CHAPTER 1

Numerical modelling of heat transfer in the food industry – recent developments and applications

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Abstract

Numerical modelling in food processing operations is receiving increasing attention in recent years. Partial differential equations describing momentum, heat and mass transfer coupled with equilibrium and kinetic equations, which usually form a model for a food processing operation, can be solved easily with today\textquotesingle s computing capabilities. In this chapter, a brief description of the main numerical techniques used in heat transfer models in food engineering, i.e. finite differences, finite volume and finite elements, are briefly presented with advantages and restrictions for each one, followed by examples of specific applications in the food industry. A brief description of the principles of computational fluid dynamics for the solution of fluid flows with heat transfer is also presented, together with examples from the food engineering literature.

1 Introduction

Heat transfer, demonstrated via heating, cooling or freezing is of primary importance in the field of food engineering. Operations involving the heating of foods are performed for cooking and also with aim to reduce the microbial population, inactivate enzymes, reduce product moisture and modify the functionality of certain compounds [1]. Operations involving cooling and freezing are performed mainly to reduce or avoid deteriorative chemical and enzymatic reactions and to inhibit microbial growth [2].
Heat Transfer in Food Processing

Understanding and quantifying the driving force of all heat transfer processes, i.e. the temperature gradient, is essential towards attaining better control and avoiding under- or over-processing which can have a detrimental effect on the food characteristics. As heat transfer in the food industry is often a transient process, an a priori determination of heating and cooling times is also of primary importance in terms of refrigeration requirements, micro-organism growth inhibition and nutritional and sensorial properties preservation [3, 4]. Moreover, heat transfer usually occurs in more than one form either simultaneously or consecutively. For example, in air blast chilling, heat exchange involves forced convective, radiative and evaporative heat transfer leading to a conductive heat flux within the sample [5, 6]. On the other hand, the preparation of sous-vide products involves a time sequence of process steps related to heat transfer such as packaging, fast cooling, cold storage and reheating [4]. To add to the complexity of the problem, foods have neither a regular form nor a homogeneous or isotropic behaviour and a number of their physical properties, such as form, size, structure, thermal conductivity, specific heat, density and viscosity, are temperature dependent and of paramount importance on the thermal behaviour of foods [7].

Other transport phenomena such as momentum and mass transfer are also present in a number of operations concerning food processing including mixing, fluidisation, pneumatic transport, sedimentation, filtration, sterilisation, drying, extrusion, packaging, frying, cooling and freezing and their coupling with heat transfer needs to be understood and accounted for [1]. Some of these processes, such as fluidisation, pneumatic transport and spray drying, also involve two-phase flows [8]. Phase change, as is the case of ice formation in freezing [9] and crust formation in frying and drying [10, 11], adds to the complexity of the problem. Finally, particular features of food being heated such as non-uniform evaporation of water or opening of pores are of such a complexity that understanding and controlling becomes a highly demanding and often impossible task [12].

To this end, numerical models and methods offer an efficient and powerful tool for simulating, comprehending and experimenting with transport processes in the food industry.

As transport phenomena in food engineering are of increased complexity and diversity, a number of numerical models accounting for a wide range of processes have been proposed. No matter the differences between the various models, the starting point is always a set of differential equations, e.g. the three-dimensional partial differential equation of heat conduction for predicting any type of heat treatment [3, 13–16], the original and modified Plank equations for predicting freezing times [17, and references therein], Fick’s law for predicting mass balance of water vapour in a wide range of applications where evaporation occurs [13, 18] and the coupled Navier–Stokes, energy and mass transport equations for predicting momentum, heat and mass transfer [19–21]. In addition, kinetic models for predicting the inactivation of enzymes and the formation of carcinogenic precursors [2, 22] and models for two-phase flow formulations are also employed [23]. One chooses an appropriate model for the target application and a solution method is usually designed for a particular set of equations. Trying to produce a general
purpose solution method, i.e. one that is applicable to all flows, is impractical if not impossible, and as with most general purpose tools they are unusually not optimum for any one application [21].

Regardless of the model adopted, a number of common steps are always followed in the solution of a transport process. In detail, after selecting the mathematical model one has to choose a suitable discretisation 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 discretisation approaches include the finite difference (FD), the finite element (FE) and the finite volume (FV) methods [17, 21]. Other approaches such as boundary elements [24], lattice gas cellular automata and lattice Boltzmann methods [25] are also gaining increasing attention.

The purpose of this chapter is to review the current state of numerical modelling of heating/cooling processes in the food industry building upon previous work by Welti-Chanes et al. [1, 12], Delgado and Sun [17], Sablani et al. [18], Scott [19], Xia and Sun [20], Wang and Sun [26], Otero and Sanz [27] and Langrish and Fletcher [28], with emphasis on some of the details of the numerical methods employed in each application. In this context the chapter is structured according to the discretisation schemes and numerical methods employed, e.g. FDs, FEs and FVs, rather than the physical phenomenon modelled, e.g. conduction, convection and evaporation. Each section commences with a brief description of the numerical technique, its advantages and restrictions, followed by examples of specific applications in the food industry.

2 Finite difference (FD) methods

This is the oldest method for the numerical solution of partial differential equations, believed to have been introduced by Euler in the eighteenth century. It is also the easiest method to use in simple geometries such as spheres, slabs or cylinders. In the food industry, FDs are commonly applied in the solution of the heat conduction equation and of Fick’s law for mass transfer:

\[ \rho C_p \frac{\partial T}{\partial t} = \nabla (k \nabla T) + \dot{q}_{\text{evap}} + \dot{q}_i. \quad \dot{q}_{\text{evap}} = \rho \lambda \frac{\partial C}{\partial t} \]

\[ \frac{\partial C_i}{\partial t} = \nabla (D_{ij} \nabla C) + R \]

In eqns (1) and (2) \( T \) is the temperature of the food sample, \( C \) the species concentration (e.g. dry air phase, vapour phase or liquid phase), \( D_{ij} \) the diffusion coefficient of phase \( i \) to phase \( j \), \( \dot{q}_{\text{evap}} \) the heat transport due to evaporation if present, \( \dot{q}_i \) any other type of heat source (e.g. microwave heating [29]), \( R \) the phase change volumetric rate [30], \( \lambda \) the latent heat of vaporisation, and \( \rho \), \( C_p \) and \( k \) are the density, heat capacity and thermal conductivity, respectively, of the food sample. Clearly eqns (1) and (2), written here in their complete three-dimensional time-dependent form, may reduce to simpler formulations (one or two dimensional in space, time dependent or steady state). Note that eqn (2) refers to a group of equations, one per
Heat Transfer in Food Processing

The actual number of mass transfer equations to be solved depends on the complexity of the problem.

Solutions of eqns (1) and (2) are obtained by dividing the computational domain, i.e. the food sample, by a rectangular or cylindrical structured grid – a grid consisting of families of grid lines with the property that members of a single family do not cross each other and cross the members of the other family only once [21]. At each grid node the differential equation is approximated by replacing the partial derivatives by approximations in terms of the nodal values. The result is one algebraic equation per grid node in which the variable values at that node, and at a certain neighbour, appear as unknown. Taylor series expansion or polynomial fitting is used to obtain approximations to the first and second derivatives [21, 31]. For example, the one dimensional in space, time-dependent heat and/or mass transfer equation can be easily solved by explicit or implicit one-step FD schemes. Implicit methods are considered to be more stable than explicit. Thus, unconditionally stable, second-order temporal and spatial accurate solutions can be easily obtained via well-established numerical algorithms such as the Crank and Nicolson scheme [31, 32]. Explicit methods can also be employed but care has to be taken in the selection of the appropriate space and time steps. Ansari [33] performed a thorough investigation on the numerical issues related to the modelling of heat and mass transfer from the surface of solids exposed to a cooling environment by use of the unsteady, normalised, one-dimensional heat transfer equation. The equation was discretised in terms of a Lagrangian interpolation scheme with a truncation error of $O(\Delta x)^3$. A fully explicit and a fully implicit FD scheme and different combinations of the two schemes with varying weighting factors were studied. Regular-shaped bodies in the form of infinite slab, infinite cylinder and sphere were considered and the study also included an investigation on the effects of the integration time (in terms of the Fourier number) and the mesh refinement on the solution. It was concluded that a simple explicit scheme with a moderately fine mesh and Fourier number increments of one-sixth of the square of the space division size can also provide highly reliable and accurate solutions.

Two- and three-dimensional heat and mass transport equations in simple geometries are commonly written in terms of an implicit FD formulation and solutions are obtained by application of the alternating-direction implicit (ADI) method [34, 35] or by the modified Keller box [31] and references therein.

