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A user-friendly general-purpose predictive software package for food safety

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ABSTRACT

Computer-aided engineering tools can help speed up food product, process and equipment design by making it easier to check "what if" scenarios, much as such tools have improved productivity in other industries. In particular, food safety is a critical area where such predictive tools can have great impact. A realistic, integrated and comprehensive software has been developed that can simulate a food process and its safety by combining a fundamental, physics-based model of the process with the kinetics of microbiological and chemical changes during processing to provide needed information at any time and at any location in the food during processing. Compositions for a large number of foods are integrated into the software, and therefore, composition-based prediction of thermophysical properties, needed for the model, can be obtained. Microbiological and chemical kinetic databases that are also built-in can cover many practical situations, based on the grouping of foods. An intuitive graphical user interface has been built with those in the food sector in mind.

1. Introduction

Computer-aided engineering (CAE) tools, where physical reality is replaced by its equivalent computer model, and which allows implementation of "what if" scenarios more quickly, can go a long way to increasing the efficiency and competitiveness of food product, process and equipment design (see, e.g., Burnham et al., 2008). However, CAE tools that are customized to food processing and integrate several disciplines (e.g., engineering, food science, food technology, etc.), need to be appropriately developed (Datta, 2008b; Sablani, 2008; Marks, 2008; Van Boekel, 2008; Banga et al., 2008; Jousse, 2008). CAE tools can improve safety and quality, reduce costs and decrease "time to market." The same tools that have made automobile, airplane and chemical process designs remarkably more efficient (Ivester, 2008) are potentially available to the food sector. However, the quality and safety aspects of food processes, and the characteristics of food materials, have many unique features compared with those in any other manufacturing sector. To make computer-aided product and process engineering more of a reality for food, so that the food sector can reap the benefits of this technology, an integrated, robust and user-friendly CAE tool has to be developed. This has been an underlying desire in the food community, as expressed in many specialized international conferences and workshops (IFT, 2009; Model-It, 2005; Eurotherm Seminar 77, 2005; FOODSIM, 2004; IFT Annual Meeting et al., 2003; AFoT, 2003; ISFTFPFFS, 2003).

In order for the food sector to increase CAE use, available generic simulation software needs to be customized for food applications, e.g., by delivering solutions to sets of equations of relevance to food processing. The need for food sector is not unique in this sense—such customization is required for other industries and involves very significant developmental time and cost. However, the current user base for the food industry is small enough that software companies are reluctant to invest the resources needed to develop specific capabilities of interest to food processing. The user base, of course, cannot increase until ready-to-use tools are available. This is a chicken-and-egg situation and the only solution is to start somewhere. The work presented here is such an attempt and it became possible with funding from the United States Department of Agriculture's National Integrated Food Safety Program for development of a software package to simulate food safety.

1.1. Physics-based models in CAE software

Typically, the basis for CAE software is fundamental physics-based or mechanistic models of processes, as opposed to observation-based models that are typically relationships fitted to observations. The relative advantages of these two broad types of models have been discussed at length (Datta and Sablani,

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2007; Datta, 2008a; Sablani, 2008). The phenomenal growth in computing power and its associated user-friendliness have allowed physics-based models to be highly realistic by including more and more of the detailed physics and have fueled rapid growth in the use of models in product, process, and equipment design and research in other sectors. The advantages of a physics-based model include: (1) a reduction in the number of experiments, thus reducing time and expenses; (2) providing immense insight into the process that might not even be possible with experimentation; (3) process optimization; (4) predictive capability, such as ways of performing "what if" scenarios; and (5) providing improved process automation and control capabilities (Datta, 2008a). On the downside, physics-based models are more restricted to the food process itself rather than food quality or food safety, since physics-based models require precise relationships between quality/safety and the process parameters, which are generally unavailable. Observation-based models can relate quality/safety to processing parameters more easily as they do not require detailed knowledge of the underlying physical process. However, observation-based models are primarily "blackbox" models that would not provide insight and they are difficult to generalize into a framework for use in multiple processes. As mechanistic models of quality and safety are continually improved (e.g., Van Boekel, 2008) these improvements can be easily integrated with physics-based process models to provide quality and safety parameters that are readily usable by the food designer.

Modeling food quality and safety requires addressing issues such as: (1) complex multiphase heat and mass transfer such as evaporation and multiphase flow as in aseptic processing; (2) multiphysics such as combined microwave or microwave-infrared heating; (3) significant changes in material property during processing; (4) significant dimensional changes and associated physics; (5) considerable variation (batch to batch or within the same material) in material properties due to a material's biological origin; (6) a large number of new processes continually being introduced; and (7) a lack of kinetic data for final variables of interest (quality and safety) as they relate to temperature and moisture (Datta, 2008a). An additional challenge in the food industry is that technical professionals who are often in charge of these issues have training in chemistry and/or microbiology as opposed to physics-based mathematical modeling. By training, the technical professionals in the food industry are more likely to be accustomed to observation-based models. These characteristics of food processing point to the requirements of a food CAE software in two broad directions—useful software would need to consider the complexities in food and processes that are unique; and such software should integrate many of the details and at the same time hide itself under a user interface that is as simple as possible. For computer-aided food process engineering (CAE applied to food processes), it would be ideal to have a scenario where a technical person, with minimal knowledge of the physics of the process and computational aspects, can use a few clicks of a mouse to define a practical food process. For example, such a user could click and choose among various container types, food material, and heating systems and ask the computer to provide the heating temperature needed for optimum quality in a sterilization process. The computer would need to formulate the physical problem (sterilization) into a mathematical one (equations), decide the best solution method, and finally do an optimization. For food processing applications, this has not yet been a reality.

Most of the modeling or CAE effort is at the research stage (e.g., Mittal, 1997; Scott and Richardson, 1997; Datta, 1998; Tijskens et al., 2001; Irudayaraj, 2001; Welti-Chanes et al., 2002; Sun, 2007; Sablani et al., 2007) and does not migrate to production or mass use in design by practicing scientists and engineers in industry, extension or education. Available software (mostly computational fluid dynamics (CFD) software that solves fluid flow, heat transfer and mass transfer problems) cannot be readily used for food for several reasons (Datta, 2008a). First, the detailed first-principle-based and experimentally validated formulations of more complex processes such as frying are generally unavailable. Second, when the problem formulations can be made, there are unique aspects of food processes (such as strong evaporation in the food matrix) that can be hard to implement in a typical commercial software. Third, when the formulation is available and the software can solve it, we often run into difficulties obtaining the appropriate material properties for specific food conditions. Until these items are resolved and hidden from a user through user-friendly interface, simulation will continue to be research rather than design project.

