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Mathematical modelling of starch oxidation by hydrogen peroxide in the presence of an iron catalyst complex

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Abstract

An advanced kinetic and diffusion model was developed and verified for the oxidation of starch by hydrogen peroxide in the presence of a homogeneous iron tetrasulphonatophtalocyanine (FePcS) catalyst. The model takes into account several experimentally confirmed observations, such as the oxidative formation of carbonyl and carboxyl groups in starch, as well as the decomposition of starch, catalyst and H_2O_2. The model is based on molecular mechanisms for the oxidation and decomposition reactions as well as on the dual structure of starch particles comprising an outer reaction layer and an internal porous layer, in which diffusion resistance retards the reaction rate. Adsorption of the catalyst on the starch surface is included in the model. The mathematical model explained very well the experimentally observed complex behavior of starch oxidation kinetics and hydrogen peroxide decomposition.

Keywords: Starch oxidation, FePcS catalyst, H_2O_2, kinetics, batch and semibatch reactor, mathematical model

1. INTRODUCTION

Starch is a native macromolecule consisting of anhydroglucose units (AGU) linked together by α-glycosidic bonds. Native starch appears in two forms, amylase (linear) and amylopectin (branched). Oxidation of starch is a very interesting and challenging process, both from the viewpoints of science and technology. The goal is to oxidize some of the hydroxyl groups in starch to carbonyl and carboxyl groups. Oxidized starch has a much better water solubility than native starch and it is used in several applications, such as paper coating and sizing as well as in textile sizing, and in in alimentary industry as gelling agent [1-9].