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Phase Behavior of Chlorinated Solvent + Water + Alcohol Mixtures with Application to Alcohol Flushing

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Alcohol flushing is a new in-situ remediation technique for the removal of water-immiscible solvents from contaminated soil and groundwater. Understanding the changes in the physical and chemical properties of chlorinated solvents and the aqueous-phase solution during flushing is prerequisite for the successful application of this technology. The overall objectives of these experiments were to characterize the ternary-phase behavior, interfacial tension, viscosity, and density for mixtures containing a chlorinated solvent, water and alcohol. Two chlorinated solvents were used: tetrachloroethylene and trichloroethylene. The alcohols studied included methanol, ethanol, and propan-2-ol. Results showed that the single-phase region of the ternary relationships increased as the molecular weight of the alcohol increased. The interfacial tension between the chlorinated solvents and aqueous solutions decreased with increasing alcohol concentration and increasing molecular weight of the alcohol. Changes in the viscosity of water + alcohol mixtures due to the addition of the solvents were only evident at high alcohol concentrations. Small changes in density were noted for the chlorinated solvents in equilibrium with water + alcohol solutions except in the case of trichloroethylene and propan-2-ol solutions, which exhibited considerable swelling.

Introduction

Chlorinated solvents, such as tetrachloroethylene and trichloroethylene are common groundwater contaminants. These chemicals, once widely used as cleaning solvents, have been released into the subsurface environment over many years and can exist as a separate liquid phase. New remediation technologies are being developed to enhance the removal of these immiscible liquids from groundwater and the subsurface environment. One new technique involves flushing alcohol solutions through the zone of contamination to enhance the solubility of the chlorinated solvents and subsequently extract the solvent-rich alcohol phase from the soil.

To understand solubility behavior during alcohol flushing, liquid−liquid equilibria must be characterized. Ternary-phase diagrams are a standard way of presenting the solubility characteristics of three-fluid phase systems such as; water, alcohol and chlorinated solvent. These diagrams have been used by petroleum and chemical engineers for decades and more recently by researchers investigating methods to remediate contaminated groundwater (Falta, 1998, Imhoff et al., 1995, Broholm and Cherry, 1994, Brandes and Farley, 1993).

The purpose of this study was to obtain liquid−liquid equilibria data for ternary diagrams and characterize the solubility enhancement, interfacial tension, density, and viscosity of tetrachloroethylene and trichloroethylene + alcohol + aqueous systems. The need to characterize the behavior of these chlorinated solvents in contact with various aqueous-phase solutions is important for a better understanding and more successful application of alcohol flushing technology.

Experimental Section

Chemicals. The chemicals were obtained by VWR Scientific and US Industrial Chemicals, with the following specifications: tetrachloroethylene and trichloroethylene (reagent grade, 99.9% and 99.8% pure, respectively), methanol and propan-2-ol (HPLC grade, 99.8% pure), ethanol (food grade, 200 proof). Water was distilled using a Corning Mega-Pure System (MP-11A).

Ternary Phase Diagrams. Ternary phase diagrams were constructed from data collected using the methods presented by Sayar (1991). The synthetic method provided the boundary between the single- and two-phase regions, and the analytical method provided the tie lines. Temperature was held at (21.5 ± 1) °C.

(a) Synthetic Method. Water and tetrachloroethylene or trichloroethylene mixtures were prepared by mass (±0.1 mg), placed in a constant-temperature bath and titrated with alcohol until the two phases disappeared.

(b) Analytical Method. Alcohol, water, and tetrachloroethylene or trichloroethylene mixtures were prepared by mass, equilibrated using a rotary mixer for at least 24 h, and centrifuged to separate the two phases. The composition of each phase was determined using a gas chromatograph and a flame ionization detector. An automated head space sampler was used to determine the mass of alcohol and chlorinated solvent in the aqueous phase. The solvent phase was directly injected into the gas chromatograph to determine the mass of alcohol dissolved in this phase. The water content of the solvent phase was determined by the Karl Fischer method using an Accumet 150 coulometric KF automatic titrator (Denver Instrument Company, Arcada, CA). The mass fraction of immiscible solvent in the solvent phase and the mass fraction of water in the aqueous phase were then determined by difference.

