Polyester in PU

Presented by
Wally Chang, Ph.D.

Coim USA Inc.
PU Applications

1. Foams
   a. Flexible Foams
   b. Rigid Foams

2. CASE
   a. Coatings
   b. Adhesives
   c. Sealants
   d. Elastomers
Polyester

Foam

CASE
### Physical Properties of Polyurethane

**Comparison between Polyester and Polyether**

<table>
<thead>
<tr>
<th>Property</th>
<th>Ester</th>
<th>Ether</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wear resistance</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>Load bearing</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>Tensile strength</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>Tear strength</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>Heat resistance</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>Solvent resistance</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>Oxidative resistance</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>Radiation stability</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>UV resistance</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>Biodegradability</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>Weathering resistance</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>Crystallization rate</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>Adhesion to substrate</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>Flame lamination</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>Energy absorption</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>Hysteresis</td>
<td></td>
<td>+</td>
</tr>
<tr>
<td>Resilience</td>
<td></td>
<td>+</td>
</tr>
<tr>
<td>Low temperature flexibility</td>
<td></td>
<td>+</td>
</tr>
<tr>
<td>Hydrolytic stability</td>
<td></td>
<td>+</td>
</tr>
<tr>
<td>Fungus resistance</td>
<td></td>
<td>+</td>
</tr>
<tr>
<td>Viscosity of prepolymer</td>
<td></td>
<td>+</td>
</tr>
</tbody>
</table>
Urethane

\[ \text{NCO} + \text{HO} \rightarrow \text{NH-C-O} \]

Polyurethane
Urea

NCO + H₂N → Polyurea
Bubble Formation

The Reaction of Isocyanates with Water

\[ \text{NCO} + \text{H}_2\text{O} \rightarrow \text{OCN} \]

\[ \text{NH}_2\text{C} \equiv \text{OH} \]

\[ \text{NH}_2\text{C} \equiv \text{NH} + \text{C} = \text{C} = \text{O} \]

Polyurea
Isocyanurate

Polyisocyanurate
Morphology

Hard domains

Soft matrix
Main Polyols for Polyurethane Application

1. Polyester Polyol
   a. PES (Diacid Based)
   b. PCL (Polycaprolactone)

2. Polyether Polyol
   a. PPG (Polypropylene Glycol)
   b. PEG (Polyethylene Glycol)
   c. PTMG (Polytetramethylene Glycol)

3. PCG (Polycarbonate Glycol)
Polyester

Ester Group
Polyether

Ether Group
Polycarbonate

Carbonate Group
Polyesterification

\[
\begin{align*}
\text{HO-R-OH}^+ &+ \text{HO-C-(CH}_2\text{)}_x\text{-C-OH} \\
\xrightarrow{(200 - 260 \degree C)} \\
\text{HO-R-O-[C-(CH}_2\text{)}_x\text{-C-O-R-O]}_n \text{H}^+ \text{ H}_2\text{O} \\
\text{DP} &= 2 \times n + 1
\end{align*}
\]
Raw Material Diols

- **Diethylene Polyol (DEG)**: 
  \[
  \text{CH}_2\text{CH}_2 - \text{O} - \text{CH}_2\text{CH}_2
  \]

- **Ethylene Polyol (EG)**: 
  \[
  \text{CH}_2\text{CH}_2\text{OH} \quad \text{OH}
  \]

- **Propylene Polyol (PG)**: 
  \[
  \text{CH}_2\text{CH} - \text{CH}_3
  \]

- **1,4-Butanediol (1,4BD)**: 
  \[
  \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OH} \quad \text{OH}
  \]

- **Neopentyl Polyol (NPG)**: 
  \[
  \text{HO} - \text{CH}_2\text{C} - \text{CH}_2 - \text{OH}
  \]

- **1,6-Hexanediol (1,6HD)**: 
  \[
  \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OH} \quad \text{OH}
  \]
Raw Material Diacids

Adipic Acid (AA)

Phthalic Anhydride (PA)
Isophthalic Acid (IA)
Terephthalic Acid (TA)
Raw Material Triols

Trimethylolpropane (TMP)