1.2. Current status of CAE in food processing

The current state of the introduction of CAE into the food industry can be described as follows: Larger food companies that can invest more resources are doing this (Jousse, 2008) but, for other than the largest multinationals, modeling is often not seen as an efficient alternative. Smaller companies that do not maintain CAE or simulation infrastructure sometimes utilize consultants to contract out simulation work. Such consultants can be those specialized for food industry (e.g., www.airflowsciences.com) or the generic CAE software companies themselves. Customized software of the type described in this manuscript can go a long way toward establishing more widespread use of CAE in the food sector. Some efforts are underway to develop customized software (Torres, 2003; CFDfood, 2004; Otles and Onal, 2004; Verdurmen et al., 2006; PROFOOD, 2009). To the best of our knowledge, these software applications are still quite limited in terms of the physics they include. For example, they may include only diffusional heat and mass transfer. There are microbiological modeling software (e.g., ComBase-PMP, 2003; Peleg, 2010) but they typically do not include the process model. In a related area, kinetic modeling of food quality has been studied extensively (Van Boekel, 2008) but not integrated in simulation software with process models.

Thus, a comprehensive software package that integrates realistic processes, products and microbiological aspects has not been available. However, such a software package has now been developed and this manuscript presents the underlying scientific principles for a fundamentally-based, easy-to-use, universal software predictive tool that is useful in a broad range of situations in the food sector (production, processing, distribution, preparation). The developed software can (1) simulate a large variety of food processes, and (2) integrate the process models with the microbiological and chemical safety models in order to predict safety information for a wide variety of food processes.

The manuscript is organized by first describing the software. This is followed by a discussion of the development steps for the software: (1) problem formulation for food processes; (2) integration of food type, composition and property estimation; (3) integration of microbiology and chemical safety simulation; (4) model validation; and (5) a short overview of software implementation and the user interface.

2. Outline of the software package

A custom-developed graphical user interface (GUI) takes various product- and process-related inputs from the user (Fig. 1). The user first selects the food process, the geometry and the dimensions of the food product to be modeled. The user then selects the food type either from the built-in database (based on the USDA National Nutrient Database (USDA – Agricultural Research Service, 2006) and which contains the composition of the food) or directly inputs the

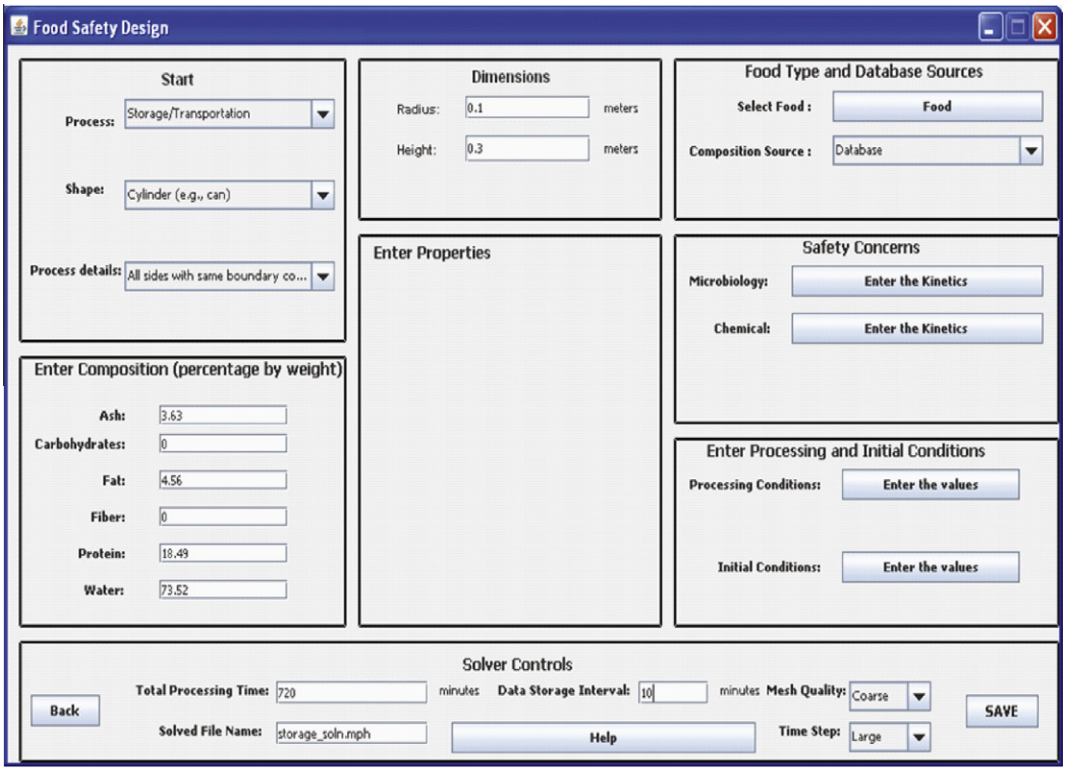

Fig. 1. The screenshot of the software GUI.

food composition. The thermal properties (density, thermal conductivity, specific heat) are then estimated from the composition. Here also, the user has the choice of specifying properties that would bypass the computer-based estimation process. Other properties required to run the process models are also entered at this step. The user then specifies the microbiological or chemical safety data or both, followed by the processing conditions. The final step in the process is to specify the solver settings. All these user inputs are then automatically fed into a commercial Finite Element solver, COMSOL Multiphysics 3.5a—which simulates the appropriate process and safety. The results of the simulation can then be processed in various ways by using the user-friendly post-processing interface of COMSOL Multiphysics.

3. Food processes

The food processes included in the software are grouped into two categories (Fig. 2) based on the physics, the computation level and the knowledge required to solve the process.

3.1. Simple process models

The first category comprises simple processes, which solve for only heat transfer (and, optionally, diffusion moisture transfer). It is assumed that the food is solid, and there can be only diffusion mass transfer of moisture inside or at the surface of the food. The only variables of interest are temperature and moisture content, and all the safety or quality analyses for these processes are associated with these variables only. The models in the simple process category cannot be used in cases where intensive heating of the food takes place and there is significant vapor generation and pressure-driven flow inside the food matrix. Currently, three industrially important thermal food process modules have been included in the simple process category—refrigeration/storage/transportation/general heating or cooling, sterilization of solid foods, and drying of solid foods. In the future versions, the software would be extended to important non-thermal processes also.

3.1.1. Refrigeration/storage/transportation/general heating or cooling

The module for these processes models conduction heating or cooling, without any evaporation/condensation (latent heat) and without any moisture loss. The governing equation is as follows:

$$\rho C_p \frac{\partial T}{\partial t} = \nabla.(k\nabla T) \tag{1}$$

where ρ is the density, C_p is the specific heat capacity and k is the thermal conductivity of the solid medium. The process module, as implemented in the software, can be applied to check the possible microbial load when there is a temperature abuse. For example, it can be used to monitor the effect of temperature abuse (resulting in bacterial growth) for a chilled product by providing any expected temperature change as a function of time. It can also estimate the maximum allowed time for a chilling process (see Section 9.1) during which bacterial growth inside the food is within the safety limit.

