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MODEL IDENTIFICATION AND ON-LINE OPTIMAL CONTROL OF FOOD PROCESSES

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Abstract. Food processes are coupled systems that involve heat, mass and momentum transfer together with kinetic processes related to quality and safety. This work is devoted to illustrate how model-based techniques offer the possibility to rationally optimise processes even in real time. The contribution is mainly based on our group experience and illustrates concepts with several examples such as the refrigeration of fruits, the deep-fat frying of potato chips, the freeze-drying of dairy products and the thermal processing of packaged foods. *Coupled Problems 2013 Conference.*

1 INTRODUCTION

Computer-aided simulation and model-based optimisation offer a powerful and systematic way to design and operate food processes. However, current industrial applications usually rely on simplified stationary models, the so called response surfaces, which are insufficient to describe the dynamic and distributed nature of food processing.

As an alternative, in recent decades there has been a growing interest in the development of rigorous models, based on first principles, that enable not only to perform experiments *in silico*, but to design and to optimise operation policies.

However, several problems arise: i) the complexity of food processes that include physical, chemical and biological phenomena on a wide range of time and space scales calls for advanced numerical methods; ii) the lack of information about specific processes and food-related thermo-physical and kinetic constants requires the implementation of identification loops incorporating parameter estimation, identifiability analyses and optimal experimental design; iii) the necessity of adapting the models to be used in real time decision making, calls for the development of techniques to obtain accurate and efficient

reduced order models and iv) the usual multimodality of the associated optimisation problems demands the development of robust and efficient global optimisation methods.

This contribution presents and describes methods to face such problems. Concepts are illustrated with the following examples: the refrigeration of fruits, the deep-fat frying of potato chips, the freeze-drying of dairy products and the thermal processing of packaged foods.

2 MODELING AND SIMULATION OF FOOD PROCESSING

2.1 Mathematical models

The mathematical modelling of food processing requires identifying and describing the physical, chemical, and biological changes experienced by the product during processing and storage. This means that, besides the heat, mass and momentum transfer mechanisms, the kinetics of quality and safety have also to be considered. As a conclusion, models of food processing typically consist of sets of coupled non-linear ordinary and partial differential (PDEs) equations:

$$\Psi(\mathbf{z}, \mathbf{z}_\xi, \mathbf{z}_{\xi\xi}, \mathbf{z}_t, \mathbf{u}, \boldsymbol{\theta}, t) = 0 \tag{1}$$

$$\mathbf{z}(\xi, t_0) = \Psi_0(\mathbf{z}(\xi, t_0), \mathbf{u}(t_0), \boldsymbol{\theta}, t_0) \quad ; \quad \mathcal{B}(\mathbf{x}, \mathbf{x}_\xi, \mathbf{u}, \boldsymbol{\theta}, \xi, t) = 0 \tag{2}$$

where $\xi \in \Omega \subset \Re^3$ are the spatial variables, $\mathbf{z}(\xi, t) \in Z \subset \Re^\nu$ are the state variables (temperature, water content, etc), $\mathbf{z}_\xi = \partial\mathbf{z}/\partial\xi$, $\mathbf{z}_{\xi\xi} = \partial^2\mathbf{z}/\partial\xi^2$, $\mathbf{z}_t = \partial\mathbf{x}/\partial t$, $\mathbf{u} \in U \subset \Re^\sigma$ are the control variables and $\boldsymbol{\theta} \in \Theta \subset \Re^\eta$, time independent parameters (thermo-physical or kinetic related constants). Eqs. (2) represent the initial and boundary conditions.

2.2 Numerical simulation

The finite element method (FEM) in combination with a suitable implicit time integration scheme is possibly the standard to handle complex geometries, and non-linear sets of PDEs in food processing simulation. In fact, commercial general purpose implementations, such as COMSOL©, are the most popular choice [1].

These software tools allow testing "what-if" scenarios to predict food product characteristics given particular operation conditions. However, the associated computational cost may be unreasonable for the purpose of design, optimisation and control. This calls for the development of methods to derive reduced order models (ROMs) which preserve the predictive capabilities of the full model and can be solved very efficiently.

