INVISTA TERRIN™ Polyols

Cost-Effective Alternative to Conventional Polyether and Polyester Polyols

Introduction

TERRIN™ polyols can be used in lieu of or in combination with conventional polyether or polyester polyols to formulate a variety of polyurethane products designed to be soft and flexible—or hard and stiff. These versatile, aliphatic, polyester polyols can be used in applications ranging from viscoelastic foam to spray coatings and adhesives to elastomeric resins. TERRIN™ polyols:

- Are cost competitive in comparison to conventional polyols
- Contain a minimum of 50% recycled or renewable[1] content
- Have similar hydroxyl values to castor oil, and can be substituted on a nearly equal weight basis
- Are REACH and TSCA compliant

In addition, TERRIN™ polyols are an easily handled, low-viscosity liquid at room temperature. TERRIN™ product offerings—especially 168 and 168G—remain pourable liquids at -15°C/5°F and below[2]. TERRIN™ polyols do not crystallize and exhibit Tg in a range of approximately -60°C to -75°C.

Application

Polyurethane Protective Coatings

This Technical Data Sheet is intended to illustrate how TERRIN™ polyols can be used in protective coatings. A simple MDI-based coating formulation is used to compare thermal and photochemical stability of coatings prepared using TERRIN™ polyols to coatings prepared using conventional polyols of similar molecular weight, including a polyether polyol, an adipate polyol, or castor oil polyol. The formulations herein are not optimized and aren't intended to cover the entire range of possibilities, but are meant to provide the experienced polyurethane formulator with ideas and starting points for coating formulations. The information set forth herein is furnished free of charge and is based on technical data that INVISTA believes to be reliable, provided that INVISTA makes no representation or warranty as to the completeness or accuracy thereof. It is intended for use by persons having technical skill, at their own discretion and risk, who will make their own determination as to its suitability for their purposes prior to use. As with any material, evaluation of any compound under end-use conditions prior to specification is essential. Nothing herein is to be taken as a license to operate under or a recommendation to infringe any patents. In no event will INVISTA be responsible for damages of any nature whatsoever resulting from the use of or reliance upon the information contained herein or the product to which the information refers.

[1]As defined by ISO 14021, Section 7.8; preliminary estimate based on small-scale production.
[2]Patents pending; consult the SDS for additional physical-chemical, safety and health information

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Coating Formulation

A coating formulation based on 4,4'-diphenylmethanediisocyanate (MDI) was used to evaluate performance of TERRIN™ polyols when substituted for conventional polyols. Polyols used in the formulations are described in Table 1, other materials in Table 2, and the coating formulations in Table 3. All coatings were prepared using 50% polyol as soft segment. The amounts of isocyanate and DEG were adjusted slightly as necessary to maintain isocyanate index at 1.05 and 50% hard segment. Multiple drawdowns were made of each formulation using a 20 mil drawdown bar (BYK 10590) on white 66 x 227 mm Weather-Ometer® cards and were cured at 80°C for at least 16 hours. Color of each drawdown was measured using a HunterLab ColorQuest® XE colorimeter in RSIN mode. Pencil hardness of the control cards was measured using a Wolf-Wilburn pencil hardness tester (BYK-Gardner cat no 5800). One card was held at in a dark oven at 100°C in air for 500 hours (thermal test). Another card was exposed in an Atlas CI65 Weather-Ometer® tester for 500 hours (UV test). A third card was stored at ambient temperature in the dark (Control). Color and pencil hardness were measured on each card after testing.

Table 1: Polyols

Polyols	Description	Supplier	Hydroxyl Value
TERRIN™ 168	Aliphatic polyester polyol	INVISTA	168.2
TERRIN™ 168G	Aliphatic polyester polyol	INVISTA	174.1
TERRIN™ 170	Aliphatic polyester polyol	INVISTA	174.4
DEG Adipate	Aliphatic polyester polyol prepared from diethylene glycol and Adipure® adipic acid	INVISTA	171.6
DB® Castor oil	Castor oil	Vertellus	165.0
POLY-G® blend	Blend of 43% Poly-G® 30-240 and 57% Poly-G® 76-120 polyether polyols	Monument	170.0

Table 2: Other Materials

Material	Description	Supplier	Function
Triethanolamine	Tertiary amine / polyol	Sigma-Aldrich	Catalyst/ crosslinker
DEG	Diethylene glycol, equivalent weight 53.06	Sigma-Aldrich	Chain Extender
Isonate® 143L (MDI)	Polycarbodiimide-modified 4,4'-diphenylmethanediisocyanate (NCO% = 32.6, equivalent weight = 128.8)	DOW	Isocyanate