Boundary conditions (BCs) to eqn (1) can be either in the form of a prescribed temperature value (referred as BC first kind or Dirichlet), a prescribed heat flux (BC second kind or Neumann) or most commonly a radiation and/or convection BC (BC third kind) [36]. The last sets the conduction heat flux from the outer surface of the food sample equal to the convective heat flux from the surrounding fluid. The heat transfer coefficient, $h$, required in the evaluation of the convective surface heat flux is estimated in terms of the process macroscale characteristics in dimensionless format, e.g. as a function of the Nusselt and the Reynolds numbers. BCs to eqn (2) usually involve a prescribed concentration value or a zero gradient assumption.

An alternative method to Taylor series expansion or polynomial fitting discretisation for the solution of the heat transport equation involves the application of energy
balances [35]. In the energy balance method, the food sample is also divided by a rectangular or cylindrical structured grid. For the one-dimensional approach, development of the FD equation is accomplished by considering a differential volume element $\Delta x$ about each node $m$ and writing the energy balance equation around that node. The method utilises the thermal resistance concept, i.e. the ratio of the differential volume element $\Delta x$ to the product of the thermal conductivity and the node cross-sectional area at distances $\pm \Delta x/2$. An advantage of the method is that it allows for a variation in the thermal conductivity and the cross-sectional area with position. For two-dimensional heat transfer the approach is similar [37, 38]. Nodes in the energy balance approach can be either capacitance surface nodes (CSNs) or non-capacitance surface nodes (NCSNs). In the former, nodes are separated by equal distances. In the latter, all interior nodes are separated by equal distances, $d_s$, while the distance between the last interior node and the surface node is set to half the interior node distance ($d_s/2$). The advantage of the NCSN approach is that it does not require knowledge of the surface temperatures to estimate internal temperatures [37] whereas the time steps for the computation of the unsteady heat transfer are larger than in the CSN approach [38]. As in the Taylor series expansion or polynomial fitting discretisation approach, BCs involve either a prescribed temperature value, a prescribed heat flux (BC second kind) or most commonly a radiation and/or convection BC. The use of energy balances allows for an explicit formulation of the FD scheme. Solution to the system is obtained by Gauss elimination or Gauss–Seidel iteration [36].

The FD method, in terms of Taylor series or energy balance approximations, has been used widely in the modelling of food processes such as heating, frying, drying, sterilisation and cooling. The following paragraphs provide examples of applications of the FD method in the modelling of heat transfer processes via conduction in the food industry. The section concludes with a critical evaluation on the limitations of the FD schemes.

2.1 FD approaches by Taylor series expansion

The unsteady, zero dimensional in space, heat and mass transfer equations have been widely used in simple models of thermal processes under the assumption that the food sample was homogeneous and isotropic. For example, Delgado and Sun [13] used the one-dimensional heat and mass transfer equations to estimate centre temperatures during the thawing of cooked meat modelled as a sphere. In their work, it was assumed that the food sample was symmetric with a uniform initial temperature. At the surface, third-class BCs were applied [39]. Results revealed a good agreement between predicted and measured centre temperatures when Schwartzberg’s equations [40] for the specific heat and thermal conductivity values were used.

The unsteady, zero dimensional in space, heat transfer equation has also been used in more complex geometries under the assumption that these could be adequately approximated by a family of simple shapes such as cylinders, slabs or bricks. For example, Davey and Pham [41] developed a model for predicting the dynamic heat load and weight loss during beef chilling in which the irregular beef geometry was
approximated by a combination of seven cylinders and slabs. The model involved the solution of the time-dependent, zero dimensional in space, heat transfer equation in each one of the seven simple shapes, modified by an empirical correction factor. Computed values of heat removed and weight loss (calculated from the latent component of the heat load) were shown to overpredict the experimental data by approximately 12% at early times.

Iguaz et al. [42] also used the unsteady, zero dimensional in space, mass transfer equations to predict moisture balance, in the grain and in the air, in a cylindrical rice grain storage bin. Temperature histories along the grain bin were predicted by solving an enthalpy balance in the grain contained in each control volume (CV). The equation for the enthalpy balance in the air was additionally solved. The model was shown to predict the grain temperature with an average error estimate of up to 0.38°C.

The unsteady, one-dimensional heat conduction equation has been widely employed to obtain insight on thermal processes in a number of practical problems that could be approximated by assuming that heat transfer is dominant along a single direction and negligible along all others. In this context, Akterian [43, 44] used the one-dimensional time-dependent heat conduction equation, modified by means of an empirical shape factor, to predict the conductive heat transfer in mushrooms during in-can sterilisation and to assess the thermal sensitivity of sausages.

The coupled one-dimensional time-dependent heat conduction and mass transport equations have also been applied in the modelling of a number of thermal processes such as frying, thawing and freezing. As in the case of the one-dimensional time-dependent heat conduction, here a single direction for the temperature gradient is also assumed and special attention is placed in the modelling of weight loss as a result of moisture evaporation and of crust formation via application of a Landau-type transformation or a temperature-enthalpy correction method as suggested by Pham [45] and Fikiin [46].

Shilton et al. [47] estimated the temperature and moisture content as a function of time and fat content along a beef patty assumed to be homogeneous and isotropic. The patty was heated by infrared radiation and modelled as an infinite slab divided into ten nodes. Solution was obtained by a commercial equation solver (DESIRE™). Thermal conductivity and density values were adjusted so as to account for both changes in temperature and fat content and an effective convection term was added to the thermal conductivity to account for the presence of fat. Computations revealed that the addition of the effective convection term enhanced the agreement between experimental data and predicted values of temperature along the patty whereas omission of the term resulted in an underestimation of the temperature rise in the patty by up to 40%.

Farkas et al. [10] used the time-dependent, one-dimensional heat and mass transfer equations to estimate the crust thickness and temperature and moisture distributions along an infinite homogeneous half slab with properties corresponding to those of a rehydrated potato mixture undergoing immersion frying. The moving boundaries between the crust and core regions were handled by a Landau transformation and the initial value of the crust thickness was obtained from an order
Numerical Modelling of Heat Transfer

of magnitude analysis that produced an equation similar to Plank’s equation for freezing. The physical and thermal properties of the potato mixture were obtained from the literature and the effects of oil flux and accumulation in the sample were neglected. Excellent agreement with the experimental data was achieved.

The problem of predicting crust formation was also addressed by Hamdami et al. [6], who used a fixed grid FD method to estimate the temperature profile, weight loss rate and moisture content during par-baked bread freezing. The food sample was modelled as an infinite two-layer cylinder comprising two composites: crumb and crust. The sample surface, directly exposed to air was assumed to be cooled by convection, radiation, evaporation or sublimation. Heat transfer in the material was treated as heat conduction with phase change. The latter was incorporated in the heat conduction process by means of the specific heat formulation and by application of the temperature-enthalpy correction method suggested by Pham [45]. The conduction equation was solved by application of the three level method proposed by Lees [48]. Enthalpy was calculated from an interpolation table using the apparent specific heat (literature values) as a function of moisture content. The thermal conductivity was modelled by a Maxwell-type model in three steps considering a continuous and a dispersed phase in each step and incorporating evaporation-condensation effects. The mass balance was formulated so as to account for the frozen water, and the mass diffusivity for crumb and crust was modelled by an Arrhenius law expression. Computed temperature values at the surface and at the centre of the food sample were in agreement with the measurements within 0.5°C and 1.8°C respectively. The precision of the computed weight loss was of the order of 10%.

A similar approach was adopted by Hamdami et al. [9], who used the heat and mass transfer equations to predict the transient thermal and evaporative behaviour of a one-dimensional sponge slab assumed to comprise of dry matter, liquid water, ice and air contained in the pores. The mass balance was formulated so as to account for the frozen water and the mass diffusivity for sponge was also modelled by an Arrhenius law expression. Results in terms of temperature profiles at the centre and at the edges of the sponge and weight loss estimates as a function of time were in good agreement with measurements obtained from a vegetable sponge of 58% initial moisture content located in an air blast freezer.

The one-dimensional approximation for the solution of the heat and mass transfer processes inherently involves the assumption of an infinite geometry. Turhan and Erdoğdu [49] estimated the error due to assuming a finite regular geometry during transient heat or mass transfer as a function of the Fourier (Fo) and Biot (Bi) numbers for a number of simple shapes including cylindrical, square and circular rods and square and rectangular slabs. They concluded that the error due to the infinite geometry assumption increases dramatically with increasing Fo number and decreases with increasing Bi number. The effect of geometry on the error was shown to depend on the Bi number for rod-shaped geometries and decreased with decreasing width over length ratio in slabs.