Solubility Enhancement. The solubility of tetrachloroethylene and trichloroethylene in various alcohol solutions was determined by placing 2.0 mL of chlorinated solvent in a 20 mL crimp cap vial containing 10 acid-

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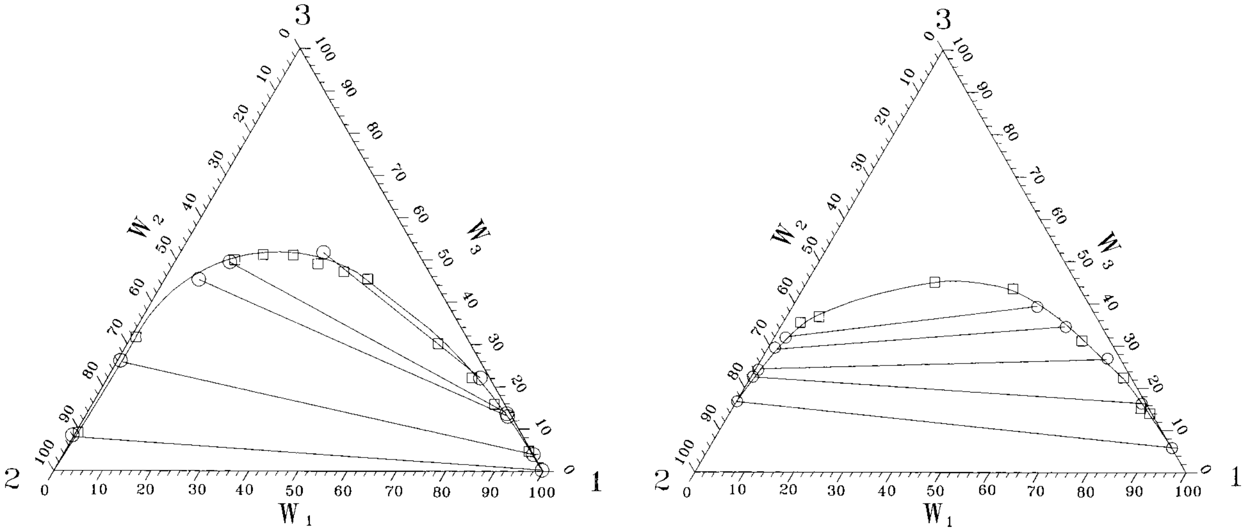

Figure 1. Ternary diagrams for experimental liquid−liquid equilibria: (left) tetrachloroethylene + water + propan-2-ol; (right) trichloroethylene + water + propan-2-ol (concentrations expressed as mass, % W_i).

washed glass beads. The aqueous−alcohol solution was filled to the top to minimize head space, and the vial was crimp capped with a Teflon-lined septum. The solutions were equilibrated on a rotary mixer (2 rpm) for 24 h and centrifuged. Initial studies indicated this was sufficient time for equilibration. The aqueous phase was sampled and analyzed using gas chromatography with a head space sampler to determine tetrachloroethylene or trichloroethylene concentrations. Replicate vials were made for each solution.

Interfacial Tension. The interfacial tension of the two chlorinated solvents in various aqueous−alcohol solutions was determined using the pendant drop technique (Ambwani and Fort, 1979). The two-phase solutions were allowed to equilibrate using a reciprocating shaker and then separate. A Rame-Hart model 100 goniometer (Rame-Hart, Inc., Mountain Lakes, NJ) was used to create and photograph the equilibrated trichloroethylene or tetrachloroethylene drops in water + alcohol mixtures. Replicate drops were photographed and subsequently measured. Tables and the equation from Ambwani and Fort (1979) were then used to calculate interfacial tension. The temperature was held at (22 ± 2) °C. Accuracy of this method was determined by comparing results of pure water in air to literature values and was within 3% of known values (Adamson, 1990).

Density and Viscosity. The aqueous-phase and solvent-phase densities were determined by filling a known volume with the solution of interest and weighing it with an analytical balance. The accuracy was determined by comparing results of pure water, propan-2-ol, ethanol, and methanol to those reported in the literature (CRC, 1990; Verschueren, 1983) and was determined to be within 0.5% of known values. The temperature was maintained at (20 ± 0.5) °C. The aqueous-phase viscosity for different equilibrated solutions was determined using a viscometer (Brookfield Dial Viscometer, Model LVT with UL Adapter 304 S/S, Stoughton, MA). The temperature was held at (21.5 ± 0.5) °C. The accuracy of this method was within 15% for water, methanol and ethanol and within 2% for propan-2-ol and was determined by comparing results of these liquids to those reported in the literature (CRC, 1990). While the accuracy of this method may not have been the best especially at low viscosity, it should be noted that one of the reasons for measuring this parameter was to evaluate the effect of the addition of the chlorinated solvent on the viscosity behavior. For comparative purposes, this method was adequate. Solutions for interfacial tension, density, and viscosity measurements were made volumetrically with an accuracy of the compositions of ±1%.

