XXII Encontro Luso-Galego

Química

9 a 11 novembro 2016

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PROGRAMA CIENTÍFICO

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Exploring oxypropylation to prepare liquid and biphasic polyols from the pine-fruit shell of *Auraucaria angustifolia*

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This work comprises the characterization of pine-fruit shell, the residue of the edible seeds of *Araucaria angustifolia*, a coniferous tree native of South America with economic importance in the South and Southwest of Brazil, and their subsequent use to produce polyols trough oxypropylation. Two different alternatives have been followed: (i) total oxypropylation to produce liquid polyols and (ii) partial oxypropylation to produce biphasic polyols (liquid polyols reinforced with biomass of the same nature). The first polyols were characterized in what concerns unreacted biomass, homopolymer content, hydroxyl number and viscosity, and their properties compared with equivalent products to foresee future applications (e.g. production of rigid polyurethane foams). The second ones were subjected to homopolymer extraction and tested to produce composite materials by hot pressing.

The used pine-fruit shell, obtained from fresh pine fruit purchased in a local market of Campo Mourão PR (Brazil), presented ash and moisture contents of 1.9% and 5.0%, respectively. The lignocellulose composition (dry-basis) comprised cellulose (26.9%), hemicellulose (13.8%) and lignin (35.0%). Moreover, the obtained extractables indicate a major presence of hydroxylated substances (5.9% extracted with methanol) and polar components (6.9% extracted with water), comparatively with nonpolar components (extraction with hexane and dichloromethane).

For total oxypropylation, a set point temperature of 160 °C was used, and 12 polyols have been produced using a pine-fruit shell to propylene oxide ratio (PFS/PO) of of 30/70, 20/80 and 10/90 (g/ml) with 4 catalyst levels (KOH, at contents of 5, 10, 15 and 20%, biomass-based). The resulting liquid polyols were characterized by an homopolymer content ranging from 4-65%, a hydroxyl number between 257-605 mg KOH/g and very high viscosities for the series 30/70 (>500 Pa.s, 20°C). The series 30/70 was the one presenting the higher amount of unreacted PFS (34.9-77.4 %) and for the series 10/90 reasonable amounts were obtained (usually inferior to 10%). In general, the use of low PFS/PO ratios favours the liquefaction process.

In comparison with total oxypropylation, partial oxypropylation was conducted under moderate process conditions, namely at lower set point temperatures (135 and 150 °C). Different PFS/OP ratios, KOH contents (5 and 10%) and productive scale (50 and 100 g) were tested. Subsequently to oxypropylation, the biphasic polyols were subjected to homopolymer extraction that ranged from 3-40%, and the obtained products hot pressed using an in-house built apparatus. The following conditions were used: 135 ºC and 50 bar during 3 minutes. In a general way the assays using a set point temperature of 150 ºC give rise to material's thermal degradation, nevertheless the used productive scale. According to these preliminary studies, the biphasic polyols produced using a PFS/PO ratio of 25/75 (100 g), and a set point temperature of 135 °C, showed good binding characteristics and adequate proportions of oxypropylated/non oxypropylated material, thus representing suitable conditions for the partial oxypropylation reaction having in view the production of composite materials.

To the best of our knowledge no other works concerning pine-fruit shell oxypropylation are available in the literature. In this context, the results presented here pointed out for the viability of using this agro-forestry residue to produce both liquid and biphasic polyols.

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