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Genetic programming approach to predict a model acidolysis system

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ABSTRACT

This paper models acidolysis of triolein and palmitic acid under the catalysis of immobilized sn-1,3 specific lipase. A gene-expression programming (GEP), which is an extension to genetic programming (GP)-based model was developed for the prediction of the concentration of major reaction products of this reaction (1-palmitoyl-2,3-oleoyl-glycerol (*POO*), 1,3-dipalmitoyl-2-oleoyl-glycerol (*POP*) and triolein (*OOO*). Substrate ratio (*SR*), reaction temperature (*T*) and reaction time (*t*) were used as input parameters. The predicted models were able to predict the progress of the reactions with a mean standard error (*MSE*) of less than 1.0 and *R* of 0.978. Explicit formulation of proposed GEP models was also presented. Considerable good performance was achieved in modelling acidolysis reaction by using GEP. The predictions of proposed GEP models were compared to those of neural network (NN) modelling, and strictly good agreement was observed between the two predictions. Statistics and scatter plots indicate that the new GEP formulations can be an alternative to experimental models.

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1. Introduction

The physical and nutritional properties of fats and oils, hence commercial value, not only depend on their fatty acid composition but also on triacylglycerol (TAG) composition (Iwasaki and Yamane, 2000), since the distribution of fatty acids on the glycerol backbone determines the structure of a TAG. Modification of fats and oils by enzymatic interesterification has long been practiced to improve their functional and nutritional properties (Macrae and Hammond, 1985). Acidolysis is the most commonly used method of interesterification. Lipids are modified by incorporation of fatty acids into specific positions of TAGs by specific or nonspecific lipases (Hoy and Xu, 2001). Production of cocoa butter equivalents from low cost fats (Wang et al., 2006), reduction of saturated fatty acid content of fats (Balcao et al., 1998) and production of structured lipids (Yankah and Akoh, 2000) are well-studied examples.

Acidolysis reactions are widely used for lipid modifications to improve functional and nutritional properties. The efficiency of the acidolysis reaction depends on reaction parameters. Major factors affecting the performance of the reaction are substrate mole ratio, reaction temperature and reaction time (Willis and Marangoni, 2002). Determination of the effect of each parameter on the reaction is required both for quality improvement and for highest economical turnover. For quality improvement and for highest economical turnover the process must be optimized. In spite of several advantages of enzymatic modification of fats and oils, because of complexity of the reactions, an exact mathematical model is not available for process optimization (Xu, 2003). Gene-expression programming (GEP) may serve as a robust approach and it may open a new area for the development of accurate and effective explicit formulation of acidolysis reactions and also for many food-related biotechnology and bioengineering problems.

Genetic Algorithms (GAs) and genetic programming (GP) have been found to offer advantages to deal with system modelling and optimization, especially for complex and nonlinear systems. GP has been applied to a wide range of problems in artificial intelligence, engineering and science, chemical and biological processes, and mechanical models including symbolic regression. In recent years only a few studies have been reported related to the use of GAs in the field of food science. Izadifar and Jahromi (2007) used GAs for the optimization of vegetable oil hydrogenation process, Dutta et al. (2005) studied optimization of a protease production process by using GAs; Hanai et al. (1999) applied GAs for the determination of process orbits in the koji making process and Liu et al. (2007) used GAs to predict moisture content of grain drying process.

An explicit neural network formulation (ENNF) that predicts the production of major reaction products of interesterification of palmitic acid and triolein as a function of experimental parameters; substrate ratio (*SR*), temperature (*T*) and time (*t*), has recently been performed by Çiftçi et al. (2008). However, a GEP-based explicit formulation for enzymatic interesterification, to the

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best knowledge of the authors, has not yet existed in the literature. Therefore, the purpose of this study is to develop a GEP-based mathematical model for the production of major products of a model interesterification reaction. For this aim, enzymatic interesterification reactions of palmitic acid and triolein were carried out and the amount of major reaction products (1-palmitoyl-2,3-oleoyl-glycero (*POO*), 1,3-dipalmitoyl-2-oleoyl-glycerol (*POP*) and triolein (*OOO*)) were determined. The data taken from experimental study were utilized in training and testing the developed models. The performance of the proposed models was compared to neural networks model developed by Çiftçi et al. (2008).

2. Materials and methods

2.1. Materials

During this research, triolein (⩾99%), palmitic acid (⩾98%) and immobilized sn-1,3 specific lipase (Lipozyme IM, immobilized from Mucor miehei, (42 U/g) were used. All solvents used were of HPLC grade.

2.2. Enzymatic acidolysis

Triolein (0.1 mM) and palmitic acid (0.2–0.6 mM) were dissolved in 5 mL hexane in 50 mL erlenmayer flasks. Reactions were carried out with 10% enzyme concentration (based on weight on substrates) in a rotary shaking incubator (New Brunswick Scientific, model Nova 40, USA) at 200 rpm, at 40, 50 and 60 °C. The progress of acidolysis was followed over a period of 72 h. In total, 50 μL aliquots were withdrawn at certain time intervals from the reaction mixtures into glass vials and stored at −20 °C prior to analysis.