3.1.2. Drying

This module can be applied for slow heating or cooling of food materials, where significant moisture loss occurs. The drying module solves for heat conduction (Eq. (2)) along with moisture loss by solving for diffusion inside the food and evaporation at the surface. The moisture diffusion equation is:

$$\frac{\partial M}{\partial t} = \nabla \cdot (D\nabla M) \tag{2}$$

where D is the moisture diffusivity through the medium and can be a function of the moisture content in the medium. The safety applications of the module are similar to those for heating or cooling situations, the only difference being that moisture transport is also important in this case.

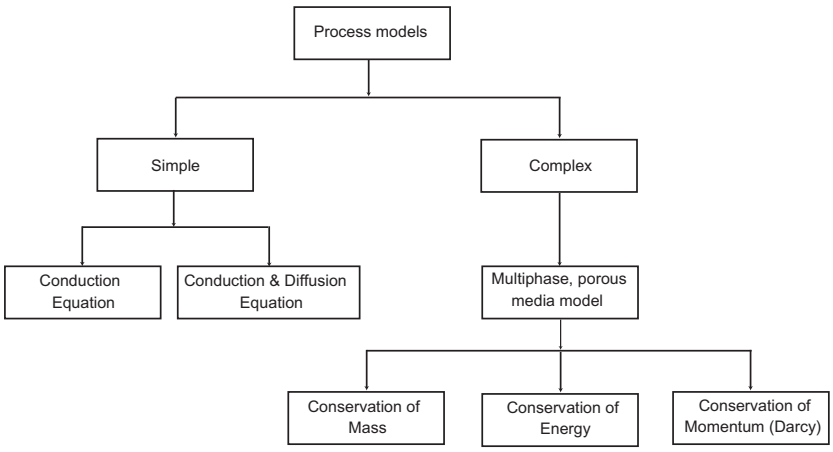

Fig. 2. Categorization of the processes depending on the level of complexities involved.

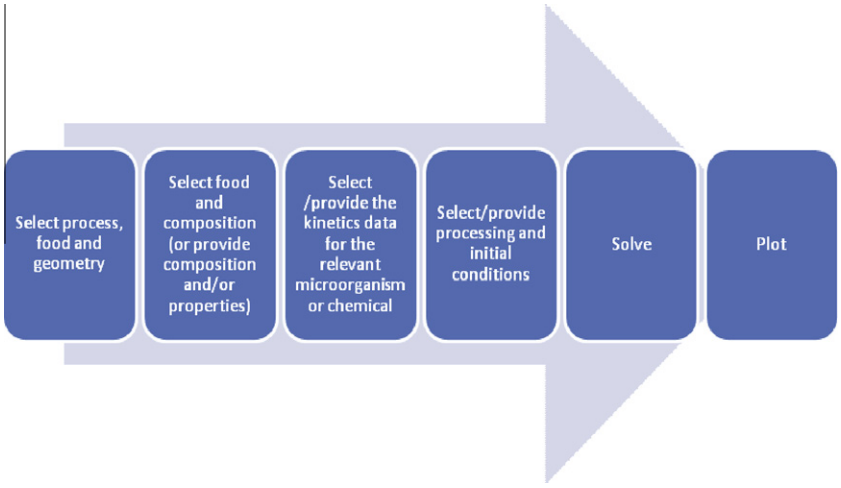

Fig. 3. Flowchart of the approach.

3.1.3. Sterilization of solid foods

The sterilization module models heating of solid foods to sufficiently high temperature using steam or hot water to inactivate microorganisms contained in the food such that it is safe to eat. The module for these processes models conduction heating (Eq. (1)), without any evaporation and moisture loss. The information from such a mathematical model can help a process designer in determining the sterilization time that retains maximum quality and safety, or planning for corrections in the processing time for unintended increases or decreases in the processing temperature.

3.2. Multiphase porous media models

In the difficult process category, food is considered as a porous medium and a multiphase, porous media problem is solved. Mass conservation equations are solved for the relevant phases inside the food (e.g., in the case of deep-fat frying of potato reported in Halder et al. (2007b), the pores inside the potato may be filled with water or gas or oil anytime during frying). So, the phases identified are solid potato, liquid water, oil and gas (a mixture of vapor and air). The solid phase conservation is not solved as the solid mass remains unchanged. The mass conservation equation for any component i can be written as

$$\frac{\partial}{\partial t}(\phi\rho_i S_i) + \nabla \cdot n_i = \dot{R} \tag{3}$$

where ϕ is the porosity of the porous medium, S is the volume saturation, n is the mass flux and $\dot{R}$ is the appropriate source term due to evaporation.

Local thermal equilibrium is assumed, which means that at a given location in the food, all the phases have the same temperature. Therefore, only one energy conservation equation is solved for the system, given as:

$$\rho_{eff} c_{p,eff} \frac{\partial T}{\partial t} + n_{fluid} \cdot \nabla (c_{p,fluid} T) = \nabla \cdot (k_{eff} \nabla T) - \lambda \dot{I} \tag{4}$$

where the subscript *eff* refers to mixture properties including the contribution by a solid and *fluid* refers to mixture properties due to fluids (transportable phases). Currently, two industrially important thermal food process modules have been included in the difficult process category—microwave heating and deep-fat frying.

3.2.1. Microwave heating

The microwave heating module solves for changes in temperature, liquid water, water vapor and pressure (from evaporation) inside the food during the microwave heating process. A multiphase porous media model, as implemented by Ni et al. (1999), has been used to simulate the process. In this problem, food geometry has been restricted to one dimension only. The model can be applied to observe the effects of microwave power level, penetration depth, product composition, surrounding temperature on the

temperature and moisture accumulation near the surface. Since the temperature can stay colder at the surface than slightly inside, safety issues arising from undercooked meat and poultry products can also be checked.

3.2.2. Deep-fat frying

The deep-fat frying model solves for changes in temperature, liquid water, water vapor and pressure (from evaporation) inside the food over the deep-fat frying duration. A multiphase porous media model, as implemented by Halder et al. (2007b), has been used to simulate the process, in which food geometry has been restricted to one dimension only. In addition to observing the temperature, moisture, pressure and oil profiles, the model can be used to obtain the effects of oil temperature, product properties, product thickness, etc., on the frying time and oil pickup. The amount of acrylamide formation can also be calculated for potato frying.

4. Composition and property estimation

4.1. Composition

After selecting the process, the geometry of the food and its dimensions, the user is asked to select the food. The software gives the user a choice of either specifying a user-defined food or selecting a food from an built-in database. The built-in food database of the software is based on the USDA National Nutrient Database for Standard Reference, Release 19, which contains data for 7293 food items and up to 140 nutrients and other components in those foods. The 7293 food items are divided into 24 food groups based on the food product type. Of the 140 nutrients listed, only 6 major food components dictate the thermal properties of a food product (discussed below). The components are those contributing to the proximate analysis and include ash, carbohydrates, fat, dietary fiber, protein and water. Upon selection of a food from the food database, the composition values are obtained from the USDA National Nutrient Database, and are used to calculate the property values based on the work of Choi and Okos (1987), as described in the following section. The user can also choose to define a food outside of the database. In such a case, the user should either know the composition (in terms of the above-mentioned proximate components) of the food so that the properties can be estimated or the properties can be entered directly.