2.3 Reduced order models

Reduced order models based on the projection of the original PDE system over a set of global spatial basis functions have emerged as efficient alternatives to classical discretisation techniques. In particular, the proper orthogonal decomposition (POD) was successfully applied in the context of food processing [2–4]. In this approach, each of the state variables is approximated by a truncated series of the form:

$$z(\xi,t) \simeq \tilde{z}(\xi,t) = \sum_{j=1}^{p} m_j(t)\phi_j(\xi) \tag{3}$$

and the terms ϕ_j are obtained by solving the following eigenvalue problem:

$$\lambda_j \phi_j(\xi) = \int_V K(\xi,\xi')\phi_j(\xi')d\xi'; \quad K = \frac{1}{k}\sum_{n=1}^{k} Z_n Z_n^T \tag{4}$$

being $\{Z_n\}_{n=1}^{k}$ a set of measurements (snapshots) representative of the system's behavior. POD basis functions can be different for each state variable (*separate basis* approach) or can be unique for all state variables (*joint basis* approach) [4]. The joint basis approach is particularly useful when the states are highly coupled.

The coefficients m_j are computed as the solution of the ODE system resulting from the projection of Eqs. (1)-(2) over the POD basis. Details on how the FEM structure can be exploited to numerically compute projections can be found in [5].

3 MODEL IDENTIFICATION

Thermo-physical properties vary considerably among food products, within products (anisotropic, heterogeneous,...) or even with the process itself. However thermo-physical properties are only a part of the story. We also need to know the rates of reactions for biochemical (nutrient, color, flavor, etc.) or microbial changes.

Even though some thermo-physical parameters may be found in the literature, most of the model parameters are not known and can not be measured. In this regard, their values must be estimated from experimental data in the so call *parametric model identification* which comprises the following steps: parameter estimation, identifiability analysis and optimal experimental design.

3.1 Parameter estimation

The parameter estimation problem is usually formulated as a nonlinear optimisation problem where the objective is to find the parameters that minimise J_{wlsq}, i.e. the sum of the weighted least squares of the residuals between the model predictions and the experimental data. The weights can be related to experimental error.

The problem is particularly challenging due to the usual presence of multiple suboptimal solutions (multimodality), or multiple equivalent solutions (lack of or poor identifiability) [6]. Multimodality may be overcome by the use of global optimisation methods. Lack or poor practical identifiability may be reduced (or even eliminated) by model-based optimal experimental design.

3.2 Identifiability analysis

In order to asses the quality of the parameter estimates, several possibilities exist. Bootstrap or jack-knife approaches allow to compute robust confidence intervals. However, the associated computational cost makes it difficult to use these methods for large scale models. Alternatively, the confidence interval of $\boldsymbol{\theta}_i^*$ may be obtained through the covariance matrix:

$$\pm t_{\alpha/2}^{\gamma} \sqrt{\mathbf{C_{ii}}} \tag{5}$$

where $t_{\alpha/2}^{\gamma}$ is given by Students t-distribution, $\gamma = N_d - \eta$ degrees of freedom and $(1 - \alpha)100\%$ is the confidence interval selected, typically 95%.

For non-linear models, there is no exact way to obtain $\mathbf{C}$. Therefore, the use of approximations has been suggested. Possibly the most widely used is based on the Crammèr-Rao inequality which establishes, under certain assumptions on the number of data and non-linear character of the model, that the covariance matrix may be approximated by the inverse of the Fisher information matrix (FIM) which is formulated as follows:

$$\mathcal{F} = \underset{\mathbf{y}_m|\boldsymbol{\theta}^*}{E} \left\{ \left[\frac{\partial J_{wlsq}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right] \left[\frac{\partial J_{wlsq}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right]^T \right\} \tag{6}$$

3.3 Optimal experimental design

In order to improve the quality of parameter estimates it is possible to use the model to define new experiments. The idea is to formulate a dynamic optimisation problem where the objective is to find those experimental conditions which result in maximum information content as measured by, for example, the FIM, subject to the system dynamics Eqs. (1-2) plus experimental constraints. The problem can be solved by a combination of the control vector parameterisation (CVP) method and a suitable optimiser enabling the simultaneous design of several dynamic experiments with optimal sampling times [7] and optimal sensor locations [5].