Results and Discussion

Ternary-Phase Diagrams. Ternary-phase diagrams for the six systems investigated are plotted in Figures 1−3 with data presented in Tables 1−6. The higher molecular weight alcohol propan-2-ol has a much greater effect on the solubilities of both trichloroethylene and tetrachloroethylene than does either ethanol or methanol, as evidenced by the greater single-phase or miscible region of the ternary diagrams.

The tie lines in all cases, except the trichloroethylene + propan-2-ol + water case, have negative slopes. This indicates the preferential partitioning of the alcohol into the aqueous phase. In the trichloroethylene + propan-2-ol + water situation, the tie lines exhibit both positive and negative slopes. The negative-sloped tie lines occur up to approximately 30% by mass propan-2-ol and indicate preferential partitioning of this alcohol into the aqueous phase. Above 30%, the slopes of the tie lines become positive, an indication of preferential partitioning of the alcohol into the trichloroethylene phase. This preferential partitioning by propan-2-ol results in a decrease of solvent density and is called swelling.

Ternary diagrams for the trichloroethylene + propan-2-ol + water and tetrachloroethylene+propan-2-ol+water systems are in agreement with those reported by Brandes and Farley (1993). The ternary diagram of the tetrachloroethylene + methanol + water compares well with both the experimental and UNIQUAC model predictions reported by Imhoff et al. (1995). The ternary diagram for trichloroethylene + methanol + water compares well with that produced using an ESP numerical simulation as reported in Broholm and Cherry (1994). Ternary-phase diagrams for the trichloroethylene + ethanol + water and tetrachloroethylene + ethanol + water systems could not be found in the literature.

Solubility Enhancement. At lower alcohol concentrations, it is impossible to read the solubility enhancement

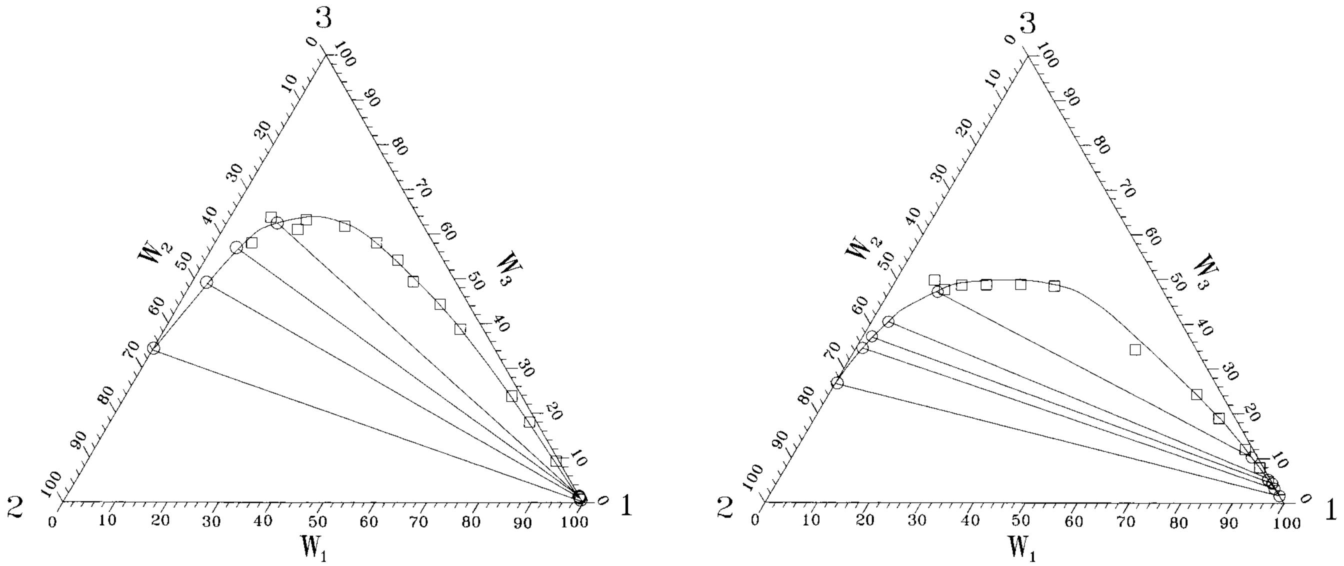

Figure 2. Ternary diagrams for experimental liquid−liquid equilibria: (left) tetrachloroethylene + water + ethanol; (right) trichloroethylene + water + ethanol (concentrations expressed as mass %, W_i).