Glycerin (GLY)
Functionality of Polyesters

HO-R-OH+ \text{HO-C-(CH}_2\text{)}_4\text{C-OH}

\text{CH}_2\text{—OH}
\text{CH—OH}
\text{CH}_2\text{—OH}
Glycerin (GLY)

HO

OH

OH
W.L. Chang's equation

\[ f = \frac{2}{1 - (n - 2) \frac{EW}{Y}} \]

- \( f \): functionality of prepolymer
- \( n \): functionality of modifier (branched raw material)
- \( EW \): equivalent weight of prepolymer
- \( Y \): yield of prepolymer based on one mole of modifier

### Polyester formulation and calculated functionality

<table>
<thead>
<tr>
<th></th>
<th>grams</th>
<th>grams</th>
</tr>
</thead>
<tbody>
<tr>
<td>EG</td>
<td>344.3</td>
<td>1,033</td>
</tr>
<tr>
<td>TMP(n=3.0)</td>
<td>44.67</td>
<td>134</td>
</tr>
<tr>
<td>AA</td>
<td>811</td>
<td>2,433</td>
</tr>
<tr>
<td>Organotin catalyst</td>
<td>0.04</td>
<td>0.12</td>
</tr>
<tr>
<td>Total weight</td>
<td>1,200</td>
<td>3,600</td>
</tr>
<tr>
<td>H2O</td>
<td>-200</td>
<td>-600</td>
</tr>
<tr>
<td>Yield</td>
<td>1,000</td>
<td>3,000</td>
</tr>
<tr>
<td>OH#</td>
<td>56.1</td>
<td>56.1</td>
</tr>
<tr>
<td>f</td>
<td></td>
<td>3.0</td>
</tr>
</tbody>
</table>

**Calculation of functionality**

\[
EW = \frac{56100}{56.1} = 1000 \quad Y = 3000
\]

\[
f = \frac{2}{[1-(3-2)\frac{1000}{3000}]} = 3.0
\]
# MDI-prepolymer formulation and calculated functionality

<table>
<thead>
<tr>
<th></th>
<th>grams</th>
<th>grams</th>
</tr>
</thead>
<tbody>
<tr>
<td>PEAG-2000</td>
<td>940</td>
<td>4,198.7</td>
</tr>
<tr>
<td>TMP(n=3.0)</td>
<td>30</td>
<td>134.0 (1 mole)</td>
</tr>
<tr>
<td>MDI</td>
<td>350</td>
<td>1,563.3</td>
</tr>
<tr>
<td>Yield</td>
<td>1,320</td>
<td>5,896.0</td>
</tr>
<tr>
<td>NCO%</td>
<td>3.78%</td>
<td>3.78%</td>
</tr>
<tr>
<td>f</td>
<td></td>
<td>2.46</td>
</tr>
</tbody>
</table>

## Calculation of functionality

\[
EW = \frac{4202}{3.78} = 1110.8 \quad Y = 5896.0
\]

\[
f = \frac{2}{[1-(3-2)1110.8/5896.0]} = 2.46
\]
Polyester Preparation

I. Uncatalyzed polyesterification

II. Catalyzed polyesterification

1. Tin compounds
2. Titanium compounds
3. Others
Side Reactions of Polyester Preparation

Unsaturated End Group Formation

\[
\text{CH-OH} \quad \xrightarrow{\Delta} \quad \text{CH} = \text{CH}_2 + \text{H}_2\text{O}
\]

\[
\text{CH}_3
\]

\[
\text{O} \quad \equiv \quad \text{O} - \text{CH}_2\text{CH}_2 - \text{O} - \text{C} - \quad \xrightarrow{\Delta} \quad \text{O} \quad \equiv
\]

\[
\text{COOH} + \text{CH}_2 = \text{CH} - \text{O} - \text{C} -
\]
Side Reactions of Polyester Preparation
Aldehyde Formation

$$\text{CH}_2\text{CH}_2\text{OH} \xrightarrow{\text{reaction}} \text{CH}_3\text{C}^=\text{O} + \text{H}_2\text{O}$$

$$\text{O} - \text{C} - \text{O} - \text{CH} = \text{CH}_2 + \text{HOOC}$$

$$\text{O} - \text{C} - \text{O} - \text{CH} - \overline{\text{O}} - \overline{\text{C}}$$

$$\text{CH}_3\text{C}^=\text{O} + \overline{-\text{C} - \text{O} - \overline{\text{C}} -}$$
Side Reactions of Polyester Preparation