4.2. Property estimation

The complex and highly heterogeneous nature of foods makes their property estimation from fundamental principles an extremely difficult task. For almost all types of foods, the physical properties are experimentally determined. Over the last several decades, efforts have been made to compile the huge amount of property data for all foods into an organized structure (Saravacos and Maroulis, 2001; Rao et al., 2005; Rahman, 2009; Nesvadba et al., 2004). However, using this huge compilation of data in software is a massive task and cannot be extended to any new food products. Another way to approach this issue is to assume that the properties of a food can be estimated as a weighted average of the properties of its constituent proximates (Miles et al., 1983; Choi and Okos, 1987). The weighing strategy depends on the nature of the property itself. This software follows the work done by Choi and Okos (1987) on predicting the properties from food composition. They compared the predicted values from the averaging technique with experimental measurements and found that the error was within 10% for all the foods that were tested.

4.2.1. Density

The bulk density of the food material is estimated by assuming that the volumes of the various proximates simply add up. So, the density for a food material which does not have any air pockets will be:

$$\rho = \frac{1}{\sum \frac{X_i^w}{\rho_i}} \tag{5}$$

where X_i^w is the weight fraction and ρ_i is the density of the ith component. If air is present with volume fraction ϵ then the density of the food material is modified to include the effect of air volume:

$$\rho = \frac{1-\epsilon}{\sum \frac{X_i^w}{\rho_i}} \tag{6}$$

4.2.2. Specific heat capacity

The net specific heat of the food material is simply the mass average of the specific heat of individual components:

$$C_p = \sum C_{p,i} X_i^w \tag{7}$$

The equation is based on the principle that the total heat required to raise the temperature of the food material by a given amount is equal to the sum of heats required to raise the temperatures of its individual components by the same amount. Here, it is assumed that there are no phase changes involved.

4.2.3. Thermal conductivity

The net thermal conductivity, k, of the food material is the volume average of the individual conductivities, k_i, given as:

$$k = \sum k_i X_i^w \tag{8}$$

where k_i is the thermal conductivity of the ith component. This is based on the fact that the thermal conductivity is a property of the volume rather than the mass. More complex models for thermal conductivity exist in the literature (Saravacos and Maroulis, 2001), but they enhance accuracy only incrementally. Therefore, we selected the simplest formulation, which gives a reasonable approximation of thermal conductivity.

4.2.4. Process-specific properties

In addition to the thermal properties of food, which are required for all food processes selected, deep-fat frying requires the porosity of the food material and the thermal properties of the cooking oil used. Similarly, the microwave heating process requires the user to specify the porosity of the food material, the microwave power supplied to the food and the penetration depth of the microwaves in the food material. The power absorbed by a food during microwave heating depends on a number of factors, which can be divided into two categories: food factors and oven factors (Zhang and Datta, 2003). The main food factors are volume, surface area and the dielectric properties of the food. The main oven factors are oven size, geometry, the location of the food inside the oven cavity, the presence of special features like a turntable and a mode stirrer, the location of the microwave feed, etc. The dependence of power absorption on so many factors makes experimental determination of the power absorbed necessary. Ni et al. (1999) used 30,000 W/m^2 as the power absorbed by the surface of a cylindrical food of radius 0.5 cm and height 2 cm in a domestic microwave oven (SHARP Carousel, Rated Power 1.5 kW). By default, this value is used in the microwave heating problem in the software. The user can scale this value to any value by using the microwave power scaling factor. The other input, penetration depth, is a measure of how deeply microwaves can penetrate into a food material. It is defined as the depth at which the intensity of the microwaves inside

the material falls to 1/*e* (about 37%) of the original value at the surface. For a given food material, it is a function of moisture content and temperature. The microwave heating model requires this value as an input. By default, the penetration depth of a potato is used.

5. Microbiological safety prediction

Quantitative microbiological modeling associated with growth or inactivation in the literature is generally not coupled to spatial variation (e.g., temperature, moisture and pH) in a food material during a process. Models typically assume one temperature for the food material or implicitly refer to one location (e.g., a cold spot) in the food material. In a typical food process, the time–temperature history would vary spatially depending on process and food thermal parameters. The absence of such growth and inactivation profiles within a food is obviously a major limitation of microbiological models (Marks, 2010). To overcome this, a process model (that provides spatial temperature–time histories) has been integrated with existing predictive microbiological models to provide for comprehensive prediction concerning food safety for many food processing situations. A part of integrating process models with microbiological growth/inactivation models was the development of a comprehensive database containing associations of foods and target microorganisms along with microbiological growth/death kinetic parameters. The database of microbial growth and inactivation kinetic parameters for various food types was developed through extensive regression analysis on decades of experimental data from the literature to facilitate predictive modeling and make the software "user-friendly" (Halder et al., 2011). Any user with a basic knowledge of food processing and no specialized background in predictive microbiological modeling can use the software. All the user needs to do is select the target microorganism (with built-in guidance) from the GUI and the software takes care of the rest. It provides, for example, the kinetic parameters as a function of temperature for the selected microorganism and food group from the built-in microbiological kinetic database.

There are several issues involved in trying to compile comprehensive microbiological kinetic information (Halder et al., 2011): (1) limited availability of data for many specific situations; (2) correlation issues between laboratory conditions and real foods; (3) variability of data on microbial inactivation reported by various researchers; (4) variability among microbial populations; and (5) evolving knowledge of appropriate predictive models that describe the data. In building a comprehensive database, a holistic approach was taken by first using a database of food products (USDA National Nutrient Database) and associating bacterial pathogens with those foods. Foods with similar composition, intrinsic characteristics and having similar pathogen associations (i.e., based on outbreak history) were grouped together and foods within a group have the same growth/inactivation kinetic parameter values. The 7294 food products from the USDA National Nutrient Database were re-grouped from the original 24 into 17 groups. Table 1 shows the original USDA National Nutrient Database food groups and Table 2 gives the rearranged food product database for the purpose of predictive microbiological modeling. After forming the food groups, experimental data on growth and inactivation from the published literature (over 1000 datasets) were analyzed using a regression technique to obtain kinetic parameters for developed food groups using the chosen models (how the model was chosen is discussed in the next section).

Table 1
USDA National Nutrient Database food groups

Category	General types of foods	Number of items
1	Dairy and egg products	183
2	Spices and herbs	60
3	Baby foods	261
4	Fats and oils	205
5	Poultry products	337
6	Soups, sauces and gravies	399
7	Sausage and luncheon meats	213
8	Breakfast cereals	409
9	Fruits and fruit juices	312
10	Pork products	289
11	Vegetables and vegetable products	776
12	Nut and seed products	128
13	Beef products	576
14	Beverages	251
15	Finfish and shellfish products	249
16	Legumes and legume products	211
17	Lamb, veal and game products	343
18	Baked products	487
19	Sweets	421
20	Cereal grains and pasta	168
21	Fast foods	309
22	Meals, entrees, and side dishes	102
23	Beef (2)	213
25	Snacks	15
35	Ethnic foods	132
42	Miscellaneous	84
43, 44, 47, 48, 80, 83, 90, 93	Miscellaneous (2)	161
Total		7294

Table 2
Rearranged food product database.