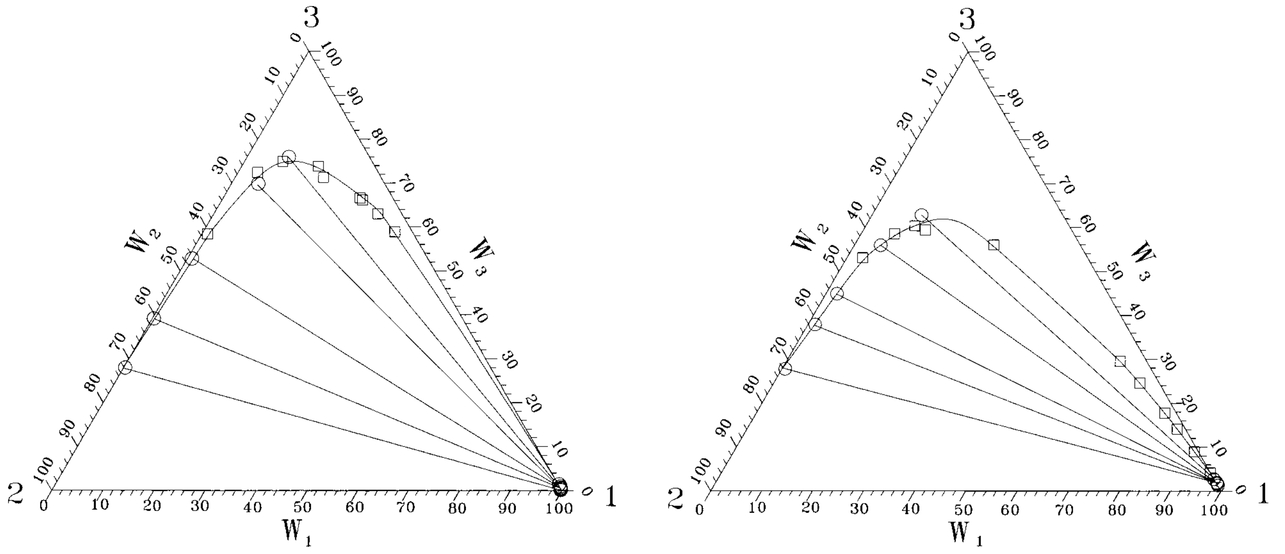

Figure 3. Ternary diagrams for experimental liquid−liquid equilibria: (left) tetrachloroethylene + water + methanol; (right) trichloroethylene + water + methanol (concentrations expressed as mass %, W_i).

Table 1. Liquid−Liquid Equilibria for Tetrachloroethylene (1) + Water (2) + Propan-2-ol (3) (Expressed as Mass Fraction W_i) at (21.5 ± 1) °C

						analytical method (tie line data)					
synthetic method (equilibrium curve data)						aqueous phase			solvent phase		
W_1	W_2	W_3	W_1	W_2	W_3	W_1	W_2	W_3	W_1	W_2	W_3
0.0016	0.988	0.011	0.356	0.173	0.472	0.0001	0.916	0.083	0.997	0.0001	0.0028
0.0044	0.905	0.091	0.413	0.133	0.455	0.0026	0.739	0.258	0.959	0.0011	0.040
0.010	0.674	0.316	0.632	0.066	0.302	0.070	0.478	0.452	0.866	0.0054	0.129
0.120	0.381	0.499	0.743	0.037	0.221	0.113	0.393	0.494	0.861	0.0076	0.131
0.172	0.317	0.511	0.820	0.021	0.157	0.291	0.192	0.517	0.761	0.019	0.220
0.232	0.256	0.511	0.948	0.0054	0.047						
0.294	0.217	0.490									

of the chlorinated solvents from the ternary diagrams. The enhancement of solubility at these lower alcohol concentrations (up to 23% by mass), however, is also of interest for environmental application of this technology and is presented in Table 7. As with the ternary diagrams, propan-2-ol had the greatest effect on enhancing the solubility of tetrachloroethylene at these alcohol concentrations. The relative increase in solubility enhancement was slightly greater with tetrachloroethylene than for trichloroethylene. For example, a solubility increase of approximately nine times was measured for tetrachloroethylene at 23% propan-2-ol compared to 0%, while only an increase of 2.6 times was measured for trichloroethylene.

