MODELLING FOOD PROCESSING OPERATIONS WITH COMPUTATIONAL FLUID DYNAMICS: A REVIEW

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Computer simulation is a powerful tool for prediction and optimal design of food engineering operations. Partial differential equations describing momentum, heat, and mass transfer coupled with equilibrium and kinetic equations, which usually form a model for a processing operation, can be solved easily with today's computing capabilities. In this paper, a brief description of the principles of Computational Fluid Dynamics (CFD) for the solution of fluid flows with heat and mass transfer is given. Selected examples from the food engineering literature including applications in baking, drying, and sterilization are presented. Some details are given for the temperature profile, the velocity profile, and the slowest heating zone in cans filled with olives. The effect of some variables, such as the number of food items, on the temperature profile, the flow pattern, and the slowest heating and cooling zone in the can are also presented with the aim of demonstrating the possibility of optimization of thermal processing in order to minimize quality losses such as texture, flavour, and nutritional value, while keeping the product safe.

computational fluid dynamics; food processing; baking; drying; sterilization

INTRODUCTION

Momentum, heat, and mass transfer take place in many unit operations in food processing, such as pasteurization and sterilization, cooling and freezing, drying, extrusion, frying, evaporation, baking, fluidization, pneumatic transport, sedimentation, etc. In applying momentum, heat, and mass transfer knowledge on food processing, one must take into account that food industry usually deals with difficult raw materials. As biological materials, in many cases they are of non-uniform and variable consistency. The shape of the products is often irregular and sometimes changes during processing. Many food products undergo physical property changes during processing, namely thermal conductivity, specific heat, density, viscosity, etc. depend on temperature and composition. Some properties depend on shear, others are time-dependent. To add to the complexity of the problem, foods very often have neither a homogeneous nor an isotropic behaviour.

In many cases, the processing results depend on the combination of time and temperature because, in addition to temperature changes, biochemical and microbiological changes take place during processing, as for example, heat transfer and reaction kinetics considerations must be taken into account in designing thermal processes of foods. As heat and mass transfer in food processing are often transient processes, an a priori determination of processing time is of primary importance. Overprocessing, by applying for example high heat treatment, has a negative effect on the product quality and its nutritional value. Underprocessing may result in spoilage of the product. Moreover, heat and mass transfer usually occurs in more than one form either simultaneously or consecutively. For example in baking, heat exchange involves convective, radiative, and conductive heat transfer, while at the same time mass transfer occurs.

Some processes such as fluidization, pneumatic transport, and spay drying involve two-phase flows. Phase change, as is the case of ice formation in freezing, add to the complexity of the problem.

Because of these complexities, the unsteady state momentum, heat and mass transfer partial differential equations can be solved analytically only with several simplifying assumptions. Numerical methods offer an efficient and powerful tool for simulating and comprehending transport processes in the food industry. Such methods have been used in canning, freezing, drying, and other food processing operations.

There are several publications on simple shape bodies using the finite difference method, while in more irregular geometries, the finite volumes and finite elements method have been used. For example, Yanniotis, Petraki (2002) used a three-dimensional model to calculate the centre temperature in a food sample of cubical shape placed in a freezer, where the temperature fluctuates around a mean temperature due to the on-off action of the compressor

doi: 10.7160/sab.2014.450101

in the freezer. The model was solved with an explicit finite difference scheme and validated experimentally for a cube of ground beef. The effect of heat transfer coefficient, size of the cube, frequency of air temperature fluctuation, and amplitude of air temperature fluctuation on the temperature variation of the cube was studied with the model.

Despite the differences between the various numerical models, the starting point is always a set of differential equations, i.e. the three dimensional Navier-Stokes equations coupled with the energy and mass transfer equations for predicting momentum, heat and mass transfer. In addition, models for two-phase flow formulations and kinetic models may also be employed. After selecting the mathematical model one has to choose a suitable discretization method, i.e. a method for approximating the differential equations by a system of algebraic equations for the variables in question at some set of discrete locations in space and time. The most common discretization approaches include the finite difference, the finite element, and the finite volume methods. Other approaches such as boundary elements (Puri, Anantheswaran, 1993), lattice-gas cellular automata, and lattice Boltzman methods (Wolf-Gladrow, 2000) are also gaining increased attention (Sardi, Yanniotis, 2007).

