Coatings Trends & Technologies SUMMIT

Engineered for Performance, Sustainable by Nature: Biobased Polyols for Performance Elastomers

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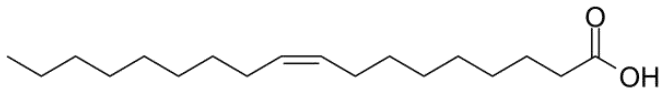
Purpose

The goal of this study was to produce a biobased polyester polyol with excellent physical properties for CASE applications—specifically elastomeric sheets and coatings.

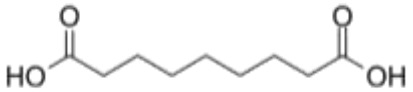
Process

Using building blocks derived from natural feedstocks like natural fats and oils, several novel polyols were generated with high tensile strength without compromising other physical/chemical properties.

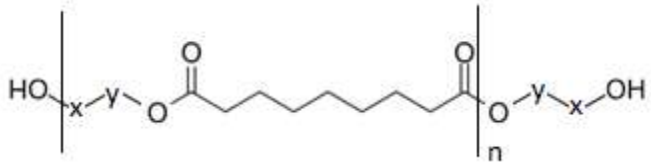
Oleic acid (from natural fats or oils)



Azelaic acid

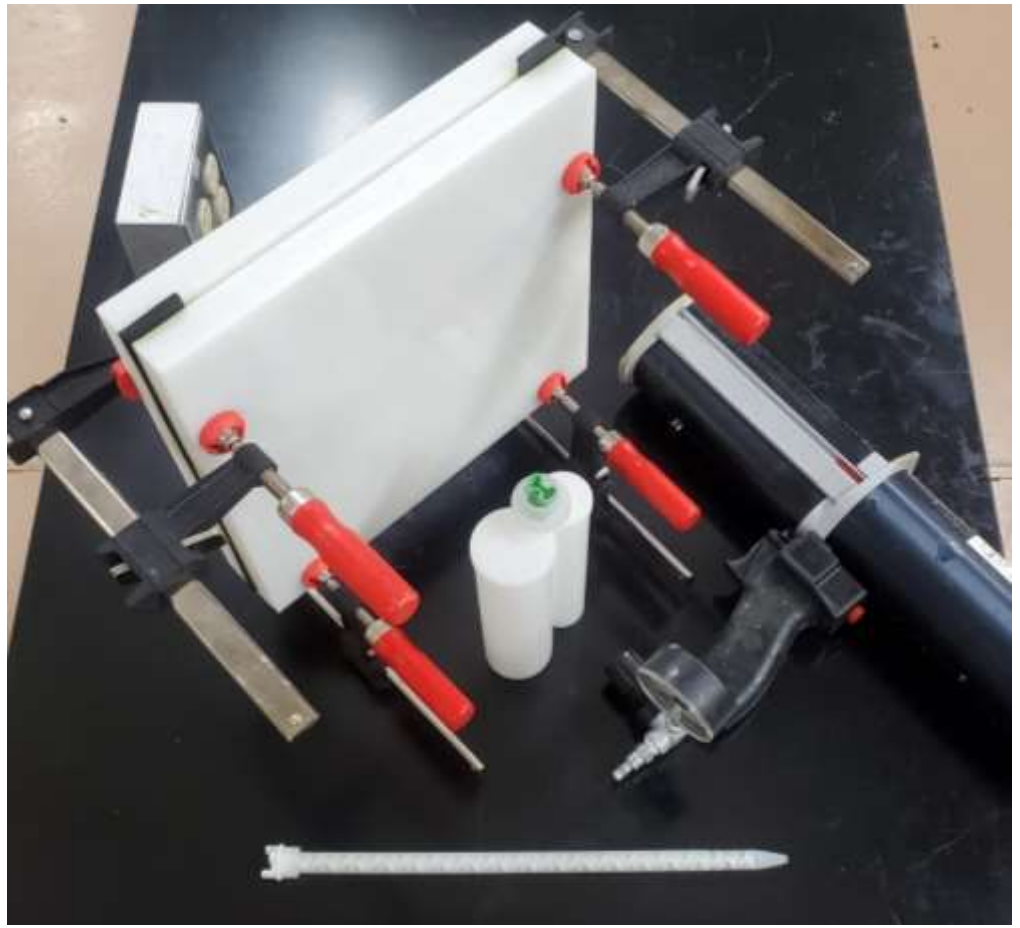


Polyester Polyol



Parts Production Method

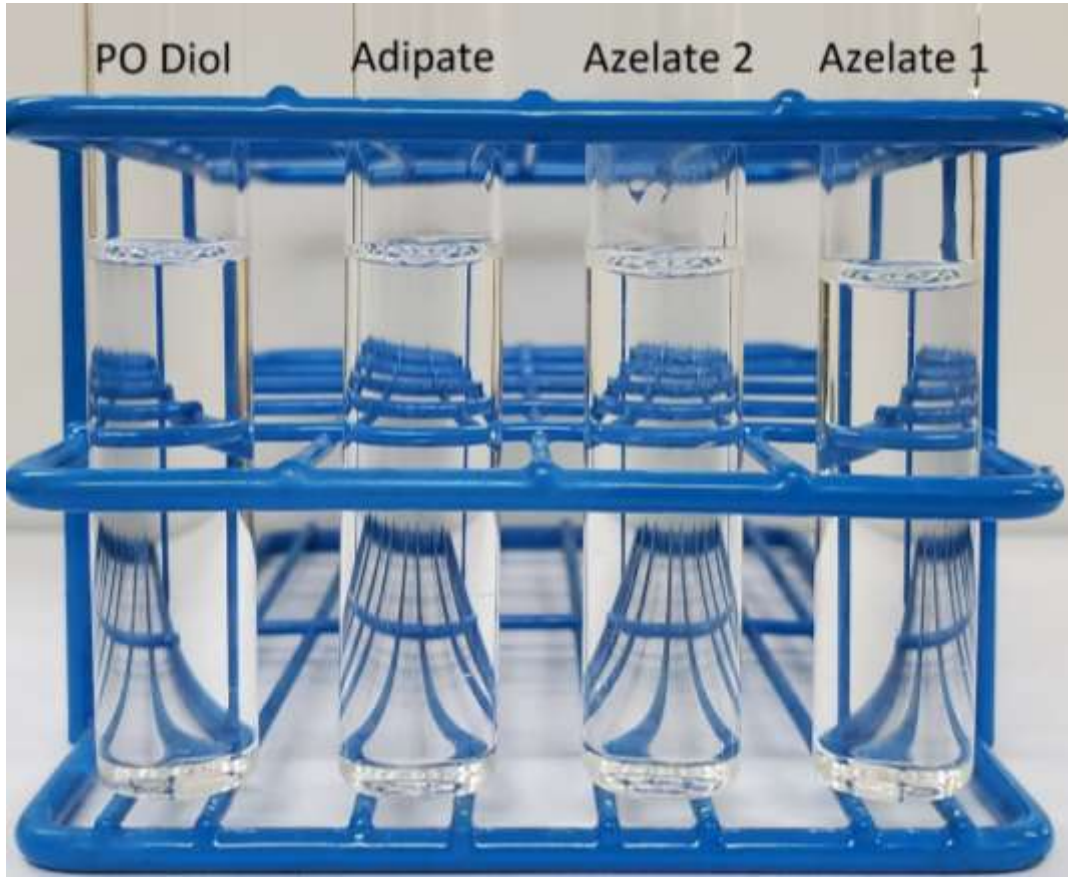
- Liquids vacuum treated prior to application
- Dispensed via cartridge gun, or centrifugal mixer
- Vertical mold used to reduce bubbles
- Force cured in 70° C oven for 2 days prior to testing
- Index was 1.0-1.05 for all formulas



Appearance

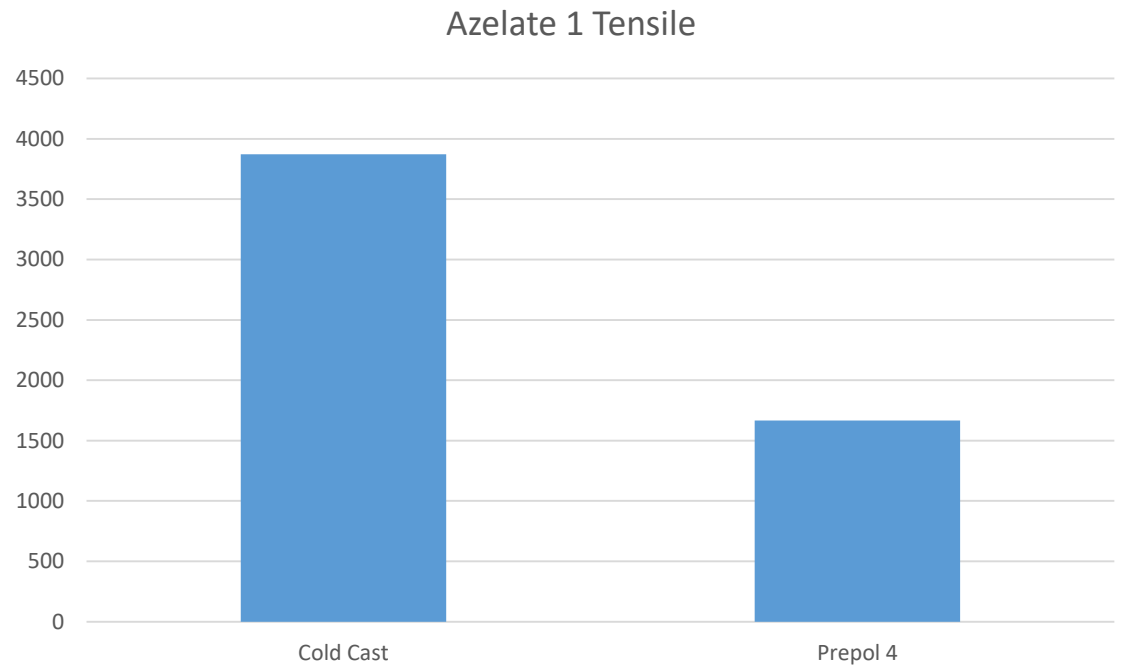
- The resultant polyols are low in color and some are liquid at room temp
- A wide range of molecular weights (OHV) is possible
- In this work we focus on 1000 mw range diols