Polyene Formation

\[
\text{O} \quad \text{CH-CH=CH}_2 + \text{CH}_3-\text{C}^\text{=O} \quad \text{H}
\]

\[\equiv (\text{CH = CH})_n\]

Polyene

(Color formation)
### Polyesters

**M.W. 2,000**

<table>
<thead>
<tr>
<th>Ingredients</th>
<th>m.p., C</th>
<th>State at 25 C</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEG-AA</td>
<td></td>
<td>liquid</td>
</tr>
<tr>
<td>EG-AA</td>
<td>52</td>
<td>solid</td>
</tr>
<tr>
<td>PG-AA</td>
<td></td>
<td>liquid</td>
</tr>
<tr>
<td>1,4BD-AA</td>
<td>54</td>
<td>solid</td>
</tr>
<tr>
<td>NPG-AA</td>
<td></td>
<td>liquid → solid</td>
</tr>
<tr>
<td>1,6HD-AA</td>
<td>56</td>
<td>solid</td>
</tr>
</tbody>
</table>
PDI (Polydispersity Index)

\[
\text{PDI} = \frac{M_w}{M_n} = 1 + P
\]

P: extent of reaction (P=100%)

<table>
<thead>
<tr>
<th>Polyester</th>
<th>Theoretical</th>
</tr>
</thead>
<tbody>
<tr>
<td>PDI</td>
<td>2.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>PEAG-2000</th>
<th>catalyzed</th>
<th>uncatalyzed</th>
</tr>
</thead>
<tbody>
<tr>
<td>PDI</td>
<td>2.8</td>
<td>2.8</td>
</tr>
</tbody>
</table>
**EW (Equivalent Weight) Calculation**

**EW of Glycol Material**

EW = \( \frac{56,100}{\text{OH}^#} \)

MW = EW \times f

<table>
<thead>
<tr>
<th>OH#</th>
<th>EW</th>
<th>f</th>
<th>MW</th>
</tr>
</thead>
<tbody>
<tr>
<td>19</td>
<td>3000</td>
<td>2.0</td>
<td>6000</td>
</tr>
<tr>
<td>28</td>
<td>2000</td>
<td>2.0</td>
<td>4000</td>
</tr>
<tr>
<td>37</td>
<td>1500</td>
<td>2.0</td>
<td>3000</td>
</tr>
<tr>
<td>56</td>
<td>1000</td>
<td>2.0</td>
<td>2000</td>
</tr>
<tr>
<td>112</td>
<td>500</td>
<td>2.0</td>
<td>1000</td>
</tr>
<tr>
<td>225</td>
<td>250</td>
<td>2.0</td>
<td>500</td>
</tr>
</tbody>
</table>

