Application of identifiability test to drying models

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Communication presented at COST-915 Copernicus CIPA CT94-0120 Workshop on Food Quality Modelling - June 4-6, 1997, Leuven, Belgium.

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Abstract

This paper deals with the problem of model identifiability. The purpose of this work is to apply Walter's method to classical food process models and identification problems. Emphasis is put on drying models where the main quality variable is the product moisture content. This method is limited to "linear in the inputs" models and so implies a linearization of models that don't satisfy this condition. The identifiability test can give a first and useful insight of the possibly identification problems.

Introduction

Modelling is a single, and thus simple, word hidding many different aspects. Modelling is not a *one step ahead* methodology. Far from this, food modelling implies good skills in:

- physics (*e.g.* thermodynamics, transfers...)
- biology (*e.g.* biochemistry, microbiology...)
- instrumentation (*e.g.* sensors...)
- computer (*e.g.* programming...)
- applied mathematics,

In general, the mathematical part of the work consists mainly in the analytical solving of the system of equation describing the model. Since, more and more models imply unmeasurable variables and parameters and parameters unavailable in the literature, optimization routines are used to identify the remaining unknowns. Since models are generally non-linear and thus numerically solved, non-linear iterative optimization routines are preferred.

Some questions arise and generally remain unanswered:

- Is the model structurally identifiable ?
- Which measurements should I add to improve parameter identifiability ?
- Guessing some starting values for the unknown parameters, would it be possible to find the best experiment design for identification purposes ?

The choice of a model structure (*i.e.* the equations, the inputs and outputs) will not be discussed here since it is basically dependent on the kind of process, product and objectives considered. Instead of that, the first question will be discussed on the basis of two examples: a diffusion-convection drying model and a compartmental-convection drying model.

Problem formulation

A very interesting survey of the two above questions is presented in [1]. Problems are dissociated in two main cases:

- Linear in Inputs (LI) models
- non-Linear in Inputs (non-LI) models.

A model is non-LI if its outputs y_m does not satisfy the superposition principle concerning the inputs u *i.e.* there exist some real scalars γ and μ, some inputs u_1, u_2 and some positive time t such that:

$$y_m(\theta, \gamma.u_1 + \mu.u_2, t) \neq \gamma.y_m(\theta, u_1, t) + \mu.y_m(\theta, u_2, t) \tag{1}$$

where θ are the parameters.

It should be noted that another, and similar, classification exists: LP and non-LP models. LP means here Linear in the Parameters. A model is non-LP if there exist some scalar values γ and μ, some parameters θ_1, θ_2 and some positive time t such that:

$$y_m(\gamma.\theta_1 + \mu.\theta_2, u, t) \neq \gamma.y_m(\theta_1, u, t) + \mu.y_m(\theta_2, u, t) \tag{2}$$

In most cases, food models are non-LP.

The general formulation of the identifiability problem is the following [2]:
if $M(.)$ is the (known) equation set of the model
θ is the (unknown beforehand) parameters of the model
The parameter θ_i is structurally globally identifiable (s.g.i.) if for almost any θ^*

$$M(\theta) \approx M(\theta^*) \Rightarrow \theta_i = \theta_i^* \tag{3}$$

The parameter θ_i is structurally locally identifiable (s.l.i.) if for almost any θ_i^*, there exists a neighbourhood $v(\theta^*)$ such that if $\theta \in v(\theta^*)$

$$M(\theta) \approx M(\theta^*) \Rightarrow \theta_i = \theta_i^* \tag{4}$$

If θ_i is not s.g.i nor s.l.i it is obviously s.n.i, Structurally Non Identifiable.
Depending on the LI or non-LI cases, four main methods can be considered.

knowledge-based approach

As a simple example, let us consider the convective heat flux:

$$\Phi = h.S.(T_a - T_p) \tag{5}$$

with both h and S unknown. Since they always appear as $h.S$ everywhere in the model equation set, these parameters are obviously non-identifiable whatever the experiment design would be. Proof: if $h'.S'$ is a solution of the identification problem then $(h'/2).(2.S')$ would be a solution as well.

This kind of approach can only work on simple problems where non-identifiability is easy to find. On the other hand it works as well on LP and non-LP, LI and non-LI problems.

