TERRIN™

Technical Data Sheet

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

Cast Polyurethanes

This Technical Data Sheet is intended to illustrate how polyurethane properties can be varied by selecting different combinations of TERRIN™ polyol, chain extender, and isocyanate. It provides polyurethane formulations and physical property data for the resulting polyurethanes as well as comparative results for polyurethanes made using reference polyols. The formulations herein are not optimized, aren't intended to cover the entire range of possibilities, and are not targeted at any specific application, but are meant to provide the experienced polyurethane formulator with ideas and starting points for application-specific 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

Preparation and Results

Use in formulations with polymeric MDI

Table 1: Materials

Designation	Description	Supplier
Adipate A	Fomrez® 11-112 aliphatic adipate polyester polyol[2]	Chemtura
Adipate B[1]	Aliphatic adipate polyester polyol[3]	INVISTA(1)
TERRIN™ 168	Aliphatic polyester polyol	INVISTA
TERRIN™ 168G	Aliphatic polyester polyol	INVISTA
TERRIN™ 170	Aliphatic polyester polyol	INVISTA
Rubinate® M[4]	Standard polymeric MDI, Functionality 2.70	Huntsman
DEG	Diethylene glycol	Shell
CLO	Caprolactone	Sigma-Aldrich
AA	Adipure® adipic acid[5]	INVISTA
GLY	Glycerol	P&G Chemicals

(1) Experimental material prepared for comparative purposes only
(2) FOMREZ is a registered trademark of Chemtura Corporation
(3) Experimental polyester polyol prepared for comparative purposes only. Not commercially available.
(4)RUBINATE is a registered trademark of Huntsman Corporation. Descriptions according to Huntsman technical data sheets
(5)ADIPURE is a registered trademark of INVISTA

Adipate A and B are reference polyols. Adipate B is an experimental adipate polyester polyol made using adipic acid, DEG, and CLO, designed to be a di-functional model compound for TERRIN™ polyols.

Table 2: Polyol Properties

Polyol	TERRIN™ 168	TERRIN™ 168G	TERRIN™ 170	Adipate A	Adipate B
Composition	Proprietary	Proprietary	Proprietary	DEG-BDO adipate	DEG-CLO adipate
Acid number	1.0 max	1.0 max	1.0 max	0.19	0.03
Hydroxyl number	160-180 spec	160-180 spec	160-180 spec	111	167
Viscosity, cP @ 25°C	350 typical	830 typical	5500 typical	1700	190
Typical functionality	<2	~2	>2	2	2

Adipate A has lower hydroxyl number (higher average molecular weight) than TERRIN™ polyols. Adipate B is an experimental material that was prepared by INVISTA to provide a reference polyol structurally similar to TERRIN™ polyols and with similar hydroxyl number / molecular weight. Adipate B is not commercially available.

Finished product specifications for all TERRIN™ polyols are:

Acid number: 1.0 max
Hydroxyl number: 160 min to 180 max
Water: 0.1 max

Table 3: Polyurethane Formulations

Formulation	Polyol		Isocyanate (Rubinate® M)	Chain Extender (DEG)	% hard segment	Isocyanate index
A	Adipate B	70.09	29.91	0.00	30	105
B	Adipate B	60.00	36.10	3.90	40	105
C	Adipate B	50.00	42.24	7.76	50	105
D	TERRIN™ 168	70.05	29.95	0.00	30	105
E	TERRIN™ 168	60.00	36.12	3.88	40	105
F	TERRIN™ 168	50.00	42.25	7.75	50	105
G	TERRIN™ 168G	70.00	29.90	0.10	30	105
H	TERRIN™ 168G	60.00	36.05	3.95	40	105
I	TERRIN™ 168G	50.00	42.19	7.81	50	105
J	TERRIN™ 170	70.31	29.69	0.00	30	105
K	TERRIN™ 170	50.00	42.18	7.82	50	105

Ingredient quantities are in parts by weight. The hard segment comprises the isocyanate and chain extender. Isocyanate index refers to moles of isocyanate per hundred moles of hydroxyl, e.g. NCO index of 105 indicates a 5% molar excess of isocyanate relative to hydroxyl.

