Modelling the Lipase-catalyzed Interesterification Kinetics of High Oleic Sunflower Oil with Stearic-Palmitic Acid Mixtures

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High Oleic Sunflower Oil was interesterified with stearic-palmitic acid mixtures of different compositions using 1,3-regiospecific lipase under constant microaqueous environment in batch operations to produce fats with high disaturated (Sat-O-Sat) TAGs. The data for the variation of TAG composition with time were used as a basis to study the kinetics of interesterification reactions, which was performed using MATLAB.

Initially, a reaction scheme was formulated allowing all possible interesterification reactions of Sat-O-Sat TAGs with stearic, palmitic and oleic fatty acids at the 1 and 3 TAG positions. However, as the presence of water in the reaction causes the formation of DAGs, a second scheme whereby all possible interesterification reactions involving DAGs was also included. In both schemes it was possible to fit the rate constants using a variety of assumptions, i.e. (i) all reactions are modelled with the same rate constant value (ii) individual reactions are modelled by different rate constants, and (iii) reactions involving palmitic acid and stearic acid in the same positions have the same rate constant.

In both schemes, fits assuming a single value of rate constant for all reactions (option i) produced poor fits, suggesting that such an approach is an oversimplification. Within the first scheme, similar levels of fits were produced with options (ii) and (iii) above. This suggests that the lipase showed little sign of fatty-acid specificity between palmitic and stearic acids, i.e. the rate constants were similar for equivalent reactions involving stearic and palmitic acid reactions. Consequently, for the second scheme option(ii) was not attempted (it required too many fit parameters), but option (iii) was found to give the best fits overall. This indicates that the DAG reactions are significant, which is not surprising, given that DAGs typically constitutes ~7-10% of the sample at equilibrium.