MW: molecular weight
f: functionality
Polyester
210 - 260 C

Time, hours

OH#
Viscosity
AN (acid number)
# Reaction Time and Acid Number

**PDEAG-2000 at 230°C**

<table>
<thead>
<tr>
<th>Time, hours</th>
<th>AN, catalyzed</th>
<th>AN, uncatalyzed</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>424.9</td>
<td>424.9</td>
</tr>
<tr>
<td>0.1</td>
<td>53.1</td>
<td>53.1</td>
</tr>
<tr>
<td>0.3</td>
<td>26.6</td>
<td>35.4</td>
</tr>
<tr>
<td>0.8</td>
<td>13.3</td>
<td>15.7</td>
</tr>
<tr>
<td>2.5</td>
<td>4.4</td>
<td>7.0</td>
</tr>
<tr>
<td>3.6</td>
<td>3.0</td>
<td>4.3</td>
</tr>
<tr>
<td>6.2</td>
<td>1.3</td>
<td>3.1</td>
</tr>
<tr>
<td>9.8</td>
<td>0.52</td>
<td>2.1</td>
</tr>
<tr>
<td>10.6</td>
<td>0.43</td>
<td>1.9</td>
</tr>
<tr>
<td>11.0</td>
<td>0.39</td>
<td>1.8</td>
</tr>
<tr>
<td>15.2</td>
<td></td>
<td>1.4</td>
</tr>
<tr>
<td>16.9</td>
<td></td>
<td>1.3</td>
</tr>
<tr>
<td>18.7</td>
<td></td>
<td>1.1</td>
</tr>
<tr>
<td>20.7</td>
<td></td>
<td>1.0</td>
</tr>
<tr>
<td>22.9</td>
<td></td>
<td>0.94</td>
</tr>
<tr>
<td>24.1</td>
<td></td>
<td>0.90</td>
</tr>
<tr>
<td>25.5</td>
<td></td>
<td>0.86</td>
</tr>
</tbody>
</table>

Hydrolytic Stability
MDI Elastomers
MDI/1,4BD/polyester (1,4BD/1,6HD-AA, OH# 56)

80°C water immersion, days

T.S. retention, %

Acid number
0.07
0.46
42
14

0
5
10
15
20
25

80 C water immersion, days
Acid Number of Polyols

Acid number >> 0.5

Trimerization

$\text{C-OH} + \text{M} + \text{NCO}$

trace amount if present

trimerization catalyst

$M = \sum M_i$ where $M_i = K, Na, Fe, \text{etc.}$

Polyisocyanurate
Pot Life Test

Viscosity, cps

Polyester 60 C
MDI 60 C
1,4-BD 60 C

Time, seconds
Effect of Polyester Acid Number on Pot Life
MDI/Uncatalyzed PBAG2000/1,4BD

Pot life, minutes vs. Acid number of polyester
Diexter Polyester

EG/1,4BD-AA polyester

eutectic point
Polyester Viscosity @ 60°C
Glycol/Adipic Acid, MW 2,000

<table>
<thead>
<tr>
<th>Glycol/Adipic Acid</th>
<th>Viscosity, cps</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEG</td>
<td>950</td>
</tr>
<tr>
<td>EG</td>
<td>1,100</td>
</tr>
<tr>
<td>PG</td>
<td>1,100</td>
</tr>
<tr>
<td>1,4BD</td>
<td>1,400</td>
</tr>
<tr>
<td>NPG</td>
<td>2,600</td>
</tr>
<tr>
<td>1,6HD</td>
<td>1,200</td>
</tr>
</tbody>
</table>
Effect of Polyester Acid Number on Polyester Viscosity

- Acid number of polyester
- Viscosity of polyester, cps
Polyester

1,4BD-AA polyester

Graph showing m.p., C as a function of M.W.
Hydrolytic Stability of PU/Polyester Elastomers

PHDG (1,6HD/dodecanedioic acid)

PHAG (1,6HD-AA)

PBAG (1,4ND-AA)

PEAG (EG-AA)

PDEAG (DEG-AA)

Reference: W.L. Chang, Polyurethanes World Congress, September 29 - October 1, 705 (1997)
Polyester Applications

DEG-AA
pigment carriers, soft elastomers, coatings, adhesives

EG-AA
cast elastomers

PG-AA
inks, radcure oligomers, coatings

1,4BD-AA
TPU, adhesives, cast elastomers

NPG-AA
outdoor coatings, radcure oligomers

1,6HD-AA
adhesives, coatings, TPU, cast elastomers

Mixed Polyols-AA
microcellular PU, TPU, cast elastomers, adhesives, coatings

Polyols-AA/IA
floor coatings, adhesives

TMP/Polyols-AA
foams, elastomers

GLY/DEG-AA
foams, elastomers
Polyester Foam Market

Garment Industry
- Clothing innerliner - composites
- Fabric adhesive - automotive
- Reasons used over ethers
  - flame lamination
  - solvent resistance
  - greater strength
  - fine uniform cell structure