Laplace-transform approach

Well described in [1] [2], the method relies on the computation of the transfer function matrix associated with the state-space representation (in its canonical form) of the problem. Thus, for linear system represented by:

$$\dot{x} = A.x + B.u \tag{6}$$
$$y = C.x \tag{7}$$

The transfer function $H(s, \theta)$ can be calculated as:

$$Y(s) = C(\theta).[s.I - A(\theta)]^{-1}.B(\theta).U(s) \tag{8}$$
$$H(s, \theta) = C(\theta).[s.I - A(\theta)]^{-1}.B(\theta) \tag{9}$$

where s is the Laplace variable and I the identity matrix.

Equation (3) is thus equivalent to:

$$M(\theta) \approx M(\theta^*) \Longleftrightarrow H(s, \theta) = H(s, \theta^*) \tag{10}$$

and the s.g.i. and s.l.i. discussions refer directly to the number of solutions from equation (10). This method can be applied to LP and non-LP models as well.

As an example, the transfer function $\frac{a.s}{s.b+c}$ (with three parameters a, b and c) is not s.g.i. since another transfer function $\frac{s}{s.\frac{b}{a}+\frac{c}{a}}$ gives exactly the same input-output map (with two parameters b/a and c/a).

Similarity-transform approach

On the basis of the local state isomorphism theorem, the similarity transformation approach primarily intended for linear models was extended to non-linear models [3], [4]. The first step consists in proving that the system is observable and controllable (whatever the parameter values) which can be quite difficult for nonlinear systems. The second step is to consider the set of all the similarity transformations that leave the model structure unchanged. The goal is then to prove that they are equal to the Identity transformation (for s.g.i.).

In the non-LI case, it makes use Lie-algebra which is barely used in food modelling.

Taylor-series expansion approach

This method is reserved for non-LI models since it requires classically more computations. Description can be found in [5]. Some examples are presented in [6]. Basically, the equation is developed as a Taylor series. Then, the goal is to find some relationships between the parameters θ and the n^{th} derivatives of the model. One of the difficulties that arise comes from the required, maybe high, order of derivation needed for the demonstration.

Linearizing approach

When it is not too complex to do, a linearizing of the model to make it LI or LP can considerably simplify the problem. There are many different ways for this purpose: using the physics of the system, multiple derivations, change of variables... Some examples can be found in [6] and [7].

Practical aspects

Whatever the preferred approach is, a computer algebra is welcome. Classical softwares used are Mathematica, Maple and MuPAD. This is especially true since obviously no method is straithforward.

Compartmental models especially in biology and pharmacokinetic are probably the most studied models concerning parameter identification. [6] discuss the identifiability of several biokinetic models with 2 methods: Taylor series and linearizing. [7] have extensively studied modelling, *on-line estimation* and control of bioreactors.

When some parameters are not structurally globally (nor locally) identifiable, the identification routine often fails finding the right s.g.i. parameters. An alternate strategy can be found in [8] to overcome these difficulties.

Application to drying

When considering drying models which take into account internal moisture content gradient and are broadly validated on a large drying domain, only diffusion based models and compartmental models appear competitive. In this paper, two examples are considered:

- diffusion model, water is assumed to diffuse in its liquid form and to evaporate at the surface. Details can be found in [9].
- compartmental model, water is assumed to be exchanged between compartments in its liquid form, evaporation takes place only in the surface compartment. Details can be found in [10].

No publications were found concerning the structural identifiability of drying models. In this paper, the preferred method for the testing of s.g.i. and s.l.i was the *Laplace transform approach* as described in [1] and [2]. A sketch of the method is:

1. write the model equation set
2. modify, if needed, the model to be LI
3. rewrite it as a linear state-space representation
4. compute the laplace transform of the system
5. simplify, if needed, the obtained transfer function to have its canonic form
6. compute the solutions of $H(s,\theta) = H(s,\theta^*)$ with θ^* fixed
7. conclude for each parameter depending on the solutions

In the following examples, the product is assumed having an internal moisture content gradient and being uniform in temperature. Within the product, mass transfers occur only in the liquid form and vapourization takes place only at the surface. The heat transfer is convective. The product is typically a grain (*e.g.* maize) with an approximately spherical shape.

The equation sets correspond to thin layer models *i.e.* models for one average grain. Initial conditions are similar: at the initial time, moisture content is assumed uniform and equal to X_0, and temperature $T_g = T_{g0}$.

