Dynamic mathematical modelling of reaction kinetics for Cyclodextrins production from different starch sources using Bacillus macerans cyclodextrin glucanotransferase

Abstract

This study relates to the mathematical modelling of enzymatic production of Cyclodextrins (CDs) by Cyclodextrin Glucanotransferase (CGTase) from Bacillus macerans. The experiments were carried out in batch mode using different starch sources and the results were used to estimate unknown parameters using linearization and dynamic simulation methods. α- and β-CD produced from tapioca were found to give the highest Michaelis-Menten constant, \(K_M,i\) of 58.23 and 54.07 g L\(^{-1}\), respectively and maximum velocity, \(V_{max,i}\) of 3.45 and 2.76 g L\(^{-1}\).min\(^{-1}\), respectively, while sago resulted in the highest \(K_M,i\) and \(V_{max,i}\) values of 342.35 g L\(^{-1}\) and 5.97 g L\(^{-1}\).min\(^{-1}\), respectively, for α-CD obtained by the linearization method. Value of product inhibition, \(K_{1,i}\) and CD degradation coefficient rate, \(\beta_{CD,i}\), were estimated using dynamic simulation, indicating that exponential reaction kinetics could be fitted better with the experimental data. Sensitivity analysis revealed that the product inhibition parameter in the exponential reaction kinetic equation is more significant in the process. For validation, the production of CDs by fed batch method was undertaken and starch and enzyme were added into the reaction medium. Then, the predicted profiles generated by simulation were compared with the experimental values. The proposed exponential reaction kinetics shows good fitting with the experimental data.

Keyword: Kinetic modelling; Cyclodextrin; Cyclodextrin Glucanotransferase; Sago; Bacillus macerans