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Table 3: Coating Formulations

Ingredient	TERRIN™ 168	TERRIN™ 168G	TERRIN™ 170	DEG Adipate	Castor oil	Poly-G® blend
Polyol	50.00%	50.00%	50.00%	50.00%	50.00%	50.00%
Triethanolamine	4.00%	4.00%	4.00%	4.00%	4.00%	4.00%
DEG	2.56%	2.35%	2.34%	2.44%	2.67%	2.49%
Isonate® 143L	43.44%	43.65%	43.66%	43.56%	43.33%	43.51%
Total	100.00%	100.00%	100.00%	100.00%	100.00%	100.00%

Results

Effects of thermal and UV exposure on coating appearance

Figure 1 is a composite image showing the tested coatings after 500 hours at 100°C (thermal), 500 hours exposure to a high-intensity xenon-arc UV light (Weather-Ometer® tester), or in the dark at ambient temperature (control). No cracking, chalking, or other obvious surface degradation was observed visually but some color changes occurred. The DEG-adipate, Castor oil, and Poly-G polyether based coatings were initially light in color but darkened moderately with thermal exposure and very dramatically with UV exposure. This behavior is expected for coatings based on aromatic isocyanates such as MDI. In contrast, the TERRIN™ polyol-based coatings are amber initially, due to the color of the polyols, but little or no color change occurs on UV exposure.

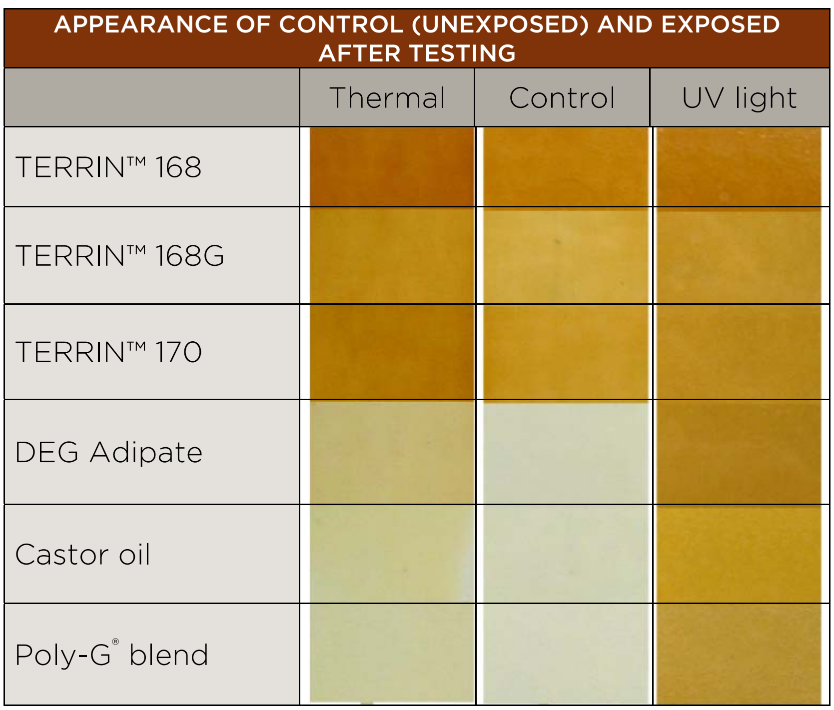

Figure 1 Effect of UV exposure on Hunter Lab "b" value (yellowness).

Hunter Lab color was measured on all the specimens shown in Figure 1. In the L a b color system, L is a gray scale (light-dark) parameter, a is a red-green scale, and b is a blue-yellow scale. The most dramatic shifts observed are in the b values of the coatings that were initially light in color, i.e. the castor oil, DEG adipate, and Poly-G® based coatings (Figures 2 and 3). In every case, b increased from ~+10 initially (slightly yellow) to over 40 (very yellow) after 500 hours in the Weather-Ometer® chamber. As shown in the figures, the b values for TERRIN™ based coatings barely changed, so that after the UV exposure all coatings had similar b (yellowness) values.

