Improved Models of Integrated Autohydrolysis and Organosolv Treatments for Lignocellulosic Residue Conversion

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Thermochemical and fractionation processes offer promising pathways for the energy recovery and valorization of biomass and waste materials. Recently, various lignocellulosic fractionation techniques have been explored to extract antioxidants, phenolic compounds, cellulose, and lignin from residues such as wheat straw or rice husk, contributing to enhanced environmental sustainability. An example is the use of the potentially eco-friendly autohydrolysis processes, which are being studied as alternatives to traditional mild acid hydrolysis. This is the focus of the Cyclevit project, which aims to investigate the transformation of lignocellulosic agro-industrial residues into valuable materials, with a particular emphasis on producing vitrimers class of recyclable and adaptable polymer networks [1]. Briefly one of the steps of the project is to develop and optimize combined treatments of autohydrolysis and organosolv for the recovery of cellulose and lignin (i.e. the basic compounds for vitrimers production) from residue in a more sustainable way compared with the traditional process which involves acid and alkaline hydrolysis. Regarding this, the development of kinetic and reactor models that can represent and simulate the two core units of the process (i.e. autohydrolysis and organosolv) is crucial to exploit the potential of the agricultural residues. In scientific literature, several mathematical models were investigated concerning both autohydrolysis and organosolv process, like the severity factor model, response surface methodology, and the kinetic model. However, these models have several shortcomings like non considering the heating and cooling phases in the case of organosolv [2] or not including the potential lignin degradation in the case of autohydrolysis [3]. Moreover, to the authors' knowledge, no study has been done combining the models of the two units to simulate the two treatments sequentially. Therefore, the aim of this work was to briefly present and comment on two improved models for autohydrolysis and organosolv process, comparing them with results obtained from models already in the scientific literature. For instance, our model includes new equations that consider heating and cooling phases during the organosolv of wheat straw or new equations for evaluating lignin degradation during autohydrolysis. In this way, it could be possible to use the obtained kinetic parameters not only for a specific case but also for different situations involving a wide range of operating conditions. Then, these models will be combined to perform an initial simulation of the internal process, evaluating the effect of varying certain operating conditions (e.g., temperature) on different key performance indicators (e.g., cellulose and lignin recovery).

Keywords: Model, Lignin, Cellulose, Autohydrolysis, Organosolv, Valorization

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