Estimating Pure Diffusion Contributions in Alkaline Pulping Processes

Vicente Costanza † and Pedro Costanza ‡

† *Grupo Tecnología de la Madera, INTEC (CONICET-UNL), Güemes 3450, 3000 Santa Fe, Argentina.*
tsinoli@ceride.gov.ar

‡ *Facultad de Ingeniería Química, Universidad Nacional del Litoral, Santiago del Estero 2654, 3000 Santa Fe, Argentina*
pedroc@intec.unl.edu.ar

Abstract— **A model that predicts isothermal alkali diffusion and reaction with acetyl groups in moist wood chips was derived and approximated. System parameters were estimated from unsteady-state experimental data. Simulation results reinforce the idea that the diffusion effect is not fully exploited in pulping processes. Traditionally, digestion is conducted at high temperature, where delignification reaction kinetics is enhanced and the reaction effect is predominant. This approach is being reviewed by modern industry since energy and environmental savings associated with low temperature operation might compensate for high-yield productivity. The concentration of alkali at the center of the chip is a measure of the completeness of wood deacetylation, which translates into the aptitude of the final product for pulping purposes. This concentration is predicted here from the solution to a pair of coupled ODE's. Since alternatives combining both low and high-temperature processes are being studied, the results in this paper provide basic data for optimization analysis.**

Keywords— **reaction–diffusion, wood pulping, alkaline pulping, impregnation, transport phenomena.**

I. INTRODUCTION

A comprehensive model for diffusion and reaction of alkali in wood chips is important for optimizing usual pulping processes in the paper industry. Alkaline treatment is increasingly replacing sulfite chemimechanical pulping due to the enforcement of environmental regulations in many countries. The alkali generates carboxylic groups in contact with cellulose and hemicellulose (an effect which is not desired for pulping purposes), and deacetylates the wood, both mechanisms resulting in a softening and swelling of the solid material needed for ulterior defibration. According to previous work (Zanuttini and Marzocchi, 1997) poplar wood (*Populus deltoides f. angulata and carolinensis*) swelling caused by alkaline treatment is related to by alkaline treatment is related to deacetylation rather than to carboxylic group content.

Experiments are time-consuming and expensive, and industrial conditions may be difficult to reproduce in the laboratory. An accurate theoretical model, on the other hand, provides a quick and inexpensive means for studying, understanding, and monitoring the pulping process and mechanisms. Our model's usefulness for optimization purposes will depend on its accuracy and robustness when temperature and bulk concentration are allowed to vary within a wide range, since these are the main operation conditions that can be manipulated.

Traditionally, pure alkaline treatment is conducted at temperatures well above 100 °C. High temperature results in an overall diffusion-controlled process with flat reaction profiles in agreement with the unreacted core model; for short reaction times, this leads to mostly unreacted chip cores. Ideally, reaction should occur as soon as the alkali reaches acetyl groups. It is therefore desired that the penetration of the alkali into the wood be reaction-driven, which happens only at high reaction rates. Perhaps one of the reasons why some researchers (Jimenez *et al*., 1989a, 1989b; Zanuttini and Marzocchi, 1997; etc.) adopted the flat front model was the familiarity with pressure treatments in wood impregnation, where diffusion is practically ignored (Costanza and Miyara, 1988, 2000). At low temperatures alkali diffusion becomes substantial, the process is no longer diffusion-controlled, and there is a reaction gradient inside the chip, so reaction occurs in all points of the material, leaving no unreacted core. The results obtained in this work suggest that the pulp and paper industries may be misusing the low-temperature diffusion effect. In other words, taking diffusion into account and allowing for a pretreatment of the chips would result in overall energy savings. The high temperatures used in common one-step reaction processes would no longer be required. Moreover, high temperatures cause important material loss together with high alkali consumption. The combination of alkaline pretreatment and sulfite final diges-