Mutual Diffusion Coefficients of VX and VM

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Introduction

Accurately predicting the fate and transport of persistent CWAs in environmental scenarios requires a better mechanistic understanding of the diffusion of persistent CWAs through soil pore water environments. Although diffusion through soils is a major factor influencing fate and transport modeling of persistent CWAs in soil environments, no data exists regarding the diffusion of persistent CWAs in liquid matrices.

The primary objective of this study was to *measure* mutual diffusion coefficients of 2 V-class agents across a range of environmentally relevant temperatures. This is the first known study to make these measurements.

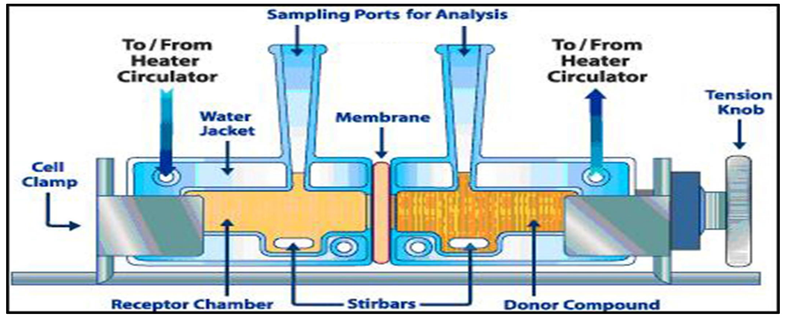
Experimental

A commercially available horizontal diffusion cell (HDC) was used during this study. The cell was constructed of borosilicate glass with each chamber having a total volume of 3.4 mL. The overall average (*n*=20) diameter of the opening was 9.26±0.043 mm. The same HDC was used for all experiments summarized in this report. Cell contents were stirred during each experiment and temperature was maintained using a recirculating water bath.

The membrane was a polycarbonate Nuclepore track-etched membrane filter. The membrane was 25 mm in diameter with 0.05 µm pores.

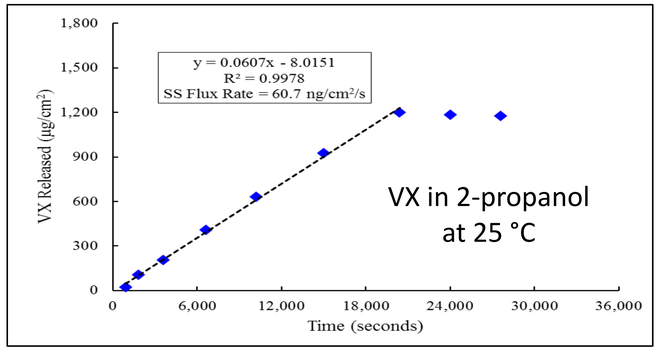
Experiments were conducted in both pH 4.5 acetate buffer and 2-propanol. Approach was validated by measuring diffusion coefficient of K^+ (as KCl) in deionized water at 25 °C.

Horizontal Diffusion Cell



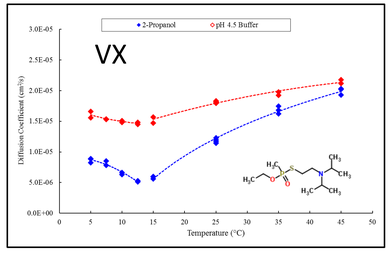
Donor chamber contained agent solution at approximately 1,800 mg/L. Small (50 µL) aliquots removed from receptor chamber and fresh solvent added to maintain infinite sink conditions. Agent determined using GC/MSD.

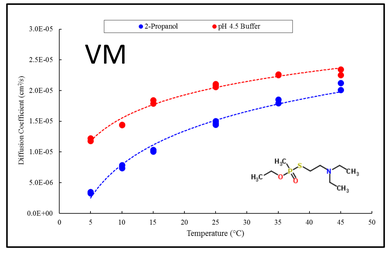
Cumulative Release Curve



1. SS Flux Rate = Slope of Linear Portion of Release Curve.
2. Permeability Coefficient (K_p) = SS Flux Rate/Donor Cell Concentration.
3. Diffusion Coefficient (D_L) = K_p × Membrane Thickness
4. Units of D_L are cm^2/s

Mutual Diffusion Coefficients





Diffusion coefficients for VX exhibit spinodal behavior, while the values for VM do not. VX has a reported lower critical temperature (LCT) of 9.4 °C, while VM has a reported LCT of 74 °C in water. Literature reports indicate diffusion coefficients go to zero at the LCT.

Discussion

Average (*n*=4) diffusion coefficients for VX and VM at 25 °C in aqueous buffer were 1.81E-5±1.738E-7 and 2.09E-5±1.790E-7 cm^2/s, respectively. The measured value for VX is approximately 3 times lower (slower) than the default value used in PEARL and other fate models. Need to do sensitivity analysis, but models could be underestimating VX clearance times.

Behavior of VX at the LCT has implications for detection strategies that rely on passive transport through membranes.

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