A powerful tool for the numerical solution of the equations governing the flow of fluids often coupled with the energy and mass transfer equations and other equations, as stated above, is Computational Fluid Dynamics (CFD), which is a relatively new approach for the food industry. However, CFD is rapidly penetrating into the field of food engineering and reports on the application of CFD in unit operations including heating, cooling, freezing, drying, baking, membrane separation, extrusion etc. are increasing in the literature. Even processes involving fluid flow, heat transfer, and liquid food product transformation have been modelled using CFD, e.g. the evolution of a starch suspension in a heat exchanger where granule swelling is represented through a kinetic equation (Plana-Fattori et al., 2013).

The purpose of the present paper is to briefly outline the principles of CFD and give specific examples of its application in the food industry by providing a short review of recent publications in certain unit operations in the food industry, built upon previous works as by Scott, Richardson (1997), Yanniotis (2000), Xia, Sun (2002), Wang, Sun (2003), Langrish, Fletcher (2003), Welti-Chanes et al. (2005), Norton, Sun (2006), Sardi, Yanniotis (2007), Jamaleddine, Ray (2010), and Chhanwal et al. (2012).

Computational Fluid Dynamics

Computational Fluid Dynamics (CFD) was firstly computer implemented in the 1950s. Ever since, it has continued to be developed contemporaneously with the digital computers (Norton, Sun, 2007).

CFD involves the solution of the diffential equation (Eq. 1), in the general form (Patnakar 1980)

$$\frac{\partial}{\partial t}(\rho\phi)+\frac{\partial}{\partial x_j}(\rho u_j\phi)=\frac{\partial}{\partial x_j}\left(\Gamma\frac{\partial\phi}{\partial x_j}\right)+S_\phi \tag{1}$$

where
ρ = fluid density
u_j = fluid velocity component
ϕ = any variant (velocity, components, enthalpy)
Γ = diffusion coefficient
S_ϕ = source term

For ϕ equal to unity, Eq. (1) reduces to the continuity equation. On the left hand side of the equation, the first term denotes the rate of change and the second the convection flux. On the right hand side, the first term stands for the diffusion flux and the second for any generation and/or destruction of variable ϕ. For the momentum conservation equations, the term S_ϕ includes the sum of any generation and/or destruction term and of the pressure gradient on the particular direction, where appropriate. Eq. (1) is usually solved by application of the Finite Volumes discretization method.

In many applications in food processing involving heat and mass transfer, simultaneous numerical solution of Eq. (2) and (3) shown below, with the appropriate boundary conditions has been used

$$\rho C_p\frac{\partial T}{\partial t}=\nabla(k\nabla T)+\dot{q}_{evap}+\dot{q}_i \tag{2}$$

$$\frac{\partial \mathrm{C_i}}{\partial \mathrm{t}}=\nabla(\mathrm{D_{ij}}\nabla\mathrm{C})+\mathrm{R} \tag{3}$$

where
T = temperature of the food sample
C = species concentration
D_{ij} = diffusion coefficient of phase i to phase j
$\dot{q}_{evap}$ = heat transport due to vapourization (if present)
$\dot{q}_i$ = any other type of heat source (e.g. microwave heating (Oliveira, Franca, 2002))
R = phase change volumetric rate (Salagnac et al., 2004)
λ = latent heat of vapourization
ρ= density of the food sample
C_p = heat capacity of the food sample
k = thermal conductivity of the food sample

Clearly Eq. (2) and (3), written here in their complete three dimensional time dependent form, may be reduced to simpler formulations (one or two dimensional in space, time dependent or steady state). Note that Eq. (3) refers to a group of equations, one per phase. The actual number of mass transfer equations to be solved depends on the complexity of the problem (Sardi, Yanniotis, 2007).

In addition to the above equations, kinetic models for predicting the inactivation of microorganisms or enzymes or the effect on quality parameters such as vitamin retention, texture, etc. may be included in the model.

