The coupling of ω-transaminase and Oppenauer oxidation reactions via intra-membrane multicomponent diffusion – A process model for the synthesis of chiral amines

In this study we consider the theoretical coupling of an otherwise thermodynamically limited ω-transaminase reaction to an Oppenauer oxidation, in order to shift the equilibria of both reactions, with the aim of achieving a significant (and important) increase in the yield of the desired chiral amine product. Using 2-propylamine as the amine donor of the ω-transaminase reaction, gives acetone as a by-product, which in turn allows the coupling of the ω-transaminase reaction with the Oppenauer oxidation. The Oppenauer reaction converts secondary alcohols into ketones, and these can subsequently be fed to the ω-transaminase reaction. In this way, one of the products of the ω-transaminase reaction becomes the reactant of the Oppenauer reaction, and vice versa, creating a cycle which shifts the equilibria of both reactions. Such coupled reactions are frequently found in nature. The purpose of this paper is to report the development of a mathematical model as a tool for the simulation and potential design of such a process for the production of a range of chiral amines. The mathematical model developed considers that each reaction is performed in a single ideally mixed isothermal reactor operating sequentially in fed batch–batch mode. Both reactors are interconnected through a semi-permeable membrane, where multicomponent intra-membrane transport takes place by diffusion and viscous flow. The kinetic modeling of both reactions has been carried out and model simulations show that in this way a significant increase in the yield of the chiral amine product may be obtained. Finally, the role of the different parameters involved in the process model has been analyzed.