Interfacial Tension. The interfacial tensions of tetrachloroethylene and trichloroethylene in water + alcohol solutions decreased for increasing alcohol concentrations, as presented in Table 8. Propan-2-ol was the most effective in reducing the interfacial tensions. This was expected on

Table 2. Liquid−Liquid Equilibria for Trichloroethylene (1) + Water (2) + Propan-2-ol (3) (Expressed as Mass Fraction W_i) at (21.5 ± 1) °C

						analytical method (tie line data)					
synthetic method (equilibrium curve data)						aqueous phase			solvent phase		
W_1	W_2	W_3	W_1	W_2	W_3	W_1	W_2	W_3	W_1	W_2	W_3
0.035	0.611	0.354	0.631	0.057	0.312	0.0021	0.831	0.167	0.940	0.0017	0.058
0.066	0.566	0.368	0.760	0.015	0.225	0.0038	0.770	0.226	0.828	0.0082	0.164
0.260	0.289	0.450	0.832	0.016	0.152	0.0056	0.751	0.243	0.704	0.025	0.271
0.428	0.137	0.435	0.856	0.0038	0.140	0.013	0.692	0.294	0.580	0.076	0.345
						0.020	0.661	0.320	0.500	0.109	0.392

Table 3. Liquid−Liquid Equilibria for Tetrachloroethylene (1) + Water (2) + Ethanol (3) (Expressed as Mass Fraction W_i) at (21.5 ± 1) °C

						analytical method (tie line data)					
synthetic method (equilibrium curve data)						aqueous phase			solvent phase		
W_1	W_2	W_3	W_1	W_2	W_3	W_1	W_2	W_3	W_1	W_2	W_3
0.070	0.350	0.580	0.425	0.081	0.494	0.0044	0.652	0.343	0.995	0.0001	0.0052
0.078	0.285	0.638	0.502	0.054	0.444	0.027	0.482	0.491	0.991	0.0003	0.0089
0.143	0.247	0.610	0.569	0.044	0.388	0.045	0.386	0.569	0.989	0.0003	0.011
0.148	0.220	0.631	0.743	0.019	0.238	0.092	0.282	0.626	0.985	0.0006	0.014
0.230	0.153	0.617	0.806	0.014	0.180						
0.310	0.109	0.581	0.902	0.0056	0.093						
0.371	0.088	0.542									

Table 4. Liquid−Liquid Equilibria for Trichloroethylene (1) + Water (2) + Ethanol (3) (Expressed as Mass Fraction W_i) at (21.5 ± 1)°C

						analytical method (tie line data)					
synthetic method (equilibrium curve data)						aqueous phase			solvent phase		
W_1	W_2	W_3	W_1	W_2	W_3	W_1	W_2	W_3	W_1	W_2	W_3
0.074	0.429	0.497	0.311	0.204	0.485	0.0041	0.730	0.266	0.984	0.0007	0.015
0.014	0.420	0.476	0.539	0.118	0.343	0.014	0.641	0.346	0.967	0.0022	0.031
0.131	0.382	0.487	0.708	0.049	0.245	0.018	0.610	0.372	0.954	0.0029	0.043
0.178	0.334	0.488	0.779	0.032	0.190	0.033	0.563	0.404	0.942	0.0049	0.053
0.244	0.267	0.488	0.865	0.015	0.120	0.093	0.436	0.472	0.885	0.0125	0.102

Table 5. Liquid−Liquid Equilibria for Tetrachloroethylene (1) + Water (2) + Methanol (3) (Expressed as Mass Fraction W_i) at (21.5 ± 1) °C

						analytical method (tie line data)					
synthetic method(equilibrium curve data)						aqueous phase			solvent phase		
W_1	W_2	W_3	W_1	W_2	W_3	W_1	W_2	W_3	W_1	W_2	W_3
0.011	0.406	0.584	0.173	0.114	0.713	0.0025	0.719	0.278	0.999	0.00004	0.00087
0.038	0.238	0.724	0.269	0.065	0.666	0.0030	0.606	0.391	0.998	0.00006	0.00154
0.075	0.176	0.749	0.276	0.062	0.662	0.0086	0.464	0.528	0.998	0.00006	0.00237
0.151	0.111	0.739	0.322	0.047	0.631	0.0529	0.249	0.698	0.996	0.00005	0.00374
			0.377	0.034	0.589	0.103	0.197	0.700	0.994	0.00005	0.00569

