**Experiment Design, Modeling and Comparative Design Optimization of the Pretreatment of Wheat Straw for the Sustainable Production of Xylitol**

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**Highlights**

* Pretreatment of Lignocellulosic Biomass with Dilute Acid Pretreatment (DAc) vs. Liquid Hot Water Pretreatment (LHW)
* Design Optimization with Response Surface Methodology vs. Artificial Neural Network - Genetic Algorithm
* Predictive Modelling to use in Process Design for Sustainable Production of Xylitol

**1. Introduction**

Xylitol has manifold beneficial health properties, e.g. possessing a low insulin index, while tasting similarly to sucrose and thus being perfectly suitable as sugar substitute for diabetics [1]. Its currently predominant production process involves extensive purification and separation steps, which makes it highly cost-expensive [2]. The feedstock for this process is lignocellulosic biomass, whose hemicellulosic fraction consists to major parts of xylose. Rather than pursuing a chemical reaction, the xylose can also be converted to xylitol by fermentation. Consequently, a sustainable, biotechnological production process for xylitol represents a possible alternative [3]. One of the bottlenecks remains the pretreatment of the lignocellulosic biomass in order to partition the hemicellulosic fraction optimally from the biomass. Therefore, the scope of this work comprises a comprehensive analysis of a pretreatment experiment design: Two pretreatment methods are analyzed in two respective design of experiments. Furthermore, the design is optimized comparatively by means of a) Response Surface Methodology (RSM) and b) an Artificial Neural Network (ANN) coupled with a Genetic Algorithm (GA), in order to provide a statement on optimal process conditions for a maximal xylitol production. This is complemented by a sensitivity analysis of both approaches [4]. On basis of the optimized design, one of the pretreatments is chosen to be implemented as a model in order to serve in an overall process design routine.

**2. Methods**

The two methods Liquid Hot Water (LHW) pretreatment and Dilute Acid (DAc) pretreatment are considered as base cases. An experimental design with a fixed temperature range for both pretreatment methods is chosen and, subsequently, for each chosen temperature experiments with both pretreatments are done. The variable considered for LHW is time, and the variables considered for DAc are time and the concentration of acid. The experiments are conducted with wheat straw as lignocellulosic biomass, chopped in a defined particle size interval. All experiments are conducted in stainless steel reactors under defined conditions. The acid used for DAc is sulfuric acid. Measured process variables are time, the concentration of xylose, glucose and the concentration of common inhibitors, such as furfural, HMF, acetic acid and phenolics [4].

The measured data from these experiments is then used to optimize the design with both RSM and the hybrid approach employing ANN-GA, with the twofold objective of a maximal xylose production and simultaneously low inhibitors formation. A local and global sensitivity analysis concludes the procedure. After the analysis of the optimized results, the pretreatment is then implemented as model based on the work of Prunescu et al. [6] and afterwards calibrated and validated with the experimental data.

**3. Results and discussion**

LHW tends to be conducted at higher temperatures than DAc. This is due to the reason of better solubility of the hemicellulosic fraction. With increasing temperature and/or acid concentration, DAc tends to yield higher concentrations of inhibitors during the course of pretreatment [5]. A main drawback of LHW is however the production of large amounts of oligomers instead of xylose monomers [4].

The main objective of the pretreatment is, as mentioned, the fractionation of the biomass. It should therefore yield a maximum amount of monomeric xylose. Other factors indicating the qualitative superiority of a pretreatment method is the amount of inhibitors produced, as well as the costs for heat and acid. In order to provide a sufficient answer for the choice of one pretreatment method or another, the design optimization gives a sufficient answer. The optimization of the design with RSM and respectively with the hybrid ANN-GA yields optimal process parameters for a maximal xylose production during the pretreatment. The comparison between both methodologies show certain differences in overall accuracy, sensitivity and optimal result. DAc yields higher amounts of monomeric xylose, although the use of acid involves cost, but still outruns LHW performance wise. The implemented, calibrated and validated model shows good predictive abilities.

**4. Conclusions**

The comprehensive analysis of the LHW and DAc pretreatment of wheat straw as lignocellulosic biomass yields ambiguous data in terms of favorability of one of them. The optimization of the design with RSM and with ANN/GA display different results considering their performance, but indicate that DAc should be chosen. This method is therefore supposed to be implemented as model for an overall process routine. Therefore, choosing DAc under optimal conditions for the pretreatment step for the biotechnological production of xylitol surmounts the bottleneck best, which makes it suitable for a sustainable process alternative.

**References**

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