Polyurethanes were prepared by the "one shot" method wherein all ingredients are combined, mixed, cast onto a flat glass plate, de-gassed, and heated to complete cure. After curing, specimens were cut for physical property testing.

Table 4: Polyurethane Test Results

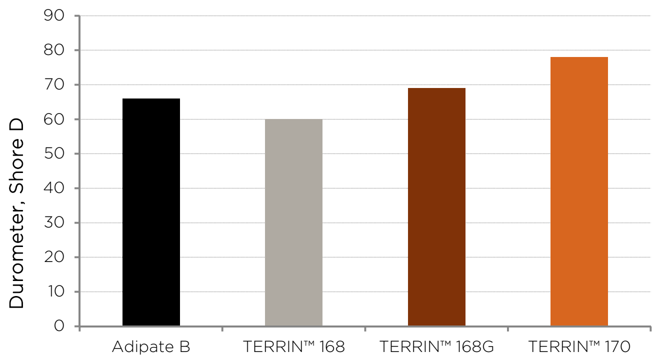
Formulation	Polyol	Chain extender	% hard segment	Shore A	Shore D	Tensile Strength, psi	Elongation at break, %	T_g (tan δ)	T_g (loss mod)
A	Adipate B		30	73	29	344	57	12	1.5
B	Adipate B	DEG	40	89	40	545	86	30	16
C	Adipate B	DEG	50		66	2379	109	47	31
D	TERRIN™ 168		30	52	29	75	103	11	-3
E	TERRIN™ 168	DEG	40	87	32	278	115	23	12
F	TERRIN™ 168	DEG	50		60	1092	72	44	27
G	TERRIN™ 168G		30	78	26	174	34	25	8
H	TERRIN™ 168G	DEG	40	93	43	421	59	34	18
I	TERRIN™ 168G	DEG	50		69	2321	41	50	34
J	TERRIN™ 170		30		57	885	26	52	22
K	TERRIN™ 170	DEG	50		78	3887	4	66	48

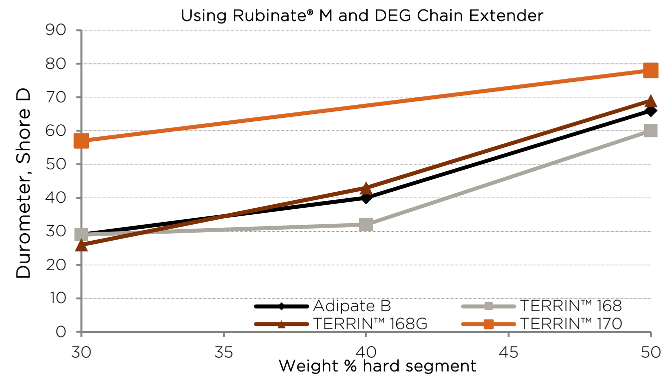
Hardness was measured by durometer on the Shore A or Shore D scales. Tensile strength and elongation were measured by testing dogbone specimens (ASTM D412 Die C) on an Instron® tester. Glass transition temperature (Tg) was measured by dynamic mechanical analysis; values are reported from the peak of the tan δ or loss modulus curves vs. temperature. Tear strength was measured on specimens cut using die C. The following pages provide graphical comparisons of the results tabulated above.

Comparison of the results using Polymeric MDI

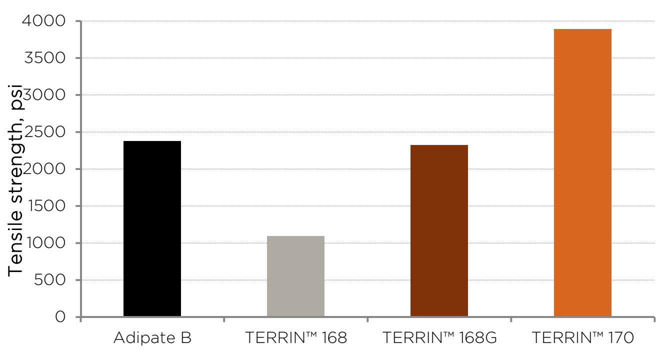
Polyurethanes made at 50% hard segment	Varying % of hard segment