A number of common steps are always followed in the solution of a problem with CFD. In particular, the geometry of the system is defined, the computational domain, i.e. the food sample, is divided into cells, the initial and boundary conditions are defined, the physical model is defined, and the solution is then obtained at each nodal point. Finally, post-processing of the results is used for the analysis and visualization of the solution. It should be clear that a reliable solution can only be expected when a meaningful description of the physical problem is used and correct initial and boundary conditions are employed along with the correct physical properties of the food material and the appropriate quality of the mesh. The higher the density of the mesh, the better the accuracy of the solution but the more computationally expensive and time consuming the solution. It is thus necessary to find the optimum mesh density before proceeding to the final solution.

Detailed descriptions of CFD and analysis of pre-processing, processing, and post-processing can be seen in standard text books and published papers, as for example in Versteeg, Malalasekera (1995), Fletcher (1991), Xia, Sun (2002), Blazek (2005), Sun (2007).

Applications

Computational Fluid Dynamics finds application in several processing operations in the food industry including baking, drying, sterilization, pasteurization, heat exchangers, mixing, refrigeration, etc. Recent publications in the first three operations will be presented here.

Baking

Bread baking is a complex process where heat is transferred to the product surface by conduction from the metal pan walls, convection from the hot air, and radiation by the hot metal walls of the cavity or heating elements. For low air speeds, radiation is often the predominant mode of heat transfer, while convection is more important for higher air speeds (Boulet et al., 2010). Heat is transferred to the centre of the bread by conduction following an evaporation-condensation cycle of water where water evaporates on the hot side of gas cells and the vapour condenses on the colder side of the cells (De Vries et al., 1989). Besides, starch gelatinization, protein denaturation, browning reactions and crust formation take place during baking. Moreover, water is removed from the surface to the air and the structure and volume of bread change. CFD has been applied to model such a complex process. If the evaporation–condensation mechanism is not included in the model, very high temperature for the bread crumb is predicted compared to experimental results. If it is included, the evaporation–condensation processes keep the temperature of the crumb below 100°C.

Moisture transfer and volume expansion are not usually included in bread modelling due to limitations of commercial CFD software. However, a numerical model for the bread baking process with heat and moisture transport and coupled with volume change was developed by Zhang et al. (2005) and Zhang, Datta (2006). Verboven et al. (2000a, b) and Therdthai et al. (2003, 2004) have also used CFD to model baking ovens. Recently, Purlis, Salvadori (2009, 2010) modelled bread baking with volume expansion using the moving boundary approach. Chhanwal et al. (2010) tested three different radiation models, namely the discrete transfer radiation model, surface to surface and discrete ordinates for the simulation of an electrical baking oven. All the models predicted almost similar results, which tallied well with the experimental measurements. Chhanwal et al. (2011) developed a 3D CFD model incorporating an evaporation–condensation mechanism of water during baking of bread in a pilot-scale electric baking oven and studied the temperature and browning profile of bread during baking as well as the air flow pattern inside the oven cavity. The evaporation–condensation mechanism was included by defining specific heat of bread as a function of temperature including enthalpy jump at the phase change, an approach used also by Purlis, Salvadori (2009). The discrete ordinate radiation model was used in this simulation but volume expansion and moisture transport have been excluded. The crumb temperature did not exceed 100°C due to incorporation of the evaporation–condensation mechanism in the model, while the crust temperature increased continuously to reach 220°C at the end of baking. Browning of bread surface was studied using a kinetic model proposed by Zanoni et al (1995a) which depends on the bread surface temperature and baking time. The degree of starch gelatinization was also calculated by integrating the kinetics model for starch gelatinization (Zanoni et al., 1995b) using the temperature profile calculated by CFD.

Arpita Mondal, Datta (2010) developed a two-dimensional CFD model for crustless bread during baking to facilitate a better understanding of the baking process. Simultaneous heat and mass transfer from the bread during baking was successfully simulated. Tank et al. (2012) developed a CFD model to study the temperature profile of the bun during the baking process. Evaporation–condensation mechanism and effect of the latent heat during phase change of water was incorporated in the model. Further, this study was extended to investigate the effect of partially (two baking trays) loaded and fully loaded (eight baking trays) oven on the temperature profile of the bun since loading affected velocity and temperature profile.

