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Optimization of production of the coffee silverskin bio-oil using a fixed bed reactor and chemical characterization of the organic fraction by GC×GC/qMS

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Coffee is one of the most consumed drinks in the world. Coffee silverskin (CS) is a tegument of coffee beans that constitutes a by-product of the roasting procedure. The pyrolysis (heating in an inert atmosphere) is one of the ways of using residues of the agro-industry, by the generation of bio-oil (condensed product), gases and solid residue (siliceous-carbonaceous material) with many utilities as energy production or as other industrial uses.

Therefore, the aim of this study was the optimization of the pyrolysis process of the CS in a fixed bed reactor and the chemical characterization of the organic fraction of the product by GC×GC/qMS. For this purpose, the present study used a 22 central composite design, with three true replicates at the center point to optimize the pyrolysis process. Two variables were investigated: final temperature of the pyrolysis process (480°C, 500°C, 550°C, 600°C and 620°C, corresponding to levels -1.41, -1, 0, +1, and +1.41, respectively), and the flow of N2 (11.3, 19.2, 38.5, 57.8, and 65.7 mL.min-1), The ranges used were selected based on previous studies in the literature. The CS used in these experiments had particle sizes of approximately 32 mesh. The evaluated response was the yield of organic fraction in the product. All experiments were conducted in random order. The organic fraction of CS bio-oil obtained were qualitatively analyzed by GC×GC/qMS. The first dimension consisted of a ZB-5 capillary column (60 m × 0,25 mm i.d. × 0.10 µm film thickness) and the second dimension consisted of a DB-17MS (2,15 m × 0,18 mm i.d.× 0.18 mm film thickness). The operational conditions were: temperature programmed conditions from 40 to 300°C at 5°C/min (hold 20 min). Injections were performed in the splitless mode. Source and interface temperature were set at 300°C. The mass spectrometer detector worked in full scan mode from m/z 50 to 400. It was used the Kratz retention index (LTPRI – linear temperature programmed retention index) combined with the mass spectrum. The LTPRI was calculated for each compound accords to Van den Dool & Kratz's equation using a standard mixture of n-alkanes (C6-C30) as external references. The values acquired were compared to literature values. The semi-quantitative analysis was made using the method of internal normalization disregarding the response factor. After obtaining a mathematical model with a good fit, it was possible to optimize the conditions for the maximum production of organic fraction of CS bio-oil, which is 568 °C for the temperature parameter and 46.7 ml.min-1 for the flow of nitrogen. The yield predicted by the mathematical model for these conditions was 15.2%. The experimental confirmation was performed in triplicate. There was no significant difference, at a 95% confidence level, between the value predicted by the model and the value obtained experimentally. A total of 231 compounds were tentatively identified in the organic fraction of CS bio-oil. The major constituents in this oil were found to be caffeine (2.45%), resorcinol (1.71%), p-creosol (1.59%), and p-ethylguaiacol (1.52%). The composition of bio-oil from CS consisted mainly of phenols (26.97%), nitrogen compounds (18.38%), saturated hydrocarbons (8.30%), and aromatic hydrocarbons (7.78%). These results represent an important contribution to the knowledge of the composition and production process of organic fraction of CS bio-oil.

Biography

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