Original categories	New food group categories	Number of items
1, 4, 19, 35, 42, 43, 44	Dairy products	224
3, 42, 43	Baby food	288
4, 35, 42, 44	Fats and oils	240
1, 5, 7, 35, 42, 43	Poultry and eggs	440
6, 35	Soups and sauces	401
8, 20, 42, 43	Cereal products	594
9, 19, 35, 43	Fruits	327
7, 10, 13, 17, 19, 23, 35, 42, 43	Red meat products	1629
11, 16, 35, 42, 43, 48	Vegetables	1012
12, 16, 42	Nuts and seeds	155
14, 35, 42, 43, 44, 47	Beverages	276
15, 35, 43, 80, 83, 90, 93	Fish and seafood	294
18, 35, 43	Baked products	492
19, 25, 42, 43, 44	Snacks	447
21	Fast foods	309
22	Entrees	102
2, 43, 44	Spices and herbs	63
Total		7294

5.1. Mathematical models

5.1.1. Growth model

The sequential stages of bacterial growth are the lag phase, the exponential phase, the stationary phase and the death phase. The lag phase is the stage at which the microorganism adapts to a new environment and the lag time (L) is the time taken by the microorganism to adapt to that environment prior to exponential growth. The exponential phase is followed by the stationary phase when the conditions are no longer favorable for rapid growth (e.g., due to lack of nutrients or a change in pH). As conditions become unfavorable and/or lethal for bacteria, the death phase begins. A growth model describes the first three stages of growth, the lag phase, the exponential phase and the stationary phase. The predictive model for the lag phase and the exponential phase using a first-order growth model is given for two different situations, isothermal and non-isothermal. A first-order model cannot predict

the stationary phase. Lag times (L_T) are available for various temperatures from the published literature. So, in a first-order model, for isothermal situations, the growth rate is zero until the lag time is over and k_T, the growth rate at temperature T, is used after the lag time has elapsed. The model is given as:

$$\frac{dN}{dt} = \begin{cases} 0 & t < L_T \\ k_T N & t > L_T \end{cases} \quad (9)$$

A methodology to predict microbial growth under fluctuating temperature conditions has been developed by Li (1988). The total adaption under fluctuating temperature conditions is given by:

$$\frac{dA}{dt} = \frac{1}{L_T} \quad (10)$$

where A is the total adaptation during the lag phase. An adaptation rate can be defined as the reciprocal of the lag time. When A equals 1, adaptation is complete and growth starts. Therefore, the growth is given by:

$$\frac{dN}{dt} = \begin{cases} 0 & A < 1 \\ k_T N & A > 1 \end{cases} \quad (11)$$

Eqs. (9)–(11) resemble equation Eq. (2) (a diffusion equation) with zero diffusivity and a non-zero source term. Therefore, the above-mentioned equations are implemented as diffusion equations in COMSOL Multiphysics, where the diffusivity is zero and the terms on the right-hand side of Eqs. (9)–(11) are added as source terms to the respective equations. The model parameters, such as k_T and L_T, are functions of temperature, and are specified as such in the software, as shown in Table 3 for *Clostridium perfringens*.

5.1.2. First-order inactivation model

For microbial inactivation, it is not practical to provide the kinetic parameters for all of the possible models in the database. After careful analysis, the first-order model was selected for the following reasons: (1) the first-order model for inactivation has been used extensively and kinetic parameter values (e.g. D-values) are available for this model for a significant number of microorganisms in specific food products; (2) there are models such as the Baranyi model and the Hills model (McKellar and Lu, 2004) which can predict both tail and shoulder effects during inactivation, but applying data from the literature to such models would be an arduous task and is not feasible given the limited presentation of the baseline data used in many studies; (3) the compilation of numerous inactivation parameters, such as D-values, over like experiments for specific microorganisms acts to normalize the impact of non-log linear effects seen in individual experiments. The important trend becomes the rate of response relative to specific food types for individual organisms under defined process conditions.

An inactivation curve following first-order kinetics (Ball, 1929) is written as:

$$log_{10}\left(\frac{N}{N_0}\right) = -\frac{1}{D_T}\int 10^{\frac{T(t)-T_{ref}}{z}} dt \quad (12)$$

where D_T is the time taken to reduce the concentration of microorganisms by a factor of 10 at temperature T, and z is the temperature change required to reduce the D-value by a factor of 10. The database for the first-order inactivation model contains the mean D_T and z values for various microorganisms in various food types. In addition to the mean kinetic values, the database also contains the upper 95% confidence interval values of D_T and the infectious dose.

6. Chemical safety prediction

Chemical safety aspects during a food process may include formation of a number of compounds, such as acrylamide, heterocyclic amines (HAs), polycyclic aromatic hydrocarbons (PAHs) and nitrosamines, from cooking food at high temperatures. Epidemiological studies have shown that humans exposed to these substances through diet and/or environment may have increased risk of cancer development (Jakszyn et al., 2004). Since these compounds are not present in raw foods, their levels in processed food depends on the amount of precursors (composition of the food) such as cooking time, temperature, cooking method and pH value. Among the physical factors, cooking time and temperature are the main parameters (Jackson and Hargraves, 1995). The amount of the chemicals generally increases with increasing cooking time and temperature, but their degradation may become significant at very high temperatures. Predicting the formation of the compounds in terms of cooking times and temperature would help producers and consumers to understand how to prevent or limit their accumulation in thermally processed foods.

The software currently includes the kinetic parameters of formation of four major chemical groups of concern (acrylamide, HAs, nitrosamines, PAHs) based on analysis of experimental data from a total of 127 scientific publications. Selection of data was limited to articles that (1) determined the concentration of the compounds using at least four time points during thermal processing for a particular food item and (2) provided the data for maximum amount of the compound that can be formed in the food under the cooking conditions—this led to a selection of only 25 publications. Furthermore, since many chemical species within each group are formed during cooking, only typical chemicals (usually formed in the largest amounts in the group) were selected for the analysis. The classification of food groups for the chemical modeling was the same as for the rearranged food product database used in the microbiological modeling, with the exception of the group 'potato (fried chips, crisps)' added as a separate entity

Table 3
First-order growth kinetic data for *C. perfringens* in various food groups, as stored in the inbuilt microbial kinetic database of the software.