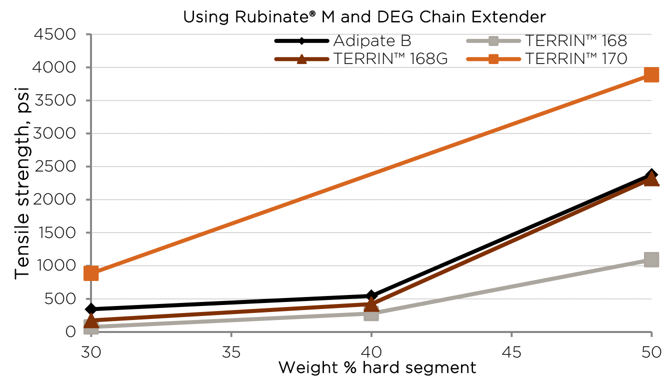
HARDNESS



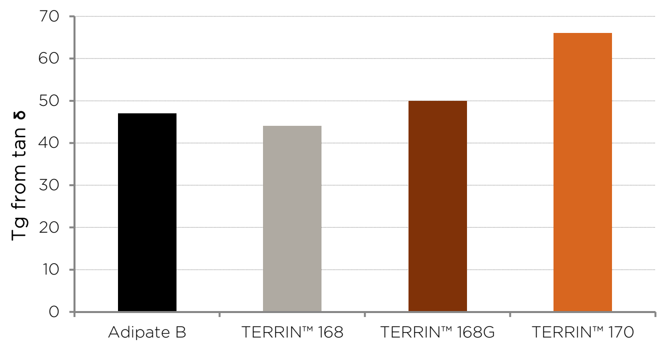


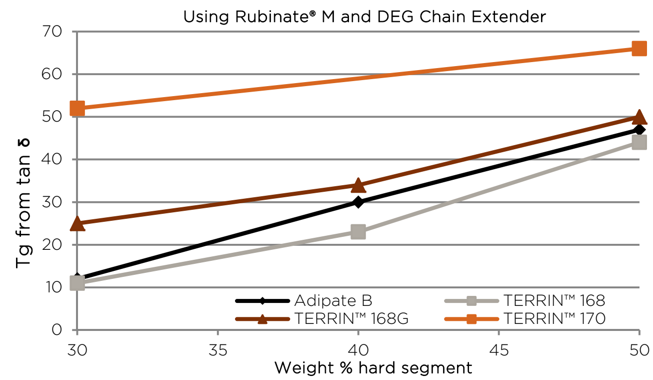
TENSILE STRENGTH



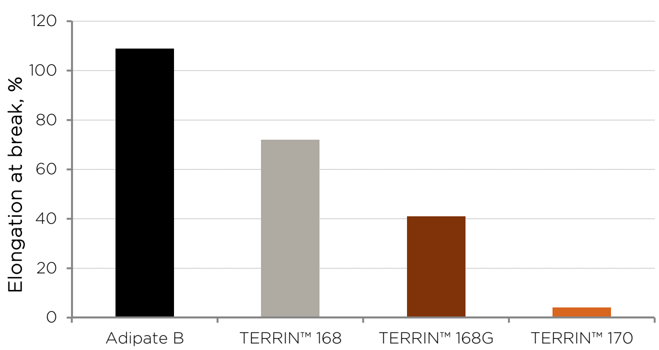


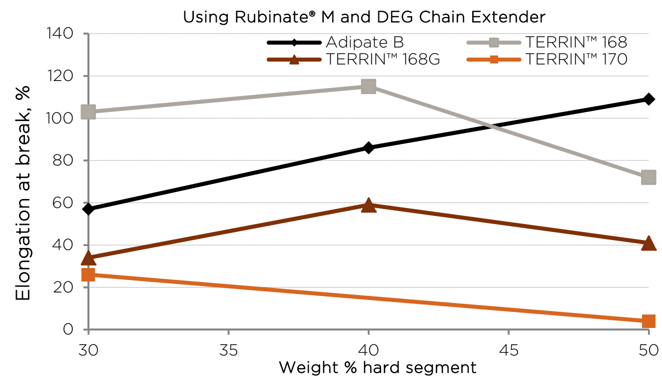
GLASS TRANSISTION TEMPERATURE





ELONGATION AT BREAK





Use in formulations with monomeric MDI

Table 5: Materials

Designation	Description	Supplier
Adipate A	Fomrez® 11-112 aliphatic adipate polyester polyol[1]	Chemtura
TERRIN™ 168	Aliphatic polyester polyol	INVISTA
TERRIN™ 168G	Aliphatic polyester polyol	INVISTA
TERRIN™ 170	Aliphatic polyester polyol	INVISTA
Rubinate® 1680[2]	Uretoneimine modified MDI, Functionality 2.12	Huntsman
BDO	1,4-butanediol	Alfa Aesar or INVISTA

(1) FOMREZ is a registered trademark of Chemtura Corporation
(2)RUBINATE is a registered trademark of Huntsman Corporation. Descriptions according to Huntsman technical data sheets

Table 6: Polyol Properties

Polyol	TERRIN™ 168	TERRIN™ 168G	TERRIN™ 170	Adipate A
Composition	Proprietary	Proprietary	Proprietary	DEG-BDO adipate
Acid number	1.0 max	1.0 max	1.0 max	0.19
Hydroxyl number	160-180 spec	160-180 spec	160-180 spec	111
Viscosity, cP @ 25°C	350 typical	830 typical	5500 typical	1700
Typical functionality	<2	~2	>2	2

Adipate A has lower hydroxyl number (higher average molecular weight) than TERRIN™ polyols.

Finished product specifications for all TERRIN™ polyols are:

Acid number: 1.0 max
Hydroxyl number: 160 min to 180 max
Water: 0.1 max

Table 7: Polyurethane Formulations

Formulation	Polyol		Isocyanate (Rubinate® 1680)	Chain Extender (BDO)	% hard segment	Isocyanate index