AMIGO (Advanced Model Identification using Global optimisation) [8], a MATLAB based toolbox that covers all model identification steps, was used in this work.

4 DYNAMIC optimisation

The dynamic optimisation (DO) problem can be formulated as: Find the controls $\mathbf{u}(t)$ subject to the system dynamics Eqs. (1-2) so as to minimize (or maximize) a given objective functional, that can be related to final product quality, energy consumption, etc. State and control variables may be also subject to constraints which force the satisfaction of safety or environmental regulations, proper operation conditions, etc. These constraints may be point constraints, that must be satisfied at certain time points during process and path constraints, that must be satisfied throughout the process.

The DO problem can be solved using the CVP method. The control variables are discretised and approximated using low order polynomials. The coefficients of these poly-

nomials become the decision variables in a non-linear optimisation problem whose solution involves the simulation of the system dynamics and the assessment of the constraints.

5 ILLUSTRATIVE EXAMPLES

5.1 Reduced order modeling: fruit refrigeration

Refrigeration is probably the most critical process in fruit storage and transport. A poor temperature/pressure control inside the storage chamber would imply a quality loss of the fruit. In this context, model-based process design may help us to compute optimal operation policies in real time. However rigorous models take into account several processes, such as hydrolysis, cellular respiration or mass and heat transport, to name a few. The result is a set of coupled nonlinear PDEs whose solution is computationally demanding. Thus preventing, its application for real time purposes.

Eight state variables were considered: temperature (T), concentration of starch (C_S), middle lamella (C_L), hexose (C_H), water (C_W), oxygen (C_{O_2}), carbon dioxide (C_{CO_2}) and nitrogen (C_{N_2}). The complete set of equations reads as follows [9]:

$$\frac{\partial C_i}{\partial t} = r_{C_i}; \quad i \in \{S, L, H\} \tag{7}$$

$$\alpha_{C_i}\frac{\partial C_i}{\partial t} + \nabla(\bar{\mathbf{u}}C_i) = \nabla(D_{C_i}\nabla C_i) + r_{C_i}; \quad i \in \{O_2, CO_2, N_2\} \tag{8}$$

$$\frac{\partial C_W}{\partial t} = \nabla(D_W\nabla C_W) + r_W; \qquad \rho c_T\frac{\partial T}{\partial t} = \nabla(K_T\nabla T) \tag{9}$$

where r_{C_i} denotes the reaction terms which are in general highly nonlinear on the corresponding states (for a detailed description see [4]).

For the solution with the FEM, linear Lagrange elements were considered and a spatial mesh of 1818 points (see Figure 1a) was used. Note that since the model consists of eight state variables, around 14500 ODEs need to be solved with this scheme.

The snapshots required for the computation of PODs in Eq. (4) were obtained by running 27 simulations of the PDE model (7)-(9) in different conditions (chamber temperature, humidity and air composition). For validation purposes a new experiment, not included in the 27 simulations, was performed. As shown in the Figures 1b&c, results obtained with ROMs are in good agreement with the ones obtained by FEM, with two orders of magnitude reduction in computational cost.

It should be also mentioned that the *joint basis* approach, which consists of 18 ODEs, is more efficient than the *separated basis* approach (31 ODEs). The solution of the ROM requires around 2 min in a PC Intel R CoreTM i7 PC, being therefore suitable for real time applications.

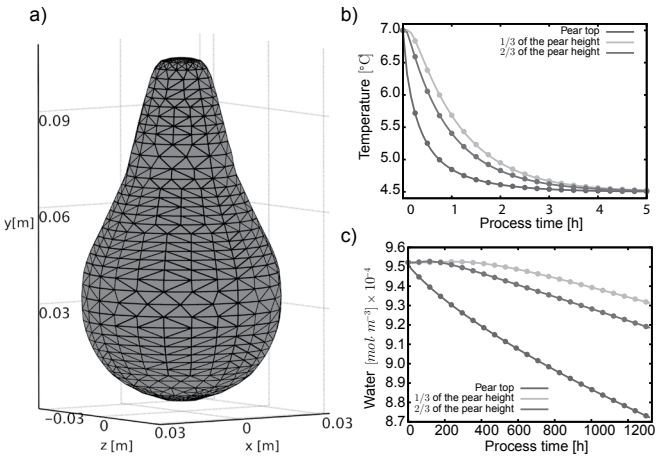

Figure 1: a) 3D geometry and FEM mesh; b) & c) Comparison of solutions achieved by FEM (continuous lines) and ROM for the validation experiment at three different spatial points.

