Polycaprolactone Polyols in 2K Polyurethane Coatings

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Coatings Trends & Technologies SUMMIT

AGENDA

1. Introduction to Ingevity
2. Chemistry of Polycaprolactone Polyols
3. Experimental Study
4. Results and Discussion
5. Conclusions

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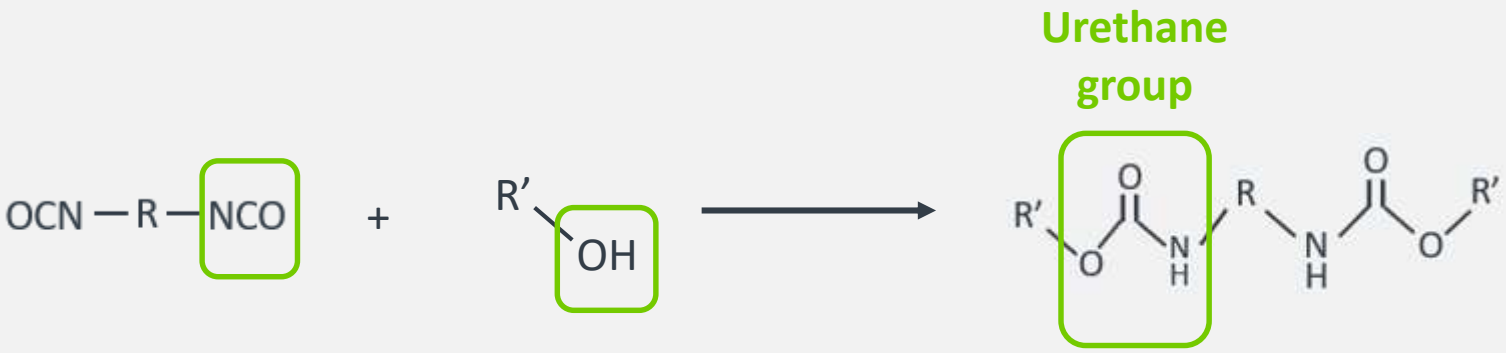
Introduction

Polyurethane Coatings

High performance, versatile coatings

Polyurethane reaction mechanism

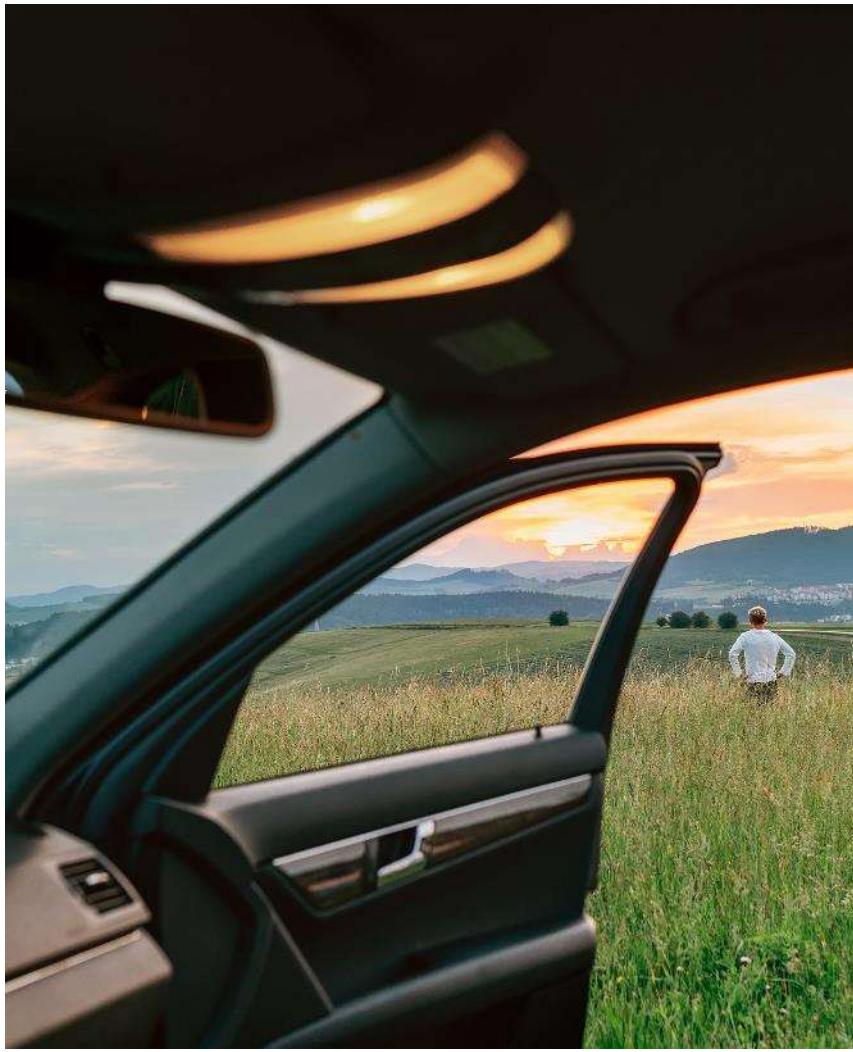


Diisocyanate

Polyol

Polyurethane

A polyurethane is created by reacting an **alcohol (polyol)** with a **diisocyanate**.



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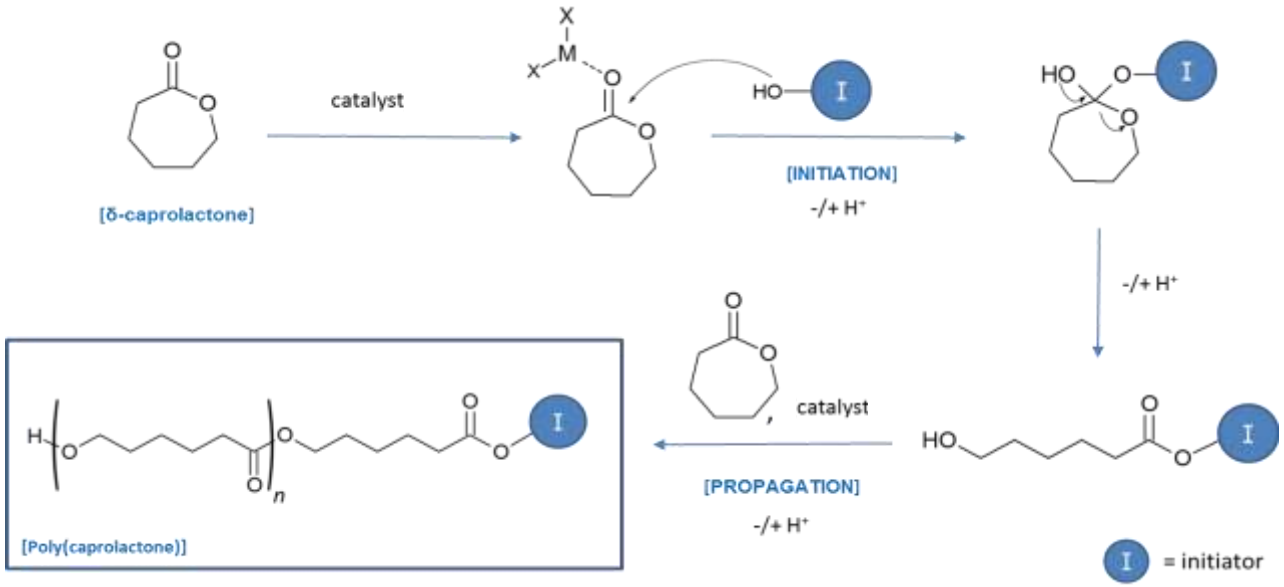
Polycaprolactone (PCL) Polyols



- Made *via* **ring opening polymerization**
- **No by-products**
- Very **low acid values** and water content
- Controlled polymerization – **all hydroxyls are primary**
- Very **narrow polydispersity**

