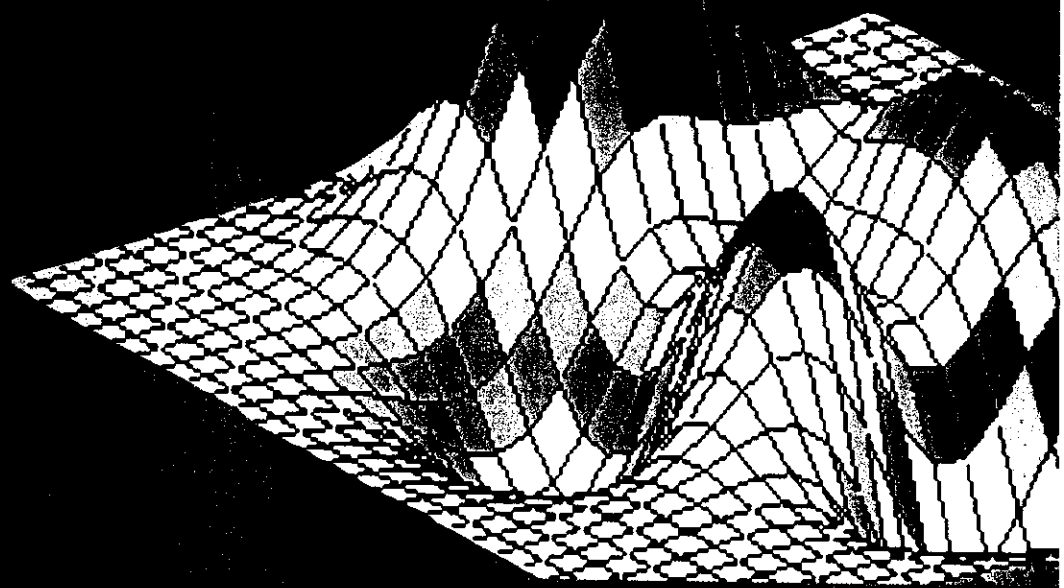
Finite Element Modelling in Chemical and Food Engineering



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The Role of Mathematical Modelling in Chemical and Food Engineering Studies

Teresa R. S. Brandão and Cristina L. M. Silva

Escola Superior de Biotecnologia, Universidade Católica Portuguesa
Rua Dr. António Bernardino de Almeida, 4200-072 Porto, Portugal
e-mail: crislui@esb.ucp.pt
phone: + 351 22 5580058
fax: + 351 22 5090351

Abstract

The role of mathematical modelling in chemical and food engineering studies is briefly and consistently presented.
The main goal was to give a short global overview of the relevant aspects involved in modelling processes. Food engineering problems are generally highlighted.
It must be emphasised that the following matter should not be analysed in a narrow perspective. The mathematical modelling field, in chemical and food engineering subjects, is very wide and this paper just presents the authors' research point of view.

Keywords: modelling, kinetics, optimisation, food processes

Introduction

Mathematical modelling is important for any process design, assessment, control and optimisation. A model is merely a mathematical expression relating a dependent variable(s) to an independent variable(s). This relationship involves "constants", usually nominated as parameters, which are often dependent on intrinsic and/or extrinsic factors. In general, the model can be written in the form:

$$y_i = f(x_{ij}, \theta_k) + \varepsilon_i \quad (1)$$

i=1,2,...,n (number of experimental runs/observations)

j=1,2,...,v

k=1,2,...,p

where y_i is the response observed at the i^{th} experimental run (e.g. dependent variable), x_{ij} are controlled variables which define the experimental conditions at the i^{th} run (e.g. independent variable(s)), θ_k are unknown parameters, f is the mathematical model assumed, and ε_i is the experimental error of the i^{th} run (assumed to be independent and normally distributed, with mean equal to zero and constant variance).

Parameters are estimated on theoretical basis or by fitting the model to experimental data.

The assumed model should predict the response variable accurately, which jointly depends on the adequacy of the model to describe the process and on the quality of the parameters estimated. It should be taken into consideration that the most complex and adequate model might not give good predictions, if it is not possible to estimate the parameters with accuracy and precision.

In figure 1 a scheme of the relevant aspects involved in modelling a process is presented. Some points will be following discussed, with particular emphasis on chemical and food engineering studies.