Two- and three-dimensional solutions of the heat and mass transfer equations arguably offer increased insight in heat and mass transfer problems. Zorrila and
Singh [50] modelled a hamburger patty as a finite cylinder comprising an inner frozen region surrounded by an unfrozen region and an outer core in both the axial and radial directions. The unsteady two-dimensional enthalpy equation and appropriate BCs at the moving interfaces formulated a system of fourteen equations that were solved numerically with an FD scheme. Because the crust thickness was small compared to the slab dimensions a linear temperature change in the crust was assumed. Nodal values of temperatures were related to the calculated enthalpy values according to the procedure proposed by Mannapperuma and Singh [51]. Following Farkas et al. [10], initial values for the moving boundaries were set to at least an order of magnitude smaller than the distance travelled by the crust–core interface in one time step. A combined radiation and convection heat transfer coefficient was assumed at the circumferential surface of the patty. Computed centre temperature values were compared to predictions obtained by Zorilla and Singh [50] using a one-dimensional model. It was shown that although no considerable differences exist between the two approaches (one and two dimensional) with regard to the temperature at the patty centre, the two-dimensional model allows for the estimation of the temperature history at the regions close to the circumferential edge. The latter was shown to be substantially different than that of the centre.

2.2 FD approaches by energy balance

Erdoğdu et al. [52] proposed an FD procedure for the estimation of heat conduction in elliptical cylinders using the energy balance approach and the so-called heat flow lines approach proposed by Eshelman [53] and Pham [54]. The approach reduces an elliptical heat transfer problem from three to two dimensional for a finite length geometry and from a two to one dimensional for an infinite length geometry by assuming that the so-called heat flow lines, which are orthogonal to the elliptic isotherms can be described by simple power curves. The intersection points between a power curve and the concentric ellipses were determined by using the Newton–Raphson method. Volume elements were defined from the volume between two concentric ellipses and power curves using the NCSN heat transfer analysis described above. The FD difference models were formulated for infinite elliptical and circular cylinders and computational results were compared to analytical solutions and experimental data. It was shown that the model could accurately predict centre temperatures in a conduction-heated elliptical cross-sectional cylinder and also in an elliptical infinite or finite cylinder if it was substituted by a circular cylinder of equal surface area to volume ratio.

In a companion article, Erdoğdu et al. [55] adapted the previous formulation to predict the temperature distribution during cooking of shrimp. The model used the NCSN approach, the shrimp cross-sectional area was considered circular and variable thermal conductivity, specific heat capacity and density were assumed. Moisture content reduction and cross-sectional shrinkage were predicted from empiric relations as a function of temperature. Elements at the same radial distance were assumed to shrink by the same amount and at each time step the nodal network was
regenerated. Calculated temperature values both at the centreline and close to the model surface were in good agreement with the experimental data.

Yanniotis and Petraki [56] 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 in the freezer. Schwartzberg’s equations [40] for the specific heat and thermal conductivity were used. The model was solved with an explicit FD 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.

2.3 Limitations of the FD approach

The most significant disadvantage of the FD approach is that it is generally limited to heat conduction problems in simple geometries that can be discretised into simple rectangular or cylindrical structured grids.

Further, in most conduction problems, the surface heat flux is due to convection. The latter requires knowledge of the heat transfer coefficient, $h$, a parameter that is in turn equal to the ratio of the surface heat flux to the temperature difference between the solid surface and the ambient air at the vicinity of the solid. Thus, the value of $h$ is related to the surface gradient of the thermal boundary layer in the surrounding fluid. The latter, in the case of a non-stagnant fluid, is in turn largely dependent on the velocity boundary layer [57, 58] so that $h$ varies along the surface as boundary layers develop. In addition, the fluid and thermal boundary layers are influenced by the solid surface geometry, the flow regime and an assortment of fluid properties such as density, viscosity and thermal conductivity. Complex aerodynamic phenomena such as boundary layer separation and reattachment, vortex shedding and turbulence can also significantly affect the heat transfer from the fluid to the solid surface.

A number of studies [59–61] have already demonstrated the importance of the local distribution of the heat transfer coefficient in a number of food processes. To this end the coupled Navier–Stokes, energy and mass transport equations for predicting momentum, heat and mass transfer can provide valuable insight and allow for a detailed estimation of the local distribution of $h$. However, the FD approach does not enforce conservation unless special care is taken [21] so that it rarely finds application in a complete flow, heat and mass transfer computation.

3 Finite element (FE) methods

The FE method is one of the most general techniques for the numerical solution of differential equations and has been astonishingly successful [62]. It uses the integral form of the conservation equations and the domain is broken in an arbitrary collection of sub-domains called FEs. In two-dimensional geometries FEs are usually triangles or quadrilaterals whereas in three-dimensional tetrahedra or hexahedra are most frequently used [21]. As long as the FEs are sufficiently small, polynomial
functions can adequately represent the local solution. Jiang [62] based on remarks by Zienkiewicz [63] and Oden [64], offers a comprehensive summary of the most important features of FEs as follows:

- **Arbitrary geometries**: The FE method is essentially independent of geometry so that it can be applied to domains of complex shape and with arbitrary BCs.

- **Unstructured meshes**: In FE analyses a global coordinate transformation is not required. FEs can be placed anywhere in physical domains and there is no restriction on the number of neighbour elements or nodes. Further, an FE can be easily added or deleted without the need to modify the global data structure. In contrast to FD approaches, in FEs the element and nodal numbering can be arbitrary without sacrificing efficiency.

- **Flexible and general purpose programme formats**: The clear structure and versatility of the FE method makes it possible to construct general purpose software for a variety of applications.

FEs are also comparatively easy to analyse mathematically and can be shown to have optimality properties for certain types of equations. Their principle drawback which is also shared by any other method that uses unstructured grids is that the equation matrices are not as well structured as those for regular grids making more difficult to find efficient solution methods [21].

The FE solution approach can be classified into three major groups: the Rayleigh-Ritz method, the Galerkin method and the least squares method [62]. The Galerkin method is the most commonly used in thermal analysis problems and thus in food engineering so that discussion in the remainder of this section will be restricted to a short presentation of its main features.

In the Galerkin method, the integral of the weighted residue over the element domain is set equal to zero by application of appropriate interpolation functions in the so-called shape functions matrix. Thus, eqn (1) may be written as

\[
\int \int V_e \left[ N^T \left( \frac{\partial}{\partial x} (k_x \frac{\partial T}{\partial x}) + \frac{\partial}{\partial y} (k_y \frac{\partial T}{\partial y}) + \frac{\partial}{\partial z} (k_z \frac{\partial T}{\partial z}) - \rho C_p \frac{\partial T}{\partial t} \right) \right] dxdydz = 0
\]

where \([N] = [N_i N_j N_k N_m]\) is the shape function matrix and \(N_i, N_j, N_k\) and \(N_m\) are the interpolation functions for a typical tetrahedron element indicated by four corner nodes \(i, j, k\) and \(m\) [65–67]. The shape function matrix is evaluated by assuming a pre-defined temperature variation inside each element (e.g. linear [65]). By use of the divergence theorem on the three terms involving a second derivative, after several manipulations and discretisation, eqn (3) reduces to

\[
\left[ \frac{[N]}{\Delta t} + a[K] \right] \{T\}_{n+1} = \left[ \frac{[N]}{\Delta t} - (1-a)[K] \right] \{T\}_n + \{P\}
\]

where \([T]\) and \([P]\) are the temperature and load vectors and \([K]\) the conductance matrix. A detailed analysis on the derivation of the individual terms of eqn (4) is...
offered by Wang and Sun [65]. Also in (4), \( \alpha \) is a weighting factor which must be chosen in the interval between 0 and 1. Note that for different values of \( \alpha \) different numerical schemes are obtained; e.g. for \( \alpha \) equal to zero, eqn (4) results to a forward difference scheme, for \( \alpha = 1/2 \) to a Crank–Nicholson scheme and for \( \alpha \) equal to unity to a backward difference scheme.

The FE method is receiving increased attention as a reliable and valuable tool for predicting temperature distributions in irregularly shaped, heterogeneous and anisotropic samples and also for obtaining insight on the effect of numerous parameters related to the heating and cooling of foods. However, it is worth pointing out that the field of FE methods in food engineering is relatively young and modelling is mostly still confined to simple geometries that could have been, in principle, adequately described even by application of FD schemes. It should also be noted that in contrast to FD schemes, FE methods can be employed for the solution of the Navier–Stokes equations. However, since most current research and commercial computational fluid dynamics (CFD) codes utilise the FV approach, FE method applications in momentum transfer are scarce. As a consequence, FE methods in food engineering are confined to the solution of heat conduction equation assuming a constant convection heat transfer coefficient as in FD approaches. Some recent examples of FE applications in the numerical modelling of heating and cooling of foods are summarised in the following paragraphs.