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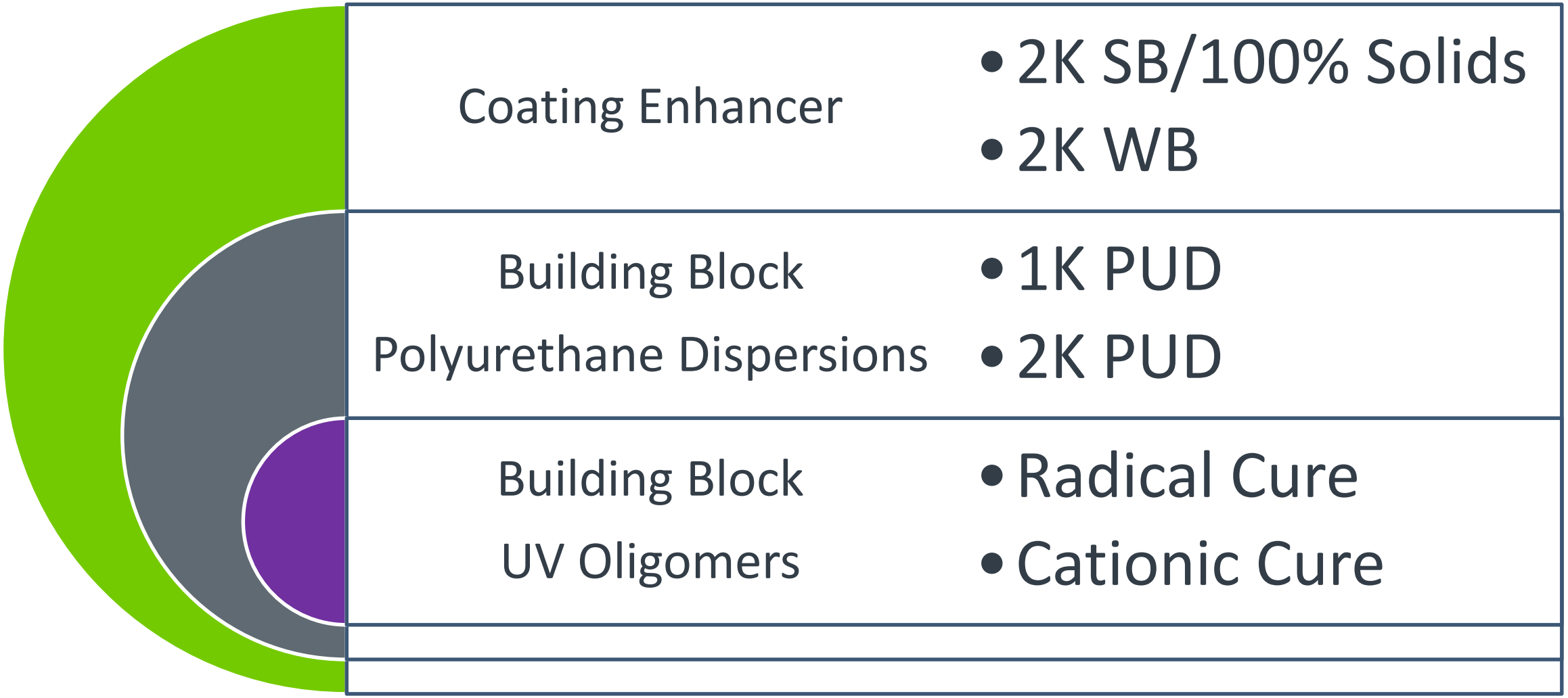
PCL Polyol Uses in Coatings



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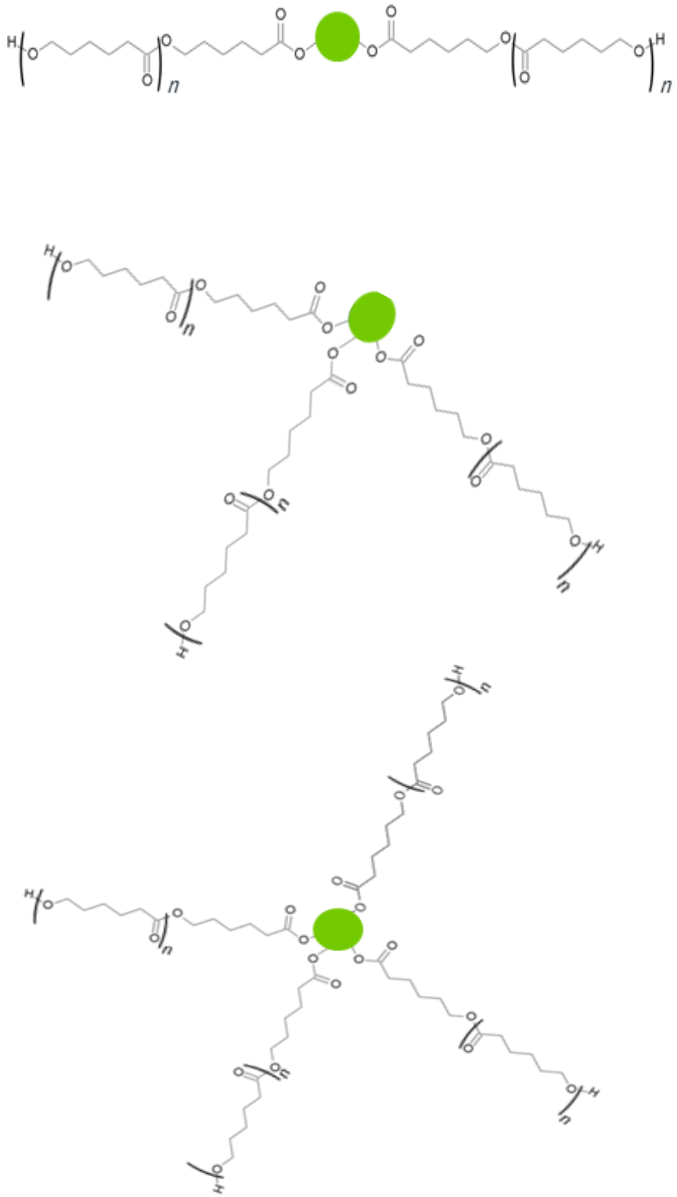
Experimental

Polyols Used for Testing

Polyol	M_w	Functionality	Solid Content (%)	Viscosity (mPa·s @ 25°C)
Acrylic polyol	1073	2.0	70	3000
PCL diol	400	2.0	100	240
PCL triol A	300	3.0	100	1600
PCL triol B	500	3.0	100	1200
PCL triol C	900	3.0	100	1250
PCL tetrol	1000	4.0	100	1800
Polyester adipate diol	400	2.0	100	705



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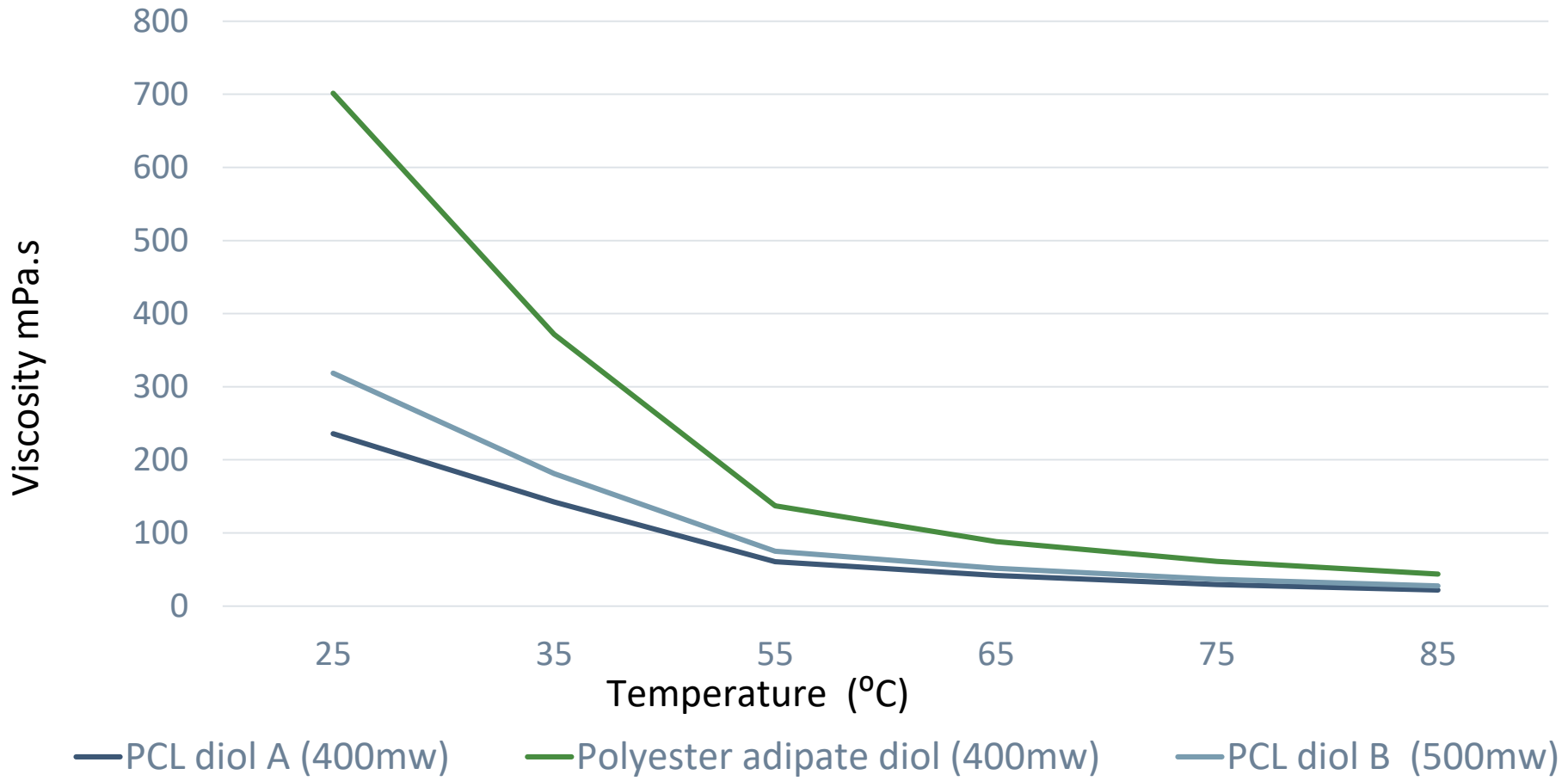
Polyol Properties