	PO Diol	Adipate	Azelate 2	Azelate 1
Hazen	3	23	68	62
Gardner	0	0.1	0.3	0.3



Azelate 1 Initial Results

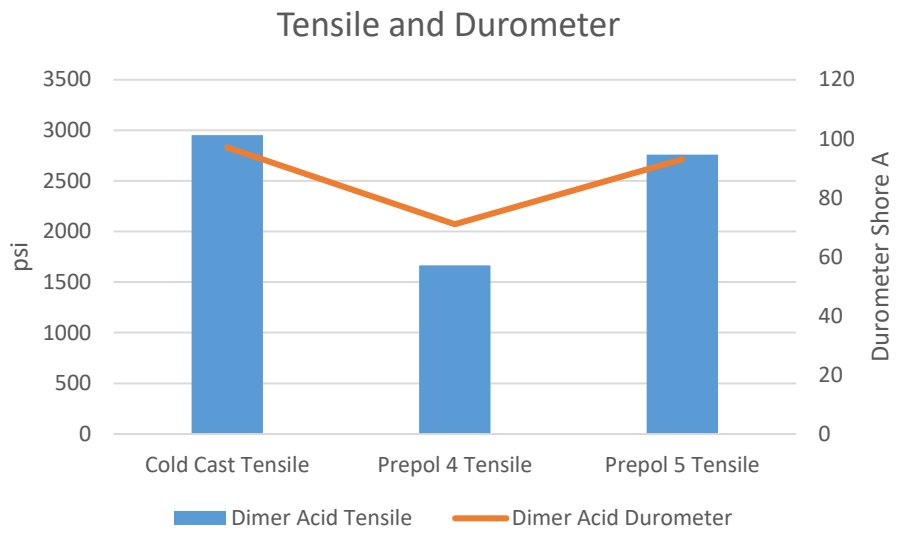
Main Polyol	Iso/Prepolymer	Durometer	Tensile psi	Elongation %	Tear lbf/in	Tabor mg/1000
Azelate 1 1000 mw						
Cold Cast	High 2,4-MDI	87 A	3871	284	327	Not Tested
Semi-Prepolymer	16% NCO Prepolymer 4	71 A	1667	238	184	Not Tested

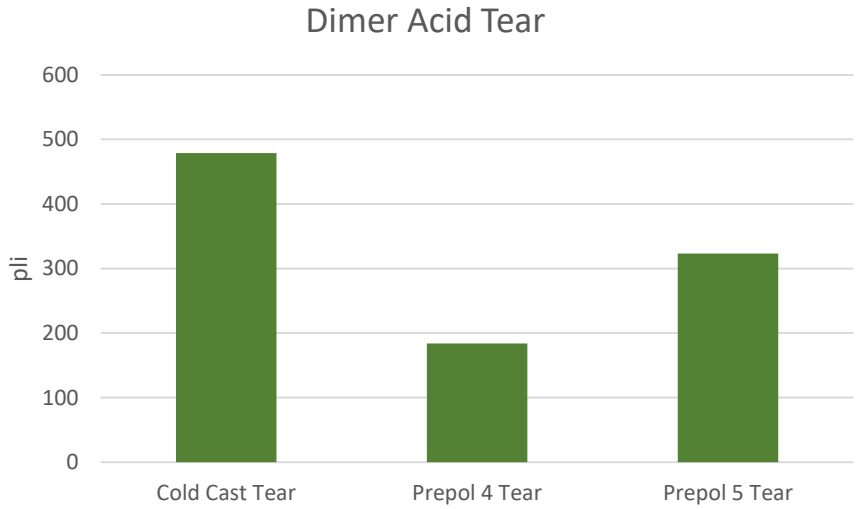


Dimer Acid Polyol Initial Results

	INGREDIENTS	Percent	Percent	Percent
A-side	Dimer Acid Polyol 1000 mw	82.0	84.8	83.0
	Dibutyltin dilaurate	0.01	0.01	0.01
	Butanediol	12.0	9.2	11.0
	4 functional ethylenediamine	2.0	2.0	2.0
	Zeolite Sieve 3A	4.0	4.0	4.0
B-Side	CDI-modified 4,4'-MDI	100.0	55	62
	3 Funct Polyether	0.0	45	0.0
	Dimer Acid Polyol 1000 mw	0.0	0.0	38
	Mix Type	**Cold Cast**	**Semi-Prepolymer 4**	**Semi-Prepolymer 5**
	Mix Ratio (vol)	2:1	1:1	1:1
	Iso/Prepol	High 2,4-MDI	High 2,4 MDI + Dimerate polyol, NCO=16%	High 2,4 MDI + Dimerate polyol, NCO=16%
	NCO/OH INDEX	1.04	1.05	1.03