Diffusion model

The model is written in spherical coordinates since a spherical shape is assumed. The diffusion coefficient D is assumed to be uniform and constant. The exact equation set follows (11-13):

$$\frac{dX}{dt} = D.\left[\frac{2}{r}.\frac{\delta X}{\delta r} + \frac{\delta^2 X}{\delta r^2}\right] \tag{11}$$

$$\frac{dT_g}{dt} = \frac{-h.a.(T_g - T_a) - K.a.(X_{equ} - X_{surface}).L_v}{\rho_g.Cp_g} \tag{12}$$

$$-D.\frac{\delta X_{surface}}{\delta r} = K.(X_{equ} - X_{surface}) \tag{13}$$

In equations (12-13), the mass transfer, at the surface, is assumed to be proportional to the distance to the equilibrium moisture content instead of a difference between product and air partial vapour pressures. This is done only for linearizing reasons since the latter has a stronger physical sense.

To fulfill the LI requirements, the $\rho_g.Cp_g$ term variations are assumed to be negligible. This is approximately true for small variations of X *i.e.* small drying ranges.

Since the equation set (11-13) is usually solved numerically through the use of finite difference scheme, the same method is applied here. The discretization allows to get rid of the space derivatives to keep only time derivatives. Classically, the spherical product is divided into n intervals of equal thickness Δr. We have arbitrarily chosen to divide the sphere into four intervals of equal thickness to have a reasonable matrix dimension. So the system becomes [9]:

$$\frac{dX_0}{dt} = D.[3.\frac{X_1 - 2.X_0 + X_1}{\Delta r^2}] \tag{14}$$

$$\frac{dX_i}{dt} = D.[\frac{X_{i+1} - X_{i-1}}{i.\Delta r^2} + \frac{X_{i+1} - 2.X_i + X_{i-1}}{\Delta r^2}],\ 1 \leq i \leq n-1 \tag{15}$$

$$\frac{dX_n}{dt} = \frac{2.K}{\Delta r}.(X_{equ} - X_n) - 2.D.[\frac{X_n - X_{n-1}}{\Delta r^2}] \tag{16}$$

$$\frac{dT_g}{dt} = \frac{h.A_g}{\rho.Cp_g.V_g}.T_a - \frac{h.A_g}{\rho_g.Cp_g.V_g}.T_p + Lv.K.X_{equ} - Lv.K.X_n \tag{17}$$

The obtained LI discrete system (14-17) can be rearranged in a matrix-vector notation:

$$\dot{x} = A.x + B.u \tag{18}$$

$$y = C.x \tag{19}$$

Two cases were tested: with or without product temperature T_g measurement. To have a reasonable matrix dimension, n was chosen small (*i.e.* 4). In the first case, it gives:

$$y = \begin{bmatrix} \bar{X} & T_g \end{bmatrix}' \tag{20}$$

$$x = \begin{bmatrix} X_0 & X_1 & X_2 & X_3 & X_4 & T_g \end{bmatrix}' \tag{21}$$

$$u = \begin{bmatrix} X_{equ} & T_a \end{bmatrix}' \tag{22}$$

$$A = \begin{bmatrix} -6.\frac{\theta_1}{\Delta r^2} & 6.\frac{\theta_1}{\Delta r^2} & 0 & 0 & 0 & 0 \\ 0 & -2.\frac{\theta_1}{\Delta r^2} & 2.\frac{\theta_1}{\Delta r^2} & 0 & 0 & 0 \\ 0 & \frac{1}{2}.\frac{\theta_1}{\Delta r^2} & -2.\frac{\theta_1}{\Delta r^2} & \frac{3}{2}.\frac{\theta_1}{\Delta r^2} & 0 & 0 \\ 0 & 0 & \frac{2}{3}.\frac{\theta_1}{\Delta r^2} & -2.\frac{\theta_1}{\Delta r^2} & \frac{4}{3}.\frac{\theta_1}{\Delta r^2} & 0 \\ 0 & 0 & 0 & 2.\frac{\theta_1}{\Delta r^2} & -2.\frac{\theta_2}{\Delta r} - 2.\frac{\theta_1}{\Delta r^2} & 0 \\ 0 & 0 & 0 & 0 & -Lv.\theta_2 & -\theta_3.\frac{A_g}{\rho_g.Cp_g.V_g} \end{bmatrix} \tag{23}$$

$$B = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 2.\frac{\theta_2}{\Delta r} & 0 \\ Lv.\theta_2 & \theta_3.\frac{A_g}{\rho_g.Cp_g.V_g} \end{bmatrix} \tag{24}$$

$$C = \frac{1}{1000}.\begin{bmatrix} 1 & 26 & 98 & 218 & 657 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1000 \end{bmatrix} \tag{25}$$

In the second case, the differences are:

$$y = \begin{bmatrix} \bar{X} \end{bmatrix} \tag{26}$$

$$C = \frac{1}{1000}.\begin{bmatrix} 1 & 26 & 98 & 218 & 657 & 0 \end{bmatrix} \tag{27}$$

The unknown parameters are $\theta_1 = D$, $\theta_2 = K$ and $\theta_3 = h$.

