MODELLING OF A LIGNOCELLULOSIC BIOMASS FRACTIONATION PROCESS IN A LAB-SCALE BIOREFINERY WITH HOT PRESSURIZED WATER

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1. Introduction – This work deals with the modelling of a hydrothermal fractionation process of lignocellulosic biomass in a packed bed reactor. The aim is to obtain a realistic physico-chemical model, taking into account the effect of temperature, water flow and biomass properties. A novel reaction pathway based on two types of hemicellulose and cellulose is proposed in order to consider structural effects in degradation. Moreover, a population of 60 oligomer is defined for each biopolymer to include the molecular weight role. Therefore, hemicellulose and cellulose oligomers have an initial length of 200 and 10,000 monomers, respectively [1-2].

2. Experimental - Samples of 5 g of holm oak (one of the most common trees in southern Spain) were treated at different temperatures and flows. The role of the operating temperature was assessed by two different ranges of temperature (140-180°C and 240-280°C) at constant flow (6 mL/min). These two ranges were selected to study the hemicellulose and cellulose extraction, respectively. The effect of the volumetric flow was considered by experiments at a constant temperature range (180-260°C) and three different flows: 11.0, 15.0 and 27.9 mL/min.

3. Results and Discussion - From the experimental results, it was observed that temperature is the main variable in the process and flow only affects the fractionation when soluble compounds are produced. Moreover, the model was validated with these results, obtaining absolute deviations around 33% (Image 1.a) for the total organic carbon (measured at the reactor outlet). In addition, the whole set of physico-chemical phenomena observed in the process (porosity and pH variations, biomass solubilisation and mass transfer) was also reproduced. Finally, the model was able to calculate successfully the biopolymers depolymerisation, simulating oligomer distribution of decreasing molecular weight (Image 1.b).



Image 1: TOC fitting (a) and oligomer molecular weight evolution (b).

4. Conclusions - A kinetic model for hydrothermal fractionation of biomass was developed and validated (deviations of 33%). This modelling also includes all the physical phenomena observed, and the effect of flow and temperature, successfully reproducing the evolution of the molecular weight distributions.

5. References

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[2] P. Harmsen, W.H., L. Bermudez, R. bakker. 2010. Literature review of physical and chemical pretreatment processes for lignocellulosic biomass. Wageningen UR Food & Biobased Res.