Wang and Sun [68] used in-house software based on a FE method (Galerkin approximation) to solve the transient, two-dimensional heat conduction equation for the specific application of cooling a cooked meat sample. The sample was assumed to be infinitely long so that only heat conduction within a cross-sectional area, elliptical in shape, was considered. Due to symmetry, the simulation was carried out on a fourth of the cross-section. Three heat transfer methods were considered: slow air cooling, air blast and water immersion cooling. Appropriate BCs to account for both convection and evaporation were set for each case. It was further assumed that the meat sample was heterogeneous but isotropic and initial temperature values were obtained from measurements. Excellent agreement between calculated and measured temperature profiles as a function of temperature at the core, surface and at an arbitrary selected node within the sample was obtained for all cooling methods. Predicted total weight loss for the slow air cooling method was underestimated by 2.8% whereas predicted and measured total weight loss values for the case of air blast cooling agreed to within 1%. In a companion article, Wang and Sun [69] also performed a detailed parametric investigation on the potential effect of the sample geometry and the surrounding air and water velocities on the cooling process efficiency. Five two- and three-dimensional simple shapes were considered (infinite cylinder, infinite slab, brick, sphere, cube) and useful conclusions that relate critical temperatures to cooling times, sample weight and weight loss were deduced.

Wang and Sun [65] extended the previous approach to model three-dimensional heat transfer on roasted meat during air blast cooling. The sample was cube shaped, comprising 6000 tetrahedron elements and composed of water, protein, fat, salt and air. The physical and thermal properties were expressed as functions of the constituents’ compositions. Temperature and weight loss predictions were generally in
good agreement with experimental data. A maximum deviation (under-prediction) of 2.4°C between predicted core temperature and the respective measured value was identified in the case of a 4.35 kg block-shaped roasted meat having an initial temperature of 48°C. The deviation between predicted and measured total weight loss was 2.5%.

Oliveira and Franca [29] also used in-house software based on the Galerkin weighed residuals technique to perform a thorough study on heat transfer by conduction and microwave heating on cylindrical and irregularly shaped beef, shrimp and pea puree samples irradiated in a frequency range of 900–2800 MHz. In their approach, the governing equations describing the electromagnetic field due to microwave power absorption (Lambert’s law and/or Maxwell’s equations) were solved in addition to the two-dimensional heat conduction equation. Note that the use of Maxwell’s equations depends on the knowledge of the dielectric properties, which are generally available for a wide range of foods. On the other hand, Lambert’s law provides a simpler formulation to the power density term but does not offer a complete representation of the electromagnetic field [70]. Computations revealed that microwave heating is significantly dependent on the radiation frequency, with power absorption and radiation penetration being more effective at lower frequencies, on sample size so that in larger samples heating occurred mainly at the outer surface and also on the dielectric properties with the addition of salt leading to an increase in the energy dissipation. The effect of rotation was also incorporated in the model through the irradiation BCs and was shown that rotation led to a decrease in the temperature gradients and thus to a more uniform temperature distribution on the sample. In the same work, Oliveira and Franca [29] also proposed a correlation to predict the minimum radius of cylindrical samples above which Lambert’s law can be employed.

Romano et al. [70] extended the previous work of Oliveira and Franca [29] in the field of Lambert’s law applicability in cylindrical geometries. In their work, heat transfer and microwave heating of a cylindrical potato sample was investigated by the application of a commercial FE package (FEMLAB) as a function of the cylinder radius and length. BCs accounted for both convective and evaporative heat loss and results also confirmed that predictions using Lambert’s law improve with increasing cylinder radius.

An example regarding the potential of FE in phase change modelling can be provided by reference to the work of Sabliov et al. [71]. In their approach, the processes of egg cooling by cryogenic carbon dioxide and the resultant ice formation between the albumen and the shell were considered. The formulation of Voller and Cross [72] was used to reduce the unsteady heat conduction equations for the liquid and solid phase into a single enthalpy equation with the thermal conductivity and density being a function of temperature. Eggs were assumed to be axisymmetric and elliptical in shape comprising of shell, albumen, air and yolk, each isotropic. The geometry was divided into a uniform mesh composed of 1247 quadrilateral elements using a commercial mesh generating software (GAMBIT). Due to symmetry, only half of the egg was considered. The FE method was based on the Galerkin approximation and solutions to the heat conduction problem were obtained by use of a commercial
FE method software (FIDAP). A convective heat flux on the eggshell surface was assumed and initial temperatures were considered to be uniform throughout the egg and equal to an experimentally determined value. Simulated centre and shell temperatures were shown to agree with measurements within 2–3°C. Differences were attributed to both experimental and simulation uncertainties. The latter were related to uncertainties regarding the model inputs, i.e. experimentally determined physical and thermal properties and environmental conditions.

Commercial FE solvers have been widely employed in the study of heat conduction problems in food engineering. For example, Zhang et al. [73] used FE to analyse the pre-cooking and cooling processes of skipjack tuna. In their approach, heat transfer by conduction in the axial direction (head to tail) was assumed to be negligible so that only a cross-section of the fish was modelled. Further, the cross-section was assumed to be elliptical in shape and symmetric in the longitudinal direction so that only one half was considered in the calculations. The geometry was divided into a non-uniform mesh comprising 2110 quadrilateral elements. The tuna body was modelled as non-homogeneous and anisotropic comprising of loin, backbone and viscera. Physical and thermal properties were adjusted accordingly with values from the literature and by use of empirical models. A convective heat flux was assumed at the sample outer surface with a zero temperature gradient symmetry BC at the tuna centreline. Weight loss due to evaporation was neglected. Simulation data were in good agreement to measurements from pilot and commercial scale experiments for all different regions in the fish (backbone, loin etc.).

In a similar context, Tewkesbury et al. [74] used FE to analyse the cooling of two-dimensional axisymmetric polycarbonate moulds containing chocolate in liquid form. Heat transfer in both the mould and the chocolate was accounted for. The mesh comprised of rectangular elements and was locally refined at the mould–chocolate, mould–air and air–chocolate interfaces. The initial condition was uniform temperature throughout and BCs were a combination of experimentally measured air temperature and two convective heat transfer coefficients for above and below the mould. The rheological behaviour of chocolate was modelled as non-Newtonian and the effect of crystallisation was accounted for by introduction of a variable, effective, specific heat capacity based on the enthalpy method and computed as a function of both temperature and cooling rate. Computed temperatures were in agreement with experimental data within a cooling rate window of 0.5–2°C/min.

Hulbert et al. [75] also used commercial software (ANSYS) to model heat conduction inside a cross-sectional carrot slice and to estimate the fluid to sample convective heat transfer coefficients. Solutions to the two-dimensional heat conduction equations were obtained by imposing initial and BCs obtained from MRI measurements.

A more complex approach was adopted by Tattiyakul et al. [76, 77], who studied heat transfer to a corn starch dispersion contained inside a circularly shaped can. The can was assumed to be stationary, continuously rotating or undergoing intermittent agitation. The problem was modelled as two dimensional. The can was meshed by a non-uniform quadrilateral grid comprising 580 elements using the same
commercial software as Tewkesbury et al. [74], Zhang et al. [73] and Sabliov et al. [71]. Various other mesh sizes were tested to ensure a grid-independent solution. The starch was considered to be in liquid form, of constant density and temperature-dependent viscosity. In addition to the heat conduction equation, the continuity and two-dimensional laminar momentum (Navier–Stokes) equations were also solved so as to account for the fluid motion inside the can, again by application of commercial software (FIDAP). Computed temperature profiles at the centre of the can were compared to experimental data for the case of intermittent rotation. It was shown that simulation results agreed with the measurements within 2% at heating times larger than 500 s but that the model under-predicted the experimental data by as much as 20% at times less than 500 s. Despite this discrepancy, the model provided useful insight in the motion of the gelatinised starch layer within the can and it was shown that intermittent rotation can lead to more uniform temperature and starch gelatinisation distributions.

The FE approach has also been successfully employed in combined simulations of heat transfer and enzyme inactivation or carcinogenic precursor formation. Martens et al. [2] used an in-house FE software (CHAMPSPACK) to simultaneously predict heat transfer and peroxidase activity on a one-dimensional axisymmetric model of a broccoli stem comprising 51 linear elements as a function of temperature. The same model was also applied to predict the inactivation of lipoxygenase in asparagus. The enzyme activity was described by a first-order kinetic model in the form of an Arrhenius expression:

$$\frac{dA}{dt} = -k_r A, \quad k_r = k_{r,ref} e^{-E_a/R(1/T-1/T_{ref})}$$

(5)

In eqn (5), $A$ is the dimensionless enzyme activity at the time $t$ relative to the initial activity, $k_r$ is the rate constant, $t$ the heating time, $k_{r,ref}$ the rate constant at a predefined reference temperature $T_{ref}$, $E_a$ the activation energy and $R$ the universal gas constant. Both equations (heat conduction and enzyme inactivation) were solved by use of the Galerkin weighted residual method.

