

Application Data

MPDiol® Glycol

MPDiol Glycol Based Polyester Polyols in Waterborne Urethane Coatings

General Information

Waterborne coatings offer the formulator low VOC alternatives for environmental and regulatory compliance. Polyurethane dispersion (PUD) chemistry is quickly becoming a preferred technology for wood and OEM formulators. PUD technology is high performance commensurate of polyurethanes in general. The properties imparted by the components of the PUD, polyol and diisocyanate, have a major impact on its use and versatility. MPDiol is a diprimary diol that can be used in polyester polyol synthesis for use in PUD formulation. Its unsymmetrical structure provides the user with a polyol that is non-crystallizable, weatherable, and extremely flexible.

Key Features and Benefits

Liquid Polyurethane Resins: MPDiol affords liquid resins even at higher aromatic diacid content. This introduces a range of easy to handle resins for coatings with good elongation and tensile strength.

Weatherable Coatings: MPDiol based polyurethane resins are weatherable and show good humidity. Other performance attributes such as stain, chemical, and corrosion resistance is equally comparable.

Excellent Performance: The formulated resins show excellent adhesion and impact resistance. Hardness in MPDiol based polyols can be tailored by increasing the amount of isophthalic acid without running into problems of crystallinity since the resulting resins are liquids.

Polyester Polyol Synthesis and Properties

MPDiol glycol and corresponding diacids were combined without the use of a catalyst. The esterification was performed at 210 °C from an acid number of 2-mg KOH/g to less than 0.5 mg KOH/g. All other polyester polyols were purchased from their respective manufacturers. The make up and properties of each of the polyols synthesized is summarized in Table 1. All polyols prepared in this manner were pourable liquids regardless of the amount of hard segment, isophthalic acid, added to the polymer backbone.

The polyurethane resin and subsequent dispersion were prepared following common procedures. (See Table 2) The polyol, dimethylol propionic acid (DMPA), solvent (N- methyl pyrrolidone NMP) and diisocyanate were added to a resin kettle with stirring and heated to 80 °C. The reaction was allowed to proceed with catalysis until the appropriate weight percent NCO was achieved, approximately 4-mg NCO/g. The prepolymer obtained was then neutralized in the presence of triethylamine (TEA), extended in the presence of a diamine, and dispersed in water. The neutralization step was performed at 50 °C to ensure reaction. The resulting dispersion was allowed to stir at 40 °C for 1 hr and then stand overnight.

MPDiol Polyester Polyol	MPDiol A	MPDiol B	MPDiol C
	moles		
MPDiol	1.0	1.0	1.0
Isophthalic Acid	0.0	0.2	0.4
Adipic Acid	1.0	0.8	0.6
Properties			
Acid Number (mgKOH/g)	<0.4	<0.4	<0.4
Hydroxyl Number (mgKOH/g)	104	102	108
Mol. Wt. No. Average	1443	1413	1400
Physical State	Liquid	Liquid	Liquid

Table 1. Compositions of MPDiol and diacids used for the synthesis of polyester polyols used in preparation of polyurethane resins.

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<i>Component</i>	<i>Wt</i>
Polyester Polyol ¹	200
DMPA	20
NMP	Variable ⁵
Desmodur W ²	Variable ⁶
T-12 catalyst ³	0.04
Formulation	
Prepolymer	200
50% TEA/Water	Variable ⁷
Deionized Water	232
DYTEK A ⁴ 2-Methylpentanediamine	11.2
NMP	Variable ⁸
VOC (lb/gal)	2.4

Table 2. Composition of polyurethane prepolymer resin based on polyols A through C in Table 1 and the formulation for these prepolymers into waterborne dispersions, respectively.

¹ Experimental A, B, C, and butanediol adipate, neopentyl adipate, 1,6-hexanediol adipate, neopentyl and 1,6-hexanediol adipate isophthalate blend, 1,6-hexanediol adipate isophthalate blend² Bayer Corporation³ 3M Corporation⁴ Dupont⁵ percent non-volatile material 75%⁶ NCO/OH ratio=1.8⁷ 90% acid neutralization⁸ percent non-volatile material 34%.

Polyurethane Polymers

Each polyurethane dispersion was prepared according to the same the basic formulation and then applied to chromate treated aluminum panel and phosphated steel panels as supplied by Q-Panel Company. Curing conditions were kept constant, 80 °C for 30 minutes, so that a direct comparison could be made between polyols. Freestanding films were prepared using wax paper and cut for tensile measurements.