Table 6. Liquid−Liquid Equilibria for Trichloroethylene (1) + Water (2) + Methanol (3) (Expressed as Mass Fraction, W_i) at (21.5 ± 1) °C

						analytical method (tie line data)					
synthetic method (equilibrium curve data)						aqueous phase			solvent phase		
W_{11}	W_{12}	W_{13}	W_{11}	W_{12}	W_{13}	W_{11}	W_{12}	W_{13}	W_{11}	W_{12}	W_{13}
0.031	0.439	0.531	0.653	0.052	0.295	0.0042	0.716	0.280	0.997	0.0011	0.040
0.065	0.350	0.586	0.717	0.038	0.246	0.0089	0.613	0.379	0.992	0.0004	0.008
0.096	0.301	0.603	0.799	0.023	0.178	0.022	0.530	0.448	0.989	0.0006	0.010
0.121	0.285	0.594	0.843	0.016	0.141	0.052	0.389	0.559	0.987	0.0007	0.012
0.271	0.167	0.560	0.903	0.0077	0.090	0.109	0.250	0.641	0.977	0.0013	0.021

the basis of solubility results. Trichloroethylene equilibrated with water had an average interfacial tension of 0.039 N m^{-1} measured in this study while 0.035 N m^{-1} was reported by Hunt et al. (1988). Tetrachloroethylene equilibrated with water had an average interfacial tension of 0.043 N m^{-1} measured in this study while 0.0458 N m^{-1} was measured by Demond and Lindner (1993). Decreases in the interfacial tension between chlorinated solvents and methanol showed about a 70% decrease at 23% by mass. The interfacial tensions of the two phases with propan-2-ol as the alcohol showed an exponential decline; with an overall decrease in interfacial tension of about an order of magnitude at 23% by mass propan-2-ol.

Density. The changes in density of the chlorinated solvents and the aqueous phase as a function of alcohol concentration are presented in Table 9. There was very little density change in the tetrachloroethylene + water + propan-2-ol system even at high alcohol concentrations. The density of the solvent phase went from an average of 1.625 g/cm^3 to 1.488 g/cm^3. The trichloroethylene phase density dramatically changed in the trichloroethylene + water + propan-2-ol system, going from 1.463 g/cm^3 to

Table 7. Average Solubility of Tetrachloroethylene (4) and Trichloroethylene (5) in Methanol (1), Ethanol (2), and Propan-2-ol (3) + Water Mixtures at (21.5 ± 0.5) °C

W_1	S_4 (mg·L^{-1})	S_5 (mg·L^{-1})	W_2	S_4 (mg·L^{-1})	S_5 (mg·L^{-1})	W_3	S_4 (mg·L^{-1})	S_5 (mg·L^{-1})
0.0	165	1065	0.0	165	1065	0.0	165	1065
0.0801	224	1477	0.0797	NA	NA	0.0781	213	1242
0.163	366	1799	0.162	354	1913	0.158	386	1532
0.248	601	2760	0.248	672	2858	0.241	1458	2866

Table 8. Average Values for Interfacial Tension of Tetrachloroethylene (4) or Trichloroethylene (5) and Methanol (1), Ethanol (2), and Propan-2-ol + Water Mixtures at (22 ± 2)°C

W_1	σ_4 (N·m^{-1})	σ_5 (N·m^{-1})	W_2	σ_4 (N·m^{-1})	σ_5 (N·m^{-1})	W_3	σ_4 (N·m^{-1})	σ_5 (N·m^{-1})
0.0	0.0430	0.0411	0.0	0.0430	0.0411	0.0	0.0430	0.0411
0.0801	0.0357	0.0302	0.0797	0.0269	0.0224	0.0781	0.0197	0.0176
0.163	0.0286	0.0239	0.162	0.0191	0.0149	0.158	0.0110	0.00796
0.248	0.0229	0.0190	0.245	0.0133	0.00928	0.241	0.00508	0.00306
0.337	0.0189	0.0130	0.335	0.00904	0.00475	0.332	0.00224	0.00118
0.430	0.0144	0.00905	0.425	0.00643	0.00217	0.424	0.00136	0.00037