5.2 Dynamic optimisation: freeze-drying of dairy products

Freeze-drying is an attractive dehydration process for preserving nutritional and organoleptic properties of valuable food goods since it helps to maintain the biological activity of their thermosensitive components. Unfortunately, it is also known to be a high demanding process in terms of time and energy, which calls for efficient tools capable of minimizing costs while attaining market quality requirements.

Classical models for freeze-drying processes are usually large-scale and computationally involved, thus unsuitable for real time applications. In order to lighten the computational efforts involved, an accurate yet simplified distributed model has been recently developed [3]. After performing a time-scale analysis of process dynamics, modelling tasks have been focused on the leading scale (the one related to the temperature within the porous matrix). The resulting 1D model for a dairy product sample describing primary and secondary drying reads:

$$\frac{\partial T_I}{\partial t}(x,t) = \alpha_I \frac{\partial^2 T_I}{\partial x^2}(x,t) \quad ; \quad \frac{\partial T_{II}}{\partial t}(x,t) = \alpha_{II} \frac{\partial^2 T_{II}}{\partial x^2}(x,t) \tag{10}$$

$$\frac{\partial}{\partial x}\left(-\rho_v(x,t)\frac{K}{\mu}\frac{\partial P_v}{\partial x}(x,t)\right) = 0, \quad \forall x \in (0, S(t)) \tag{11}$$

with the following boundary conditions:

$$k_I \frac{\partial T_I}{\partial x}(0,t) = \sigma e f \left(T_c^4 - T_I^4(0,t)\right) \quad ; \quad k_{II}\frac{\partial T_{II}}{\partial x}(L,t) = h_L\left(T_L - T_{II}(L,t)\right) \tag{12}$$

$$T_{I_s} = T_{II_s} = T_s(P_v(S(t)) \; ; \; k_{II}\frac{\partial T_{II}}{\partial x}(S(t),t) - k_I \frac{\partial T_I}{\partial x}(S(t),t) = \Delta H_s(\rho_{II} - \rho_I)\frac{\partial S(t)}{\partial t} \tag{13}$$

$$P_v(0,t) = P_c \quad ; \quad -\rho_v(S(t),t)\frac{K}{\mu}\frac{\partial P_v}{\partial x}(S(t),t) = \frac{\partial S(t)}{\partial t}\left(\rho_{II} - \rho_I\right) \tag{14}$$

where, T regards temperature, P the pressure, L the sample length, $S(t)$ the moving front position, C_b the water content and T_g the glass transition temperature. The subscript I refers to the dried region, II to the frozen region, c to the chamber, L to the shelf, v to the vapour and s to sublimation. The secondary drying is only governed by the Fourier equation in the dried region, while boundary conditions are defined by fluxes in Eq. (12). For a complete description of the time-scale analysis and the derivation of this simplified model (including the definitions of model parameters and the GAB-based desorption model) readers are referred to [3]. The system of Eqs.(10-14) was solved by FEM with an Arbitrary Lagrangian-Eulerian method so as to track the moving front [11]. An adaptive mesh of 73 nodes was used and the simulation takes around 20 s in COMSOL©.

The model was used to compute the temperature in the shelf ($223K \leq T_L \leq 323K$) and the pressure in the chamber ($10\ Pa \leq P_c \leq 60\ Pa$) that minimise the freeze-drying cycle time t_f, while satisfying process dynamics in Eqs. (10)-(14) simultaneously with the product stability specifications ($C_b^{ave}(t_f) = 0.02$, $T(x,t) \leq T_g$).