Williamson, Wilson (2009) used CFD to test and optimize the design of a novel gas-fired radiant burner suitable for incorporation into industrial tunnel ovens. Computational fluid dynamics simulations have been used to model the burner and baking chamber environment, and in particular to predict radiation heat fluxes incident on the top surface of the food, both across the width of the baking chamber and along its length. The model developed in this work included heat transfer from coupled radiation and natural convection only. The Shear Stress Transport (SST) k-ω based turbulence model was used for this heat transfer system.

Khatir et al. (2012) used a Reynolds Averaged Navier Stokes (RANS) turbulence CFD model to predict the flow and temperature distribution within a 3-zone small scale forced convection bread-baking oven and showed how regions of recirculating flow depend on the speed of the impinging jets. Khatir et al. (2013) carried out a design parameterization of a three-dimensional generic oven model for a wide range of oven sizes and flow conditions to optimize desirable features such as temperature uniformity throughout the oven, energy efficiency and manufacturability in high-speed air impingement bread-baking ovens.

Drying

Successful drying is often based on empirical knowledge and operator experience. Improving product quality, increasing dryer throughput, and reducing energy costs requires a mathematical model for optimization which will address the heat and mass transfer aspects as well as the air flow pattern and pressure drop. CFD can be applied to model these phenomena and aid in the optimal design of a dryer. However, as Jamaleddine, Ray (2010) pointed out, CFD cannot completely replace pilot-scale testing and the partly empirical nature of the design process. Moreover, dryer simulations should be considered as qualitative and not purely quantitative.

Spray drying is one of the most important methods of drying liquid foods. Most of the existing reports on the application of CFD in drying are related to spray drying, as for example those of Langrish, Fletcher (2001), Goula, Adamopoulos (2005), Lin, Chen (2007), Woo et al. (2008). Kuriakose, Anandharamakrishnan (2010) reviewed the existing literature on CFD applications in spray drying and concluded that CFD can be used to successfully predict the air flow pattern and particle histories such as temperature, velocity, residence time, and impact position. They also concluded that the Eulerian-Lagrangian model is suitable for the spray-drying operations, as it has the advantage of being computationally cheaper than the Eulerian-Eulerian method for a large range of particle sizes.

Recent reports for other drying methods include those of Assarie et al. (2007) who used CFD to simulate the drying of wheat in a fluidized bed dryer and reported a good agreement between theoretical and experimental results and Wang et al. (2008) who also used CFD on a fluidized bed dryer. The later simulated the moisture diffusion in the air and solids phases using a user defined scalar transport equation in the FLUENT® software package and their model was integrated into an online process control system for a batch fluidized-bed drying application in the pharmaceutical industry. Da Silva et al. (2012) used CFD to simulate drying of soybean meal in a fluidized bed dryer incorporating heat and mass transfer into the fluid dynamics model.

Keshavarz et al. (2010) used CFD to simulate heat and mass transfer during food drying via an ohmic heating process. The effects of electrical field intensity, electrical conductivity, solid heating, liquid-solid conductivity, and some parameters such as drying rate, moisture content, and temperature changes on the drying process of potato were investigated. In this modelling, simultaneous solution of the equations of heat transfer, moisture, and electrical field was achieved. Also Marra et al. (2010) analyzed, using a CFD model, the transient distributions of temperature and moisture during the combined treatment of microwave and convection heating and applied it in potato drying.

Margaris, Ghiaus (2006) simulated an industrial air dryer using CFD and stated that they better understood the air flow pattern. Amanlou, Zomorodian (2010) and Darabi et al. (in press) used the FLUENT® software package to design a cabinet dryer and achieved a more uniform air and temperature distribution inside a pilot dryer they had constructed.