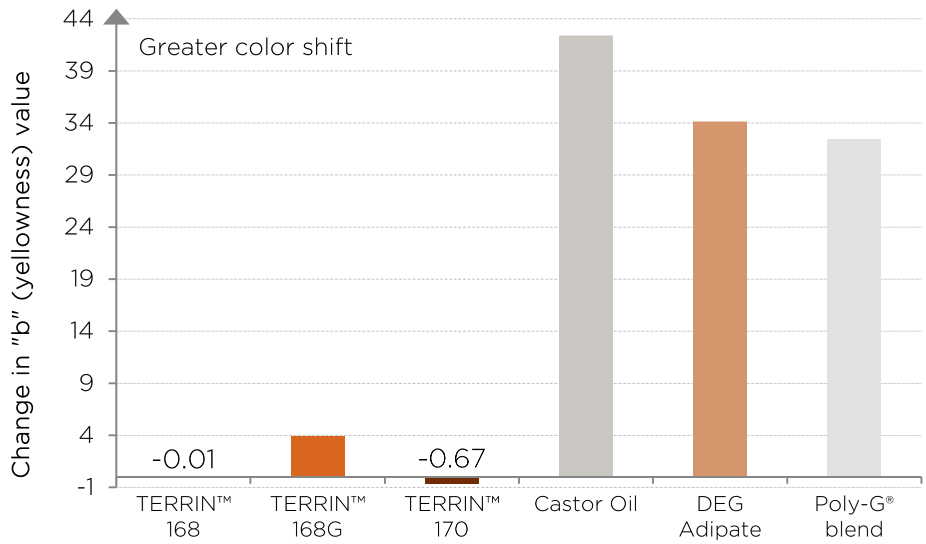

Figure 2: Effect of UV exposure on Hunter Lab "b" value (yellowness)

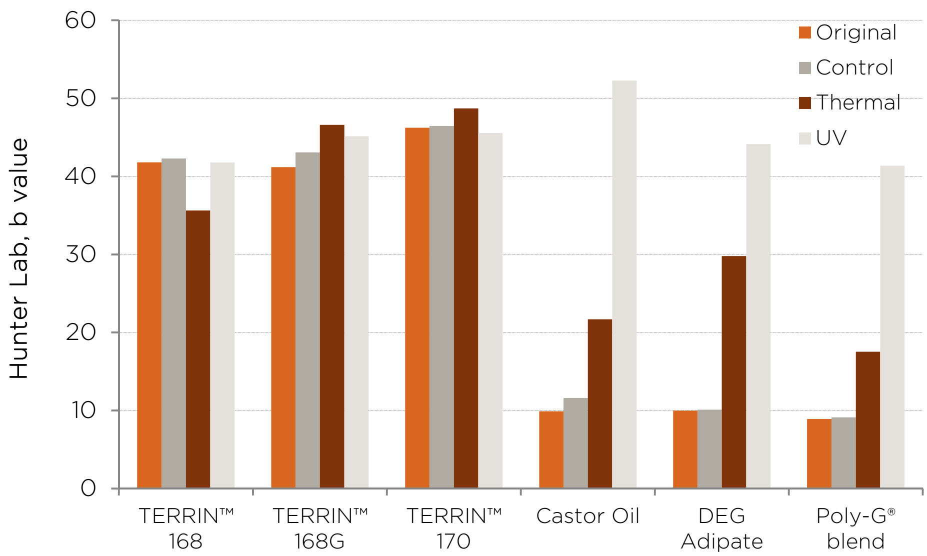

Figure 3: Hunter Lab "b" color coordinate of control (unexposed) and exposed coatings before and after testing.

All coatings except those based on Castor oil or Poly G® blend exhibited 60° gloss > 70 even after UV exposure and can be considered "high gloss." Gloss measurements reported in Figure 4 were made at 20° in accordance with standard practice to magnify differences between high gloss samples.

