Predictive Modelling of Fat Compositions

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Very rarely do two fats, when blended together, interact in a truly linear way. Even when they are closely related to each other in terms of their triacylglycerol composition there is often some deviation away from linearity when they are mixed. This can make it difficult to predict physical properties such as solid fat contents. When there are more than two fats in a blend the difficulty is compounded.

Various models have been proposed to enable the prediction of multi-component fat compositions purely from a knowledge of each of the binary interactions. The simplest of these is the Constrained Quadratic Model in which the linear terms are constrained to the values of each individual fat and a quadratic term is introduced to take account of any non-linearities. Because of the constrained nature of the model it is relatively easy to add other binary systems to make a truly multicomponent model.

Such a model is of great benefit in then predicting the physical properties of new blends. It is, however, more difficult to use it to optimize blend compositions to meet various requirements other than by multiple calculations. The technique of linear programming does, though, offer a quick and easy way of carrying out such optimizations. The problem here is that the non-linear terms cannot be incorporated into such simple models (but can be in the much more complex non-linear programming models). By placing some formulation constraints on the system it is possible to make a good approximation to linearity which then permits the use of the simpler models.

Examples will be given of the conversion of binary data into a Constrained Quadratic Model format to enable multicomponent prediction and of a simple linear programme model based on a subset of such information.