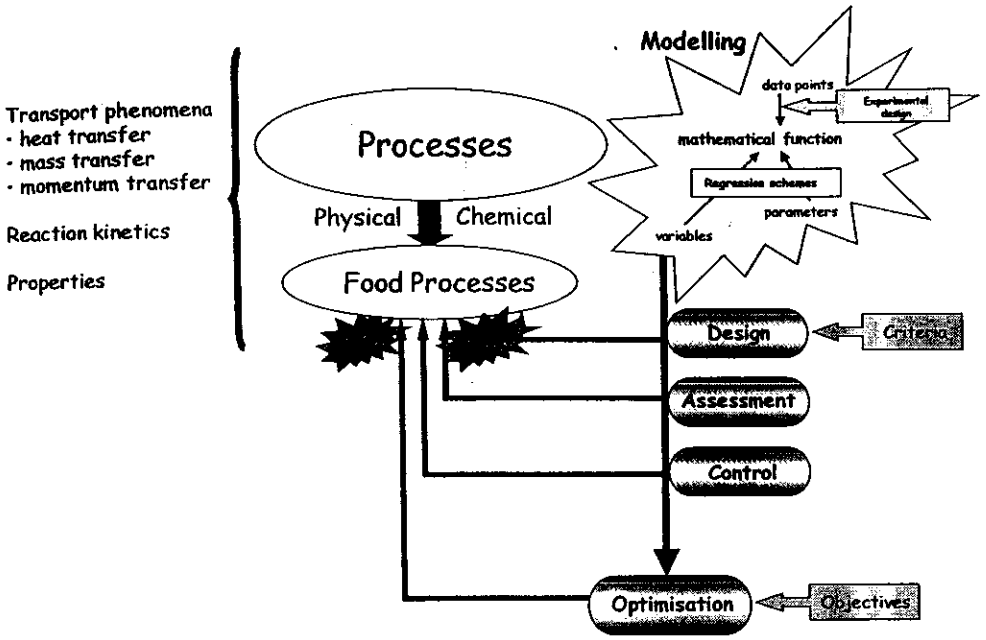

Figure 1. *Scheme of relevant aspects involved in modelling processes*

Modelling processes

The development of mathematical models can be done on a mechanistic basis (e.g. on the knowledge of the fundamental mechanisms involved in a process), on infinitesimal balances of the material properties involved (which gives the properties change as a function of time and space) or simply by an empirical approach.

The relevant transport phenomena involved in chemical and food engineering processes can be divided into heat, mass and momentum transfer. A universal equation rules all transport phenomena and, in general, the dependence of any property (I) with time and space co-ordinates can be given by the expression:

$$\frac{\partial \Gamma}{\partial t} = \delta\left(\frac{\partial^2 \Gamma}{\partial x^2} + \frac{\partial^2 \Gamma}{\partial y^2} + \frac{\partial^2 \Gamma}{\partial z^2}\right) \quad (2)$$

where δ is a generalized diffusion coefficient (assumed to be constant in the previous expression), *x*, *y* and *z* are the orthogonal space coordinates, and *t* is the time.

By assuming adequate initial and boundary conditions and for simple geometries, analytical solutions of the preceding equation can be obtained. Those solutions are often a sum of terms of infinite series, and difficulties arise in obtaining an exact analytical resolution.

Another approach is based on numerical methodologies, by replacing the differentials of equation 2 to an algebraic equation and discretising the independent variables of time and space (finite differences or finite elements numerical solutions).

Applying transport phenomena theory to food processes is not an easy task. This is one field in which modelling becomes a great challenge. Food processes involve a large number of industrial processes, applied to a larger variety of food products. Difficulties arise due to the complexity and heterogeneity of foods and to their structural and physicochemical changes, when subjected to processing conditions (Gekas, 1992). Besides all this complexity, the fundamental equations of the transport phenomena, or simpler empirical models, usually give good description of the processes and consequently are often used for predictive purposes.

Heat and momentum transfer becomes the fundamental phenomena in thermal processes of foods. Heat transfer is governed by the well-known Fourie's law, which can be attained by replacing the property Γ (in eq. 2) with temperature. Available solutions for this equation are commonly applied for conduction heating foods (Silva *et al.*, 1993; Ávila, 2001).

In the mass transfer domain, and by analogy with heat transfer, one obtains Fick's 2nd law by substituting Γ with concentration. Food processes, such as acidification, blanching, drying, leaching, or salting, are controlled by mass transport phenomena, occurring in unsteady-state conditions. The analytical solutions of Fick's 2nd law often yield satisfactory description of those processes, if adequate boundary conditions are applied (Garrote *et al.*, 1988; Oliveira and Silva, 1992; Moreira *et al.*, 1993; Bourani *et al.*, 1994; Gomes *et al.*, 1998).

Interfacial resistances can restrict heat and mass transfer. Interfacial transfer is the controlling step in many unit operations, which is generally accounted by a transfer coefficient between the bulk and the interphase.

Modelling safety and quality

Kinetic studies are related to the change of any process characteristics with time (x_{ij} becomes the time variable, in eq. 1). These studies allow quantifying the extension of the production/consumption of any substance or quality attribute, and also the assessment of the rate at which those changes occur. This is particularly important regarding safety and quality of food products.

