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MATHEMATICAL MODELLING FOR PHENOLATION OF SPENT SULFITE LIQUOR

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Abstract

In this study major factors affecting the phenolation process of lignosulfonate (LS) waste liquor (recovered from pulp and paper industry) were optimized in order to improve LS substitution for replacing petroleum-based phenols during phenolic resin manufacturing. Four different parameters, namely phenol/lignosulfonate ratio, time, temperature and lignosulfonate waste liquor concentration, were varied in an experimental program having as response function the reaction yield. Response Surface Methodology (based on central composite or Box-Behnken designs) and Artificial Neuronal Network were applied for establishing the process parameters impact on phenolation yield.

The developed mathematical models presented a high accuracy being able to adequately estimate the phenol conversion and adduct formation. Yields over 80 % were obtained when lignosulfonate waste liquor with a concentration in lignosulfonate between 35 % and 45 % was used in a ratio of 1:1 with phenol and the reaction was conducted at temperatures in a range of 100 °C – 110 °C for a period of time of 3.0 – 3.5 hours.

Key words: Artificial Neural Network, lignosulfonate, mathematical optimization, resin, Response Surface Methodology

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