2.3. Triacylglycerol analysis by HPLC

The triacylglycerol composition of the products obtained from reactions was followed by reversed phase high performance liquid chromatograph (HPLC). Samples were diluted in acetone, filtered and injected to HPLC. HPLC system consisted of quadratic pump (model LC-10ADVP; Shimadzu, Japan) equipped with a column (Sphereclone 5 μ ODS (2), 250 × 4.6 mm; Phenomenex, USA) with an accompanying guard column (40 × 3 mm id) of the same phase and an ultraviolet (UV) detector (Hewlett Packard Series 1100). Elution was monitored by UV absorbance at 215 nm. The mobile phase consisted of acetone and acetonitrile (50:50, v/v) with a flow rate of 1.0 mL/min. The column temperature was set at 50 °C with a column heater (Eppendorf CH-30 column heater).

3. GEP model development

3.1. Overview of GP and GEP

GP is a search technique that allows the solution of problems by automatically generating algorithms and expressions. These expressions are coded or represented as a tree structure with its terminals (leaves) and nodes (functions) (Koza, 1992). GP applies GAs to a "population" of programs—typically encoded as tree-structures. Trial programs are evaluated against a "fitness function" and the best solutions selected for modification and re-evaluation. This modification–evaluation cycle is repeated until a "correct" program is produced.

GEP technique, which is an extension to GP, evolves computer programs (mathematical expressions, decision trees, polynomial constructs, logical expressions and so on). GEP utilizes computer programs all encoded in linear chromosomes, which are then expressed or translated into expression trees (ETs). ETs are sophisticated computer programs that are usually evolved to solve a particular problem and are selected according to their fitness at solving that problem. Via genetic modification, population of ETs is capable of discovering traits and therefore adapting to the particular problem they are employed to solve. This means that, within enough time and setting the stage correctly, a good solution to the problem will be discovered (Ferreira, 2001a, b).

GEP is a full-fledged genotype/phenotype system, with the genotype totally separated from the phenotype, while in GP genotype and phenotype are one entangled mess or more formally, a simple replicator system. As a consequence of this, the full-fledged genotype/phenotype system of GEP surpasses the old GP system by a factor of 100–60,000 (Ferreira, 2001a, b).

Fig. 1 shows a brief flowchart of GEP. Initially, the chromosomes of each individual of the population are randomly generated. Then the chromosomes are expressed and each individual is evaluated based on a fitness function, and selected to reproduce with modification, leaving progeny with new traits. The individuals of new generation are, in their turn, subjected to some developmental process as, expression of the genomes, confrontation of the selection environment, and reproduction with modification. The process is repeated for predefined number of generations or until a solution is achieved (Ferreira, 2001a, b)

Typical notation of a GEP model is Karva language or Karva-expression (Ferreira, 2001a). An example for Karva-expression of a two-gene GEP chromosome can be: $*\mathbf{ln}.\mathbf{a}.\mathbf{b}.\mathbf{b} + */.\mathbf{a}.\mathbf{b}.\mathbf{a}$, where "." Is used to separate elements, **ln** is the natural logarithm

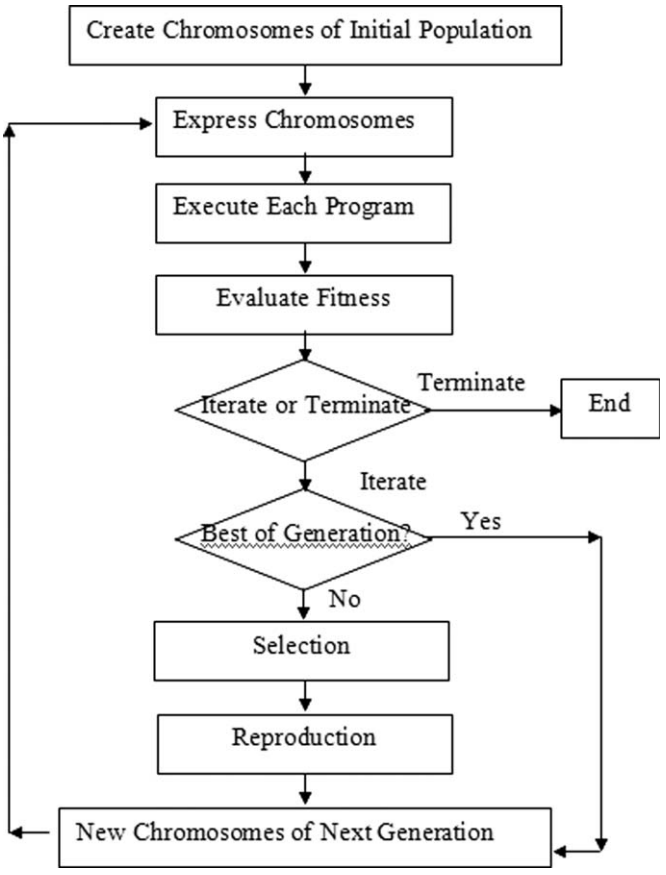

Fig. 1. Brief algorithm of gene-expression programming (Ferreira, 2001a).

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