Tran et al. [22] used a similar approach to estimate heat transfer and heterocyclic amine (HA) formation in a pan-fried ground beef patty without flipping. The FE analysis was carried out by the use of commercial FE software (FlexPDE) and HA predictions were shown to be in good agreement with experimental data.

A more complex approach was adopted by Lian et al. [78], who used commercial software (FIDAP) to solve the continuity equation, the standard Darcy equation [79] for a low Reynolds number fluid flow in a porous media and the volume averaged energy conservation equation for a packed bed:

$$\frac{\partial \rho}{\partial t} + (\rho u_i) = 0$$

(6)

$$\frac{\rho \partial u_i}{\alpha} + \frac{\mu u_i}{\kappa} = -p_i$$

(7)

$$(\rho c_{el}) \frac{\partial T_j}{\partial t} + \rho c_i u_j = (k_{j})_{ij} + H$$

(8)
Numerical Modelling of Heat Transfer

and obtained the special distributions of the air flow, temperature and enzymatic oxidation of polyphenols during black tea fragmentation. In eqns (6)–(8) $u_i$ is the volume averaged velocity component, $\alpha$ is the porosity, $\kappa$ the permeability, $\mu$ the viscosity, $c$ the air heat capacity, $(\rho c)_e = \alpha \rho c + (1 - \alpha) \rho_s c_s$ the effective heat capacity, $k_e = \alpha k + (1 - \alpha) k_s$ the effective conductivity, $H$ the heat generated by the enzymatic oxidation, $p$ the pressure and $i$ (or $j$) is the tensor notation. For instance, for a two-dimensional axisymmetric flow $u_i = (u_r, u_z)$ and $u_{ij} = \partial u_z / \partial r + \partial u_r / \partial z$. It follows that $T_{ij} = \partial T / \partial r + \partial T / \partial z$ and $(k_e T)_{ij}$ is the second derivative. Twelve enzymatic reactions were used to model the tea fermentation and the rate of depletion of catechins was modelled by a Michael–Menten equation [80]. Results showed that the air flow through the packed bed exhibits a plug flow type behaviour, the temperature distribution in the radial direction was uniform and that heat transfer during fermentation was dominated by the enzymatic reactions and heat removal by the air flow. More importantly, it was also shown the rate of theaflavin accumulation was a non-monotonic function of temperature and time. A main conclusion of the work was that computational methods can provide not only a means to analyse fluid and temperature fields but also a valuable tool in the understanding of complex enzymatic reactions.

FE simulations have also been applied in plate heat exchanges. Fernades et al. [81, 82] used commercial software (POLYFLOW) to model the thermo-rheological behaviour of yoghurt in a three-dimensional corrugated channel. The simulations were carried out considering stationary, incompressible laminar flow and involved the solution of the conservation equations for mass, linear momentum and energy in the form:

$$\text{div}(\vec{u}) = 0$$  \hspace{1cm} (9)
$$\text{div}([S]) + \rho b - \rho \text{div}(\vec{u}) = 0$$  \hspace{1cm} (10)
$$\|S\| \nabla \vec{u} + \rho h - \text{div}(q) = 0$$  \hspace{1cm} (11)

where $\vec{u}$ is the velocity vector, $\|S\|$ the total stress tensor and $h$ refers to the heat supply strength of an internal heater. A Herschel–Bulkley model for the yoghurt viscosity and an Arrhenius-type term for temperature dependence were used. Numerical results concerning the difference between the inlet and outlet yoghurt temperature were shown to agree with experimental data within 7%. It was further concluded that the presence of corrugations induced a sinusoidal behaviour in the main flow direction in the yoghurt velocity, temperature, viscosity and shear rate.

Application of FEs in the food industry for understanding and controlling the heating and cooling of foods remains a field of ongoing research.

4 Finite volume (FV) methods

As in the FE method, the FV method also uses the integral form of the conservation equations and the solution domain is sub-divided into a finite number of contiguous elements, here referred to as CVs. Conservation equations are applied to each CV [21]. The principal difference between the FE and the FV method is that in
the latter differential equations are integrated directly, i.e. without the application of weighting factors. Equation (12) presents the discretised form of the unsteady conduction equation integrated over a CV of volume $\Delta x \times 1 \times 1 \ [83]$.

$$\alpha_p T_P^1 = \alpha_E [f T_E^1 + (1 - f)T_E^0] + \alpha_W [f T_W^1 + (1 - f)T_W^0]$$
$$+ [\alpha_p^0 - (1 - f)\alpha_E - (1 - f)\alpha_W] T_P^0 \quad (12)$$

where

$$\alpha_E = \frac{k_e}{(\delta x)_e} \quad (13a)$$
$$\alpha_W = \frac{k_w}{(\delta x)_w} \quad (13b)$$
$$\alpha_p^0 = \frac{\rho c_p \Delta x}{\Delta t} \quad (13c)$$
$$\alpha_p = f \alpha_E + f \alpha_W + \alpha_p^0 \quad (13d)$$

In eqns (12) and (13), superscripts 0 and 1 denote ‘old’ (known) values at time $t$ and ‘new’ (unknown) values at times $t + \Delta t$, respectively, $f$ is a weighting factor between 0 and 1, $P$ is the centroid of the CV where $T_P$ is currently being calculated and $E$ and $W$ are the centroids of the CVs to the left (east) and right (west) of $P$. Also in eqn (13a) and (13b), the letters $e$ and $w$ denote CV faces so that $(\delta x)_e$ and $(\delta x)_w$ denote the distance of node $P$ from the respective faces.

From the above it is clear that in the FV method, at the centroid of each CV lies a computational node at which the variable values are to be calculated. Interpolation is used to express variable values at the CV faces in terms of the nodal (CV-centre) values. Face and volume values are approximated using suitable quadrature formulae. As a result one obtains an algebraic equation for each CV in which a number of neighbour nodal values appear. The FV method can accommodate any kind of grid so it is suitable for complex geometries [21].

As in FD and FE, the algebraic forms of the conservation equations in FV are solved with iterative methods such as TDMA or ADI [35, 83].

FV methods are present in most in-house and commercial CFD codes incorporating the two- or three-dimensional transient or steady solution of the Navier–Stokes equations and are increasingly finding applications in the food industry [84–87].

Application of FV methods for the solution of solely heat conduction or species conservation equations (eqns (1) and (2)) is generally scarce. One of the rare examples in this direction is provided by the work of Zorilla and Rubiolo [88] who used the CV approach and a logarithmic mesh for the mathematical modelling of immersion chilling of cheese in the shapes of a one-dimensional infinite slab, an infinite and a finite cylinder, an infinite rectangular, a rectangular parallelepiped and a sphere. The enthalpy method was used to account for the phase change from liquid to ice and a total of four differential equations (one for enthalpy, one for the ice phase and two for the liquid phase) were solved. As expected, multi-dimensional
Numerical Modelling of Heat Transfer

Geometries were shown to improve heat and mass transfer with a penalty regarding CPU time.

Pajonk et al. [89] also used the FV approach to model various Emmental cheese samples during ripening by application of eqn (1). Overall heat transfer flux at the external surface was considered as the sum of convective, evaporative and radiative contributions. The cheese was cylindrical in shape with thermal properties that were experimentally determined as part of the work. Simulated and experimental temperature profiles were in excellent agreement when the temperature variations were small. For temperature changes that exceeded 15°C discrepancies between experimental and computational results were detected and were attributed to the fact that melting enthalpies of the different fat fractions were neglected in the modelling approach.

5 Computational fluid dynamics (CFD)

The advantages of CFD as a tool towards obtaining a complete characterisation of all transport properties during the heating or cooling of foods have been already outlined. This section aims to provide a brief summary of the principles and challenges of CFD for the solution of laminar and turbulent fluid flows with heat transfer. As previously, the section concludes with appropriate references to specific examples of the application of CFD in food engineering. Note that the use of CFD by the food industry is relatively young [19] so that not all of the currently, otherwise, widely available techniques, methods and models have yet been applied. However, for the sake of completeness and also because CFD is rapidly penetrating the field of food engineering (so that techniques, methods and models currently widely available in other scientific and practical areas of engineering and science are indeed expected to find application in the food industry in the coming years), this section includes a more general approach towards the current, commercial and research, state-of-the-art status of CFD.