Compartmental model

The model is written assuming 3 compartments (without any assumption about a particular shape). The product is assumed to be uniform (negligible internal temperature gradient). The evaporation takes place only in the third compartment (at the surface). The exact equation set follows (28-31):

$$\frac{dX_1}{dt} = \frac{B_1}{\rho_g.\tau_1}.(X_2 - X_1) \tag{28}$$

$$\frac{dX_2}{dt} = \frac{B_1}{\rho_g.\tau_2}.(X_1 - X_2) + \frac{B_2}{\rho_g.\tau_2}.(X_3 - X_2) \tag{29}$$

$$\frac{dX_3}{dt} = \frac{B_2}{\rho_g.\tau_3}.(X_2 - X_3) + \frac{K.a}{\rho_g.\tau_3}.(X_{equ} - X_3) \tag{30}$$

$$\frac{dT_g}{dt} = \frac{-h.a.(T_g - T_a) - K.a.(X_{equ} - X_3).L_v}{\rho_g.Cp_g} \tag{31}$$

Compared to [10] and [11], there is a slight difference in the way evaporation is represented. As for the diffusion model, the mass transfer at the surface is represented in equations (30-31) in terms of moisture content distance to equilibrium instead of vapour partial pressure difference.

To fulfill the LI requirements, as for the diffusion model, the $\rho_g.Cp_g$ term variations are assumed to be negligible.

The obtained LI system (28-31) can be rearranged in a matrix-vector notation:

$$\dot{x} = A.x + B.u \tag{32}$$

$$y = C.x \tag{33}$$

Two cases were tested: with or without product temperature T_g measurement. In the first case, it gives:

$$y = \begin{bmatrix} \bar{X} & T_g \end{bmatrix}' \tag{34}$$

$$x = \begin{bmatrix} X_1 & X_2 & X_3 & T_g \end{bmatrix}' \tag{35}$$

$$u = \begin{bmatrix} X_{equ} & T_a \end{bmatrix}' \tag{36}$$

$$A = \begin{bmatrix} \frac{\theta_1}{\rho_g.\tau_1} & -\frac{\theta_1}{\rho_g.\tau_1} & 0 & 0 \\ \frac{\theta_1}{\rho_g.\tau_2} & -\frac{\theta_1}{\rho_g.\tau_2} - \frac{\theta_2}{\rho_g.\tau_2} & \frac{\theta_2}{\rho_g.\tau_2} & 0 \\ 0 & \frac{\theta_2}{\rho_g.\tau_3} & -\frac{\theta_2}{\rho_g.\tau_3} - \frac{\theta_3.a}{\rho_g.\tau_3} & 0 \\ 0 & 0 & \frac{\theta_3.a.Lv}{\rho_g.Cp_g} & -\frac{\theta_4.a}{\rho_g.Cp_g} \end{bmatrix} \quad (37)$$

$$B = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ \frac{\theta_2}{\rho_g.\tau_3} & 0 \\ \frac{Lv.a.\theta_3}{\rho_g.Cp_g} & \frac{a.\theta_4}{\rho_g.Cp_g} \end{bmatrix} \quad (38)$$

$$C = \begin{bmatrix} \tau_1 & \tau_2 & \tau_3 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad (39)$$

In the second case, the differences are:

$$y = \begin{bmatrix} \bar{X} \end{bmatrix} \quad (40)$$

$$C = \begin{bmatrix} \tau_1 & \tau_2 & \tau_3 & 0 \end{bmatrix} \quad (41)$$

The unknown parameters are $\theta_1 = B_1$, $\theta_2 = B_2$, $\theta_3 = K$ and , $\theta_4 = h$.

Discussion

Doing the calculation without a computer would be a heavy duty job. Hence, the computations were done on MuPAD 1.3 from Paderborn University. It takes about 10 minutes before having the result. Conclusions for diffusion model are presented on table 1 while those for the compartmental model are on the table 2.

