Coupling Agents and Surfactants for the Preparation of Aqueous Solutions of DOWANOL™ PPh Glycol Ether

Introduction

DOWANOL™ PPh glycol ether is a slow evaporating, very hydrophobic glycol ether with applications in household and specialty cleaners where the solvent acts as an oil and grease remover, and textile baths, where the solvent act as a plasticizer and allows water-based dyes to penetrate hydrophobic fibers. This product has low odor. With its aromatic structure, DOWANOL™ PPh glycol ether is an excellent match for phenolic coatings and linings; it is also an excellent coalescent for acrylic-based latexes. DOWANOL™ PPh glycol ether is also used extensively in dyeing applications, where it can function as a dye carrier. DOWANOL™ PPh has superior viscosity reduction properties in metalworking fluids. However, the limited solubility of this solvent in aqueous solutions often hinders its use in applications where water is the predominant media.

Challenge

In this technical data sheet we describe two ways to improve the solubility of DOWANOL™ PPh in aqueous media. One method relies on the use of surfactants and the other on the use of coupling agents.

Materials Used

Product Designation	Description	Abbreviation	Supplier
DOWANOL™ PPh Glycol Ether	Assay-99.9% phenoxypropanol	PPh	Dow Chemical
TERGITOL™ 15-S-7 Surfactant	Mixture of linear secondary alcohols	15-S-7	Dow Chemical
TERGITOL™ 15-S-9 Surfactant	Mixture of linear secondary alcohols	15-S-9	Dow Chemical
TERGITOL™ 15-S-15 Surfactant	Mixture of linear secondary alcohols	15-S-15	Dow Chemical
TERGITOL™ 15-S-20 Surfactant	Mixture of linear secondary alcohols	15-S-20	Dow Chemical
TERGITOL™ 15-S-30 Surfactant	Mixture of linear secondary alcohols	15-S-30	Dow Chemical
TERGITOL™ TMN 6 Surfactant (90% aqueous)	Nonionic Surfactant	TMN 6	Dow Chemical
TERGITOL™ TMN 10 Surfactant (90% aqueous)	Nonionic Surfactant	TMN 10	Dow Chemical
Sodium Lauryl Sulfate	Anionic Surfactant	SLS	Fisher Scientific
DOWFAX™ C10L surfactant	Anionic Surfactant	C10L	Dow Chemical
Cetyltrimethylammonium chloride (25wt% aqueous)	Cationic Surfactant	cetyl	Aldrich
Butyl CELLOSOLVE™ Solvent	Assay 99.9% 2-butoxyethanol	BuCs	Dow Chemical
Methoxytriglycol	Assay 99% triethylene glycol methyl ether	MTG	Dow Chemical
Butyl CARBITOL™ Solvent	Assay 99.9% diethylene glycol n-butyl ether	BuCb	Dow Chemical
DOWANOL™ TPM Glycol Ether	Assay 99% tripropylene glycol methyl ether	TPM	Dow Chemical

Solubility and Compatibility in Presence of Surfactants

Aqueous surfactant solutions containing 0.5%, 1.0%, 2.5% and 5.0% surfactant were prepared. The solutions were mixed for 5 seconds. If bubbles formed during mixing, the solutions were allowed to sit until the bubbles dissipated. A burette was filled with the DOWANOL™ PPh and clamped in place. The surfactant solution was stirred at 2 rpm and the DOWANOL™ PPh was added drop wise to a **cloudy end point that persisted after 5 minutes**. The total weight of the solvent added was obtained by difference and recorded. It was then converted to weight %. All titrations were conducted at room temperature (25°C). To determine solubility of water in solvent, the same procedure was used except that the surfactants were dissolved in the solvent and water was added as the titrant. Results can be found in Tables 1 and 2.

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Table 1: Solubility of DOWANOL™ PPh in Water at Various Surfactant Concentrations

	Weight % Solvent			
Surfactant	**@ 0.5% Surfactant Concentration**	**@ 1.0% Surfactant Concentration**	**@ 2.5% Surfactant Concentration**	**@ 5.0% Surfactant Concentration**
15-S-7	1.2	1.2	1.2	1.2
15-S-9	2.3	2.8	2.2	2.2
15-S-15	2.8	2.3	2.2	3.3
15-S-20	2.3	2.3	3.3	4.3
15-S-30	2.3	3.4	3.3	4.3
TMN-6	1.2	1.2	1.1	2.2
TMN-10	1.2	2.3	2.8	3.3
SLS	3.4	3.4	5.4	7.4
C10L	2.3	2.3	3.3	4.3
cetyl	2.3	2.3	3.4	3.4
Note: The Solubility of neat PPh in water is 2.3%				

Effects of surfactants on the solubility of DOWANOL™ PPh glycol ether in water

DOWANOL™ PPh is very hydrophobic and therefore difficult to solubilize in water. SLS was the most effective surfactant for this solvent, although 2.5% by weight surfactant was needed to double the solvent solubility (Table 1). Solvent solubility increased with increasing surfactant concentration reaching 7.4% when the SLS concentration was adjusted to 5% by weight. DOWFAX™ C10L and the TERGITOL™ surfactants 15-S-20 and 15-S-30 doubled the solvent solubility when used at the maximum concentration of 5% by weight. The rest of the surfactants afforded very little improvement in solubility.