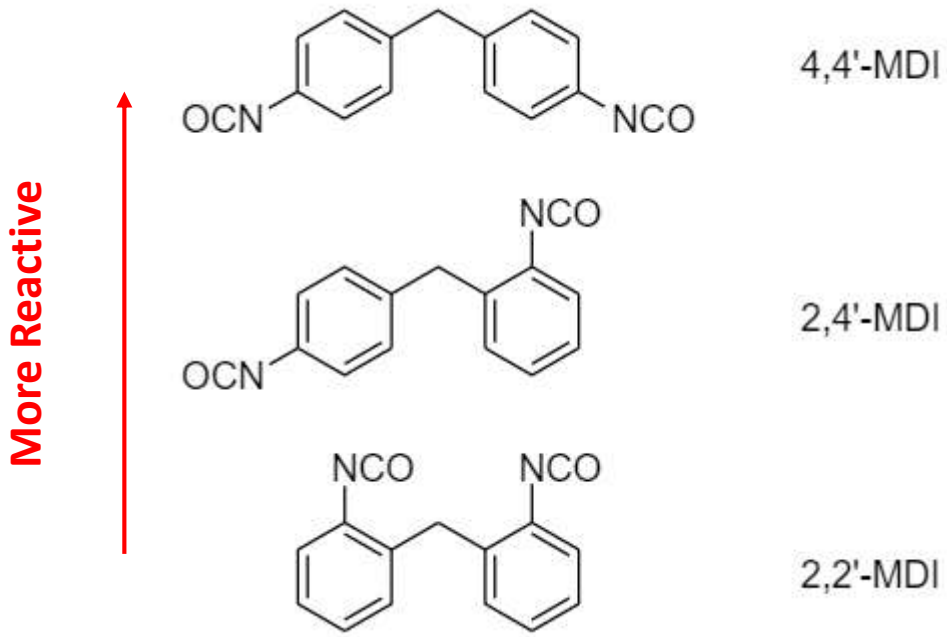
Durometer	97 A	71 A	93 A
Tensile psi	2953	1667	2759
Elongation %	96	238	170
Tear lbf/in	479	184	323
Tabor mg/1000	Not Tested	Not Tested	Not Tested





2,4 MDI vs 4,4 MDI Content

- The reactivity of the isocyanate group in the para-position is about 4 to 6 times higher than that of the ortho-positioned isocyanate group.



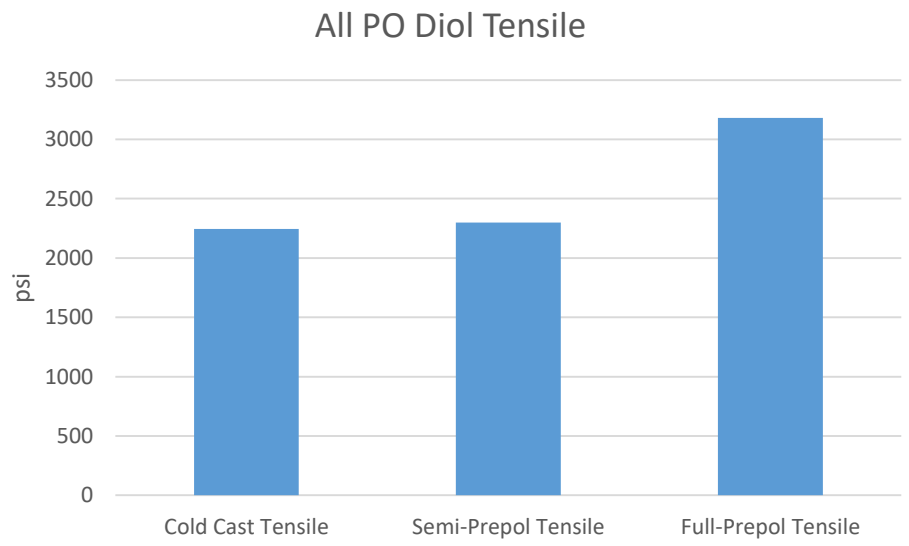
All PO Diol Control

	INGREDIENTS	Percent	Percent	Percent
A-side	All PO Diol 1000 mw	84.0	76.3	0.0
	Dibutyltin dilaurate	0.01	0.01	0.005
	Butanediol	10.0	16.5	81.2
	4 functional ethylenediamine	2.0	2.5	14.8
	Zeolite Sieve 3A	4.0	4.0	4.0
B-Side	CDI-modified 4,4'-MDI	100.0	73.0	44.2
	Azelate 1 (1000 mw)	0.0	27.0	55.8
	Mix Type	**Cold Cast**	**Semi-Prepolymer**	**Full Prepolymer**
	Mix Ratio (vol)	2:1	1:1	1:10
	Iso/Prepol	High 4,4-CMDI	High 4,4 CMDI + PO Diol, NCO=19%	High 4,4 CMDI + PO Diol, NCO=6-7%
	NCO/OH INDEX	1.03	1.04	1.05

Cold Cast	Durometer	Tensile psi	Elongation %	Tear lbf/in	Tabor mg/1000
	87-88 A	2245	128	221	28

Semi-Prepol	Durometer	Tensile psi	Elongation %	Tear lbf/in	Tabor mg/1000
	91 A	2300	134	324	33

Full Prepol	Durometer	Tensile psi	Elongation %	Tear lbf/in	Tabor mg/1000
	90-92 A	3181	156	Not Run	Not Run