Food groups	Temperature range (°C)	Rate (CFU/h)	r^2/N	Lag (h)	r^2/N
Poultry, eggs and red meat	15–18	0.067		39	
	18–24	0.0305T−0.504	0.991/7	158.54−6.49T	
	24–35	0.0305T−0.504	0.991/7	12.44−0.341T	0.900/3
	35–40	0.0305T−0.504	0.991/7	0	0.712/4
	40–50	0.75		0	
Soups, sauces, spices, herbs	15–18	0.073		55	
	18–24	0.0376T−0.641	0.988/8	223.86−9.21T	
	24–35	0.0376T−0.641	0.988/8	15.81−0.442T	0.892/3
	35–45	0.0376T−0.641	0.988/8	0	0.725/4
	45–50	0.94		0	

Table 4
Summary of information collected for determining chemical safety of acrylamide, heterocyclic amines (HAs), polycyclic aromatic hydrocarbons (PAHs) and nitrosamines in cooked foods.

Groups of compounds	Compound	Publications	Food groups included
Acrylamide	Acrylamide	18 (6)	Potatoes (fried chips, crisps) Nuts and seeds (coffee) Baked products
Heterocyclic amines (HAs)	MeIQx, PhIP, 4,8-DiMeIQx	52 (14)	Poultry and eggs Red meat (beef, pork, bacon), Sea food
Polycyclic aromatic hydrocarbons (PAHs)	B(a)P	32 (4)	Poultry and eggs
Nitrosamines	NDMA, NDEA, NYPR	25 (1)	Red meat

Table 5
Example of data collected from literature for determination of the kinetic parameters of PhIP in beef products.

Beef	Temperature (°C)	Cooking time (min)	Conc. of PhIP (ng/g)	C_0 (ng/g)	k_g (per min)	k_d (per min)	References
Meat extract	175	120 180	19.5 16.7			−0.0026	Bordas et al. (2004)
Beef burger	180	6 10	1.2 0.7			−0.1347	Johansson and Jagerstad (1994)
Ground beef	180	5 10 15 20	1.5 1.5 1.5 7	8.6846	0.082		Ahn and Grun (2005)
Ground beef	200	5 10 15 20	1.5 1.5 4 12	13.3372	0.115		Ahn and Grun (2005)
Ground beef	220	5 10 15 20	3 5.5 10.5 15	16.1527	0.132		Ahn and Grun (2005)
Beef patties	230	3 3.75 4.5 5.25 6	3.2 6.8 9.9 25 33.1	57.0154	0.1448		Jautz et al. (2008)
Beef patties	250	5 7	3.1 0.1			−1.717	Gross et al. (1993)

for acrylamide (Table 4). Table 5 presents a summary of the information included in the database.

6.1. Mathematical models

The formation of chemicals at constant temperature was described as a first-order reaction (Arvidsson et al., 1997, 1999; Persson et al., 2008):

$$\frac{dc}{dt} = -k_g(c_0 - c) \tag{13}$$

where c is the concentration of the chemical (ng/g or mg/kg), c_0 is the estimated maximum concentration of the chemical (ng/g or mg/kg), k_g is the rate of formation of the chemical (per min), and t is the cooking time (min).

Eq. (13) resembles equation Eq. (2) (a diffusion equation) with zero diffusivity and a non-zero source term. Therefore, it is implemented as a diffusion equation in COMSOL Multiphysics where diffusivity is zero and the term on the right-hand side of Eq. (13) is added as a source term. The model parameters, such as k_g and k_d, are functions of temperature and are specified as such in the software.

7. Software platform

The software package graphical user interface is built using Java script with the process, microbiological and chemical kinetic models (equations in Sections 3–5) solved in the background using COMSOL Multiphysics (Burlington, MA), a finite-element-based commercial modeling package. Some of the reasons for choosing the software COMSOL Multiphysics as the computational engine were: (1) the ease at which we could implement food processes with rapid evaporation and resulting Darcy flow, for example, of water and vapor; implementing such processes in some other software required solving the Navier–Stokes equivalent of the fluid momentum equation for porous media that is computationally far more intensive; (2) flexibility with which the transport equations and their boundary conditions can be programmed; and (3) a more user-friendly interface of the software itself.

8. Implementation details

8.1. Geometry

For simpler processes, a 2-dimensional heat transfer model has been implemented and the geometry has been restricted to

cylindrical or rectangle shapes. Simulation of frying and microwave heating in 2- or 3-dimensions is much more involved than a 1-dimensional problem. Such simulations are very sensitive to parameters for solution convergence and require a lot of computational time. Due to these reasons, complex processes, like frying and microwave problems, are restricted to solving 1-dimensional heat and mass transfer. For these two processes, we have used the 2-dimensional shape (a rectangle) for better visualization, and have insulated one direction so that all the changes happen in the other direction only.

8.2. Meshing

Since a finite element method is used to solve the governing equations, the relevant geometry is discretized into elements and the equations are solved at the vertices of the elements (called nodes). The discretized geometry is called a mesh and the meshing of the geometry is done automatically with the help of COMSOL Multiphysics. For all the processes and geometries, structured meshing with quadrilateral elements is used. The user gets the option of having a coarse, medium or fine mesh. The finer the mesh, more accurate is the solution but at the expense of increased computation time.

8.3. Solver

The direct UMFPACK solver of COMSOL Multiphysics has been used for all processes. The time stepping has been decided for each process after careful analysis. Similar to meshing, the user gets a choice of large, medium or small time step, with the recommendation that a small time step should be used for processes that involve rapid changes of variables such as temperature and pressure, for example in deep-fat frying and microwave heating processes. For slower processes, such as storage, a small time step is recommended when the processing conditions such as ambient temperature are changing rapidly.

8.4. Post-processing

COMSOL Multiphysics has a well developed post-processing module, which is very intuitive, and does not require modeling expertise for its use. Therefore, the built-in COMSOL Multiphysics post-processing module was used for the software package. Although, this may be seen as a disadvantage of the software being reported here, the user-friendliness and functionalities offered by COMSOL combined with tutorial-type directions developed by us for food-specific quantities are deemed very adequate for a non-specialized user. Some of the examples of post-processing capabilities of the software are (Datta and Rakesh, 2010):

Information at a location (temporal history): at a given location, value of a parameter of interest (temperature, moisture content, microbial concentration, etc.) or its variation with time are basic forms of information that may be necessary.
Spatial variation: a simple form of spatial variation is the information pertaining to maximum and minimum value. A more comprehensive way of getting spatial information is to plot the contours of the parameter of interest.
Spatial integration and averaging: integration or averaging over a region can give useful information such as average temperature or moisture content of the food or the total microbial load in the food.
Secondary quantities: secondary quantities such as heat or mass fluxes at a surface location and variation in such quantities with time can give information about rates of heat or moisture loss (or gain) from (or by) the food.

Apart from the quantities mentioned above, any kind of customized parameter which is a function of parameters being solved for can be defined and plotted in various ways in COMSOL Multiphysics.

9. Software validation

Validation is essential for any modeling effort. In the context of predictive microbiological modeling, a model is evaluated on the basis of how well the model predictions match with the observed phenomena. Often, the model is applied to make predictions only in the experimentally studied range of conditions only. However, if the predictive capabilities are applied only to the experimentally verified conditions, the use of modeling will be seriously limited. The power of modeling technology can be leveraged effectively by making predictions for a wide variety of conditions, of course, after we have gained confidence in the model by applying it to available experimental observations. In this section, we validate the approach by applying the model to two food processes.