A	Adipate A	51.51	42.13	8.35	50	102
B	TERRIN™ 168	53.11	44.58	6.88	50	102
C	TERRIN™ 168G	52.89	46.05	7.10	50	102
D	TERRIN™ 170	52.89	46.05	7.10	50	102

Ingredient quantities are in parts by weight. The hard segment comprises the isocyanate and chain extender. Isocyanate index refers to moles of isocyanate per hundred moles of hydroxyl, e.g. NCO index of 105 indicates a 5% molar excess of isocyanate relative to hydroxyl.

Polyurethanes were prepared by the "one shot" method wherein all ingredients are combined, mixed, cast onto a flat glass plate, de-gassed, and heated to complete cure. After curing, specimens were cut for physical property testing.

Table 8: Polyurethane Test Results

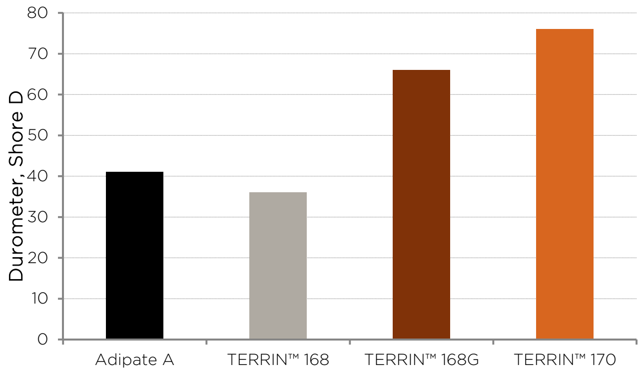
Formulation	Polyol	Chain extender	% hard segment	Shore		Tensile Strength psi	Elongation at break, %	Hysteresis % 1st cycle / 10th cycle	T_g (tan δ)	T_g (loss mod)	Tear Strength (N/cm)
				A	D						
A	Adipate A	BDO	50	88	41	4732	377	56 / 36	12	1.5	1209
B	TERRIN™ 168	BDO	50	50	36	1214	61	72 / 56	30	16	404
C	TERRIN™ 168G	BDO	50		66	3027	116	85 / 83	47	31	1162
D	TERRIN™ 170	BDO	50		76	9731	10		11	-3	2338

Hardness was measured by durometer on the Shore A or Shore D scales. Tensile strength and elongation were measured by testing dogbone specimens (ASTM D412 Die C) on an Instron® tester. Glass transition temperature (Tg) was measured by dynamic mechanical analysis; values are reported from the peak of the tan δ or loss modulus curves vs. temperature. Tear strength was measured on specimens cut using die C.