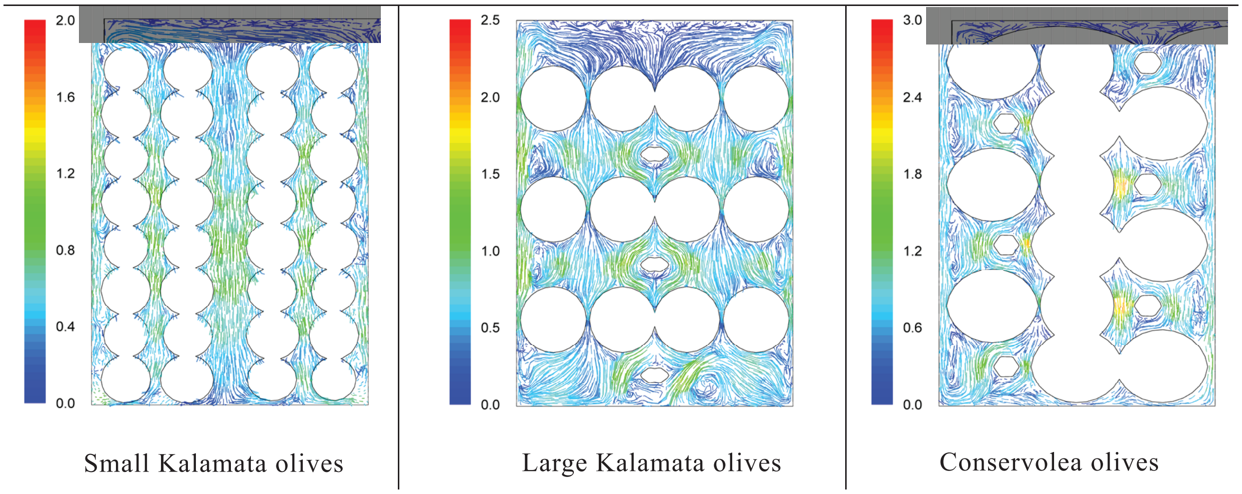
Sterilization

In sterilization, it is important to locate the critical point, the point which receives the least thermal treatment in the container, and make sure that processing time is enough for even this point to receive adequate thermal treatment for spores to be destroyed. The required processing time in commercial canning can be calculated by the analytical solution of the heat conduction equation for simple cases of solid foods where the slowest heating point coincides with the geometric centre of the can. Numerical solutions have been also applied to the sterilization problem with most focusing on solid foods or very viscous foods like purees and concentrates which are usually assumed to be heated by pure conduction. One of the earliest applications of numerical methods in thermal processing of foods was that of Teixeira et al. (1969).

The mathematical analysis in sterilization of stationary cans containing liquid foods is more difficult because in this case the heat is transferred inside the can by natural convention. Since the fluid motion is due to the buoyancy force, the velocity in the momentum equations is coupled with the temperature in the energy equation. Therefore, the momentum equations must be solved simultaneously with the energy equation in order to calculate the temperature profile, the velocity profile, and the slowest heating zone of the can. Datta, Texeira (1988) numerically predicted transient temperature and velocity profiles during natural convection heating of canned liquid foods. Yang et al. (1997) used a CFD code for the simulation of natural convection heating of starch dispersions in a cylindrical still can. Abdul Ghani et al. (1999a) have applied CFD to calculate transient temperature and velocity profiles in sterilization of canned liquid foods in a still-retort. Quarini, Scott (1997) used a CFD package to predict the thermal-hydraulic behaviour of a non-Newtonian liquid food heated in a vertical still can. Other examples include analysis of natural convection heating and bacterial destruction in canned liquids (sodium carboxy-methyl cellulose (CMC) and water (Abdul Ghani et al., 1999a, b)), study of the thermal sterilization of a canned food in a 3-D pouch (Abdul Ghani et al., 2001), analysis of the thermal destruction of vitamin C in food pouches (Ghani et al., 2002), heat transfer coefficient determination during natural convection heating of CMC solutions in cylindrical containers (Kannan et al., 2008), pasteurization of beer (Augusto et al., 2010) or milk (Anand Paul et al., 2011). Recently Erdogdu, Tutar (2012) applied a 2-D simulation associated with a volume of fluid element model and reproduced accurate numerical results for the temperature evolution in air–water and air–food material two-phase rotational fluid systems in cans.

Problems dealing with thermal processing of liquids containing solid particles of food have been also successfully approached through CFD. In these applications, particle size and shape as well as particle orientation, arrangement, and packing density are important as they influence liquid motion and therefore heat transfer from the liquid to the particles and the exact location of the critical point in the can. Examples include the heating of large food particles in water (Rabiey et al., 2007), pineapple slices in juice (Abdul Ghani, Farid, 2006), asparagus in brine (Dimou, Yanniotis, 2011) and peaches in syrup (Dimou et al., 2011). Kiziltas et al. (2010) studied the temperature changes inside a can containing peas in water. They used the axi-symmetric assumption, leading to the formation of torus volumes of solid phase inside the liquid which reduced the problem from 3D to 2D without affecting the results significantly. Their simulation results were in a good agreement with experimental data.