9.1. Growth of C. perfringens during air chilling of ready-to-eat ham

Clostridium perfringens is a bacterium of particular concern in cooked meat products. The microorganism is a spore former and is one of the more rapidly growing bacteria, with doubling times as short as 7.1 min at around 44 °C (Amezquita et al., 2005). In this case study, the chilling process of boneless cooked cured ham is modeled along with the growth of *C. perfringens*, to determine whether the number of *C. perfringens* would be kept sufficiently low during the process. The ham is in the shape of a cylinder (radius 10 cm and height 30 cm) and is cooled by air at 7 °C. Blowing of the air over the ham leads to a surface heat transfer coefficient of 50 W m^{-2}. The flow chart (Fig. 4) shows the sequence of the solution process using the software. The specific food, boneless cooked cured ham, is selected by the user from the USDA composition database from within the software. From the composition, thermal properties needed for the simulation are estimated by the software following the discussion in Section 4. The heat conduction equation (Eq. (1)) is solved to describe the temperatures inside the ham at any point and at any time. A non-isothermal first-order growth model (Eq. (10) and (11)) is solved using the temperature history at any location inside the ham to obtain the growth of *C. perfringens* with the lag phase equation (Almonacid-Merino et al., 1993). The kinetic data for the growth of *C. perfringens* is obtained by the software from the microbiological database contained in it

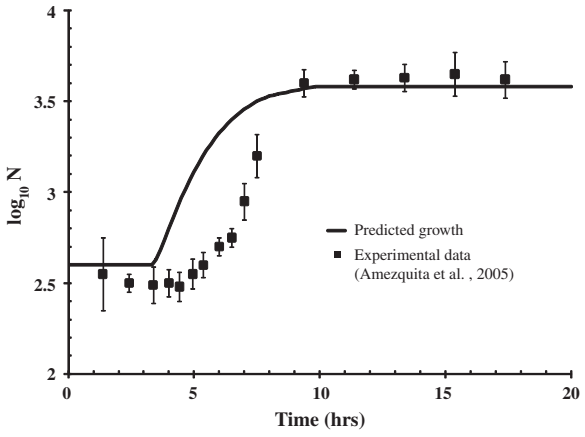

Fig. 4. Predicted and observed *C. perfringens* growth during cooling of boneless cooked and cured ham.

(Table 3). In the database, the growth kinetics data for ham belong to a red meat group (pH 5.5; beef, pork and ham), and is the most conservative estimate within this group. Fig. 4 shows the comparison of predicted and observed *C. perfringens* growth during cooling of the ham, assuming the cooling process is in compliance with FSIS stabilization performance standards for cured products. The prediction made by taking the database value for the red meat group (pH 5.5; beef, pork and ham) is always on the conservative side (as can be seen in Fig. 4), which is acceptable for evaluation of the safety of the process. The difference between experimental and predicted values can be attributed partly to the selection of the kinetic data as the most conservative value in the food group. This serves to validate predictions related to microbiological safety.

9.2. Safety prediction during deep-fat frying of a potato slice

Deep-fat frying is one of the most important industrial processes, with crust thickness and oil pickup being two quality parameters of importance associated with frying. In this case study, the goal is to estimate the total oil picked up and thickness of the crust developed during deep-fat frying of a potato slice. Formation of acrylamide, a probable carcinogen, is also modeled as the food safety parameter. The potato slice is 3 cm thick. It is being heated equally from both sides by oil at 180 °C. The surface heat transfer coefficient for frying is taken as 300 W m^{-2} K^{-1}. The flow chart (Fig. 3) shows the sequence of the solution process using the software. The user selects the type of potato from the database. The thermal properties of the slice are estimated by the software, following the discussion in Section 4. The oil properties are entered by the user. Processing conditions and initial conditions are then specified. A multiphase porous media model developed by Halder et al. (2007b) is solved to describe the temperature, moisture and oil content inside the potato slice at any point and at any time. Fig. 5 shows the comparison of predicted and temporal history of temperatures at different locations and the overall moisture content during potato frying. Also, the total concentration of acrylamide with time is plotted. Such close agreement between experimental measurements and model prediction confirms the effectiveness of the model and serves to validate it.

10. Limitations of the predictive software

Although the software is based on fundamental models and is intended to cover a large range of processes, there are limitations to its predictive capabilities. Some of the limitations are:

Process models: modeling complex food processes such as those involving shrinkage (Mayor and Sereno, 2004; Katekawa and Silva, 2006) is still in the research stage. The models in the software do not include shrinkage, but the transport properties used in the models are obtained from experiments and they contain some of the effects of shrinkage in their values. Therefore, the error due to not including shrinkage is balanced to some extent by using these transport properties.
Geometry of the food: the simpler processes (such as refrigeration and sterilization) are limited to 2-dimensional geometries