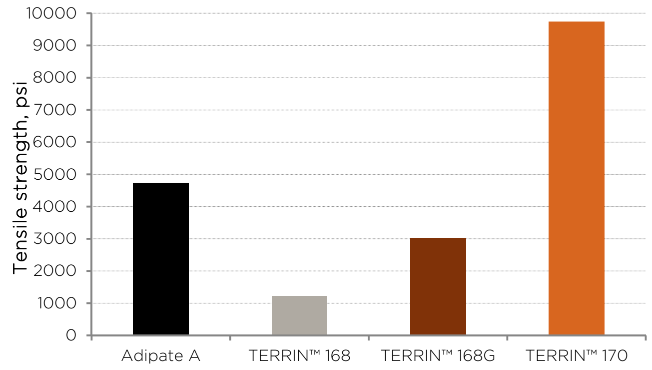
Comparison of the results using Monomeric MDI

Polyurethanes made at 50% hard segment

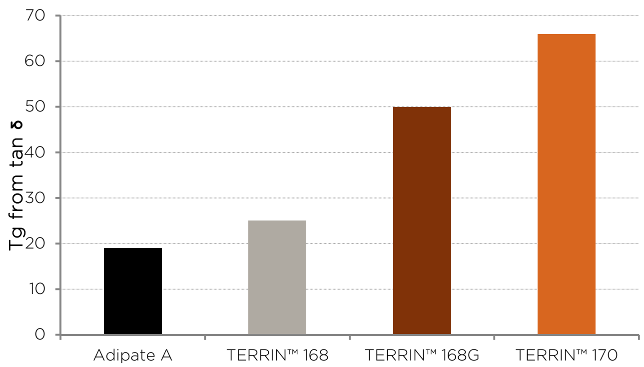
HARDNESS



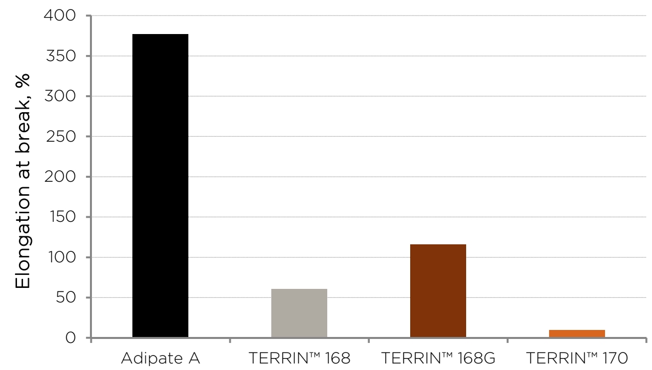
TENSILE STRENGTH



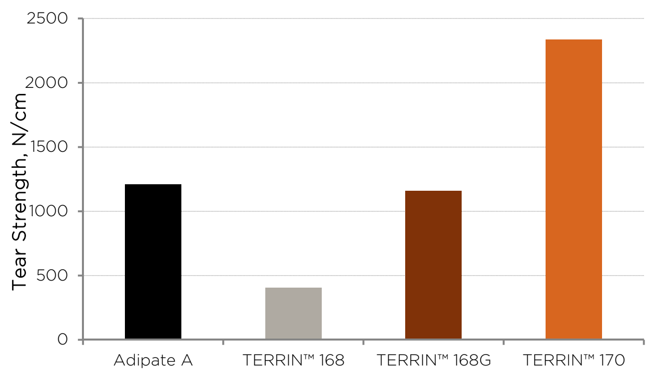
GLASS TRANSITION TEMPERATURE



ELONGATION AT BREAK



TEAR STRENGTH



TERRIN™

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