The safety and quality of any food product is a result of the several intrinsic and extrinsic factors. The final safety is a cumulative effect of handling and processing conditions, since the first handling and harvesting steps at primary production, till storage, distribution and consumers home. Kinetic studies, that quantify safety and quality changes of food products, have been carried out since several decades. Kinetic models can be used as a great and useful tool for prediction, and have been used in a relatively narrow group of handling, storage and processing unit operations.

Modelling quality (e.g. nutritional content, sensory characteristics, physic-chemical attributes) of processed foods is often attempted by researchers (Villota and Hawkes, 1986, 1992). For a total control of the process variables effect on the final product, it is also important the study the environmental factors influence, such as temperature, pH and water activity among others, on the rate constant. With technological enhancements, quality attributes are more recently studied at microscopic level. Drying of fruits is one area in which modelling microstructural changes is emerging (Ramos *et al.*, 2003).

The bacterial spoilage of foods and the survival of pathogens are of major importance to the food industries, because it directly affects the consumer's health and safety. The development of accurate models, that describe the inactivation behaviour of microorganisms (*predictive microbiology*), is a considerable tool to predict target pathogen's survival within specific environmental conditions. It may also help to determine if the extent of existing thermal processes could be modified, in order to obtain major quality retention. Modelling microbial kinetics, that lead to reliable predictions of safety and shelf-life of foods, is not commonly used by microbiologists. On the other hand, the majority of works deal with the growth behaviour and only a limited number of publications approaches the inactivation process (Reichart, 1994; Geeraerd *et al.*, 2000; Peleg *et al.*, 2001).

Experimental design and data analysis

After a mathematical model is chosen for a process (eq. 1), it should be experimentally validated. The collection of experimental data points (e.g. values of the response variable(s) for the experimental imposed conditions) should be carefully chosen, so that the measured response(s) and its(their) errors are compatible with the selected method of analysis (Johnson and Frasier, 1985).

The wise selection of the sampling pattern is also an important issue. Heuristic sampling (e.g. based on empirical sense: equally spaced in time range, in the logarithmic of the time range or in the response scale) is commonly used to assess the model adequacy. Even so, when there is no conscious about the process rate, only a small extension of the process can be covered or not enough amount of data was collected to describe the initial period of the process. These situations are critical in kinetic studies and results obtained on the basis of such experimental designs could be seriously affected.

Experimental sampling could also be planned to reach the most precise statistical inference, which is based on statistical background theory. The soundest criteria aim at minimising the variance of the predicted response or the variance of the parameter estimates (Steinberg and Hunter, 1984). These types of designs, usually referred to as optimal designs, are based on the knowledge of the mathematical function and the precise estimation of the response or the model parameters are the merely final objective (Atkinson and Donev, 1992).

Experimental design plays an important role in the mathematical modelling of any process. As Box *et al.* (1978) wisely stated, no sophisticated analysis can provide good results if experimental data are poor *a priori*.

After experimental data have been collected according to the established experimental design, model fitting is the subsequent procedure. Regression

schemes are used to estimate the model parameters, by establishing a suitable measurement between the experimental data and the model function. Least-squares method is the most popular and widely used regression scheme (Bard, 1974). It relies on the minimisation of the sum of the square of the deviations or residuals (SSR) between the experimental points and the predicted values of the response variable:

$$SSR = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} \left[y_i - f(x_{ij}, \theta_k) \right]^2 \qquad (3)$$

If the model is suitable, the residuals (e_i) should present the same properties assumed for the experimental error (ε_i) previously referred (eq.1). Thus, the analysis of the residuals provides a simple tool for detecting model deficiencies (Chatterjee and Price, 1991).

The regression analysis procedure yields estimation of the model parameters. Nevertheless, the procedure is not fulfilled if precision of the estimates is not measured.

The calculation of the confidence intervals of the estimates (e.g. the limits within the real values are expected to lie, by means of a certain probability (Box *et al.*, 1978)) allows quantifying the precision of the estimates. For systems of more than one parameter, a better interpretation of precision is achieved by the construction of joint confidence regions (Bates and Watts, 1988; Seber and Wild, 1989).

The improvements of modern computer technology and software (Statistica® 2001 is one good example) allow a complete analysis of the regression procedure. The researcher has only the role of interpreting the reported results, and the effort of programming all the regression analysis is avoided.

List of symbols

e_i	-	residual at i^{th} experimental observation
f	-	mathematical form of the model
n	-	number of experimental observations or points
p	-	number of the model parameters
t	-	time [s]
T	-	temperature [K]
v	-	number of the model independent variables
x, y, z	-	orthogonal space co-ordinates [m]
x_{ij}	-	independent variable j at i^{th} experimental observation
y_i	-	observed response at i^{th} experimental observation

Greek symbols

δ	-	generalised diffusion coefficient ($m^2\ s^{-1}$)
ε_i	-	experimental error of the i^{th} run
Γ	-	general property
θ_k	-	model parameters

Abbreviations

SSR	-	Sum of squares of residuals

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