FOOD PROCESS MODELING

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Contents

Summary

Modeling, particularly numerical and observational models of food processes, has come a long way and has become an integral part of research and design. Although analytical models were the main mode of modeling before the days of faster computers, computer-based numerical and empirical models are the primary types of models in development today. Food processes are often complex, with variation in properties due to natural biological variability and transformation of the materials during processing. The numerical and empirical models are highly versatile and can cover a wide range of input and output parameters and process types, thus providing flexibility in developing a more realistic description of the process. It is important to bear in mind the limitations of each modeling method. In so doing, the judicious use of these models is expected to provide improved efficiency of the food sector by providing a better understanding of the processes and shortening the cycle for product and process design.

1. Modeling and Its Various Uses

A model is a mathematical analog of a physical process. An accurate model is expected to work just like a physical prototype, but its engine is mathematical rather than physical. Models have two major uses. The most common use of a model is to provide a better understanding of the physical process, by seeing the relationships between its input and output parameters. This is referred to as the research objective of modeling. For example, in modeling a sterilization process, one would need to know the effect of steam temperature (input parameter) on the extent of lethality or bacterial death (output parameter). As computing techniques and computational hardware and software underwent a revolution, the second major objective emerged: to use the model in design or in checking the “what if” scenarios. As applied to the sterilization problem, one can now easily check if the sterilization process improves in quality if the process temperature (input variable) is varied in some way. Better yet, in the future, optimization software is likely to become available that would provide a process temperature profile for optimum quality. Product processes and equipment designs are rapidly becoming the major driving force for the use of modeling. In this article, the discussions refer to both research and the design use of models.

2. Types of Process Modeling

For simplicity, modeling can be divided into three groups:
1. Analytical Models
2. Numerical Models
3. Observational (Empirical) Models

2.1. Analytical Models

Analytical models usually refer to models that have analytical or closed-form solutions, which can often be developed without the aid of a computer. The heyday of analytical solutions was generally before the advent of high-speed computers when large amounts of memory became available. Analytical models continue to be of great importance because of their potential power to provide a complete understanding of the system when used. The cost of this power is in its limited applicability, as much of food processing is simply too complicated to describe using such models. However, approximate analytical models that do require computers are still used in active areas of research. For example, pieces of analytical solutions can make numerical models (described later) more effective. In food processing applications, until very recently, modeling has mostly been based on simple analytical solutions. The best analytical solution was that of Ball in 1923, applied to heat sterilization. It involved combining the solution to partial differential equations describing heating and cooling with the first-order kinetics of bacterial death, and obtaining approximate closed-form solutions. Today, most sterilization of canned foods, pouches, etc., is based on this analytical solution. Another widely used analytical solution in food processing is the solution of the mass diffusion equation, applied to moisture transport in drying and similar processes. In this article, models of this type will not be covered in any further detail, and the reader is referred to textbooks, the references for which are given in the Bibliography.

2.2. Numerical or Computational Models

The analytical models described in the previous section have major limitations, such as the requirements of a simple geometry, constant processing conditions, constant properties, and so forth. Numerical, computer-based solutions are highly versatile and can avoid the limitations just mentioned. A numerical model typically involves solving the set of partial differential equations that describe the physics of the model more exactly than an analytical one. Access to fast computers with vast amounts of memory has made the reliance on these types of models almost the default in recent years, especially in food process modeling. Numerical models will be described in detail later in this article.

2.3. Observational (Empirical) Models

Analytical and numerical models assume that the model (process description) is known, and tries to find the detailed behavior of the system. Frequently, finding the model in the first place is the most difficult, so difficult that one begins inferring a model from measured data. These models coming from introspection or observation (or both) can be called observational or empirical models. Such models are used to characterize and classify the data, to generalize from the measurements in order to make predictions about new observations, or to learn something about the rules underlying the observed behavior. An example of this type of model is the neural network model that will be described in detail later. These models do not attempt to explain the workings of the process represented on a chemical or physical level. They simply predict on the basis of known data, without determining more about the underlying process. As such, they can model complex processes easily, but also have certain inherent limitations.

3. Other Models Used in Food Plant Design and Operation

In addition to examples of models provided in this article, there are many other models used in the design of large-scale industrial food processes. For an overview of computer-aided engineering in the food industry, see the references given in the Bibliography. There are process modeling software packages that can combine various operations of a food process as modules and help identify the optimum combination of operations for improved quality and reduced cost of the overall process. These models provide the next higher scale of integration, as compared to the numerical or observational model described later in this article, which are typically applied to a single operation. The multi-operation modeling software packages mostly have their roots in chemical processing. On the production floor, modeling is also used for inventory control, statistical process control, machine vision, and expert systems for maintenance and scheduling. These other types of models are beyond the scope of this article.

4. Computational or Numerical Models

Computational or numerical models based on the detailed physics of the process have gone through a revolution in recent years, primarily due to the availability of faster and cheaper computers with vast amounts of memory. New computational branches of existing disciplines have appeared, for example, computational solid and fluid mechanics, computational heat transfer, and computational electromagnetics. In this section, numerical models in a number of areas with application to food processing are described. This section is intended for the food product, process, and equipment design, an application area that is rapidly increasing.

4.1. Computer-based Engineering as a Design Tool

Computer models of food processes have been developed mostly from research activity in the past, starting with perhaps the earliest study by Teixeira *et al*. in 1969. Design typically requires frequent computations with more frequent changes in parameters. Such intensive computations have only recently been practical due to the availability of high-powered desktop workstations, PCs, and advanced, user friendly, software (see *Software for Food Engineering Applications*). These advances have made computer models a practical tool for product and process design. Consequently, modeling for design purposes has been shown or suggested for food applications in research.

Use of computer modeling or computer-prototyping has several advantages for food products and the process development environment:

1. Testing “what-if” scenarios is quick and inexpensive, thus shortening the design cycle (quicker turnaround), which should result in reduced costs and increased profits.

2. Modeling can provide insights into complex processes that are otherwise difficult to understand. It provides a clearer understanding of the interactions between the physical processes and their sensitivity to various operational parameters. This can enable the designer to be more creative.

3. Modeling allows front-end engineering before physical prototyping, making the prototypes closer to the optimum and reducing the number of prototypes.

4. Modeling makes possible concurrent design and analysis, also shortening the design cycle. While an experiment is underway, the results can be used simultaneously to further optimize the process on the computer, also reducing the amount of experimentation.

Computer-aided engineering (CAE), simulation-based engineering, and computer prototyping all refer to the use of computers to build and test computer models of products and processes to reduce the extent of physical prototypes. Computer prototyping can help today's competitive product and process design by a) reducing cost, b) reducing the time needed to market, and c) making more dramatic changes possible.

Industries, such as automotive and chemical processing, have been exploiting the advantages of computer-aided engineering in a very significant way. The food industry also stands to benefit from the use of this tool. Although the total application is still somewhat small, use of computational software is also rapidly increasing in food process engineering. The food industry, however, is generally behind other processing industries in such CAE applications.

4.2. