A COMSOL Multiphysics® Study of the Temperature Effect on Chemical Permeation of Air Supply Tubes

R. Kher, C. Gallaschun, D. Crockill, R. Pillai

Department of Chemical Engineering, University of Pittsburgh, Pittsburgh, PA, USA

Introduction: Air hoses are predominantly used in the medical industry to aid in patient oxygen intake. In many situations, the outside of the hose can be contaminated with chemicals, especially if the hose lies on the ground in an environment where chemicals are easily found. An experimental test method was developed by Bromwich and Parikh(1) in which chemical permeation through homogenous hoses could be calculated by sealing a short section of the hose with the chemical and weighing it at different time intervals to show the chemical had permeated the hose wall and evaporated. Testing was performed at 19, 30, 40, 50, 60, and 70° C to represent possible workplace environments. The trials lasted between 25-360 hours and cumulative permeation was calculated in milligrams per meter of hose.

Computational Methods: A 2-D axisymmetric geometry was selected to create the model due to assumed cylindrical symmetry of the PVC pipe. The physics selected in the COMSOL time-dependent study included heat transfer in fluids and chemical species transport. Parameters that were required to be input into COMSOL (MEK and PVC)are listed in Table 1**:**

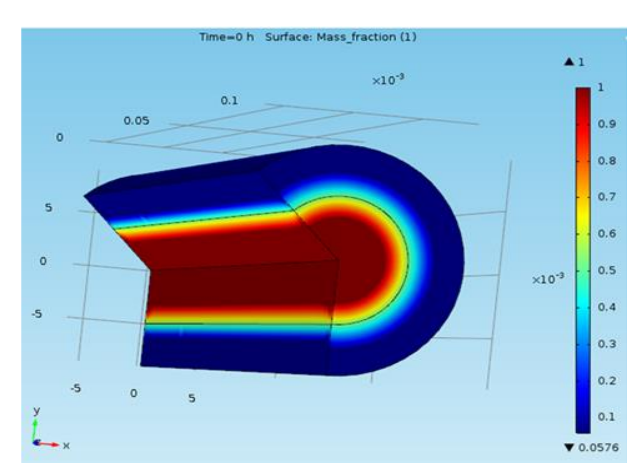
Property	Name	Value	Unit
Thermal Conductivity	k	0.000358	cal / (cm.s.ºC)
Density	rho	0.8037	g/cm^3
Heat Capacity at constant pressure	Cp	0.549	cal/(g. ºC)
Ratio of Specific Heats	gamma	1	1

Property	Name	Value	Unit
Thermal Conductivity	k	1.1	(BTU.in) / (h.ft^2. ºF)
Density	rho	1.4	g/cm^3
Heat Capacity at Constant Pressure	Cp	0.25	BTU / (lb.ºF)
Ratio of Specific Heats	gamma	1	1

Table 1. Model inputs

Since the tube is initially completely filled with MEK solute, the first assumed boundary condition is that initially the inner radius of the tube, $r < R2$, is assumed to have a weight fraction of 1, $\omega 1 = 1$, the second boundary condition is at the outer radius, $r = R1$, where it is assumed the mole fraction of MEK is zero, $Xw1 = 0$, due to presence of the air flow which continuously sweeps away any permeate and maximizes the gradient.

Results: Figure 1 depicts the diffusion of the solvent MEK across the PVC pipe. As can be seen in the figure, the mass fraction of the solvent MEK is at a maximum at the center of the PVC pipe and a gradual decrease in the mass fraction is observed when moving along the radial coordinate to the outer surface of the pipe. All the experimental results from Bromwich and Parikh(1) are plotted with all the COMSOL results and are shown in Figure 2.When comparing the full set the overall prediction of the model is good. The simulation model predicts a higher cumulative permeation than the experimental data in all temperature cases. The offset of the experimental and simulation data decreases as the temperature decreases since the assumptions made in the model are a better fit to reality.



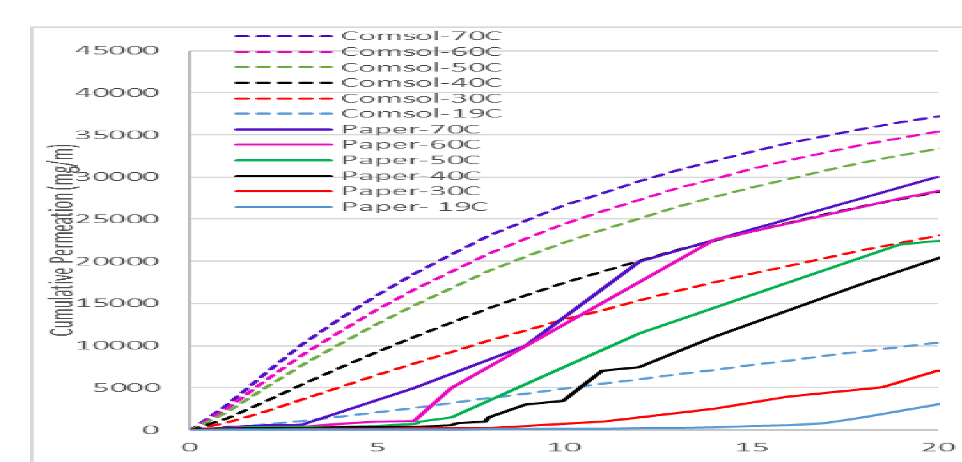


Figure 1.3-D View of Mass Diffusion of MEK Across PVC Pipe ; Table 2. Comparison of Cumulative Permeation Versus Time for different temperatures.

Conclusions: The model predicts higher cumulative permeation values for all temperatures at the various times. In addition, the proposed simulation model is better at fitting the experimental data over long time compared with at a short time. This may mean that the diffusion coefficient may change, possible due to the low molecular weight species in the PVC migrating out along with the MEK.

References

[1] B.David, and J.Parikh,Journal of Occupational and Environmental Hygiene 3.3 (2006): 153-60. Web.

[2] "PHYSICAL AND CHEMICAL PROPERTIES OF MEK."Sevas Educational Society, 2007. Web. 08 Mar. 2016.