Lower viscosity enables higher solids (and lower VOCs)

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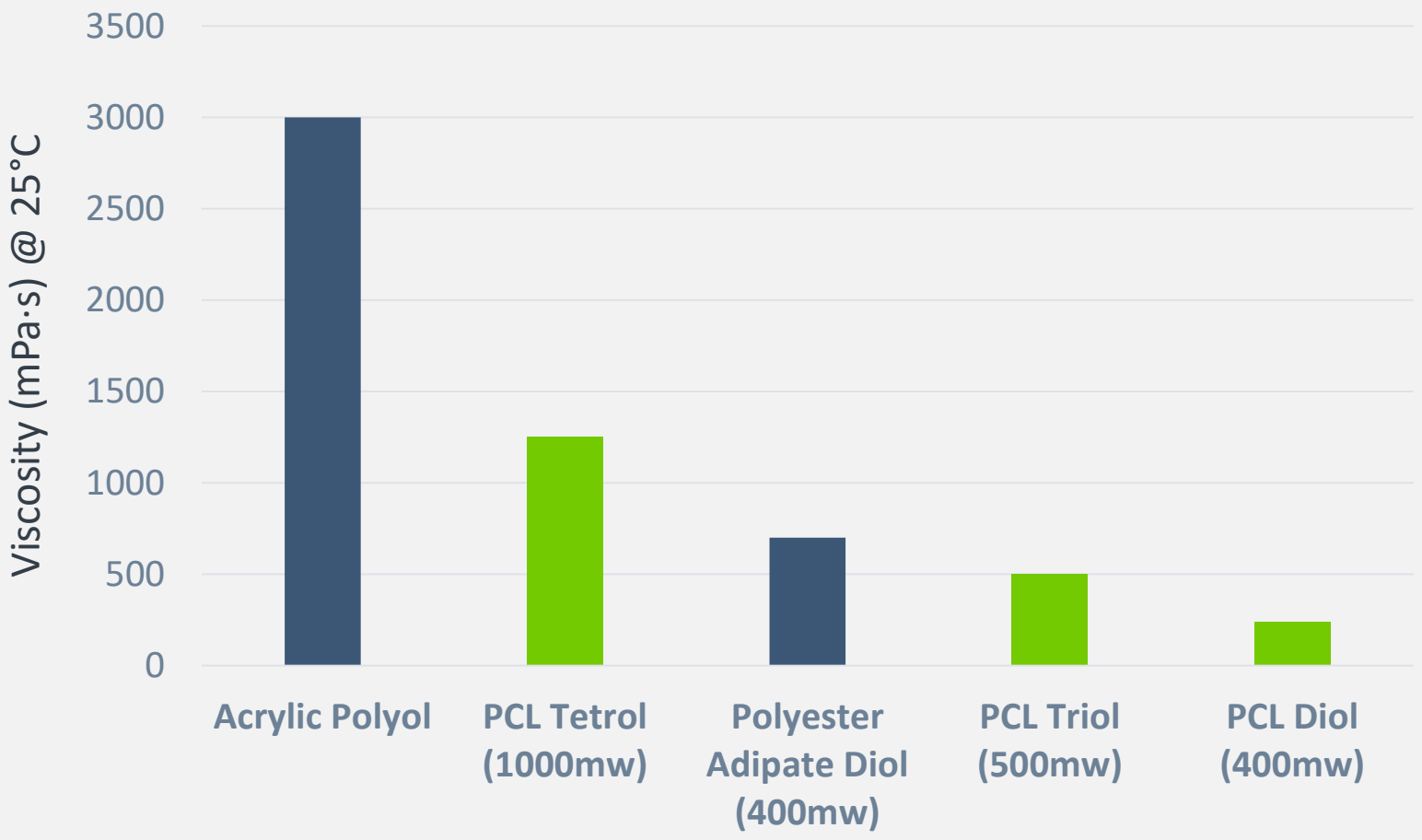
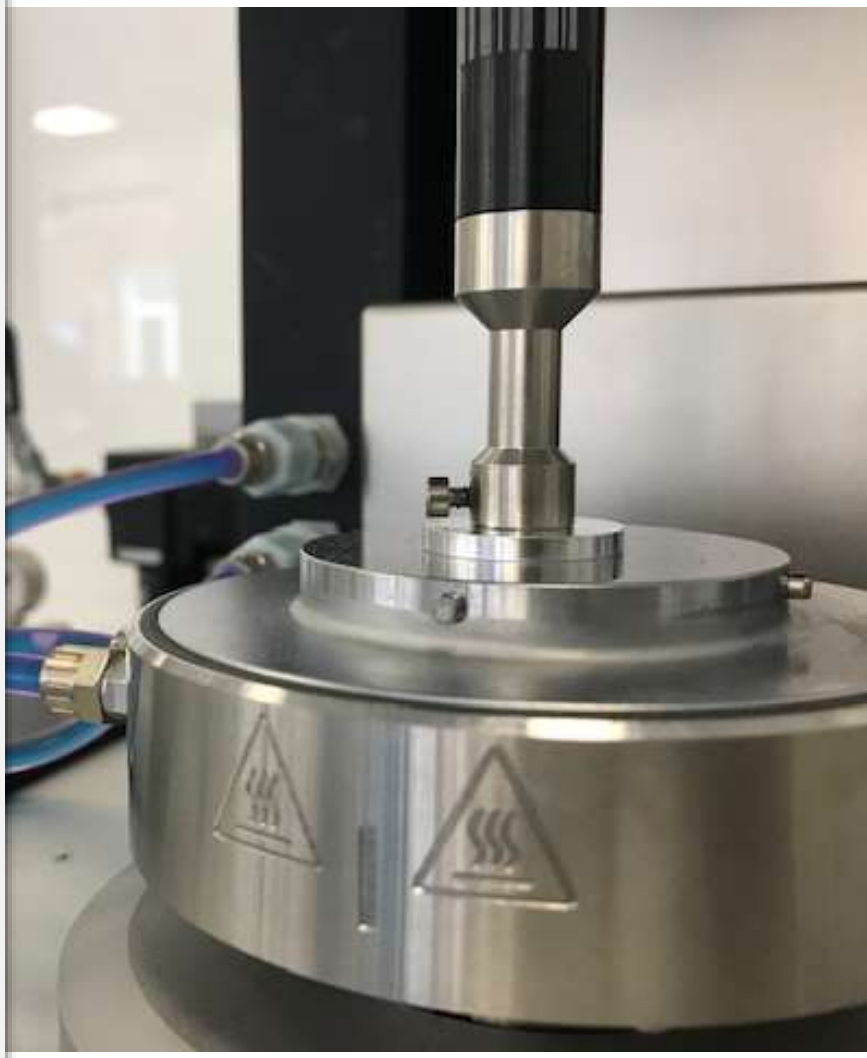
Polyol Properties