Novelty / Industrial
- High strength
- High elongation
- Diecuttability

Technical Foams
- Reticulated foams
- Cell size variations
- Post treated foams
- Low perm gasketing
- Hydrophilic foams
- Sponge foams
Polyester Flexible Foam for Shock Absorption

Polyester Flexible Foam
Polyester Flexible Foam for Filter Application

Polyester Flexible Foam
Polyester Flexible Foam for Packaging Application

Polyester Flexible Foam
Polyester Flexible Foam for Bras Application

Polyester Flexible Foam
Polyester Flexible Foam for Shoulder Pad Application

Polyester Flexible Foam
Polyester Flexible Foam for Paint Brush Application

Polyester Flexible Foam
Polyester Flexible Foam for Scrubbing Pad

Polyester Flexible Foam
## Comparison of Polyester vs. Polyether Foams

<table>
<thead>
<tr>
<th>Polyester Foam</th>
<th>Polyether Foam</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Positive</strong></td>
<td><strong>Positive</strong></td>
</tr>
<tr>
<td>• good green strength</td>
<td>• hydrolytic stability</td>
</tr>
<tr>
<td>• less burn-off</td>
<td>• good compression sets</td>
</tr>
<tr>
<td>• fine cell foam</td>
<td>• better clickability</td>
</tr>
<tr>
<td>• high tensile strength</td>
<td>• lower price</td>
</tr>
<tr>
<td>• high tear strength</td>
<td>• coarser foam / cell size control</td>
</tr>
<tr>
<td>• high elongation</td>
<td>• lower tensile strength</td>
</tr>
<tr>
<td>• pin-hole free</td>
<td>• lower tear strength</td>
</tr>
<tr>
<td>• solvent resistance - dry cleaning</td>
<td>• lower elongation</td>
</tr>
<tr>
<td><strong>Negative</strong></td>
<td><strong>Negative</strong></td>
</tr>
<tr>
<td>• hydrolytic instability</td>
<td>• swelling in dry cleaning solvents</td>
</tr>
<tr>
<td>• poor compression sets</td>
<td>• higher price</td>
</tr>
</tbody>
</table>
Cellesters for Flexible Foam

- Solvent resistance
- Heat resistance
- Flame lamination
- Tensile strength
- Tear strength
- Wear resistance
- Load bearing
- Energy absorption
Formation of Cyclic Structure
from Diethylene Glycol (DEG)

\[
\text{Diethylene Glycol (DEG)} \quad \rightarrow \quad \text{Adipic Acid (AA)}
\]

\[
\text{13 - membered ring}
\]

\[
\text{formation of cyclic structure}
\]

\[
\text{8,13-Dioxo-1,4,7-Trioxacyclotridecane}
\]

m.p. 79 – 81°C

CAS#: 6607-34-7
Cellesters for **Low-Fogging** Flexible Foam

<table>
<thead>
<tr>
<th>OH#</th>
<th>Viscosity, 25C, cps</th>
<th>Applications</th>
</tr>
</thead>
<tbody>
<tr>
<td>52.0</td>
<td>21,000</td>
<td>Textile</td>
</tr>
<tr>
<td>60.0</td>
<td>20,000</td>
<td>Clickable</td>
</tr>
</tbody>
</table>
Elastomers

I. CPU (Cast PU)
   • slightly crosslinked
   • I.I. (isocyanate index) 105 - 115

II. TPU (Thermoplastic PU)
   • linear structure
   • I.I. (isocyanate index) 98 - 100

III. Microcellular elastomer
TPU (Thermoplastic PU)

Applications

• **Film and sheet**
  - conveyor belts
  - welded hollow bodies
  - textile lamination
  - protective coverings
  - sealing of foams
  - abrasion resistant coatings

• **Hose**
  - inner liner of fire hoses
  - inner layer of tubes

• **Shoes**
  - outer materials of ski boot
  - ice hockey boots

• **Automotive**
  - exterior body parts
  - bearing bushings
  - gaskets
  - tie rod
  - shock absorbers
  - tank bleeding tubes

