Utilization of β-farnesene distillation and evaporation residues for the production of green polyol and its subsequent conversion to polyurethane foams

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Introduction

Polyurethane are traditionally produced with fossil-based non-renewable feedstock. To mitigate problems concerning sustainability and negative environmental impacts, there have been increased efforts to synthesize biobased polymers from natural feedstock like vegetable oils and fermentation products amongst others.

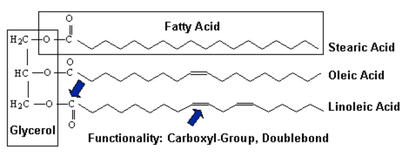
Objectives

Valorization of β-farnesene distillation and evaporation residue (FDR) through transformation into bio-based polyols.

Production of rigid polyurethanes using green methodologies.

Methodology

FDR Evaluation



Iodine value = degree of unsaturation

Synthesis

FDR Epoxidation (oxirane ring formation)

↓

Epoxide

↓

Hydroxylation (ring-opening)

↓

Polyol

↓

Polyurethane Foam

Polyol & Polyurethane characterization

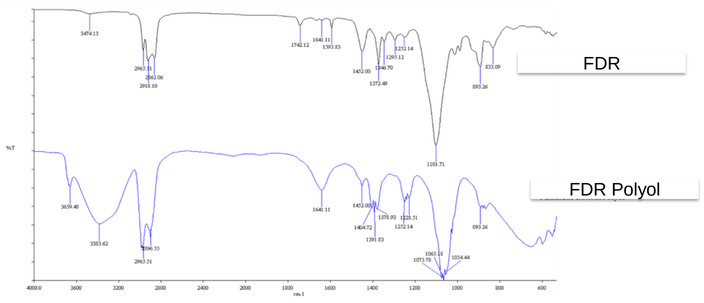
Quantitative analysis

- -OH value (ASTM D1957-86), acidity value (ASTM D4662-08)
- Texture test (ASTM 1621)
- Density evaluation (ASTM 3574)
- Fourier-transform infrared spectroscopy (FTIR)
- Flammability test (ASTM D 4986-03)

Results & Discussion

Polyol Characterization

Formulation/Hydroxylation agents	$[-OH]_{av.}$ (mg KOH/g sample)	Acidity value (mg KOH/g sample)
F1 (PEG400)[1]	106	23
F2 (PEG 600) [2]	146	42
F3 ($HClO_4$) [3]	145	3
F4 (Methanol) [4]	166	33
F5 (1,3-Propanediol) [5]	265	9
F6 (Sorbitol) [6]	40	12
F7 (Glycerol) [7]	84	11
F8 (H_3PO_4) [8]	50	32



FT-IR spectra from FDR before and after the transformation into polyols.

Polyurethane Characterization

Polyurethane composition: Polyol, 4,4'MDI, PDMS (blower), glycerol (plasticizer), DBTDL (catalyst), water

Density (Kg/m^3) of the polyurethane foams

	Density (kg/m^3)
PU Foam	110.1 ± 7.1
Soudafoam 1K	22.7 ± 4.3
Soudafoam B1_Flame retardant	29.6 ± 2.3

Compressive strength of polyurethane foams measured with a texturometer

	Compressive Strenght at 13% (MPa)
PU Foam	0.022 ± 0.014
Soudafoam 1K	0.0049 ± 0.001
Soudafoam B1_Flame retardant	0.0129 ± 0.001

Horizontal Burning Characteristics

Samples	Burning time after flame (s)	Burning Length (mm)	Time Extinguishment (s)	PMR (%)	Burning rate (cm/min)	Density (Kg/m3)
PU Foam	251	132	255	57	3.25	135
Soudafoam 1K	80	140	139	17.03	9.43	26.7
Soudafoam B1_Fire retardant	0	31	60	90.74	0	27.9

T extinguishment - time between application of burner flame and specimen flame extinguishment, s. Afterglow shall not be included in this time.
PMR- percent mass retained by entire specimen. PMR=(S2/S1) * 100, where S2 is the mass of specimen after ignition (g) and S1 before ignition (g).

SoudaFoam 1K | PU Foam Mix | Soudafoam B1_Fire retardant

Conclusions

- The chemical characterization of hydroxyl (-OH) and acidity values have variations between 50 to 265 mg_{KOH}/g and from 3 to 42 mg_{KOH}/g, respectively.
- The best results attending the volume, color and porosity of final foams were synthesized with the polyols with the lower -OH values.
- Rigid polyurethanes were obtained after reaction of the polyols with isocyanate (4'4-MDI), presenting high density (~110kg/m^3), suitable compressive strength (0.022 MPa at 13% strain) and interesting findings related with flammability showing a lower burning rate (3.25 cm/min) than a commercial rigid foam (Soudafoam K1; 9.4 cm/min)

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