T-P22 Modeling and simulation of fructo-oligosaccharides production

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It is foreseen that Systems Biology will have a great impact not only in Metabolic Engineering and Drug Discovery efforts, but also in Bioprocess development and optimization. In fact, the computational tools developed in this area made possible to simulate a biochemical process with a mathematical model comprising dynamical equations based on first principles as well as empirical kinetic equations and parameters that can be estimated from experimental data.
Fructo-oligosaccharides (FOS) have become important as healthy food ingredients because of their beneficial characteristics to the health of human (Lee, 1999). They can be obtained biotechnologically using the enzyme Beta-fructofuranosidase, produced by some fungi.
The main purpose of this work was to develop a mathematical model able to simulate the formation of FOS in a bioreactor, in order to perform a faster optimization of the FOS production process, allowing to identify which parameters can influence the final amount of FOS. An empirical model presented by Kow Jen Duan *et al* (1994) was used to obtain the first set of reactions. Several hydrolysis equations were added in order to achieve a general mathematical model of the occurring enzymatic reactions.
After the reformulation of the Kow Jen Duan model, the kinetic parameters were determined from experimental data using the System Biology toolbox [2] with the Simulated Annealing method for curve fitting. Several experiments in bioreactors were performed with two different FOS producing fungi for that purpose. The time evolution of 7 state variables (Sucrose, Glucose, Fructose, 1-Kestose, Nystose, 1-Fructosyl Nystose and Biomass) was considered. After parameter fitting, several simulations were performed in MatLab and the simulation results were compared with experimental data, exhibiting a very satisfactory correlation for both fungal cultures. Correlation coefficients of 0.9980 - 0.9549 between simulated and experimental data were obtained. This model will be used to optimize the production process, using an optimization tool that has been developed in our research group.

1. *Kow Jen Duan, J. S. (April 1994). Enzyme Microb. Technol, 16, 334-339.*
2. *Schmidt, H. et al. (2006). Bioinformatics, 22(4), 514-515*