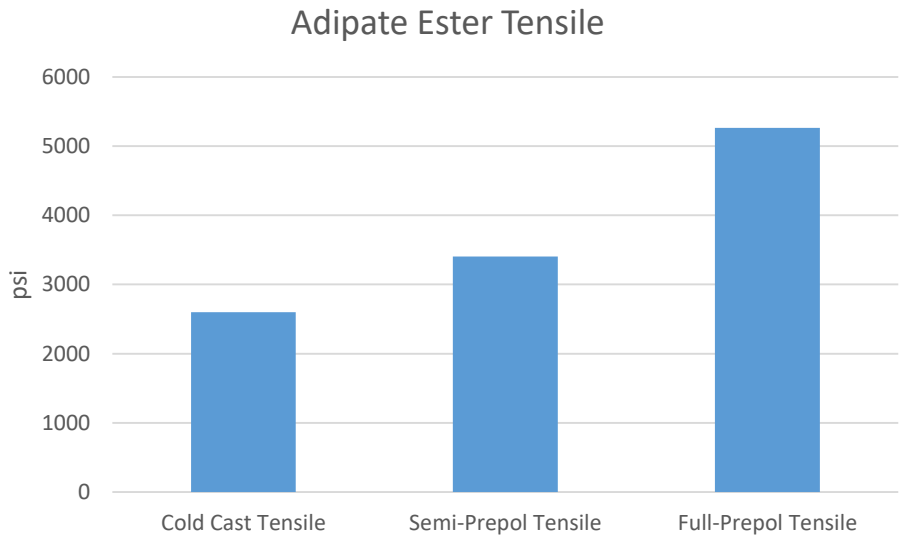
Adipate Ester Control

	INGREDIENTS	Percent	Percent	Percent
B-side	Adipate Ester 1000 mw	86.0	81.5	0.0
	Dibutyltin dilaurate	0.03	0.03	0.005
	Butanediol	7.0	12.0	96.0
	4 functional ethylenediamine	2.0	2.5	0.0
	Zeolite Sieve 3A	4.0	4.0	4.0
A-Side	CDI-modified 4,4'-MDI	100.0	73.0	40.0
	Adipate Ester (1000 mw)	0.0	27.0	60.0
	Mix Type	**Cold Cast**	**Semi-Prepolymer**	**Full Prepolymer**
	Mix Ratio (vol)	2:1	1:1	1:11.9
	Iso/Prepol	High 4,4-MDI	High 4,4 CMDI + Adipate polyol, NCO=19%	High 4,4 CMDI + Adipate polyol, NCO=6-7%
	NCO/OH INDEX	1.01	1.02	1.05

Cold Cast	Durometer	Tensile psi	Elongation %	Tear lbf/in	Tabor mg/1000
	87-88 A	2245	128	221	28.4

Semi-Prepol	Durometer	Tensile psi	Elongation %	Tear lbf/in	Tabor mg/1000
	90 A	3403	178	333	12.43

Full Prepol	Durometer	Tensile psi	Elongation %	Tear lbf/in	Tabor mg/1000
	85 A	5264	335	321	5.67



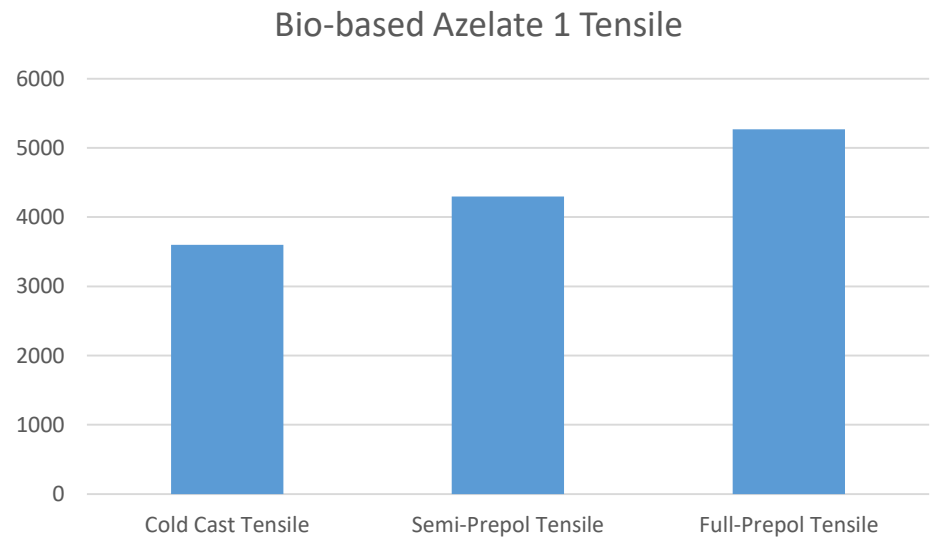
Bio-based Azelate 1

	INGREDIENTS	Percent	Percent	Percent
B-side	Azelate 1 (1000 mw)	85.0	80.4	0.0
	Dibutyltin dilaurate	0.01	0.01	0.010
	Butanediol	9.0	12.0	96.0
	4 functional ethylenediamine	2.0	2.6	0.0
	Zeolite Sieve 3A	4.0	5.0	4.0
A-Side	CDI-modified 4,4'-MDI	100.0	73	41.5
	Azelate 1 (1000 mw)	0.0	27	58.5
	Mix Type	**Cold Cast**	**Semi-Prepolymer**	**Full Prepolymer**
	Mix Ratio (vol)	2:1	1:1	1:11.5
	Iso/Prepol	High 4,4-MDI	High 4,4 CMDI + Azelate 1 polyol, NCO=19%	High 4,4 CMDI + Azelate 1 polyol, NCO=6-7%
	NCO/OH INDEX	1.03	1.06	1.05

Cold Cast	**Durometer**	**Tensile psi**	**Elongation %**	**Tear lbf/in**	**Tabor mg/1000**
	87 A	3600	176	262	7.48

Semi-Prepol	**Durometer**	**Tensile psi**	**Elongation %**	**Tear lbf/in**	**Tabor mg/1000**
	92 A	4300	156	345	4.5

