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Models Analysis of the Hydrogenation Reaction of Sucrose for the Production of Sorbitol and Mannitol

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Abstract – The modeling of the hydrogenation reaction of sucrose for the production of mannitol and sorbitol represents the chance to obtain representative models that can be used in the scale-up of the industrial processes of such important substances. The model analysis of different reaction configurations indicates the presence of hybrid autocatalytic kinetic terms representing the reaction network of the formation of sorbitol and mannitol. The simulation results from such models represented adequately the experimental data, showing autocatalytic behaviors in the concentration profiles of sorbitol and mannitol. The inverse routine applied showed to be effective in the estimation of multiple parameters, showing good correlations between the experimental data and the simulation results from the autocatalytic kinetic models. From the calculations were possible the determination of kinetic parameters of the hydrogenation for both the catalysts utilized.

The use of sucrose to obtain products with great industrial application as polyols (See Fig. 1) has been broadly reported in the literature [1, 2]. Sucrose is a di-saccharide that turns into glucose and fructose by hydrolysis. The hydrogenation of glucose and fructose produces both sorbitol and mannitol. Sorbitol is a valuable addictive used in foods, medicines and cosmetics, besides being an intermediary in the production of vitamin C. Mannitol possesses larger commercial value than sorbitol due to their properties as sweetener and for being less hygroscopic. It is used in the food industry as sweetener, in diet products and in products for diabetics. Mannitol can also be used in the production of medicines.

The reaction network was modeled through the superficial kinetic concepts for batch processes. The Fig. 2 presents the experimental data of hydrogenation of glucose and fructose (points) and the simulation results (lines) utilizing the Ruthenium catalyst supported on Alumina. From Fig. 2 it is observed after a long time (about 4 hours) a decrease in the amount of sorbitol produced, indicating a possible formation of isomers or others secondary products.

The kinetic models below represent the accumulation terms of mannitol and fructose, respectively. These kinetic models depends on the kinetic parameters, that are represented by the kinetic constants (*k*).

$$\frac{dC_M}{dt} = k_2.C_G + k_4.C_F.C_M - k_6.C_M.C_I \qquad -\frac{dC_F}{dt} = (k_3 + k_4).C_F{}^m$$

From Fig. 2, it can be observed the increase in the rate of reaction with time for sorbitol and mannitol compounds, being it an indication of autocatalytic behavior. The sigmoidal aspect of the concentration profiles of sorbitol and mannitol is an indication of autocatalysis. Differently, the concentration behavior of glucose and fructose presented exponential profiles, indicating reactions without autocatalysis.

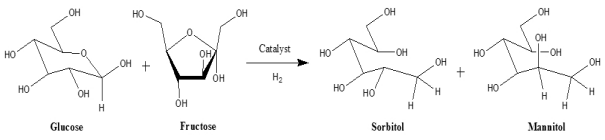

Figure 1: Reaction molecular representation of the catalytic hydrogenation of sucrose for the production of sorbitol and mannitol

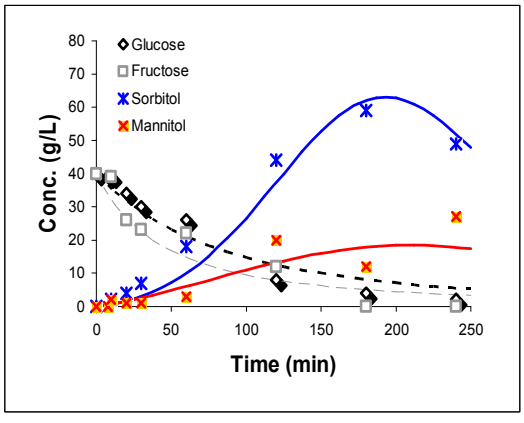

Figure 2: Correlation between the kinetic models and the experimental data from the hydrogenation using the Ru/Al2O3 catalyst

[1] L.C.A. Maranhão, F.G. Sales, J.A.F.R. Pereira, C.A.M. Abreu, React. Kinet. Catal. Lett., 81, (2004) 169.

[2] F. Lichtenthaler, Carbohydr. Res., 313, (1998) 69.