Viscosity differences at room temperature





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Experimental Formulation

Raw Material	Function	Weight % (in total formulation)
Hydroxyl functional Acrylate	Solventborne acrylic polyol	57
PCL triol C (900mw)	**Polycaprolactone polyol**	**6**
Add above in order under medium shear mixing. Mix for 10 minutes.		
Defoamer additive	Defoamer	0.75
Wetting agent additive	Wetting agent	0.25
DBTL (10% in butyl acetate)	Catalyst	1
Xylene/Butyl Acetate/MPA (1:1:1)	-	9
Add above in order under medium shear mixing. Mix for 10 minutes.		
HDI based Diisocyanate	Crosslinker	21
Butyl Acetate/Xylene (1:1)	-	5

Weight solids: 67% Viscosity: 45-55 cps Isocyanate index: 1.00

Application Parameters

Method of Application	D.F.T (Dry film thickness - µm)	Substrates	Environmental
K- Bar – 100 µm	50-55 µm	Degreased Aluminum, Degreased Mild Steel	23°C ± 3°C 50% RH ± 5%

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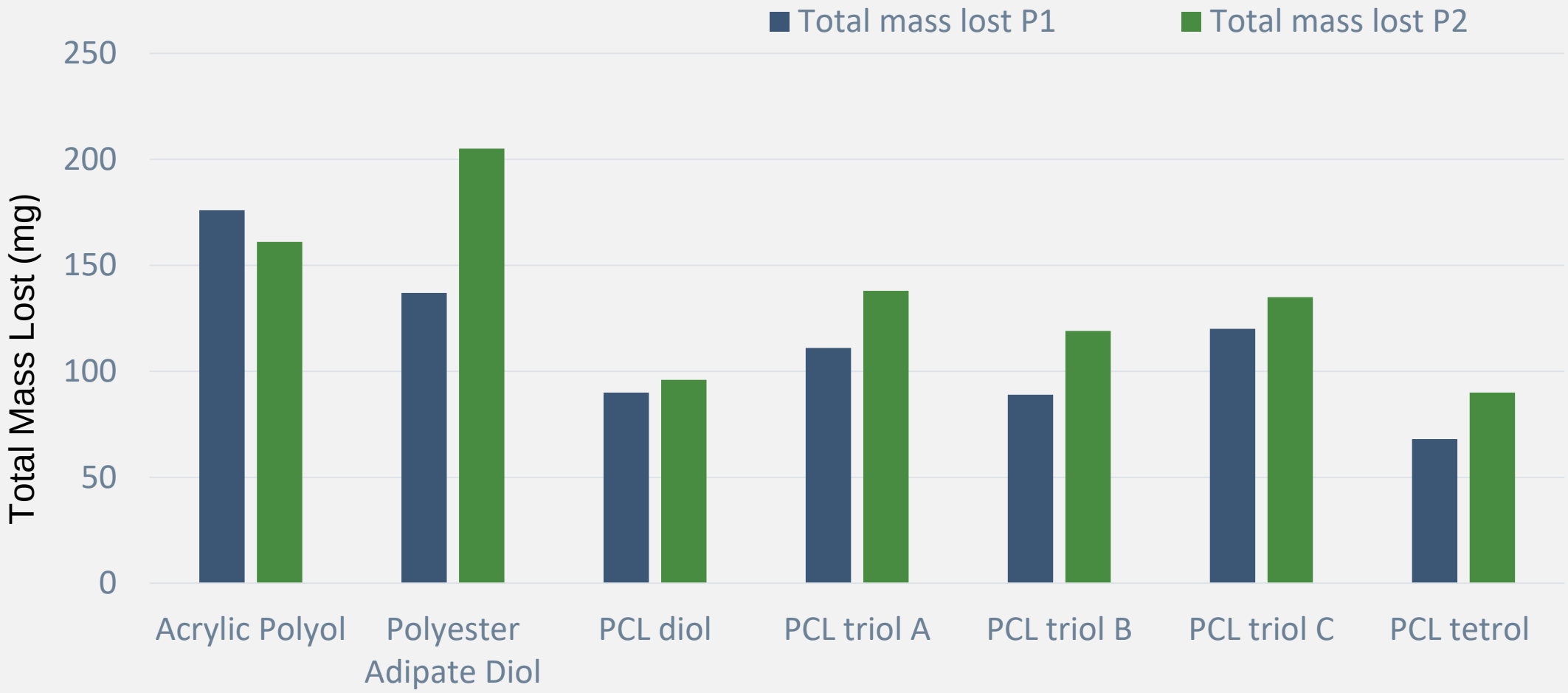
Results & Discussion

Taber® Abrasion Testing



- Acrylic-based 2K coatings modified with PCL polyols show **improved abrasion resistance**
- **Increased cross-linking**, provided by the PCL tetrol, shows the best results

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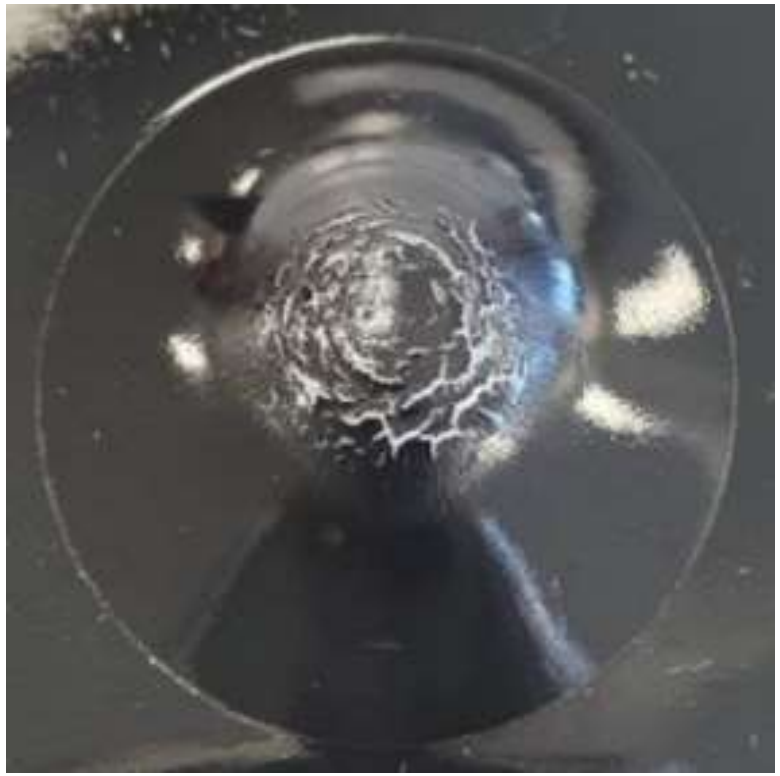
Rapid Deformation Impact Resistance Test (ISO 6272-1)

