245c Preferential Permeability of Methanol into Water Using Polysilicone and Polytrimethylsilylpropyne Membranes

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The relative permeability of alcohols, water, and gases find relevance in industrial processing and consumer applications. In the beverage industry, for instance, alcohol and air impermeable containers present opportunities for safe consumer packaging with minimal loss of product or overpressurization. In consumer personal care applications, such as product cleaning or miniature heating apparatus, alcohol or hydrocarbon delivery are crucial features. For medical and biological research, membranes offer the opportunity to control semi-passively the dispensing of alcohols. Where multiple fluids are involved either in the permeate or the feed, preferential permeability is important. For evaluation of the use of membranes and barriers for such applications, fundamental property measurements and interpretation can be used to guide and to drive consideration for present and new applications.

Here, measurements and calculations of permeation of methanol into water permeate have been undertaken. Three membranes were evaluated for delivery of initially pure methanol from a closed, pressure-relieved feed container into liquid water or humid vapor permeate. Feed volume was monitored with time with a final concentration determination per experiment. Commercially available 5-mil polysilicone membrane demonstrated the ability for preferentially permeation of methanol with limited water uptake (7 mol methanol delivered: 1 mol H_2O accepted). Similar preferential permeation at higher flux was obtained with a custom polytrimethylsilylpropyne (PTMSP) with 2 support layers. An analogous custom trilayer version of PDMS demonstrated both the flux and preferential delivery (11 mol methanol delivered : 1 mol H_2O accepted). Calculations are undertaken to investigate if the ratio of methanol delivered to water accepted from permeate exceeded the ratio based on the respective driving forces. This can indicate that the membrane provides preferential methanol delivery. Furthermore, transport calculations are intended to estimate whether the forward flux of methanol inhibits water uptake from permeate to feed. Thus, the result is expected to scale to different membrane thicknesses.

The numerical analysis is implemented using a model of lumped mass transfer coefficients (k). The following differential equations arise for the transport of initially pure methanol (m) in a closed, pressure-relieved feed container and continually replenished pure water (w) permeate through a membrane:

$$d(n_m)/dt = - k_m * A * P_{s,m} * x_m \quad \text{(Equation 1)}$$

$$d(n_w)/dt = k_w * A * P_{s,w} * x_m \quad \text{(Equation 2)}$$

where n = moles in the feed; t = time; area = membrane area; Ps = saturated vapor pressure; x = mole fraction in feed. The following analytical solution results:

$$t = (n0 - n)/A + [B / (A^2)]*\log[(B – A\, n0)/(B – A\, n)] \quad \text{(Equation 3)}$$

$$n_m = n0 [(B – A\, n) / (B – A\, n0)] \quad \text{(Equation 4)}$$

where n0 = initial moles in feed vessel; n = total moles in feed; $A = k_m*area*P_{s,m}$; and $B = n0*k_w*area*P_{s,w}$. An expression for the excess volume of methanol-water mixtures provides the final equation for fitting the mass-transfer coefficients to the volumetric data.