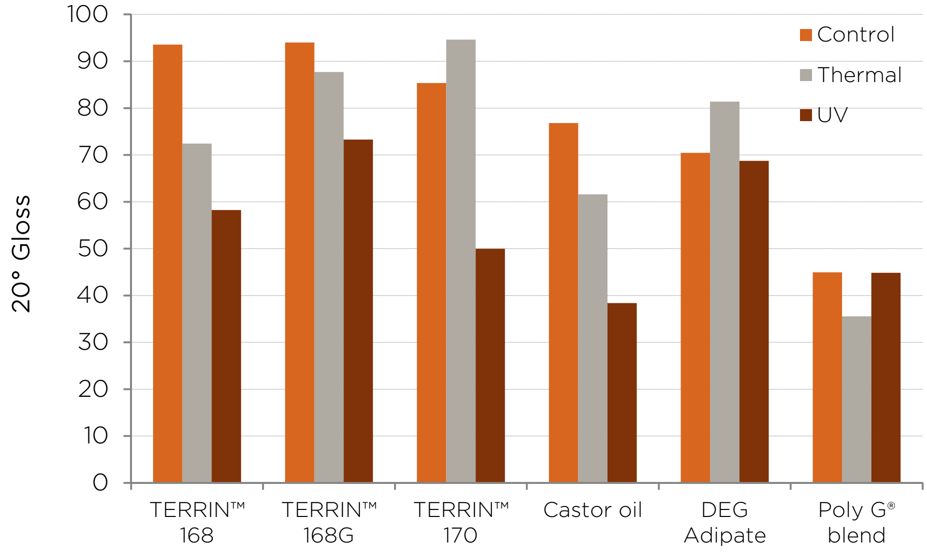

Figure 4: Gloss measured at 20° using a BYK-Gardner micro-TRI-gloss meter 200 days after coating preparation and exposure as described in the text. All samples except Poly G® blend exhibited 60° gloss > 70 and are considered high gloss.

Effects of thermal and UV exposure on coating hardness

Figure 5 shows pencil hardness of the original, control, thermal- and UV-exposed coatings. All of the control samples had pencil hardness 2H except for the one based on TERRIN™ 168, which was considerably softer at hardness HB. All thermally-exposed coatings had hardness 2H. All Weather-Ometer®-exposed coatings had hardness 2H except for those based on TERRIN™ 168G and 170, which had hardness 3H and 4H respectively after the test.

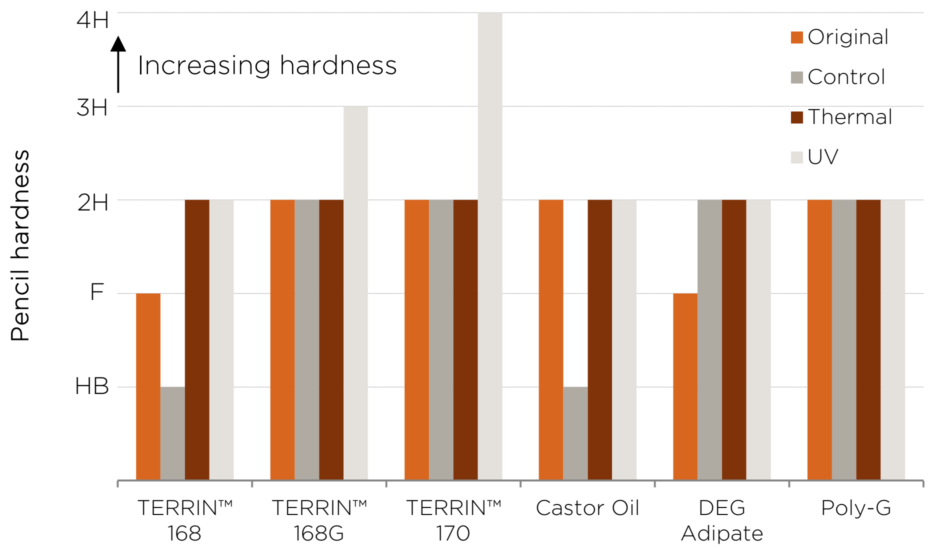

Figure 5: Pencil hardness of control (unexposed) and exposed coatings before/after testing.

Thermal Analysis – Glass transition temperature & thermal stability

The coating formulation used here was not optimized or designed for any particular application, but only to show differences between the polyols tested. Glass transition temperatures (T_g) measured by differential scanning calorimetry (DSC) are summarized in Table 4. The three comparison polyols fell within a fairly narrow range of ~20-24°C. The three TERRIN™ polyols cover a much wider range of ~10-40°C. TERRIN™ 168, with the lowest average functionality of ~1.8, gave the lowest T_g while TERRIN™ 170, with the highest average functionality of ~2.2, gave the highest T_g.

Polyurethanes are known to thermally decompose, typically at temperatures above 200°C. It is known, for example, that the polyurethane linkage can revert to isocyanate and alcohol. Thermogravimetric analysis (TGA) done in air shows that polyurethane coating made using TERRIN™ aliphatic polyester polyols are not dramatically different than coatings made using the three comparison polyols studied here. All coatings show an initial event in the TGA scan between 250-300°C and display similar weight loss profiles, as can be seen from the temperatures corresponding to 10%, 50%, or 90% weight loss.

Table 4: Polyol Glass Transition Temperature

Polyol	T_g
TERRIN™ 168	10.1
TERRIN™ 168G	26.8
TERRIN™ 170	38.2
Castor Oil	23.4
DEG Adipate	20.3
Poly-G blend	21.2

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For samples and further information please contact:

1.800.231.0998 | TERRIN@INVISTA.com

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