Different configurations in the equipment were considered, leading to different operational scenarios. The CVP approach was used in combination with a scatter search based global optimiser [10] to solve the associated problems. Optimal profiles (Figure 2a)&b)) resulted in a 25% reduction of the cycle time: from $t_f = 38.4\ h$ to $t_f = 28.6\ h$ achieved with constant and dynamic P_c and T_L optimal profiles, respectively.

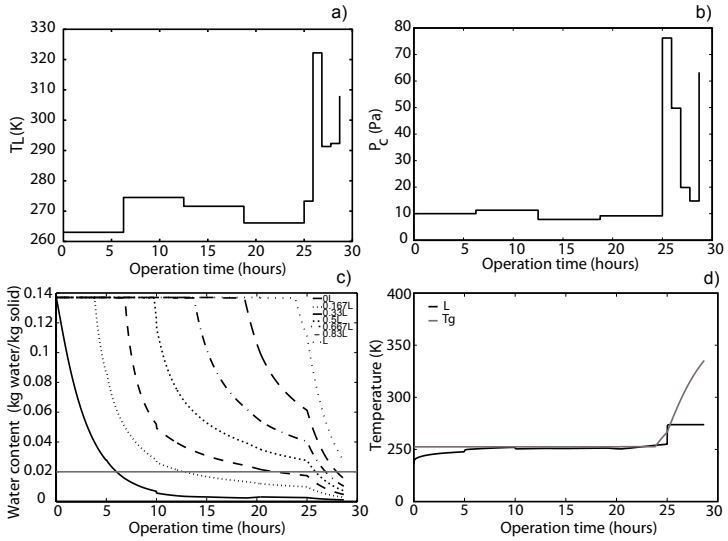

Figure 2: a) & b) Optimal operation profiles, c) & d) Satisfaction of operation constraints

5.3 Identification and dynamic optimisation: frying of potato chips

In deep-fat frying foodstuff is immersed into oil at high (constant) temperature. This induces water evaporation and the formation of a thin crust. As the temperature increases and moisture is lost, the typical deep-frying sensory characteristics (colour, flavour, texture) are developed. However, the use of high temperatures results in the production of acrylamide, a carcinogen compound. Thus model-based optimisation may assist in the design of those operating conditions that provide the best compromise between quality and safety.

A multiphase porous media based model was formulated to describe heat, mass and momentum transfer and acrylamide kinetics within a potato chip [12]. The model consists of a set of coupled nonlinear PDEs describing the evolution of the saturation of water, oil and vapor (S_w,S_o, S_g), product temperature (T), moisture content (M), pressure (P), water vapour mass fraction (ω_v) and acrylamide content (c_{AA}). The potato chip is assumed to be cylindrical and heated from outside therefore axi-symmetry can be assumed.

The model was solved in COMSOL©. The *Convection and Diffusion* module was used to solve for water, oil and acrylamide mass conservation while *Maxwell-Stefan Diffusion and Convection* was used to gas mass fraction and *Darcy's Law* and *Convection and Conduction* were used to solve for pressure and temperature respectively. The selected mesh consists of 20×10 rectangular elements. The simulation of 1.5 *min* frying takes around 40 *s* in a standard PC 3.25GB RAM and 2.83GHz.

Unknown parameters, the heat transfer coefficient (h) and the surface oil saturation $S_{o,surf}$, were identified from experimental data using AMIGO [8]. The final model exhibits good predictive capabilities enabling the possibility to analyse alternative operating conditions.

The objective was then to compute the oil temperature profile ($T_{oil_{min}} \leq T_{oil} \leq T_{oil_{max}}$) that guaranties the desired moisture content ($M(t_f) \leq 2$) while minimizing final acrylamide content subject to the process dynamics. The problem was solved by means of a combination of the CVP approach and a scatter search based global optimiser [10].

Results show that using two heating zones significantly reduces the final acrylamide content with respect to typical constant operating profiles (Figure 3a). Under constant optimally designed T_{oil}, the minimum acrylamide content would correspond to a longer process at a lower temperature. However, a longer process leads to an increase of oil uptake as well as to a reduction of the production rates. The optimal profile corresponds to the use of a higher temperature at the beginning of the process, this helping to satisfy the constraint on the moisture content, followed by a lower temperature to minimise the final acrylamide content (Figure 3b).