CFD by application of FV involves the solution of integrated Navier–Stokes conservation equations in the general form of [83]:

\[
\frac{\partial}{\partial t}(\rho \phi) + \frac{\partial}{\partial x_j}(\rho u_j \phi) = \frac{\partial}{\partial x_j} \left( \Gamma \frac{\partial \phi}{\partial x_j} \right) + S_\phi
\]

(14)

where \( \rho \) is the fluid density, \( u_j \) the air velocity component, \( \phi \) any variant (velocity components, enthalpy), \( \Gamma \) a diffusion coefficient and \( S_\phi \) a source term. For \( \phi \) equal to unity, eqn (14) 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 \( \phi \). For the momentum conservation equations, the term \( S_\phi \) includes the sum of any generation and/or destruction term and of the pressure gradient on the particular direction, where appropriate. Conjugate heat transfer, in the context of coupled fluid-solid temperature and enthalpy calculations, is obtained by simultaneous solution of the FV form
of eqns (1) and (2) together with eqn (14) and application of appropriate BCs at the common boundaries.

For laminar flows, integration and discretisation of a group of equations as in (14), i.e. for $\phi$ equal to unity, equal to the velocity components and equal to enthalpy, respectively, leads to a system of closed algebraic equations that can be solved by a well-established numerical method such as ADI. Note that for both laminar and turbulent flows that will be subsequently discussed, special attention needs to be placed on the discretisation scheme employed, in particular for the convection and diffusion terms, and also on the treatment of the pressure gradient in the momentum equations. A thorough discussion on both issues and descriptions of a number of well-established algorithms (e.g. SIMPLE, SIMPLER, SIMPLEC and PISO) are offered by a number of seminal works, e.g. Ferziger and Peric [21], Patankar [83], Roache [90], Issa [91], Hirsch [92], Vandoormaal and Raithby [93] and Oliveira and Issa [94].

For turbulent flows, which are indeed the ones most commonly encountered in engineering applications, including food engineering, three levels of CFD computations are identified and may be applied [95, 96].

The first level [Reynolds averaged Navier–Stokes (RANS)] has been historically the first possible approach for the solution of turbulent fluid flows. In RANS, the conservation equations for the Reynolds or Favre (mass weighted) time-averaged values of variable $\phi$ are obtained by averaging the respective instantaneous conservation equations (i.e. eqn (17)). However, the resulting averaged equations contain unclosed terms and call for specific closure rules, namely a turbulence model to deal with fluid dynamics and additional models for energy and chemical species conversion. In detail, the RANS approach to turbulence modelling requires that the so-called Reynolds stresses (i.e. the mean of the product of the turbulent velocity fluctuations, $u_i''u_j''$ and the species and enthalpy mean turbulent fluxes ($u_i''Y_k''$ and $u_i''h_k''$, respectively) appearing in the RANS averaged momentum, enthalpy and species conservation equations, respectively, be appropriately modelled. A common method in this direction employs the Boussinesq hypothesis [97] to relate the Reynolds stresses and species and enthalpy fluxes to an eddy viscosity and also to the mean velocity, species and enthalpy gradients. To this end, a number of turbulence models have been proposed [98–102]. The most popular turbulent model in this context remains the so-called standard $k-\varepsilon$ model [99, 103] due to its robustness, economy and reasonable accuracy for a wide range of turbulent flows. However, the $k-\varepsilon$ model is semi-empirical while the derivation of the model equations for the turbulent kinetic energy $k$ and for the dissipation rate $\varepsilon$ of the turbulent fluctuations (which are also of the general form of eqn (14)) relies on phenomenological considerations and empiricism [104]. As the strengths and weaknesses of the standard model have become known, advancements and modifications have been made to the model to improve its performance. Two of these popular variants include the RNG $k-\varepsilon$ model and the realisable $k-\varepsilon$ model [100, 101]. An alternative approach to the Boussinesq hypothesis includes the solution of transport equations for the Reynolds stresses and the turbulent fluxes [105–107]. An additional scale-determining equation (normally for $\varepsilon$ and also for the dissipation $\chi$ of the scalar
fluctuations) is also required. This means that at least five additional transport equations are required in two-dimensional flows and at least seven additional transport equations must be solved in three dimensions. Note that in many cases, models based on the Boussinesq hypothesis perform very well, and the additional computational expense of the Reynolds stress model is not justified. However, the RSM is indeed superior for situations in which the anisotropy of turbulence has a dominant effect on the mean flow. Such cases include highly swirling flows and stress-driven secondary flow.

Of all models mentioned above only the standard $k-\varepsilon$ model has been employed in the field of food engineering. Note that despite the turbulence model employed, the solution of the RANS equations provides averaged quantities corresponding to averages over time for stationary mean flows, averages over different realisations (or cycles) for periodic flows [95] or averages over a particular time interval for time evolving mean flows.

The second level of CFD involves the so-called large eddy simulations (LES) and is currently gaining increased attention in a number of turbulent flow calculations [95, 108]. In LES, the larger three-dimensional unsteady turbulent motions are directly represented, whereas the effects of the smaller scale motions are modelled. In terms of computational expense, LES lies in-between Reynolds stress models and the third level of CFD, namely direct numerical simulations (DNS) discussed below [108]. Because large-scale motions are explicitly represented in LES, the approach is expected to be more accurate than RANS (even with a Reynolds stress model) in the case of flows where large-scale unsteadiness is significant, e.g. the flow over bluff bodies. In principle LES can find several applications in food engineering, e.g. during air blast cooling or heating of food samples. However, to the authors’ knowledge no publications on LES computations with relation to the food industry are yet available. One reason for the complete absence of LES in the modelling of food products may be attributed to the fact that until quite recently, i.e. the last 3–4 years, LES CFD codes were confined to only a few research groups focusing on specialised issues of turbulence, aerodynamics, meteorological applications and combustion [109–113] and were not available in the form of commercial CFD software. Currently, however, most commercial CFD codes are equipped with the LES approach. For the sake of completeness and also because it is recognised that it is not unlikely for LES to penetrate the field of food engineering in the coming years, a short overview on the general concept of the LES approach, divided into four conceptual steps, is provided [108].

The first step for LES calls for the definition of a filtering operation to decompose the variable $\phi$ of the instantaneous Navier–Stokes conservation equation [eqn (14)] to a sum of a filtered (resolved) component and to a residual (or sub-grid scale, SGS) component. The filtered value which is three dimensional and time dependent represents the motion of turbulent eddies.

The second step involves the derivation of the equations for the evolution of the filtered value of $\phi$ from eqn 14. These new equations are of a standard form (i.e. similar to the ones obtained in the RANS approach) and contain the residual stress tensor (or SGS tensor) and the residual species and enthalpy fluxes that arise from
the residual turbulent motions. As in RANS these terms are unclosed and modelling is required.

As in RANS, the third step involves modelling of the unknown terms. Closure is obtained by appropriate approximations, most simply by an eddy viscosity model [114–117] conceptually similar to the one obtained by the Boussinesq hypothesis in RANS.

Finally a numerical solution of the filtered equations that provides a single realisation of the large-scale turbulent motion is obtained.

Additional details on the application, modelling and numerical issues related to the LES method are outside the scope of this work. Comprehensive and critical reviews on the topic may be found in the works of several researchers in the field including Brandt [118], Pope [108], Poinset and Veynante [95], Galperin and Orszag [109] and Mason [110]. Research on SGS modelling and other aspects of LES is on-going.

The third and most advanced level of CFD is based on DNS. In DNS, the full instantaneous Navier–Stokes equations are solved without any model for turbulent motions: all turbulence scales are explicitly determined [95]. Thus, DNS is able to predict, for example, all time variations of temperature at a particular location in the flow exactly like a high resolution sensor would measure them in an experiment. In DNS, pseudo-spectral methods [108, 119, 120] are the preferred numerical approach (instead of the conventional finite differencing schemes employed in all other approaches discussed up to now) and the solution domain is represented by finite Fourier series. The major drawback of the DNS method is its excessive computational cost since the number of grid points required to resolve all scales of three-dimensional motion is proportional to the nine-quarter power of the characteristic Reynolds number, $Re^{9/4}$ [96, 121]. Nevertheless DNS studies have been extremely valuable in supplementing fundamental understanding of turbulent flows [122, 123]. However, with computer times that exceed 200 h on a supercomputer for flows of low and moderate Reynolds numbers and with 90% of the total effort devoted to small scales of the dissipation range, rather than on the mean flow and the statistics of the energy-containing motions [108], the wide application of DNS in practical problems, including those arising in the food industry, remains questionable.