Acrylic Polyol

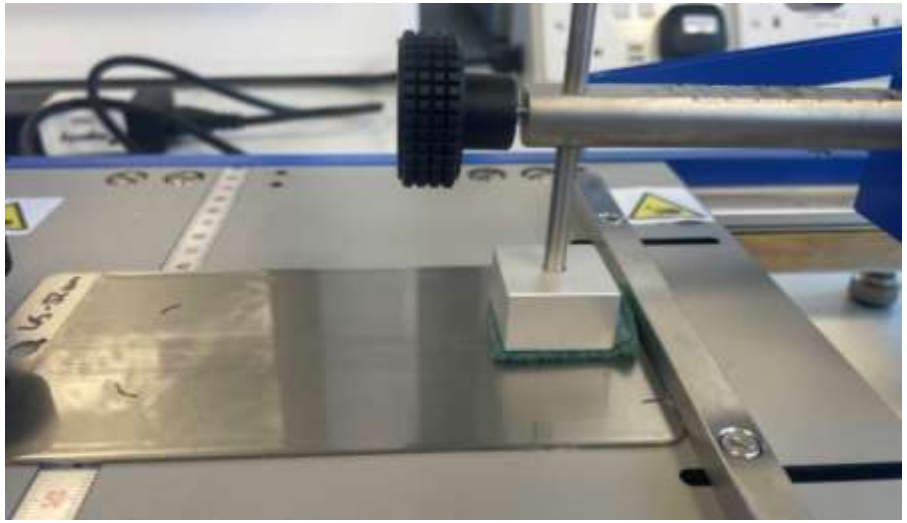


Acrylic Polyol + PCL Diol

Acrylic Polyol + Polyester Adipate Diol

Enhancement with PCL polyols give improved indirect impact resistance

Mar Resistance



40 Double Rubs with a Scrub Pad

Acrylic Polyol + PCL diol

Acrylic Polyol

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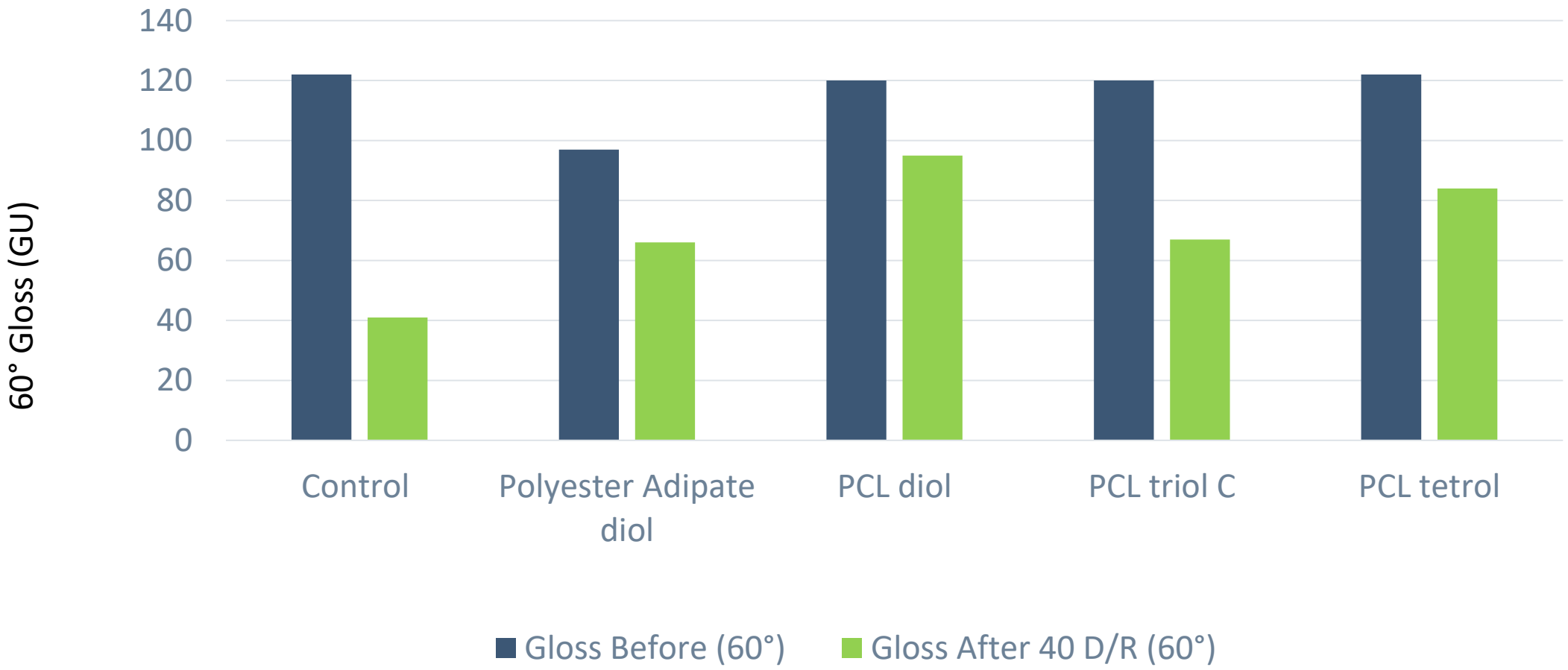
Mar Resistance – Pre & Post Rub



PCL diol showed the best resistance to gloss reduction

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Gloss Recovery – Post Rub

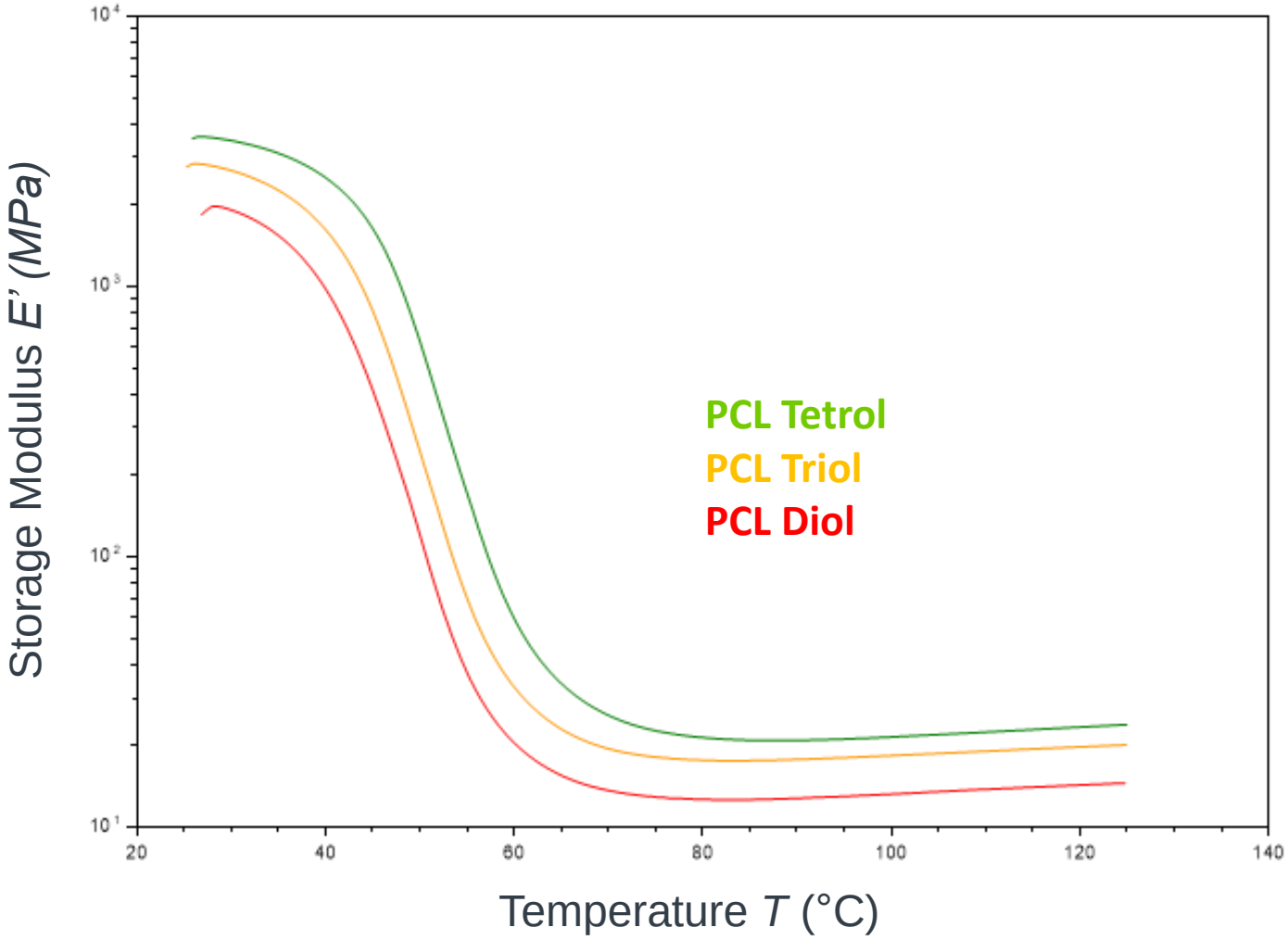
- PCL triol showed the largest gloss recovery
- PCL diol and PCL tetrol showed the best abrasion resistance
- Longer chains present in PCL triol help chain mobility

Intrinsic Self-Healing Properties

Polyol Used	40 Scotch-Brite® Double Rubs	5 mins @ 50°C	10 mins @ 50°C
Acrylic Polyol			
Acryic polyol + **PCL triol**			

2.5X magnification

DMA (Dynamic Mechanical Analysis) – Crosslinking Density



- The degree of crosslinking is related to the storage modulus (E') at the rubbery plateau region.
- The value of the rubbery plateau region can be closely related to the chain entanglement.