Recently, fluid flow and heat transfer phenomena during thermal processing of table olives in brine, in a stationary tin can, have successfully been simulated through CFD (Dimou et al., 2013). The movement of the brine in the can was assessed. During the heating cycle, the heated brine near the wall is moving upwards, towards the top of the container due to buoyancy forces, forcing the brine sitting on the top of the container to move downwards at the interior of the can through the layers of olives. This circular flow is repeated until the brine approaches the temperature of the heating medium. The presence of the olives substantially affects the flow of the brine. Fig. 1 shows such a pattern after 30 s of heating for the different cases examined.



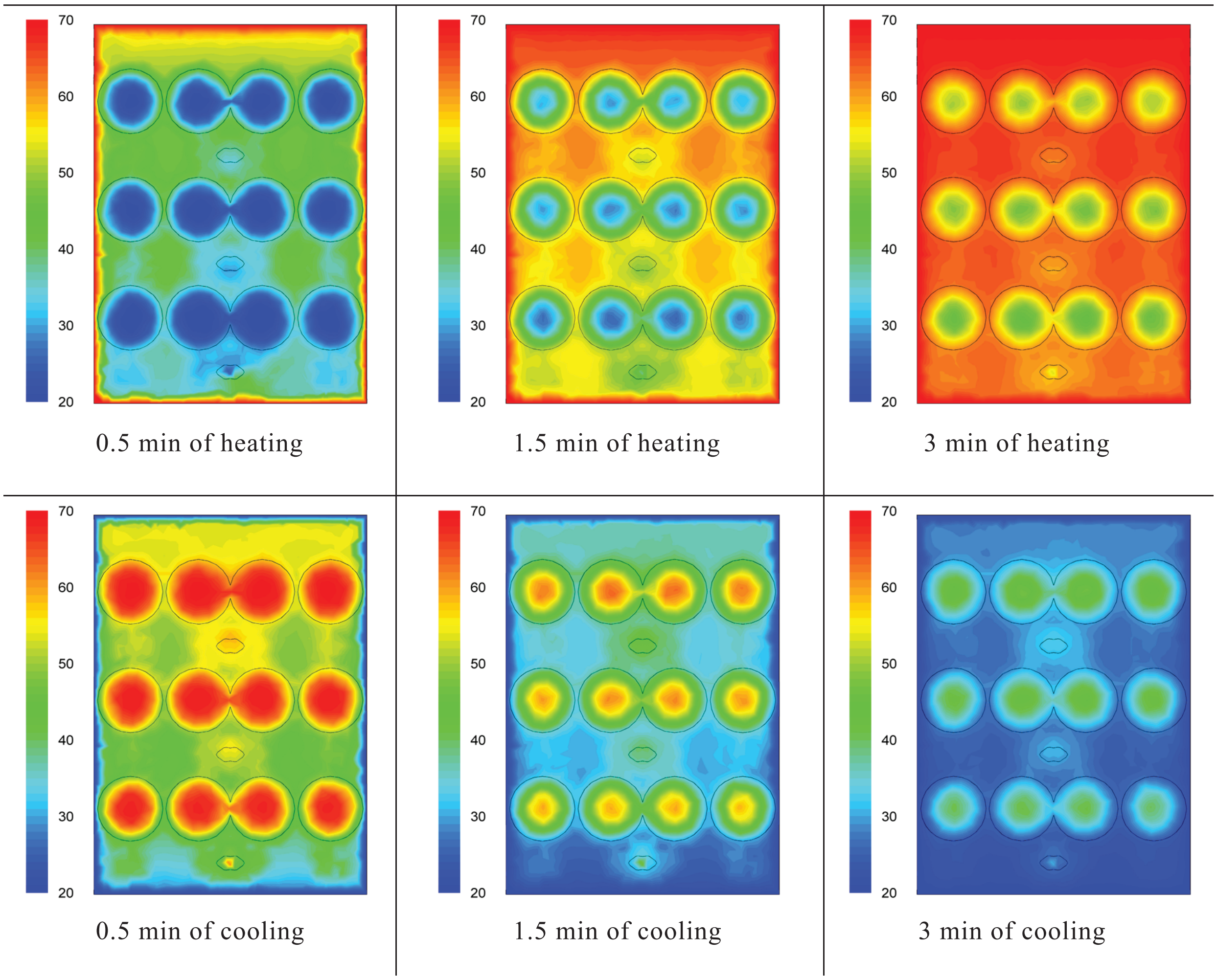
Small Kalamata olives

Large Kalamata olives

Conservolea olives

Fig. 1. Velocity profiles of 4% brine (initially held at 20°C) in a stationary cylindrical can filled with table olives (80 small-size Kalamata olives, 48 large-size Kalamata olives and 48 Conservolea olives) after 30 s of heating at 70°C (velocity in cm/s) (after Dimou et al., 2013)

The distribution of temperature and the location of the slowest heating zone were also calculated. The olives located at the second row from the bottom and at the central region of the can were the slowest heating olives within the container. The interior of these olives represented the slowest heating region of the system under investigation. Due to the brine motion, the same olives were the fastest cooling olives during the cooling cycle of the process. Typical temperature contours for Kalamata olives in 4% brine at different heating and cooling times are shown in Fig. 2. The distribution of the *F* values (values of equivalent heat treatment received by the product, in min) and the location of the critical point within the product, the point with the minimum microbial destruction, were also assessed. For the cases studied, the critical point was located at the interior of the olives at the second, or between the first and the second olive row from the bottom of the container. It was also found that the critical point did not exactly coincide with the point of the slowest heating zone (SHZ), due to the lethal contribution of the cooling cycle. On the other hand, the olives on the top of the can which are the first to be heated and the last to be cooled receive much more heat treatment, as for example in one case $F_{62.4^\circ C}^{5.25^\circ C}$ = 20 min (for the interior of the olives located at or close to the slowest heating point) and $F_{62.4^\circ C}^{5.25^\circ C}$ = 145 min (at the surface of the olives located at the top of the