Table 9. Density of Tetrachloroethylene (4) and Trichloroethylene (5) Phases Equilibrated with Methanol (1), Ethanol (2), and Propan-2-ol (3) + Water Mixtures at (20 ± 0.5) °C

W_1	ρ_4 (g·cm^{-3})	ρ_5 (g·cm^{-3})	W_2	ρ_4 (g·cm^{-3})	ρ_5 (g·cm^{-3})	W_3	ρ_4 (g·cm^{-3})	ρ_5 (g·cm^{-3})
0.0801	1.603	1.445	0.0797	1.630	1.476	0.0781	1.608	1.437
0.163	1.603	1.445	0.162	1.633	1.470	0.158	1.594	1.400
0.248	1.605	1.445	0.245	1.640	1.464	0.241	1.562	1.290
0.337	1.602	1.443	0.335	1.631	1.443	0.332	1.532	1.144
0.430	1.602	1.439	0.426	1.628	1.403	0.424	1.488	1.036

Table 10. Viscosity of Alcohol + Water Phase Alone (4), Equilibrated with Tetrachloroethylene (5), and Equilibrated with Trichloroethylene (6) at (21.5 ± 0.5) °C

W_1	η_4 (mPa·s)	η_5 (mPa·s)	η_6 (mPa·s)	W_2	η_4 (mPa·s)	η_5 (mPa·s)	η_6 (mPa·s)	W_3	η_4 (mPa·s)	η_5 (mPa·s)	η_6 (mPa·s)
0.0	1.08	NA	NA	0.0	1.09	NA	NA	0.0	1.14	NA	NA
0.0801	1.31	1.33	1.34	0.797	1.47	1.50	1.49	0.781	1.50	1.54	1.53
0.163	1.59	1.57	1.57	0.162	1.90	1.93	1.95	0.158	2.12	2.23	2.21
0.248	1.93	1.79	1.77	0.245	2.40	2.42	2.42	0.241	2.82	2.80	2.69
0.337	2.04	1.90	1.88	0.335	2.68	2.74	2.73	0.332	3.19	3.33	2.98
0.430	1.98	1.92	1.93	0.426	2.83	2.80	2.81	0.424	3.48	3.57	3.10
0.526	1.90	1.89	1.81	0.521	2.74	2.73	2.68	0.513	3.59	3.61	3.34
0.629	1.62	1.61	1.60	0.625	2.56	2.51	2.48	0.622	3.65	3.26	2.89
0.743	1.37	1.36	1.33	0.736	2.27	2.13	1.66	0.733	3.35	2.73	2.08
0.866	1.07	1.06	1.01	0.854	1.84	1.64	1.32	0.849	2.93	2.26	1.65
1.00	0.67	0.89	0.86	1.00	1.33	1.23	1.07	1.00	2.40	1.93	1.41

[a] Initial methanol (1), ethanol (2), and propan-2-ol (3) concentrations are given in mass fraction.

1.036 g/cm^3. This phenomenon is called swelling and is also reflected in the slope of the tie lines in the ternary diagram. Minimal changes in trichloroethylene and tetrachloroethylene densities were noted in the ethanol and methanol cases.

Viscosity. The aqueous-phase viscosity is affected by both its alcohol and chlorinated solvent concentrations. Viscosity results are presented in Table 10 and show both the effect of alcohol concentration on viscosity and the effect of the dissolved chlorinated solvent in the solution on viscosity. The dissolution of the chlorinated solvent did not affect viscosity until a high alcohol concentration was reached in the case of propan-2-ol resulting in a reduction of viscosity over those of the water−alcohol systems.

Conclusion

The purpose of this study was to obtain liquid−liquid equilibria data for ternary diagrams and to characterize the solubility enhancement, interfacial tension, viscosity, and density of two chlorinated solvents in alcohol + water systems which are important for the application of in-situ alcohol flushing as a remediation strategy. An alcohol flushing strategy relies primarily on enhanced solubility; however, an understanding of viscosity, density, and interfacial tension changes is also important. The results presented in this paper suggest that alcohol concentrations of 23% (mass) or greater are required in order to substantially enhance the solubility of either trichloroethylene or tetrachloroethylene. This corresponds to a significant decrease in the interfacial tension between the chlorinated solvent and the water + alcohol phases which may be important from the standpoint of mobilizing these trapped chlorinated solvents in the soil.

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