Up to now, discussion in this section has been confined to single-phase flows as in the case of modelling of air flow around a particular food sample. Two-phase situations as in the case of thawing, freezing and frying are treated as conjugate heat transfer problems with, for example, a RANS CFD approach for the fluid flow and by solving eqns (1) and (2) on the food sample.

However, practical problems in food engineering also involve the presence of two-phase flows in the sense of a dispersed secondary phase within the primary gaseous phase, e.g. the case of spray drying of milk powder and other instant beverages [8], the creation of air bubbles inside liquid foods and sedimentation. Computational modelling of two-phase flows is usually defined in either an Eulerian or a Lagrangian frame of reference and has also considerably advanced over the past 20 years. However, as in other aspects of CFD, applications of two-phase
CFD simulations in food engineering remain limited and mostly confined to the use of the Lagrangian approach. The following paragraphs, and again for the sake of completeness, provide a brief overview of two-phase CFD modelling. Specific references to applications of CFD in food engineering are provided in the next two subsections.

In detail, in the **Euler–Lagrangian approach**, the fluid phase is treated as a continuum by solving the time-averaged Navier–Stokes equations, while the dispersed phase is solved by tracking a large number of particles, bubbles or droplets through the calculated flow field. The dispersed phase can exchange momentum, mass and energy with the fluid phase \([104]\) through the addition of extra terms in the group of eqn (14). A fundamental assumption made in this approach is that the dispersed second phase occupies a low volume fraction, \(\alpha_p\), per volume, \(V\), defined as [124]:

\[
\alpha_p = \frac{\sum N_i V_{pi}}{V}
\]  

(15)

where \(N_i\) is the number of particles in the size fraction \(i\), having a particle volume \(V_{pi}\). Since the sum of the volume fraction of the dispersed phase and the continuous phase is unity, the continuous volume fraction is \(\alpha_F = 1 - \alpha_p\).

The particle or droplet trajectories are computed individually at specified intervals during the fluid phase calculation through the solution of ordinary differential equations that account for the particle instantaneous location, \(\vec{X}\) and the linear, \(\vec{u}_p\) and angular velocities and may be expressed in vector form as [124]:

\[
\frac{d\vec{X}}{dt} = \vec{u}_p
\]  

(16)

\[
m_p \frac{d\vec{u}_p}{dt} = \sum \vec{F}_j
\]  

(17)

\[
l_p \frac{d\vec{\omega}_p}{dt} = \vec{T}
\]  

(18)

where \(m_p\) is the particle mass, \(I_p\) the moment of inertia, \(\sum \vec{F}_j\) represents the sum of the different forces acting on the particle (e.g. drag force) and \(\vec{T}\) is the torque. Equations (16)–(18) are usually solved by FD discretisation and application of the fourth order Runge–Kutta scheme and rotation is commonly neglected.

Additional sub-models accounting for further two-phase flow effects such as evaporation, inter-particle collisions and agglomeration can also be incorporated in the Lagrangian approach [125–131].

The Lagrangian approach is appropriate for the modelling of spray dryers but quite unsuitable for the modelling of liquid–liquid mixtures, fluidised beds or any application where the volume fraction of the second phase is not negligible. Note that according to Sommerfeld [128] and Elgobashi [132], two-phase flows with volume fractions of the order of, or less than, \(10^{-3}\) are considered as adequately dilute.
In the **Eulerian approach**, the different phases are treated mathematically as inter-penetrating continua [104]. Since the volume of a phase cannot be occupied by the other phases, the concept of a phasic volume fraction is introduced. These volume fractions are assumed to be continuous functions of space and time and their sum is equal to unity. Conservation equations for each phase are derived to obtain a set of equations, which have similar structure for all phases. These equations are closed by providing constitutive relations that are obtained from empirical information, or, in the case of granular flows, by application of kinetic theory. There are three main categories of Eulerian multi-phase models: (1) the volume of fluid (VOF) model, the mixture model and the Eulerian model; (2) the mixture model and (3) the Eulerian model. The following paragraphs provide an outline of each one of the three approaches.

The VOF model is a surface-tracking technique applied to a fixed Eulerian mesh [133–135]. It is designed for two or more immiscible fluids where the position of the interface between the fluids is of interest. In the VOF model, a single set of momentum equations is shared by all fluids, and the volume fraction of each of the fluids in each computational cell is tracked throughout the domain. Applications of the VOF model include stratified flows, free-surface flows, filling, sloshing, the motion of large bubbles in a liquid, the motion of liquid after a dam break, the prediction of jet break-up (surface tension) and the steady or transient tracking of any liquid–gas interface [104].

The mixture model is designed for two or more phases (fluid or particulate). As in the Eulerian model described below, the phases are treated as inter-penetrating continua. The mixture model solves for the mixture momentum equation and prescribes relative velocities to describe the dispersed phases. Applications of the mixture model include particle-laden flows with low loading, bubbly flows, sedimentation and cyclone separators.

Finally, the full Eulerian approach is the most complex of multi-phase models. It solves for each phase a set of conservation equations in the general form of (14). Coupling between phases is achieved through the so-called pressure and inter-phase exchange coefficients and differs between granular (fluid–solid) and non-granular (fluid–fluid) flows. Applications of the Eulerian approach include bubble columns, risers, particle suspensions and fluidised beds [132, 136–139].

### 5.1 Single-phase flow problems

This section attempts to provide a review on the application of CFD in food engineering. As with FEs, application of FVs and CFD in the food industry remains a field of ongoing research.

Examples of the use of CFD in food engineering for calculating the heat transfer rate from the surrounding air flow to specific food samples are provided in the works of De Baerdemaeker and Nicolai [4], Moureh et al. [140], Olsson et al. [141], Hu and Sun [5], Therdthai et al. [142] and Mirade et al. [85].

In detail, De Baerdemaeker and Nicolai [4] used commercial CFD software (CFDS) to calculate the effect of the stacking pattern of one or two packages on the
Numerical Modelling of Heat Transfer

air flow field inside an oven with application to equipment considerations for sous
vite cooking. They concluded that spatial variations in the flow field are indeed
present and are dependent on the stacking pattern with implications on the heat
transfer coefficient.

Moureh et al. [140] also used commercial CFD software (Phoenics) to assess
the effectiveness of insulating devices in reducing the rate of temperature changes
during product transportation on vehicles in the absence of refrigeration. The com-
putational domain was three dimensional and comprised of one and a half pellets
located at the rear end of a vehicle and covered by an insulating canvas. Each pellet
was represented as a succession of air and product layers. Inside the pellet heat was
assumed to be transferred by conduction. Solar flux, external radiative heat flux
and convective heat flux were exchanged between the pellet and the canvas. The
model was used to estimate the tolerable time for transport or storage of sensitive
products and the computations were in excellent agreement with experimental data
also presented in the article.

Two-dimensional steady-state calculations of slot air jets impinging on cylinder-
shaped food products were carried out by Olson et al. [141]. Note that understanding
of flow interactions and heat transfer characteristics from multiple slot jets is a topic
of great practical implication during the heating, drying, freezing and cooling of
foods as the high velocity of the air jets enhances the momentum, heat and mass
transport. In the particular work of Olson et al. [141], commercial CFD software
(CFX) and the $k-\omega$ turbulence model of Menter [102] were used to calculate
the flow field around one and two cylindrical food products. They concluded that the
heat transfer to the cylinder surface is uneven, resulting in local dehydration of
the product and that the use of single, two or three impinging jets and the distance
between the jets’ exit and the food product have a tremendous effect on the local
heat transfer.

Emphasis on the local heat transfer rate and coefficients was also placed by Hu
and Sun [5] who used commercial CFD software (CFX) to predict the turbulent
flow field and the heat and moisture transfer in a three-dimensional air blast chiller
containing cooked meats of cylindrical and elliptical shapes. Hu and Sun used for
their simulations three turbulence models (standard $k-\varepsilon$, low Reynolds number
and RNG $k-\varepsilon$) and assessed the effect of the three models on the accuracy of
the local heat transfer predictions. Results were compared with experimental data
which showed that the RNG model provided the best selection due to its easiness
in use, comparatively low computation time and good prediction accuracy.

Therdthai et al. [142] used CFD (CFDACE+ code) to simulate a two-dimensional
cross-section of a bread baking oven fitted with a burner and a convection fan. Few
details on the CFD simulation and modelling approach are provided in the article so
that it is unclear whether a laminar or turbulent flow was considered. The simulation
provided information on the temperature and air flow pattern in the oven and allowed
for a sensitivity study on the positioning of the controller sensors.