Effects of surfactants on the solubility of water in DOWANOL™ PPh

The solubility of water in DOWANOL™ PPh in the presence of the surfactants is shown in Table 2. None of the surfactants tested increased the solubility of water in the solvent above the solubility observed in the absence of surfactants. DOWFAX™ C10L and cetyltrimethylammonium chloride actually decreased the water solubility in the solvent.

Table 2: Solubility of Water in DOWANOL™ PPh at Various Surfactant Concentrations

	Weight % Water			
Surfactant	**@ 0.5% Surfactant Concentration**	**@ 1.0% Surfactant Concentration**	**@ 2.5% Surfactant Concentration**	**@ 5.0% Surfactant Concentration**
15-S-7	8.1	8.1	8.0	7.8
15-S-9	8.1	8.1	8.0	7.8
15-S-15	8.1	8.1	8.0	7.8
15-S-20	9.0	8.1	8.0	7.8
15-S-30	7.6	8.1	8.0	8.7
TMN-6	8.1	8.1	8.0	6.9
TMN-10	8.1	8.5	8.0	7.8
SLS	**	**	**	**
C10L	5.2	6.2	7.0	4.1
cetyl	6.2	7.1	5.1	4.1
Note: The Solubility of water in neat PPh is 9.1 % **SLS is not soluble in DOWANOL PPh				

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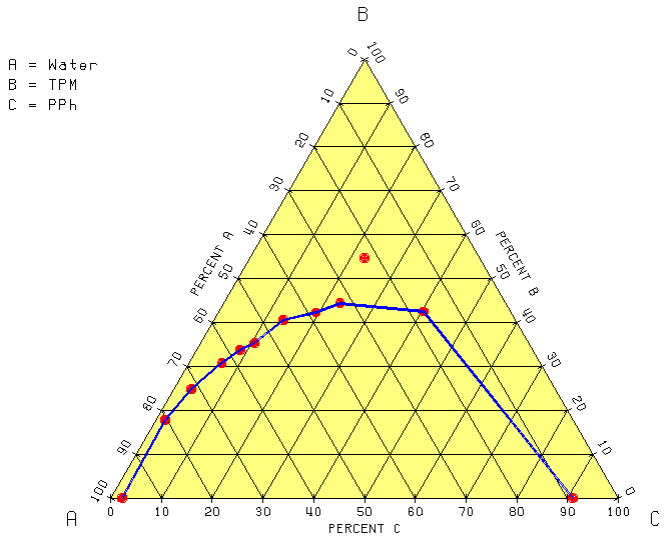
Solubility in Presence of Coupling Agents

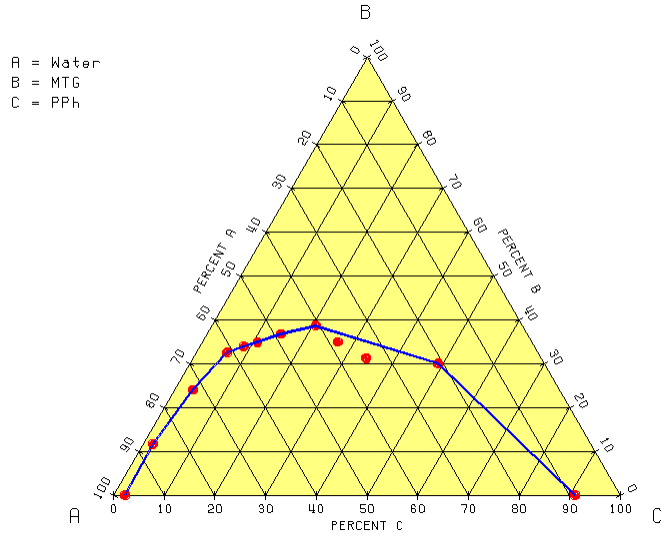
Four glycol ethers previously established as excellent coupling agents for hydrophobic solvent-water systems were evaluated as coupling agents for the phenolic glycol ether-water system. The solvents were mixed in the appropriate ratios and the water titrated with the coupling glycol ether until **a clear endpoint** was reached. Results for the phase diagrams can be found in Figures 1-4. In these diagrams, solvent compositions falling under the area of the curve represent a 2-phase system and those above the curve are single phase systems.