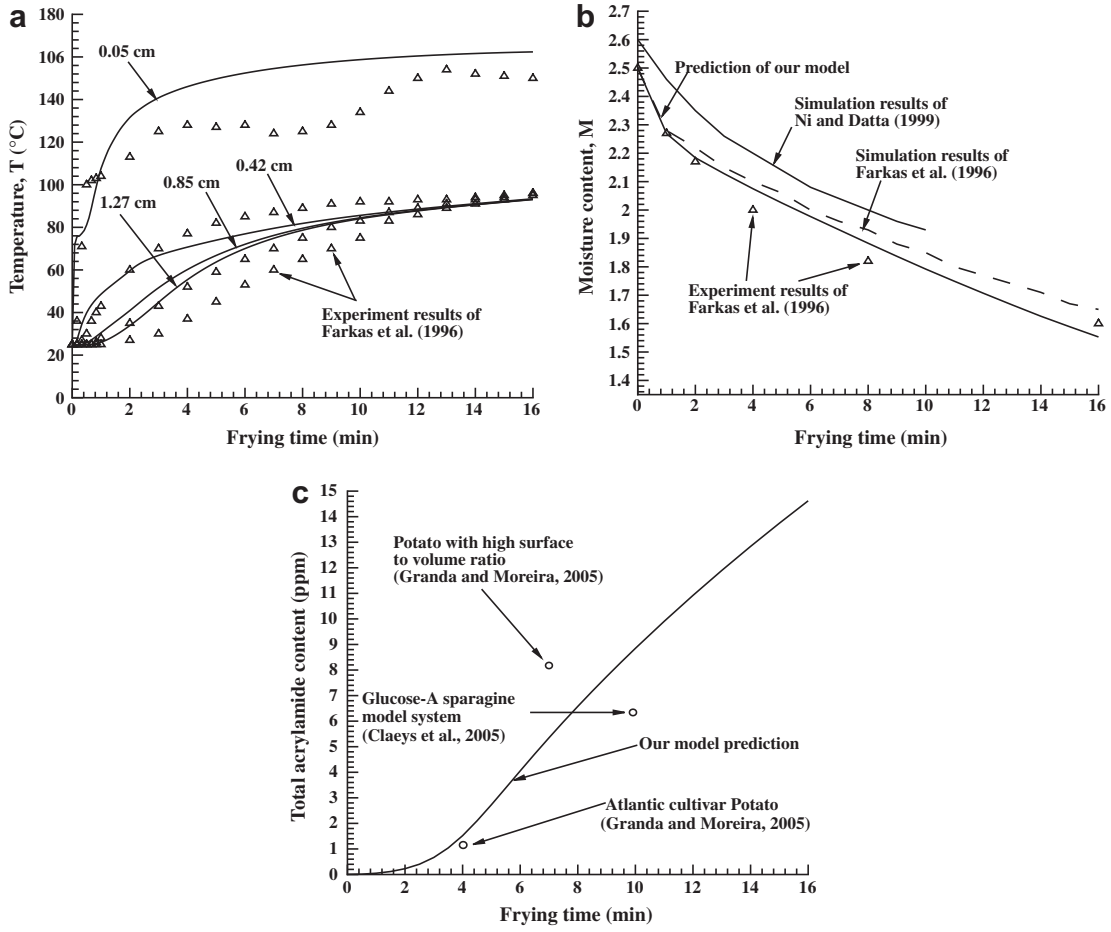

Fig. 5. Comparison of model predictions with the experimental data from the literature for (a) temperature; (b) moisture content (dry weight basis); (c) total acrylamide concentration.

Table 6
Example of determination of dependence of k_g and k_d on temperature for PhIP in red meat

Chemical	C_0 (ng/g)	Generation		Degeneration	
		k_g (per min)	Upper k_g values (per min)	k_d (per min)	Upper k_d values (per min)
PhIP in red meat	57.0154	0.0012T−0.1299	0.0015T−0.0742	0.0227T−3.9695	0.0255T−3.3976

and the more complex multiphase porous media models are limited to 1-dimensional geometry. These limitations arise from the need to either make the software available to a user with little knowledge of simulation (restrictions on geometry) or restrict the computational time.

Property estimations: the Choi and Okos (1987) relations used to estimate food properties are based on compositions, and therefore may have an error of around 10%. Also, there can be significant variation in compositions of different samples of the same food material. An estimation of the implications of this variability (e.g., by Monte Carlo techniques applied by Halder et al., 2007a) cannot be performed from within the GUI developed here, but can be performed using the COMSOL Multiphysics interface directly.

Microbial models: the microbiological kinetics database developed here has some drawbacks, as was discussed in detail in Halder et al. (2010). There can be instances in which there is a difference in composition within a food group and, therefore, it is likely that there are also differences in kinetic parameters. For example, some foods may not clearly belong to any one group. The decision to put them in a particular group was made on the basis of outbreak history, pathogen-food association literature, pH, or other intrinsic or extrinsic factors. Moreover, the estimated growth/inactivation kinetic parameters are conservative estimates, but there can be situations in which kinetic parameters will vary significantly due to the formation of micro-environments, which protects the microorganisms against extreme conditions. The effects of such variability can be included using the COMSOL Multiphysics interface directly, as already mentioned under property estimation. Finally, there are a number of risk factors associated with microbiological food safety which have not been modeled to date and that could contribute to the overall safety of a food product (Black and Davidson, 2008).

11. Summary and expected benefits

A software program has been developed that can simulate food safety by combining a physics-based model of food processes with the kinetics of microbiological and chemical changes in foods during processing to provide bacterial or chemical amounts at any time and any location in the food during processing. Physics-based modeling ranges from simple conduction or diffusion to multiphase porous media model that can keep track of multiple components such as moisture and oil, and multiple phases such as water and water vapor. The thermophysical properties needed for the models are predicted from composition, based on available correlations. The compositions themselves, available from published sources, are integrated into the software. Microbiological kinetic data corresponds to that for a food group, as opposed to individual foods, available from published sources. Similarly, the data for the kinetics of chemical changes was also grouped. An intuitive graphical user interface has been built with those in the food sector in mind. This interface sits on top of a general purpose commercial computational software, thus delegating the detailed computation to the software. This enabled the development of this highly versatile software over a relatively short period of time. Because of the fundamentals-based framework on which the computations are built, it will be somewhat routine to extend the approach to newer processes or combinations of processes.

The software is intended to be a comprehensive tool for speeding up food product, process and equipment design for improved safety and quality. With the help of a simple interface provided by the software, it is now easier and quicker to check "what if" scenarios. A food scientist with little knowledge of simulation engineering can use the software with the help of the documentation provided and thus have this potential tool available. Apart from direct use by the food industry, the beneficiaries of such a comprehensive software tool might include food extension educators, university food science/engineering courses, and food science researchers. Such a tool can be incorporated into a food science/food engineering curriculum following details outlined in Datta and Rakesh (2010). Extension will benefit by having customized instruction capabilities for microbiological safety with respect to arbitrary products, processes and handling situations. The tool, with the ability to present highly detailed visualizations, will make difficult concepts of process more easily comprehensible. In university classroom education, the advantages of the proposed tool include (1) incorporating safety issues for more realistic food product/process/equipment situations; (2) gaining much greater insight into processes; and (3) introducing a concept that is rapidly becoming part of the design process. The tool also has the potential to increase food research productivity in academia.

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Appendix

The method by which chemical kinetics data was estimated is shown. The formation of chemicals at constant temperature was described as a first-order reaction (Arvidsson et al., 1997, 1999; Persson et al., 2008):

$$c = c_0(1 - e^{k_g t}) \tag{14}$$

where c is the concentration of the chemical (ng/g or mg/kg), c_0 is the estimated maximum concentration of the chemical (ng/g or mg/kg), k_g is the rate of formation of the chemical (per min), and t is the cooking time (min). A series of chemical concentrations (c) in a certain food group (red meat, poultry, etc.) at various cooking times (t) at constant temperature can be obtained from the literature. Based on the minimum of four time-concentration points, the values of the maximum concentration (c_0) and the rate constant for formation/generation (k_g) were determined by using nonlinear regression and the first-order equation with Matlab 7.7 (MathWorks Inc., Natick, MA).

The rate constant for degradation of the compound k_d (per min) was calculated based on the following equation:

$$c_2 = c_1 e^{k_d(t_2 - t_1)} \tag{15}$$

where c_2 is the concentration of the chemical degraded (ng/g or mg/kg) after time t_2 and c_1 is the concentration of the chemical degraded (ng/g or mg/kg) after time t_1.

For each type of food, the values of k_g and k_d were determined for at least three temperatures for regression analysis (Excel, MS Office 2007) in order to determine the respective 95% upper and lower confidence values. After the analysis, the rate constants, k_g and k_d, as functions of temperature for each chemical in different food products were determined, as shown in Table 6 as an example.

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