A detailed study on the transient thermal behaviour of large food chillers was
carried out by Mirande et al. [143]. A commercial CFD code (FLUENT) was used
to simulate the flow patterns inside a three-dimensional computational model of a
chiller filled with pork carcasses. Results revealed that the calculated air velocity agreed with measurements and that the use of CFD correctly depicts the effect of a change in the ventilation level and direction on the air flow pattern. Heat and mass transfer coefficients around the carcass hindquarters with respect to the air velocity fields were also determined and subsequently used into a chilling model which permitted the calculation of chilling kinetics and carcass weight loss as a function of the different ventilation conditions.

In addition to the CFD studies that analysed the temperature and flow fields inside food-related practical applications, a number of CFD simulations were focused on the particular problem of heat transfer in heat exchangers. For example, Grijspeerdt et al. [144] carried out two- and three-dimensional CFD simulations of the flow of milk between corrugated plates in the FINE-Turbo software environment [145]. In all simulations the flow was considered as turbulent of a Reynolds number of 4482 (based on a characteristic velocity on 1 m/s) and turbulent shear stresses were modelled using the Baldwin–Lomax model [146]. They showed that CFD computations can successfully identify regions with the heat exchanger where backflows and thus higher temperature and fouling may occur and that CFD can provide a useful tool for optimal design of plate heat exchangers.

5.2 Two-phase flow problems

This section summarises previous attempts to predict two-phase flows with particular application to food engineering. Note that here, as discussed in Section 5 earlier, the term ‘two phase’ refers to a dispersed secondary phase within the primary gaseous phase rather than the presence of two or more phases on the same food sample. As already emphasised, most existing work with two-phase flow in the food industry refers to industrial spray dryers for the drying of dairy and other food products. Further, here the focus is mostly on the understanding of the flow patterns inside the dryers rather than on the heat transfer inside the food sample and for simplicity, most of the existing studies consider either water droplets or solid particles of arbitrarily selected constant physical properties.

Notably, one of the earliest attempts to predict the flow pattern within a laboratory spray dryer was reported in the pioneering work of Crowe [147] who used the Particle-Source-in-Cell model to calculate gas flow patterns and particle trajectories within a laboratory spray dryer. Oakley et al. [148] predicted the flow pattern inside a pilot scale co-current spray dryer as a function of the angle of the swirl vanes in the inlet annulus around the atomiser and reported periodic oscillations in the size of the recirculation zones in agreement with experimental data. Similar findings were reported by Levesley et al. [149] and Langrish et al. [150]. Oakley and Bahu [151] using commercial CFD software (CFDS-FLOW3D) confirmed the existence of low frequency oscillations for conditions where significant swirl in the inlet air leads to vortex breakdown and the formation of a central recirculation zone with a processing vortex core. They also predicted the trajectories of water droplets injected from a hollow-cone nozzle and noted cooling of the central gas jet in the region below the atomiser and significant evaporation in a recirculation zone located...
in the outer regions of the chamber. The existence of a self-sustained quasi-flapping oscillation inside a simple short-form spray dryer configuration was also confirmed by the more recent works of LeBarbier et al. [152] and Guo et al. [153].

Wall deposition in a co-current spray dryer with a rotary atomiser was examined computationally by Goldberg [154] who suggested that powder deposition is greater in the annular area around the roof and in the region below the height of the atomiser for medium and larger droplets, respectively. Langrish and Zbicinski [155] also explored the use of CFD towards the reduction of wall deposition by examining the effects of the inlet air swirl velocity and the spray cone angle on the particle deposition rate. Kieviet and Kerhof [156] simulated the air flow pattern (no spray) and the temperature and humidity patterns (water spray) in a co-current spray dryer. Further, Kieviet [157] and Kieviet et al. [158] correlated wall deposition with the particle residence time distribution and concluded that the time taken for particles to slide down the conical wall of a co-current cylinder-on-cone dryer was the most important factor in determining residence times in spray dryers with high wall deposition rates.

In a similar context, Goula and Adamopoulos [159] used a commercial CFD code (FLUENT) to assess the effect of feed concentration oil spray drying of tomato pulp and of pre-conditioned humidity levels. To this end they investigated the trajectories of evaporating water droplets inside a pilot scale co-current spray dryer fitted with a two-fluid nozzle atomiser as a function of the drying and atomising air velocities. Their results revealed increased residue accumulation on the dryer walls with decreasing the velocity of either the drying or the atomising air.

Huang et al. [160] also used commercial CFD software (FLUENT) to investigate the effects of operating pressure, heat loss and inlet air conditions on the flow pattern, the particle trajectories and the temperature and humidity profiles inside a co-current spray dryer fitted with a pressure atomiser. They concluded that a decrease in the operating pressure or an increase in the ambient air humidity calls for an increase in the air mass flow rate in order to obtain the same product capacity. In an accompanying article, Huang et al. [161] reported additional results in a co-current spray dryer fitted with a rotary disk atomiser.

The use of CFD to evaluate alternative spray dryer configurations was examined by Southwell et al. [162] and Huang et al. [163]. In particular, Southwell et al. [162] used commercial CFD software (CFX) to investigate alternative ways of obtaining a uniform flow inside a co-current cylindrical spray dryer with a single off-axis inlet pipe. Huang et al. [163] reported gas flow and temperature profiles, droplet trajectories, residence times and drying times in four co-current configurations (cylinder on cone, conical, hour glass shaped and lantern shaped) as a function of the particle wall BCs (i.e. trap or reflect). Their results revealed increased and decreased evaporation intensities for the cylinder-on-cone and conical configuration, respectively, and a strong dependency upon the choice of particle wall BCs.

Closely linked to the effect of wall deposition is that of particle stickiness. Stickiness is a phenomenon that reflects the tendency of some materials to adhere to contact surfaces and/or to agglomerate [164]. Although wall particle stickiness is undesirable, the formation of larger particles as a result of droplet/droplet,
droplet/semi-dried particle, droplet/particle or particle/particle collisions is a necessity in a number of spray drying applications including milk powder, coffee and detergents [165]. For these products, a larger and uniform particle size is generally preferred as it facilitates collection, packaging and post-processing and can enhance solubility. However, the understanding and successful modelling of the mechanism that leads to coalescence or agglomeration has proven to be a most challenging task due to the complex physics of the process and also due to a number of numerical difficulties. In particular, coalescence and agglomeration are governed by a number of major phenomena [166]. These include (1) glass transition temperature and moisture evaporation effects both of which influence particle stickiness and thus their propensity to agglomerate and (2) turbulent dispersion effects which produce relative velocities between particles so that they approach each other and may potentially collide.

Collision, coalescence and agglomeration can be modelled either via the Eulerian or the Lagrangian approach described in Section 5. In the former, coalescence of droplets is modelled by solving a population balance equation [167, 168]. In the latter, particles trajectories are calculated by solving the Lagrangian equations of mass and momentum with collision and coalescence modelled from semi-empirical relations stemming from experimental observations [169, 170] that relate the collision outcome to the Weber number, the impact angle and the diameter ratio of the colliding particles. Two-phase flow modelling and particular issues related to inter-particle interactions are a field of ongoing research.

Yanniotis and Xerodemas [171] used commercial CFD software (FLUENT) to simulate the operation of a pad humidifier. The flow inside a 'unit cell', the repeating geometry structure, was solved for a wide range of air velocity magnitudes and for all three directions so that a library of the hydrodynamic losses was established. The governing equations of the momentum, heat and mass exchange between the main phase (air and water vapour mixture) and secondary phase (water) were solved for the whole pad humidifier with the dispersed phase model.

6 Conclusions and outlook

The purpose of this work was to provide a general overview of the current state of numerical modelling in the food industry with emphasis on some of the details of the numerical methods. From the selected cases presented herein, which by no means offer an extensive listing of the enormous amount of computational work currently undertaken by the food engineering R&D sectors, it has become clear that simple one-dimensional numerical methods for the estimation of heat and mass transfer in food samples have reached an extensive degree of reliability. However these methods are limited to simple geometries and are bound by a number of assumptions and approximations. On the other hand, the evolution of FEs and CFD coupled with the now well-established ability of setting up complex and unstructured meshes that can accommodate geometries of arbitrary shapes, currently provide a mature, useful, reliable and comparatively simple tool to extend knowledge and understanding on most food-related processes including momentum, heat and mass transfer, phase change and multi-phase flow phenomena. To this end, an effort has been made to
highlight in this work not only methods and models that have already found application in the food industry (e.g. CFD by application of the $k-\varepsilon$ model for the determination of the heat transfer coefficients) but also methods and models that have either reached a certain degree of maturity or are still a subject of ongoing research on other disciplines (e.g. LES, DNS, two-phase flow modelling) but yet relevant in many aspects of food engineering currently and in the near future.

References