• **Mechanical goods**
  - toothed belts
  - couplings
  - screens
  - cables

• **Medical**

• **Adhesives**
Very low APHA of polyester color

Very low acid number of polyester

No pink color of polyester

Tailored polyester backbone for improving TPU physical properties

Consistent reactivity for TPU manufacturing

Low yellow index of PU product
TPU (Thermoplastic PU) continuous process - reaction extruder process

MDI
- polyester
- chain extender
- additives
- catalyst

feed zone
mix zone
extrusion zone

90 C
150 C
200 C

twin screw extruder

cutter
water bath
conveyor
dryer
pellets
Formation of Cyclic Structure
Impurity in PBAG [Poly(butylene adipate) Glycol]

1,4-Butanediol (1,4BD) + Adipic Acid (AA)

12-membered ring
0.30 wt% in PBAG2000
Microcellular Elastomers

- polyester
- chain extender (EG, etc.)
- water
- amine catalysts (Dabco EG, etc.)
- surfactant (L5305, etc.)
- pigment (TiO2, etc.)
- additives

MDI
Isonate 2143L (optional)
polyester

NCO% ~ 19.0% (quasi prepolymer)

mold

shoe soles

post cure
Polyurethane Fibers

Spandex

Melt spinning

polyester + MDI

polyester

HO-\text{-}OH + X \text{OCN-}CH_2\text{-}CH_2\text{-}NCO

MDI

1,4BD

CH_2CH_2CH_2CH_2\text{OH} \quad \text{OH}

TPU

melt → Spandex

spinnerets → spinning

Spandex
Polyester for Rigid Foam

DEG/aromatic acid based polyester

- Phthalate
- Terephthalate
Chemical Structure of Main Raw Materials

Glycol: DEG (diethylene glycol)

2,2'-Oxybis[ethanol]  
Diethylene Glycol  
(DEG)
Chemical Structure of Main Raw Materials

Acid:  PA (phthalic anhydride)
       TPA (terephthalic acid)

Phthalic Anhydride  (PA)  

Terephthalic Acid  (TPA)
Chemical Equation of DEG/PA Polyester Preparation

\[
\text{HO-} \quad \text{O-} \quad \text{HO} + \quad \text{PA (phthalic anhydride)}
\]

200 - 280°C catalyst
- \( \text{H}_2\text{O} \) (under vacuum)

Poly(diethylene phthalate) glycol
state @ 25°C: liquid

+ free DEG
10 - 15%
Chemical Equation of DEG/TPA Polyester Preparation

DEG (diethylene glycol) + TPA (terephthalic acid)

200 - 280°C catalyst
- H₂O (under vacuum)

Poly(diethylene terephthalate) glycol
state @ 25°C: solid

+ free DEG
10 - 15%
Chemical Equation of DEG/TPA/PA Polyester Preparation

\[
\text{HO-} \quad \text{O} \quad \text{HO} + \text{HO-} \quad \text{C-} \quad \text{OH} + \text{HO-} \quad \text{C-} \quad \text{OH}
\]

DEG (diethylene glycol)  
TPA (terephthalic acid)  
PA (phthalic anhydride)

200 - 280°C  
catalyst  
- H₂O (under vacuum)

\[
\text{DEG-TPA-DEG-PA-DEG} + \text{DEG-TPA-DEG} + \text{DEG-PA-DEG} + \text{free DEG}
\]

state: liquid @ 25°C  
state: solid @ 25°C  
state: liquid @ 25°C  
10 - 15%
Shelf Life

PA/DEG Polyester: 6 years

TPA/PA/DEG Polyester: 1 year
Rigid Foam

Boardstock PIR foam

- Polyisocyanurate (Polyiso) is a closed-cell, rigid foam insulation board used in commercial roofing
- Polyiso insulation is the best choice as a cost-effective, energy efficient and environmentally responsible insulation product
Rigid Foam
Boardstock PIR foam
## Rigid Foam