Full Prepol	**Durometer**	**Tensile psi**	**Elongation %**	**Tear lbf/in**	**Tabor mg/1000**
	91 A	5270	219	385	7.7



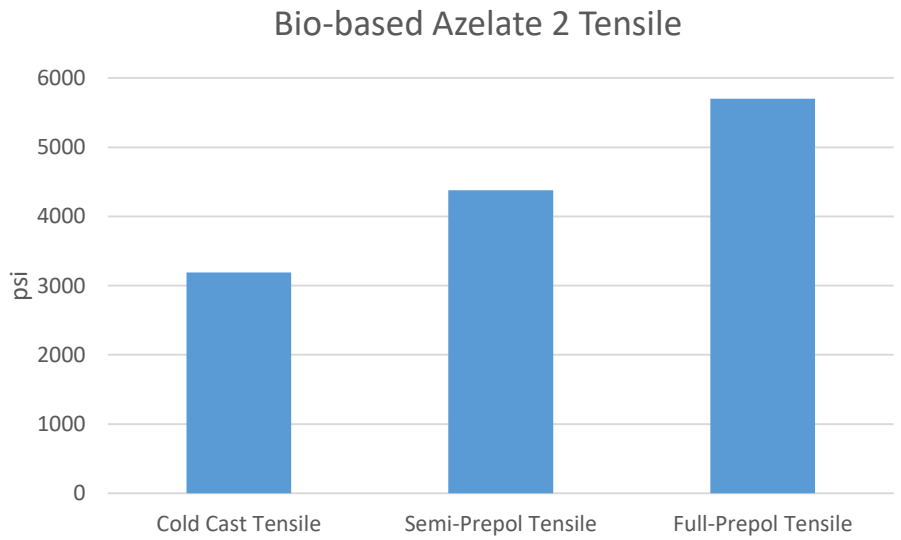
Bio-based Azelate 2

	INGREDIENTS	Percent	Percent	Percent
A-side	Azelate 2 1000 mw	84.0	80.0	0.0
	Dibutyltin dilaurate	0.01	0.01	0.005
	Butanediol	9.0	12.0	96.0
	4 functional ethylenediamine	2.0	3.0	0.0
	Zeolite Sieve 3A	5.0	5.0	4.0
B-Side	CDI-modified 4,4'-MDI	100.0	72.0	41.5
	Azelate 2 (1000 mw)	0.0	28.0	58.5
	Mix Type	**Cold Cast**	**Semi-Prepolymer**	**Full Prepolymer**
	Mix Ratio (vol)	2:1	1:1	1:11.5
	Iso/Prepol	High 4,4-MDI	High 4,4 CMDI + Azelate 2 polyol, NCO=19%	High 4,4 CMDI + Azelate 2 polyol, NCO=6-7%
	NCO/OH INDEX	1.03	1.06	1.05

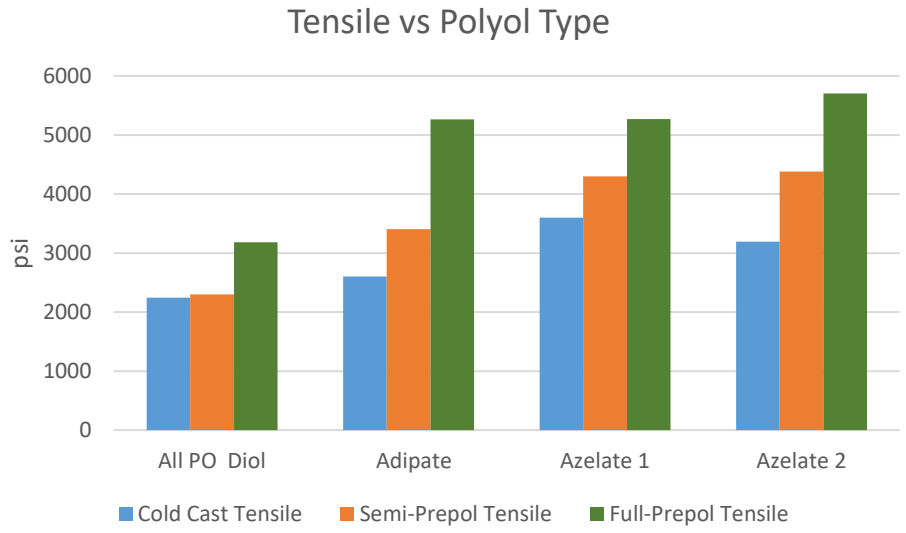
Cold Cast	Durometer	Tensile psi	Elongation %	Tear lbf/in	Tabor mg/1000
	90 A	3192	153	277	10.18

