}$ for D_{keff} where n_1 is the porosity of the porous material, D is the diffusivity of the trace gas in the stagnant carrier, and $\hat{O}$ is the tortuosity. For completeness, the author will include the final flow equations.

B. 3. 1 Diffusive Flow on a Hemishell

$$P_{pole} = P_b - \frac{\dot{m} RT}{2\delta n_1 D \hat{O} h} \left\{ \ln \left[\tan \frac{\hat{E}_{pole}}{2} \right] - \ln \left[\tan \frac{\hat{E}_b}{2} \right] \right\} \quad (\text{B.28})$$

B. 3. 2 Diffusive Flow on a Disk

$$\dot{m} \ln \frac{r_{in}}{r_{out}} = \frac{2\delta h}{RT} n_1 D \hat{O} (P_{in} - P_{out}) \quad (\text{B.29})$$

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