Figure 1: Phase Diagram for DOWANOL™ PPh, Water and DOWANOL™ TPM Ternary System



Wt % TPM	Wt % PPh	Wt % Water
0.00	2.30	97.70
17.80	1.79	80.41
24.87	3.48	71.65
30.72	6.51	62.77
33.75	8.62	57.63
35.28	10.70	54.02
40.63	13.73	45.64
42.29	19.27	38.44
44.39	22.95	32.66
54.70	22.64	22.65
42.54	40.32	17.15
0.00	91.00	9.00

Figure 2: Phase Diagram for DOWANOL™ PPh, Water and Methoxytriglycol Ternary System



Wt % MTG	Wt % PPh	Wt % Water
0.00	2.30	97.70
11.70	1.88	86.42
24.10	3.61	72.29
32.55	6.14	61.31
34.02	8.68	57.30
34.96	10.91	54.13
36.81	14.65	48.54
38.69	20.55	40.75
34.99	26.74	38.28
31.32	34.20	34.49
30.04	49.05	20.91
0.00	91.00	9.00

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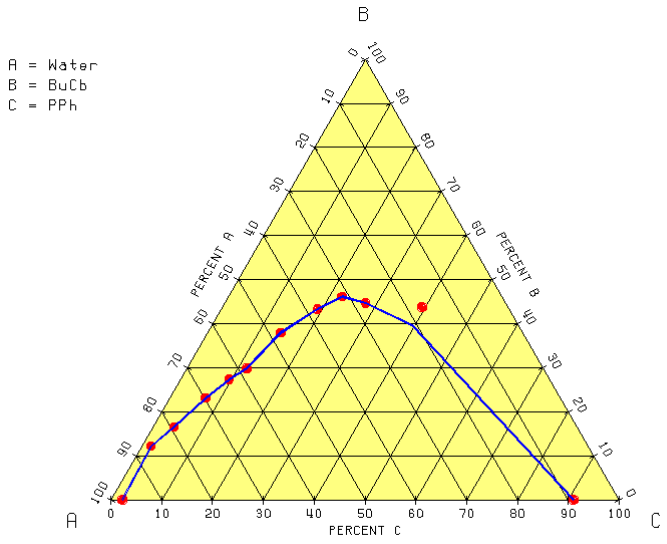
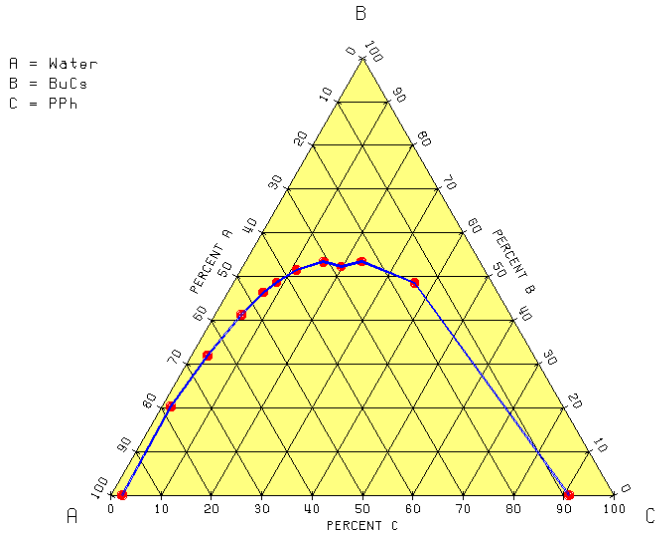
Figure 3: Phase Diagram for DOWANOL™ PPH, Water and Butyl CARBITOL™ Ternary System



Wt % BuCb	Wt % PPh	Wt % Water
0.00	2.30	97.70
12.21	1.79	85.99
16.53	4.13	79.34
23.12	7.08	69.79
27.43	9.58	62.99
29.84	11.80	58.37
37.96	14.45	47.58
43.26	18.99	37.75
46.13	22.45	31.42
44.74	27.70	27.56
43.75	39.32	16.93
0.00	91.00	9.00

Figure 4: Phase Diagram for DOWANOL™ PPh, Water and Butyl CELLOSOLVE™ Ternary System



Wt % BuCs	Wt % PPh	Wt % Water
0.00	2.30	97.70
20.27	1.78	77.95
31.94	3.28	64.78
41.25	5.32	53.43
46.37	7.06	46.58
48.68	8.58	42.74
51.55	11.10	37.36
53.40	15.57	31.03
52.31	19.62	28.07
53.47	23.13	23.40
48.54	36.09	15.37
0.00	91.00	9.00

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Summary

In general, the solubility of phenolic glycol ethers in water can be improved by adding surfactants to the water. SLS was the most effective surfactant for DOWANOL™ PPh, although 2.5% by weight surfactant was needed to double the solvent solubility. Solvent solubility increased with increasing surfactant concentration reaching 7.4% when the SLS concentration was adjusted to 5% by weight. DOWFAX™ C10L and the TERGITOL™ surfactants 15-S-20 and 15-S-30 doubled the DOWANOL™ PPh solubility when used at the maximum concentration of 5% by weight. The rest of the surfactants afforded very little improvement in solvent solubility.

In general, the solubility of water in DOWANOL™ PPh glycol ether is not improved by the addition of surfactants tested.

The best coupling agents for the DOWANOL™ PPh-water system were methoxytriglycol (MTG) and Butyl CARBITOL™. MTG would be the preferred coupling agent when trying to couple equal amounts of solvent and water. Alternatively, Butyl CARBITOL™ would be the preferred coupling agent to couple about 10% solvent into the water.

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