Table 1: Structural identifiability of the diffusion model.

T_g	$\theta_1 = D$	$\theta_2 = K$	$\theta_3 = h$
measured	s.g.i.	s.g.i.	s.g.i.
unmeasured	s.g.i.	s.g.i.	**s.n.i**

Table 2: Structural identifiability of the compartmental model.

T_g	$\theta_1 = B_1$	$\theta_2 = B_2$	$\theta_3 = K$	$\theta_4 = h$
measured	s.g.i.	s.g.i.	s.g.i.	s.g.i.
unmeasured	s.g.i.	s.g.i.	s.g.i.	**s.n.i**

The major conclusion is that the heat transfer coefficient h can only be identified if the product temperature T_g is measured. It appears obviously since h disappears in $H(s, \theta)$ if T_g isn't measured. This is a very interesting point since this kind of measurement is very difficult to obtain without any bias. For instance, putting a micro-thermocouple in the center of the product is known to lead to biased measures (due to the resulting heat shortcut). On the other hand, h can be *a priori* fixed from literature as a given constant or as a K-related parameter (using Colburn analogy for instance).

This also means that such models shouldn't be expected to simulate precisely the product temperature T_g. Hence, since quality models strongly rely on this prediction, increased errors may appear in the quality estimate.

A minor conclusion is that measuring a single and global apparent moisture content of the product is sufficient to identify all mass transfer coefficients. This was heavily expected since most authors adjust their (unknown) parameters on the basis of weight measures.

Some discussion arises when remembering the strong assumptions made to force the model linearity. Probably the most arguable point is the the assumption concerning the mass transfer coefficients being constants. For instance the dependency of D on X is well accepted. It can be shown easily that this dependency does not change the conclusion concerning h. The only thing that can change the result is a T_g temperature dependency.

Similarly, the B_1 and B_2 coefficients depend on the air temperature T_a in [10] and [11] and not on the grain temperature T_g. So, it shouldn't change the s.n.i. conclusion for h. In fact, it would be interesting to show that replacing the $K.(X_{equ} - X_3)$ by its equivalent expression in terms of partial pressure of vapour should make h s.g.i. instead of s.n.i. This comes from the dependency of the grain partial pressure of vapour on the grain temperature T_g.

Taking into account the full complexity of the previous models would lead to heavy duty jobs whose practical interest is not proven. A point of view could be to use the simplified structural identifiability test for better understanding more than for the obtaining of definitive proofs.

And it shouldn't be neglected that the experiments often add much more limitations. For instance, drying kinetics under constant conditions can be regressed as one or two exponentials leading to two to four parameters. Hence, it would be a non sense to try to identify more than four parameters on this data.

Although relying on strong simplifying assumptions, this methodology, can be a useful tool prior to any experimentation. Its conclusions concern the instrumentation of the experimental apparatus and the identification expectations. Since most calculations can be done on a computer algebra, the implied work is limited.

Notation

latin letters

A, B *and* C	matrix used is state-space representation
a	grain surface area / volume ratio (m^{-1})
A_g	single grain surface area (m^2)
B_i	water exchange coefficient between compartments i and $i+1$ $(kg.s^{-1}.m^3)$
Cp	specific heat at constant pressure $(J.kg^{-1}.K^{-1})$
D	liquid water diffusivity in the product $(m^2.s^{-1})$
H	transfer function matrix
h	convection heat transfer coefficient $(W.m^{-2}.K^{-1})$
I	identity matrix
K	mass transfer coefficient at the product surface $(m.s^{-1})$
L_v	latent heat of vapourization $(J.kg^{-1})$
$M(.)$	model structure
r	radius in diffusion model (m)
s	Laplace variable †
S	section area (m^2)
t	time (s)
T	temperature $(°C)$
U, u	model input vector †
V	volume (m^3)
X	grain moisture content (dry basis) †
$\bar{X}$	grain mean moisture content (dry basis) †
x	model state vector †
Y, y	model output vector †

greec letters

Φ	heat flux (W)
ρ	product density ($kg.m^{-3}$)
τ	volume ratio of compartment †
θ	(unknown) model parameters

subscripts

0	initial
1	central compartment
2	medium compartment
3	peripheral compartment
a	air
equ	at equilibrium
f	final
g	grain
p	product
t	at time t
w	water

†No dimension

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