can). Such differences in heat treatment may have deleterious effect on the quality of the product. Given the kinetics of key quality parameters, one can evaluate, using CFD, different time–temperature schedules, leading to an optimization scheme that will produce a safe product with the least quality degradation. Similar results have been also reported for the case of asparagus (Dimou, Yanniotis, 2011) where the SHZ lies at a height of about 13.5% of the can height from the bottom and for peaches in syrup (Dimou et al., 2011). Also Datta, Teixeira (1988) found the SHZ for a can filled with water to be in a region that is at about 15% of the can



0.5 min of heating

1.5 min of heating

3 min of heating

0.5 min of cooling

1.5 min of cooling

3 min of cooling

Fig. 2. Typical temperature contours for Kalamata olives (arranged in 6 rows with 8 olives per row – 6 olives at the perimeter and 2 olives at the centre of the container) in 4% brine in a stationary cylindrical metal can, initially held at 20°C, at different heating and cooling times during heating (at 70°C) and cooling (at 20°C) in water (after Dimou et al., 2013)

height from the bottom, Zechman, Pflug (1989) located SHZ at about 10% height from the bottom, and Abdul Ghani et al. (1999b) found it at about 10–12% height from the bottom. Abdul Ghani, Farid (2006) found SHZ in a can filled with pineapple slices at about 30–35% of the can height from the bottom. In this case, the presence and the shape of the solid apparently reduced the effect of natural convection in the fluid causing the SHZ to be located at a higher point.

CONCLUSION

A short outline of the principles of Computational Fluid Dynamics and a short review of its applications in baking, drying, and sterilization was presented in this article. Reports on such applications have become more frequent in the literature in recent years, mainly due to available user-friendly commercial packages of CFD and increased computational capabilities. From the scientific reports in the literature, it is obvious that CFD is a valuable tool that can be used to optimize processes and design equipment in the food industry where fluid flow and heat and/or mass transfer take place, replacing expensive and time-consuming experimentation, but models should always be validated against experimental results. It can also be used for troubleshooting and optimization of processing conditions including the assessment of the effects of design and operating parameters on the process.

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Received for publication on December 19, 2013
Accepted for publication on January 16, 2014

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