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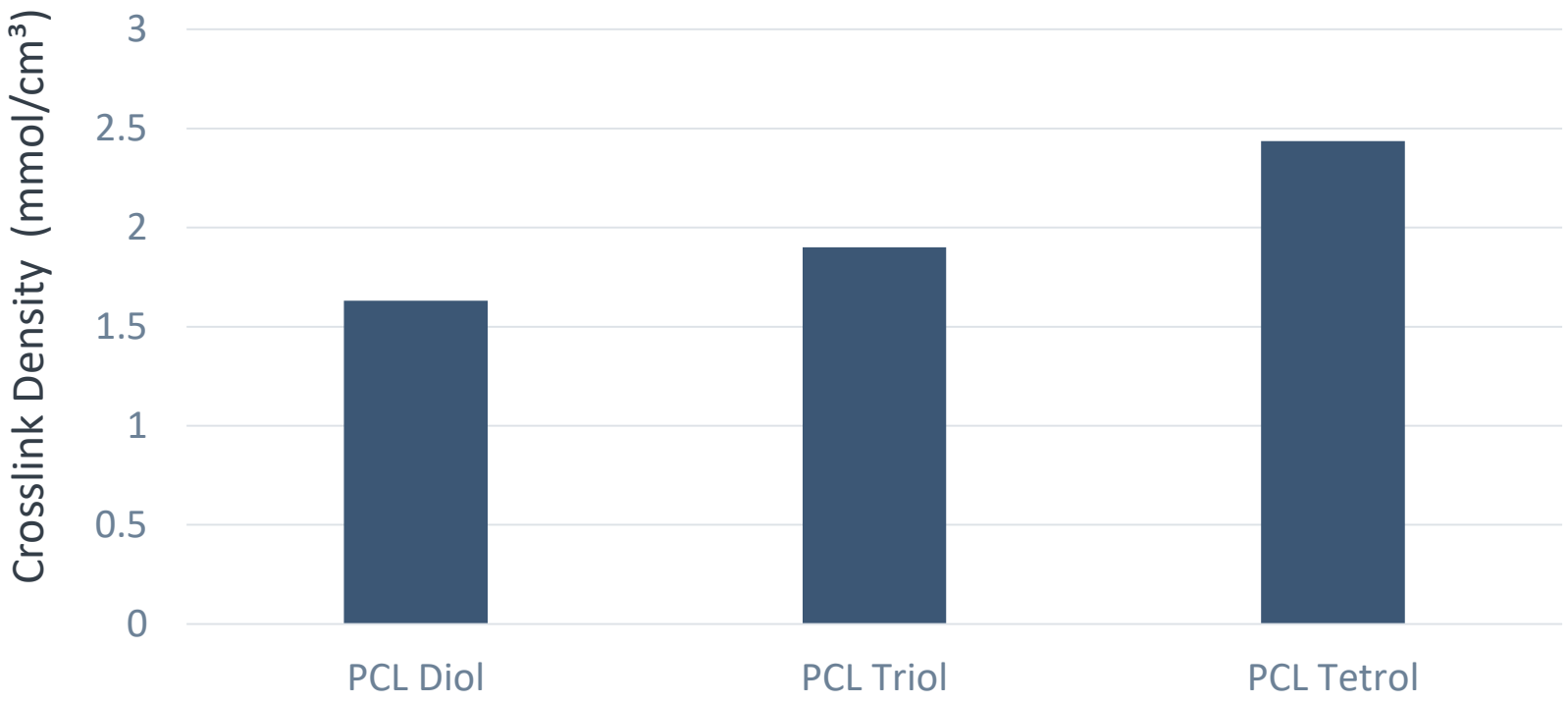

PCL tetrol promotes better chemical resistance

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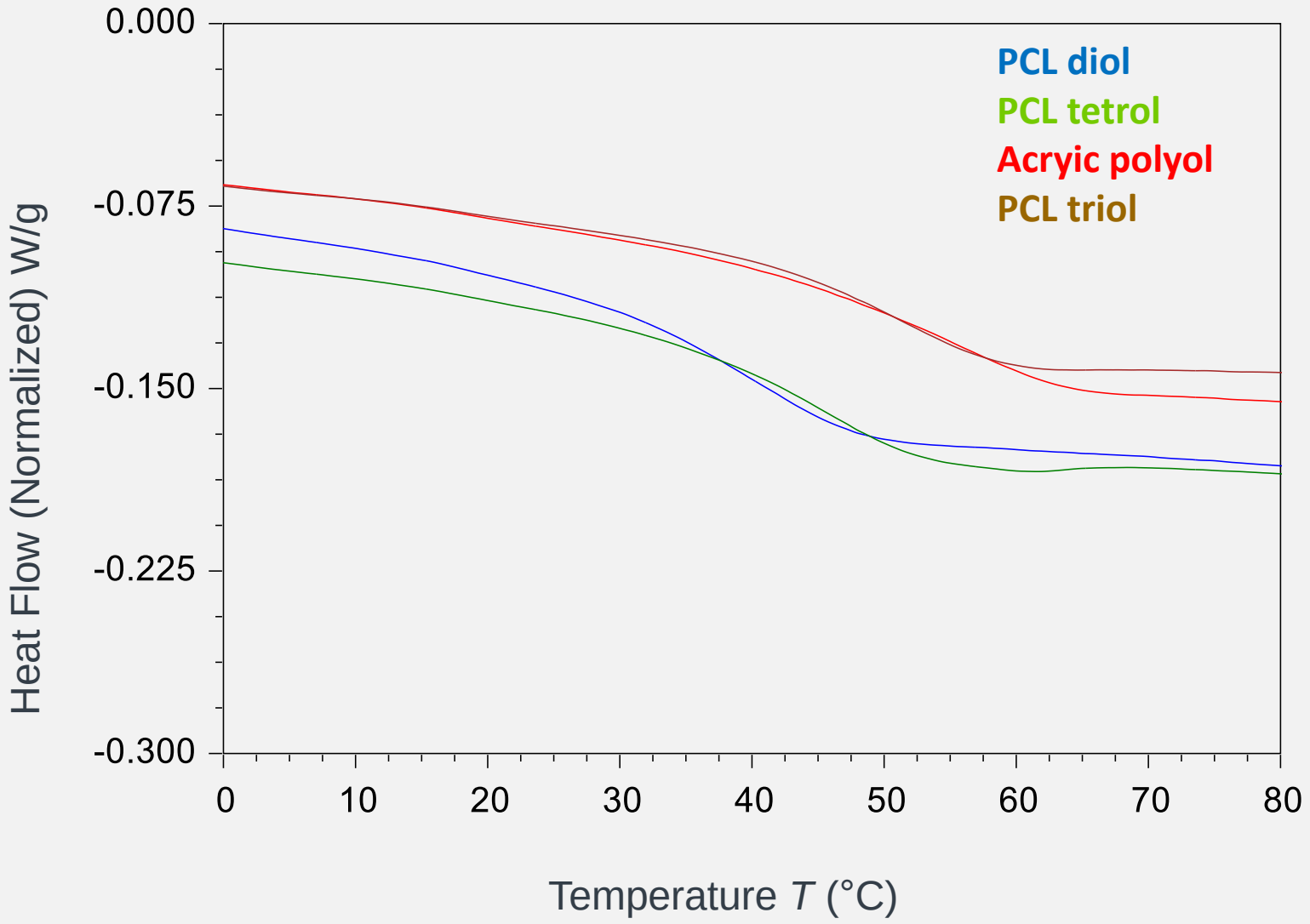
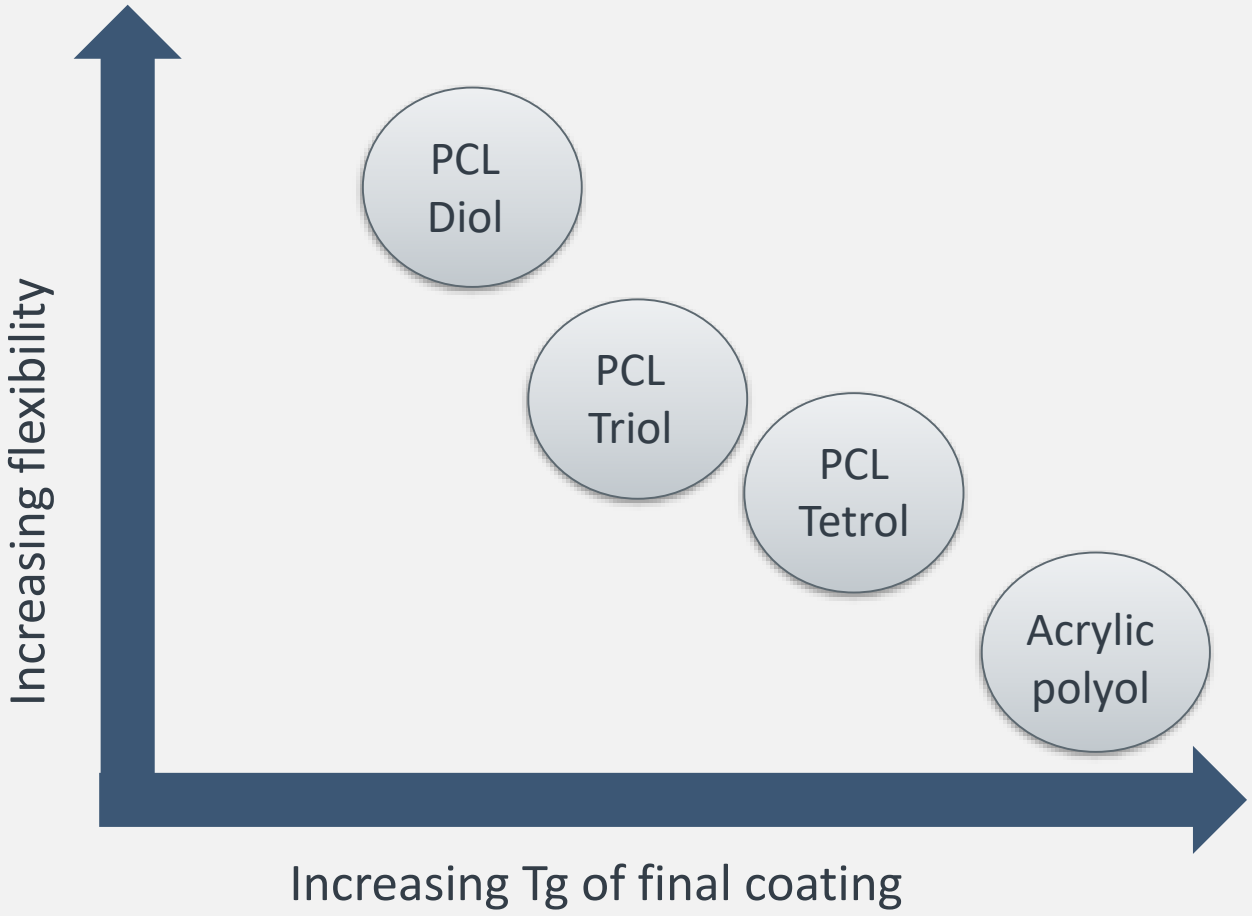
DSC Analysis (Differential Scanning Calorimetry)