In general, all films showed excellent adhesion and impact resistance. (See Table 3) MPDiol based polyols' pencil hardness followed the expected trend, increasing as the amount of isophthalic acid added increased. The benefit of this trend is in resin design latitude since they can be designed according to the desired properties without running into problems of crystallinity. This is often not the case with neopentyl and 1,6-hexane diols based polyols. In the free films, MPDiol adipate when compared to the other commercial adipates, showed increased elongation with out loss of tensile strength. In the mixed isophthalate/adipate samples, increasing the amount of isophthalate made the films tougher as evidenced by the increase in tensile strength going from Resin B to C. The elongation in this case stays comparable to the commercial mixed acid polyester polyols.

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<i>Polyester Polyol</i>	<i>Pencil Hardness</i>	<i>Adhesion</i>	<i>Reverse Impact (Lb/Lb)</i>	<i>Tensile Strength (psi)</i>	<i>Elongation (%)</i>
MPDiol A	B	5B	160	2970	205
MPDiol B	F	5B	160	2890	78
MPDiol C	H	5B	160	3199	147
1,4-BDO Adipate	B	5B	160	2372	108
NPG Adipate	F	5B	160	4036	132
1,6-HDO Adipate	2B	5B	160	2631	142
NPG/HDO Blend*	HB	5B	160	2853	129
HDO Blend*	F	5B	160	3159	139

* Blend means both adipic and isophthalic acids were used in the synthesis of the resin

Table 3. PUD film properties

The coatings were also subjected to accelerated weathering tests and showed good resilience. (See Figures 1 and 2) Cycling conditions for QUV-A weathering test was kept constant for all samples at eight hours light with 100% humidity at 60 °C followed by four hours of 100% humidity at 50 °C. The MPDiol adipate showed the best humidity resistance of the adipate-based resins as shown in the right hand side plot in Figure 1. The exterior weatherability shown in Figure 2 is also good. It is narrowly outperformed by NPG but comparable to BDO and HDO adipate. On the other hand, as the amount of isophthalic acid is increase in the case of Resin B and C; MPDiol based resins show the same humidity resistance as the NPG/HDO and HDO mixed acid resins as depicted in the left handed plot in Figure 1. The weatherability of these types of resins is significantly enhanced by the addition of isophthalic acid. In fact, the MPDiol based resin, Resin C, shows to be as weatherable as the NPG/HDO blend and better than the HDO blend.

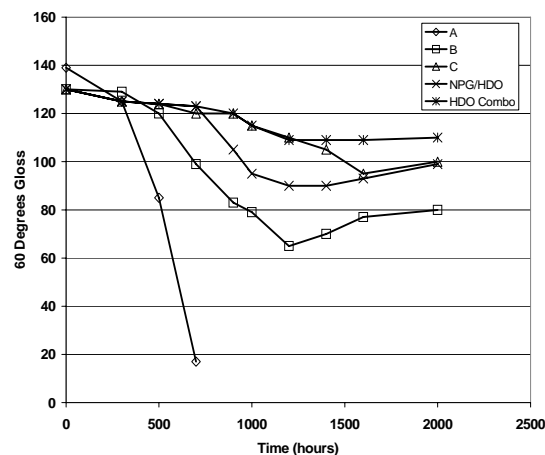
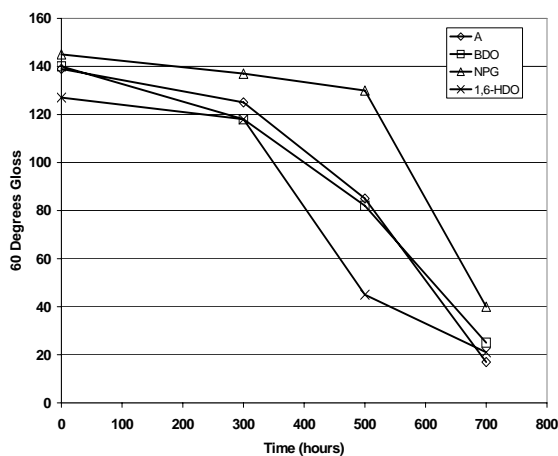


Figure 1. Accelerated humidity testing of MPDiol based polyester polyols versus commercially available polyols as used in PUD.

Figure 2. Accelerated weathering QUVA-340 testing of MPDiol based polyester polyols versus commercially available polyols as used in PUD.

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Summary

In general, MPDiol is a viable substitute to comparable, commercially available polyester polyols. One added benefit is that the diol structure contributes to non-crystallinity in the resulting resins. The diol imparts toughness and flexibility to formulated PUD coatings. The resulting PUD coatings are comparable to those commercially available and present an option to, if necessary, lower volatile content in the final coatings through a lower initial viscosity in the prepolymers.

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