5.4 Real time optimisation: thermal sterilisation of packaged foods

The thermal processing of packaged foods is intended to inactivate possible spores, microorganisms or enzymes present in the foodstuff which may have a negative impact

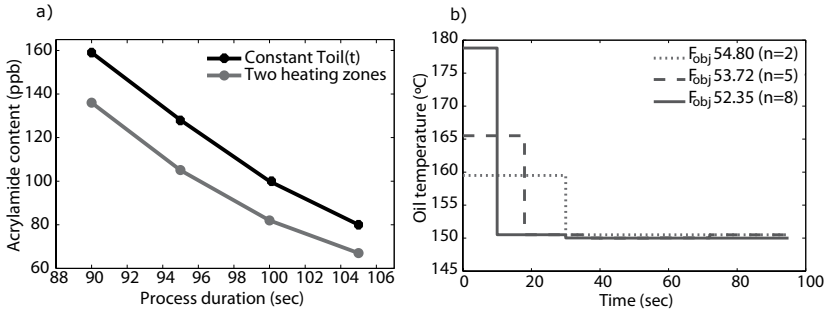

Figure 3: a) Acrylamide content versus process duration for optimally designed 1 and 2 heating zones. b) Optimal operation profiles (oil temperatures) using different numbers of heating zones ($t_{final} = 95\ s$).

on consumer's health or product quality. To that purpose, the product is introduced in a steam retort where it is subjected to a given heating-cooling cycle so as to get a pre-specified degree of inactivation indicated by the microbiological lethality. However, some organoleptic properties or nutrients can be negatively affected by the heat action. The objective is, therefore, to optimise operation conditions to maximise quality while guaranteeing safety. In this example, we go a step further, and propose a real time optimisation (RTO) architecture to handle the optimisation during processing and in the presence of uncertainty or sudden disturbances. The performance of the proposed RTO architecture was experimentally validated for tuna paté at the pilot plant in the IIM-CSIC.

The dynamic representation of the plant couples the description of the temperature and pressure inside the retort, the temperature distribution inside the food product and the corresponding distribution of nutrients and microorganisms:

Retort dynamics

$$\frac{d\mathbf{z}}{dt} = \mathbf{f}(\mathbf{z};\boldsymbol{\theta}) + \mathbf{g}(\mathbf{z},\mathbf{u};\boldsymbol{\theta}), \tag{15}$$

here $\mathbf{f}$ and $\mathbf{g}$ are nonlinear vector fields of appropriate dimensions; $\mathbf{z}$ denotes the temperature and pressure in the retort $[T_R, P_R]$; $\mathbf{u}$ stands for the control variables: valve positions for input and output streams. Finally, $\boldsymbol{\theta}$ denotes the vector of unknown parameters.

Temperature distribution inside the food product

$$\frac{\partial T_{prod}}{\partial t} = \alpha \Delta T_{prod} \quad , \quad n(k\Delta T_{prod}) = h(T_R - T_{prod}) \tag{16}$$

where T_{prod} is the temperature of the food stuff and h, k, α stand for the heat transfer coefficient of the package and the food thermal conductivity and diffusivity, respectively.

Quality and safety models

$$\frac{dC_i(t)}{dt} = -(\frac{\ln 10}{D_{i,ref}})C_i(t)\exp(\frac{T_{prod}(\xi,t) - T_{\xi,ref}}{z_{i,ref}}) \tag{17}$$

where subindex C_i refers to the concentration of either microorganisms or nutrients.

The unknown parameters of the model, the functional dependencies of fluxes on valves openings and the valves related constants were identified by means of parameter estimation, identifiability analysis and multi-experimental optimal design, using AMIGO toolbox [8].

For the case of the evolution of temperature inside the retort, the resulting model presents excellent predictive capabilities taking into account that a maximum error of around 3% is observed in fast transitions.

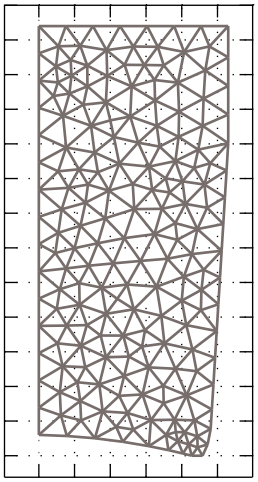

Figure 4: Geometry of the food package.