Test Method:

1. Heat 10°C/min to 100°C
2. Cool 10°C/min to -50°C
3. Heat 10°C/min to 100°C
4. Cool 10°C/min to -50°C

Tg Impact - Improved Low Temperature Performance



- **PCL diol** shows the largest reduction in T_g of the coating 2K coating system
- **A lower T_g** of the coating helps **durability** at **lower temperatures** and influences **crack bridging properties**
- **PCL tetrol** has a good balance of reducing the T_g while **incorporating cross-linking**

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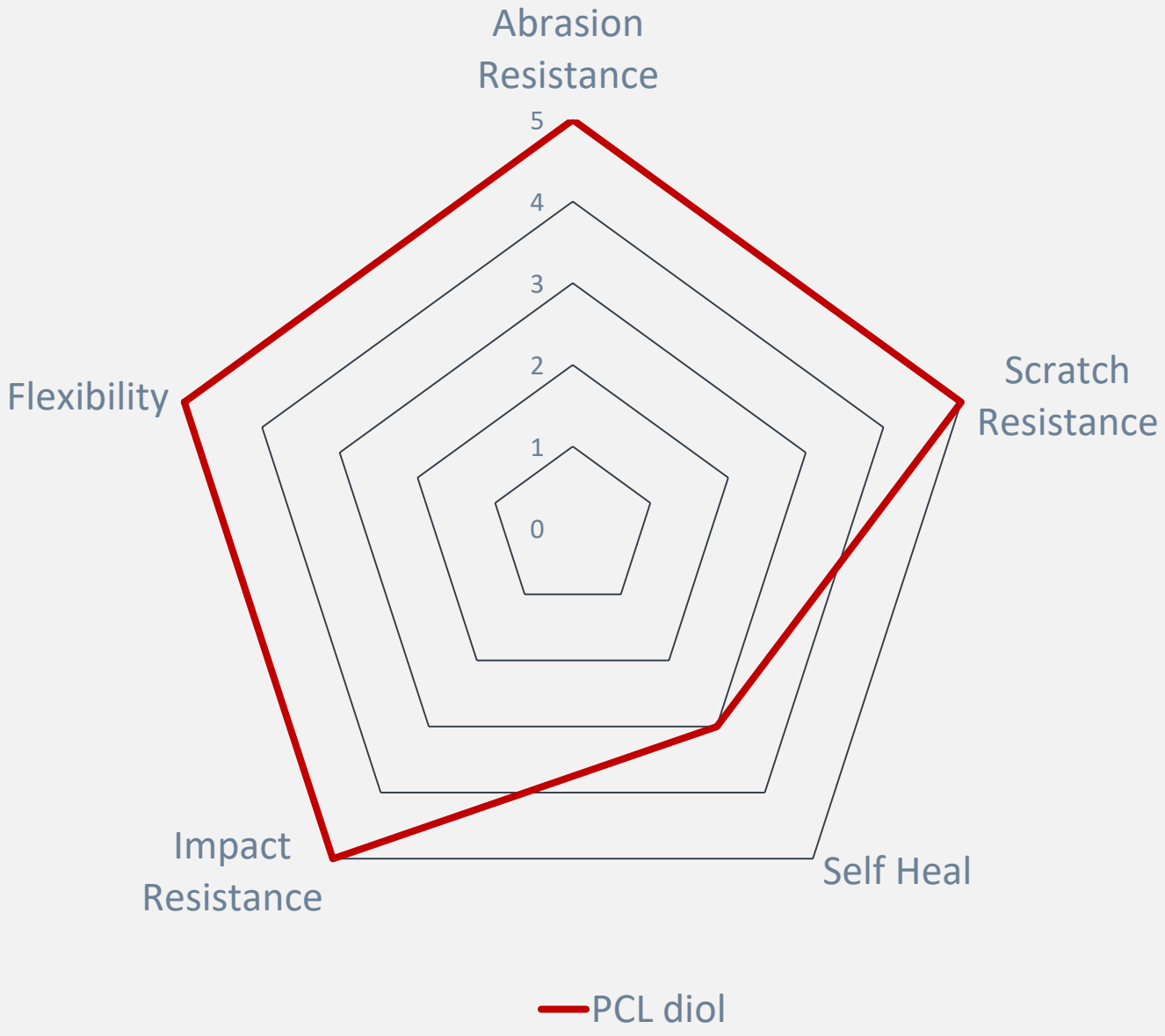
Polycaprolactone Polyol Properties – Summary

- **PCL diols** improve **impact resistance**, and can help improve **resistance to wear** mechanisms