**Typical formulation of PIR boardstock rigid foam**

<table>
<thead>
<tr>
<th>ingredients</th>
<th>wt., phr</th>
<th>wt%</th>
</tr>
</thead>
<tbody>
<tr>
<td>aromatic polyester (OH# 240)</td>
<td>71</td>
<td>31%</td>
</tr>
<tr>
<td>K octoate</td>
<td>3</td>
<td>1.5%</td>
</tr>
<tr>
<td>K acetate</td>
<td>0.2</td>
<td>0.3%</td>
</tr>
<tr>
<td>amine catalyst (PMDETA)</td>
<td>0.14</td>
<td>0.1%</td>
</tr>
<tr>
<td>surfactant</td>
<td>1.4</td>
<td>0.6%</td>
</tr>
<tr>
<td>n-pentane</td>
<td>15</td>
<td>6%</td>
</tr>
<tr>
<td>water</td>
<td>0.3</td>
<td>0.2%</td>
</tr>
<tr>
<td>flame retardant (TCPP)</td>
<td>9</td>
<td>5%</td>
</tr>
<tr>
<td>B-side, total</td>
<td>100</td>
<td>44%</td>
</tr>
<tr>
<td>Isocyanate (PMDI, f=3.0)</td>
<td>125</td>
<td>56%</td>
</tr>
<tr>
<td>Isocyanate Index (I.I.)</td>
<td>250</td>
<td></td>
</tr>
</tbody>
</table>
Rigid Foam
Bun stock PIR foam
Rigid Foam
Spray Polyurethane Foam (SPF)
Rigid Foam
Spray Polyurethane Foam (wall foam) (SPF)
Rigid Foam
Spray Polyurethane Foam (roof foam) (SPF)
### Rigid Foam

**Spray Polyurethane Foam (SPF)**

Currently foamers use 3 polyols mix for SPF.

<table>
<thead>
<tr>
<th>Polyol Type</th>
<th>wt%</th>
<th>func.</th>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aromatic polyester</td>
<td>~70</td>
<td>2.2</td>
<td>high aromaticity</td>
<td>low func.</td>
</tr>
<tr>
<td>Mannich polyether</td>
<td>~20</td>
<td>3.3</td>
<td>increase reactivity</td>
<td>increase smoke</td>
</tr>
<tr>
<td>Sucrose-initiated polyether</td>
<td>~10</td>
<td>5.0</td>
<td>high func.</td>
<td>increase smoke</td>
</tr>
</tbody>
</table>
Mannich polyether polyol is an auto-catalytic polyether polyol used for SPF to increase SPF reactivity
**Typical formulation of PUR spray rigid foam**

<table>
<thead>
<tr>
<th>ingredients</th>
<th>wt., phr</th>
<th>wt%, B-side</th>
</tr>
</thead>
<tbody>
<tr>
<td>aromatic polyester</td>
<td>70</td>
<td>50.4</td>
</tr>
<tr>
<td>Mannich polyether</td>
<td>20</td>
<td>14.4</td>
</tr>
<tr>
<td>sucrose-polyether</td>
<td>10</td>
<td>7.2</td>
</tr>
<tr>
<td>TCPP flame retardant</td>
<td>7</td>
<td>5.0</td>
</tr>
<tr>
<td>Br flame retardant</td>
<td>9</td>
<td>6.5</td>
</tr>
<tr>
<td>amine catalyst, 1</td>
<td>0.6</td>
<td>0.43</td>
</tr>
<tr>
<td>amine catalyst, 2</td>
<td>0.2</td>
<td>0.14</td>
</tr>
<tr>
<td>water</td>
<td>2.5</td>
<td>1.8</td>
</tr>
<tr>
<td>blowing agent</td>
<td>18</td>
<td>13</td>
</tr>
<tr>
<td>surfactant</td>
<td>1.5</td>
<td>1.1</td>
</tr>
<tr>
<td>PMDI (f=2.7)</td>
<td>134</td>
<td></td>
</tr>
<tr>
<td>Index</td>
<td>110</td>
<td></td>
</tr>
</tbody>
</table>
Rigid Foam
Pour-in-Place Foam
designed to fill and insulate large voids and blind cavities
Aromaticity%

Coim USA, based on C6H4 (phenyl)

Competitor, based on aromatic molecule

\[ y = 1.7601x \]
What are the advantages from TPA?

- better flammability resistance than PA
- higher compressive strength than PA
Thank you!