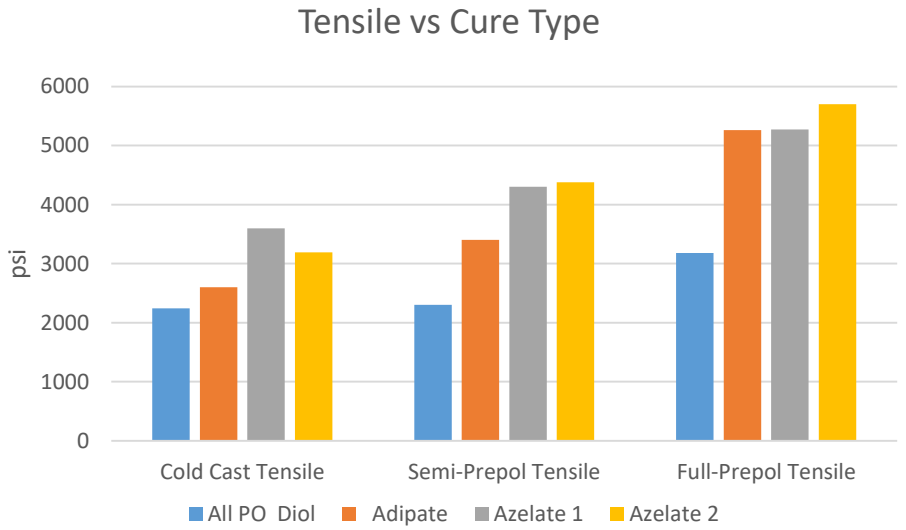
Semi-Prepol	Durometer	Tensile psi	Elongation %	Tear lbf/in	Tabor mg/1000
	91 A	4380	171	331	6.07

Full Prepol	Durometer	Tensile psi	Elongation %	Tear lbf/in	Tabor mg/1000
	91 A	5700	238	408	9.37