The product was packed in glass containers with metal top. The corresponding geometry and the FEM mesh used for simulation purposes are depicted in Figure 4. Selected mesh consists of 184 nodes which translates into 553 ODEs. Three model parameters were estimated from the temperature measurements, namely, the product thermal conductivity, and the glass/steam and the metal/steam heat transfer coefficients. After the model identification, the differences between model predictions and experimental data are lower than 1%.

Once a satisfactory model became available, a POD-based ROM model was developed to be used within the RTO scheme, it should be noted that each simulation of the ROM takes less than 1 s. In addition, the optimal operating conditions were computed off-line using the CVP and scatter search [10] methods.

Real time implementation of the optimal control needs to consider the effect of unmeasured disturbances not being part of the prediction model. To that purpose, feedback was implemented by regularly measuring the current retort variables and observing the relevant variables of the packaged product to compute efficient on-line optimisation. Optimal operation conditions are then re-computed any time a difference between predicted value and off-line optimal solution is detected. A combination of a local optimiser and SSm was designed so as to guarantee feasibility and optimality of the solution even in the presence of significant perturbations or plant/model mismatch (see details in [14]).

Figures 5 illustrate the performance of the RTO architecture in an experimental case were large perturbations occur. The implementation of the optimal off-line heating profile leads to a product that does not fulfil the lethality requirement ($F_c = 8min$). The RTO architecture proposed in the work was able to drive the system to feasibility and optimality by means of re-computing optimal profiles on-line and slightly extending the duration of the heating phase.

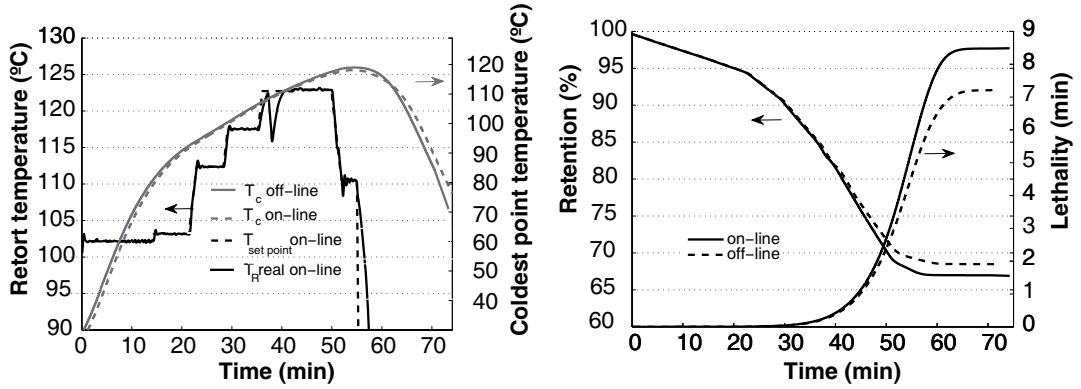

Figure 5: a)Comparison of off-line and on-line optimal profiles under large perturbations in the retort at the pilot plant (IIM-CSIC). b)Comparison of off-line and on-line optimal profiles surface nutrient retention and lethality value at the coldest point.

6 CONCLUSIONS

This work presented an overview of recent developments of our group in the context of food process modeling, model identification and reduction and real time dynamic optimisation through a number of cases of interest such as food refrigeration, freeze-drying, deep-fat frying and packaged food thermal processing.

Mechanistic models of the processes were identified for specific food products and simulated via the finite element method; reduced order versions were obtained by means of the proper orthogonal decomposition approach; quality and safety optimal operation conditions were computed using advanced global optimisation techniques and, for some cases, a real time optimisation architecture was designed and tested in pilot-plant.

Results revealed that the use of model-based process design largely improves process performance in terms of final quality and reductions on process time and energy consumption with respect to traditional operations. Proposed methodologies are general therefore opening new venues for the design of emergent or minimal food processing techniques.

Acknowledgements

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