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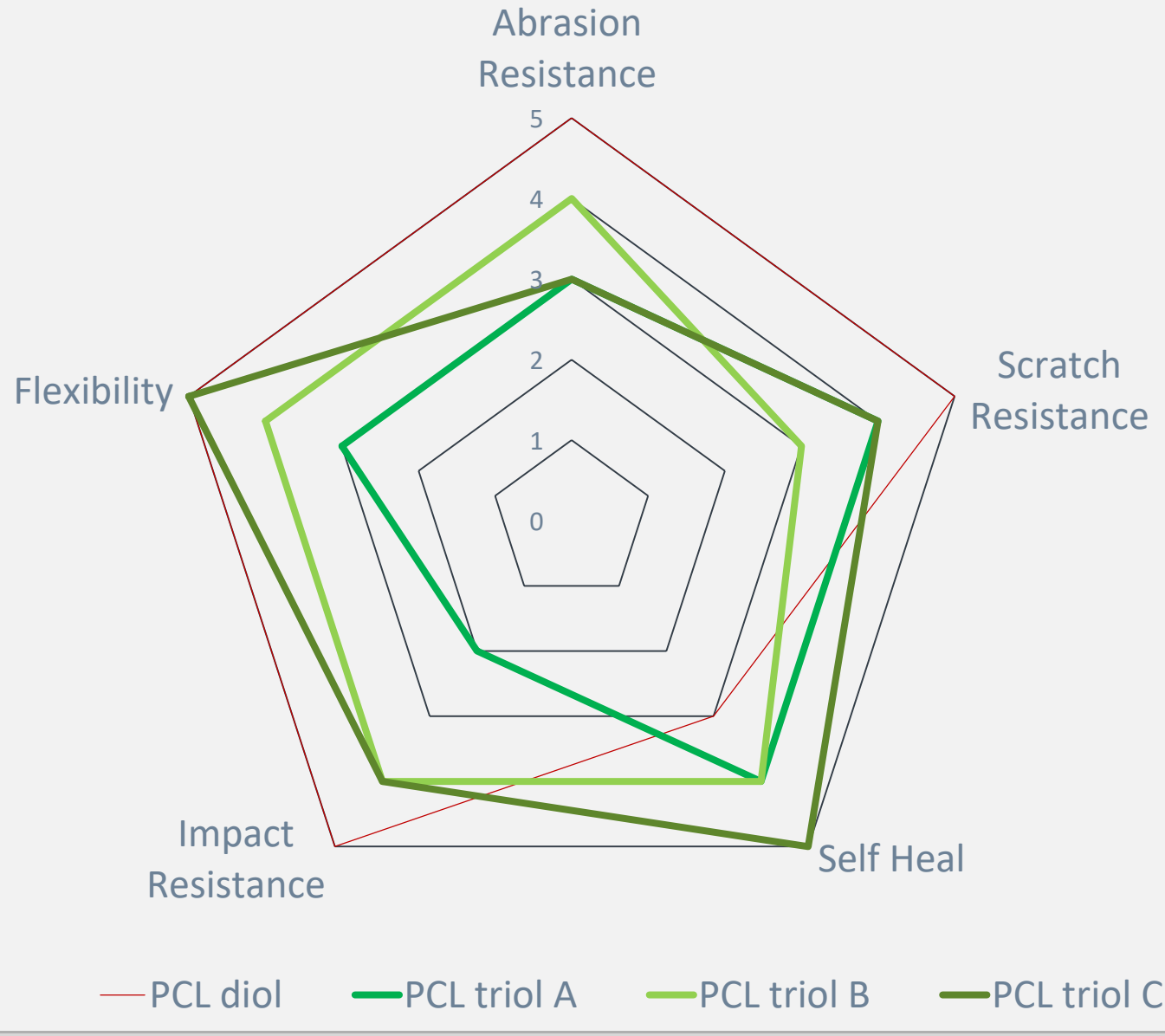
Polycaprolactone Polyol Properties – Summary

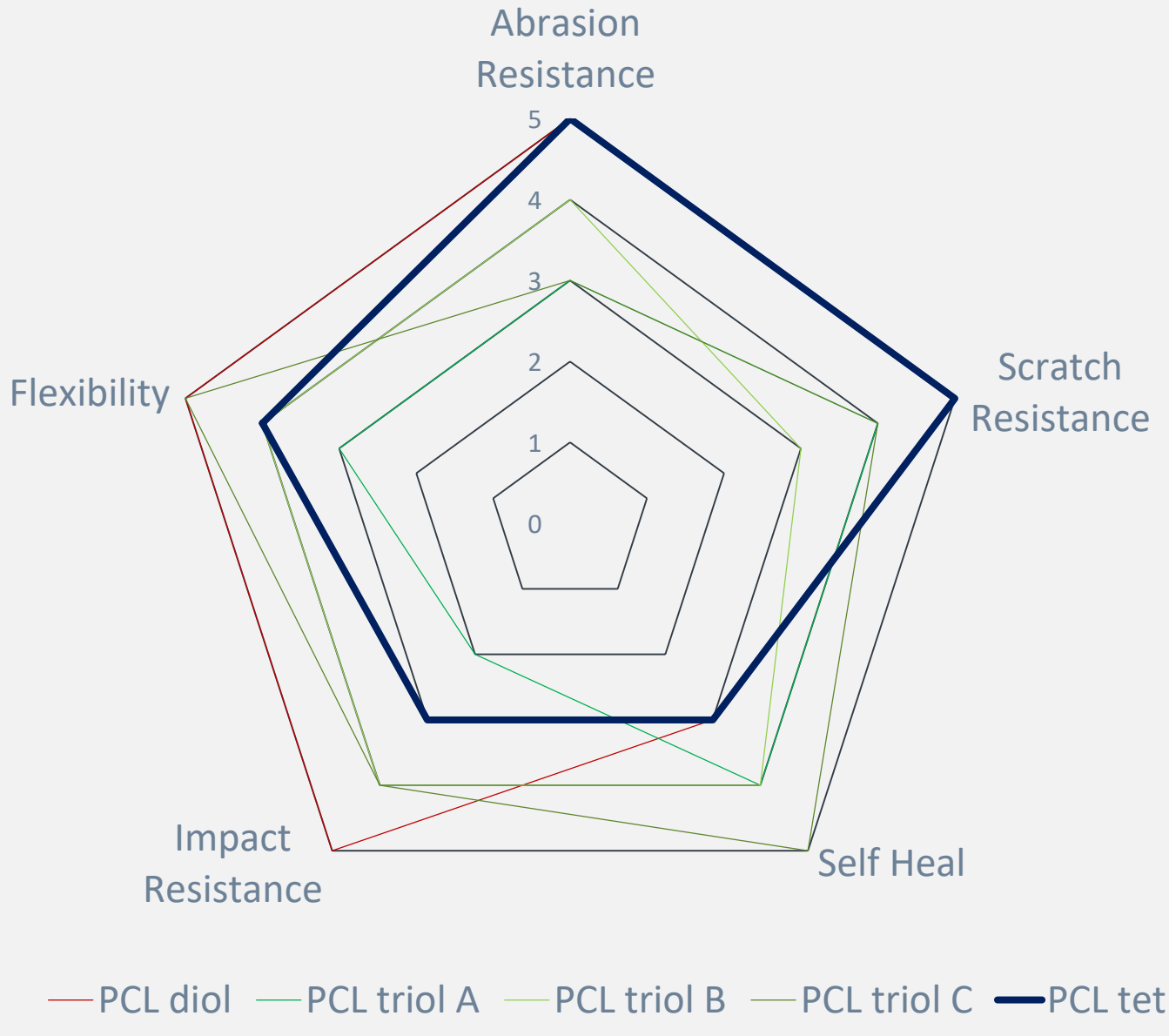
- **PCL diols** improve **impact resistance**, and can help improve **resistance to wear** mechanisms

- **PCL triols** will **improve crosslinking**, along with adding **flexibility** – this can help **adhesion**



Polycaprolactone Polyol Properties – Summary

- **PCL diols** improve **impact resistance**, and can help improve resistance to **wear** mechanisms
- **PCL triols** will **improve crosslinking**, along with adding **flexibility** – this can help **adhesion**
- **PCL tetrol** can help improve with its additional cross-linking but greatly improve **chemical resistance**



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THANK YOU