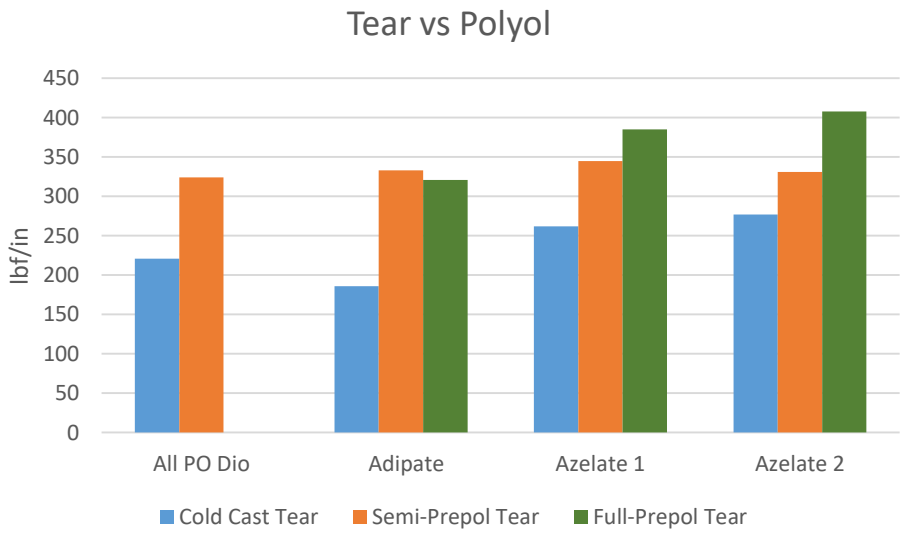


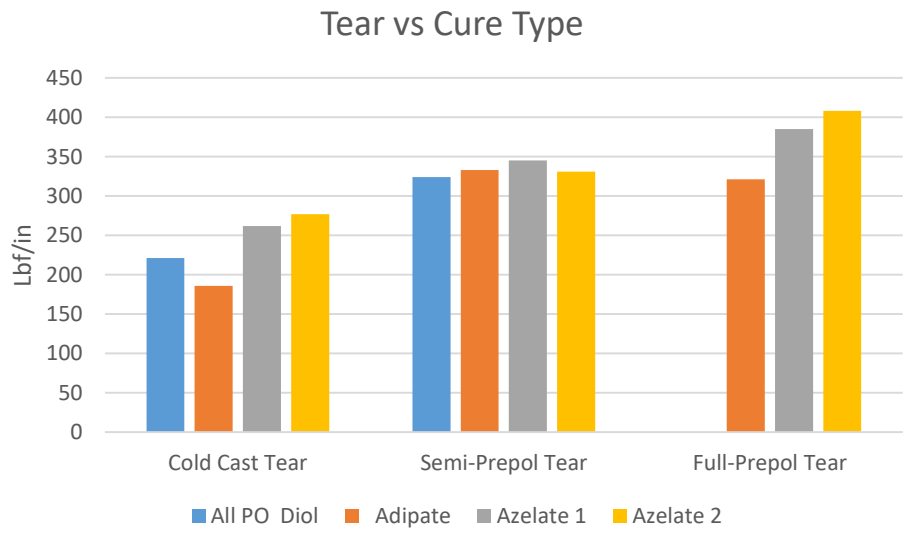
Physical Properties Comparison





Physical Properties Comparison





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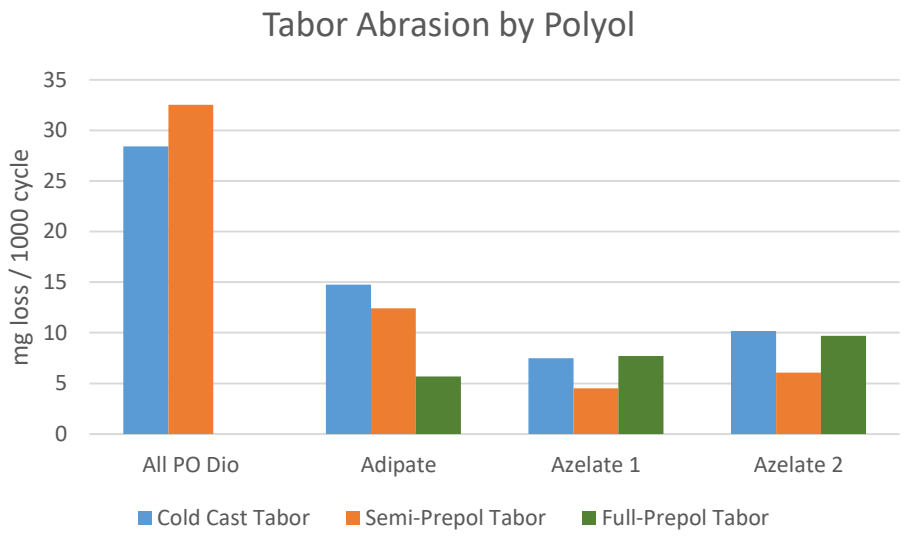

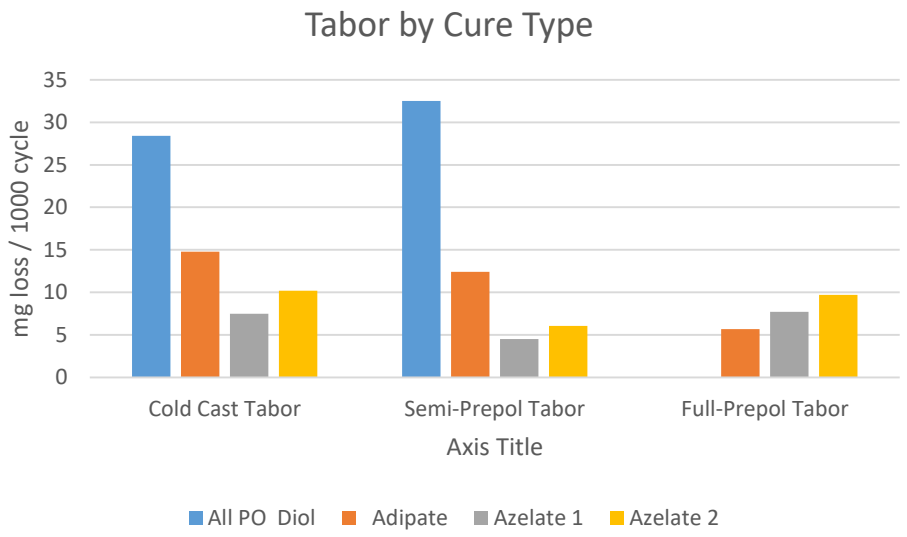

Conclusion

Biobased Polyols are:

- High Tensile
- Low in Color
- Liquid at room temperature

Future Research

- Evaluate 2000 MW Diols
- Evaluate other chain extenders
- Hydrolytic stability

Questions?

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Summary of Results

Main Polyol	Iso/Prepolymer	B side Blend Description	Index	Mix Method	Durometer	Tensile psi	Elongation %	Tear lbf/in	Tabor mg/1000
All PO Diol 1000 mw									
Cold Cast	Carbodiimide Modified 4,4-MDI	All PO Diol, BDO, Quadrol	1.02	Static Mixer 2:1	87-88 A	2245	128	221	28.4
Semi-Prepolymer	prepolymer 7	All PO Diol, BDO, Quadrol	1.04	Static Mixer 1:1	91 A	2300	134	324	32.52
Prepolymer	Prepolymer 77	BDO, Quadrol	1.05	Hand Mix	90-92 A	3181	156	Not Run	Not Run
Adipate Ester 1000 mw									
Cold Cast	Carbodiimide Modified 4,4-MDI	ADP1000,BDO,Quadrol	1.01	Static Mixer 2:1	80 A	2600	226	186	14.77
Semi-Prepolymer	19% NCO Prepolymer 9	ADP1000,BDO,Quadrol	1.02	Static Mixer 1:1	90 A	3403	178	333	12.43
Prepolymer	6-7% NCO Prepolymer 99	BDO	1.04	Hand Mix	85 A	5264	335	321	5.67
Azelate 1 1000 mw									
Cold Cast	Carbodiimide Modified 4,4-MDI	Azelate 1,BDO,Quadrol	1.03	Static Mixer 2:1	87 A	3600	176	262	7.48
Semi-Prepolymer	19% Prepolymer 8	Azelate 1,BDO,Quadrol	1.06	Static Mixer 1:1	92 A	4300	156	345	4.5
Prepolymer	6-7% Prepolymer 88	BDO	1.04	Hand Mix	91 A	5270	219	385	7.7
Azelate 2 1000 mw									
Cold Cast	Carbodiimide Modified 4,4-MDI	Azelate 2,BDO,Quadrol	1.02	Static Mixer 2:1	90 A	3192	153	277	10.18
Semi-Prepolymer	19% Prepolymer 9	Azelate 2,BDO,Quadrol	1.04	Static Mixer 1:1	91 A	4380	171	331	6.07
Prepolymer	6-7% Prepolymer 99	BDO	1.04	Hand Mix	91 A	5700	238	408	9.37

Appearance Additional

	Dimer Acid	PO Diol	Adipate	Azelate 2	Azelate 1
Hazen	>1000	3	23	68	62
Gardner	6.7	0	0.1	0.3	0.3

Physical Properties Considered in this Study

- Tensile
- Tear
- Elongation
- Tabor Abrasion
- Durometer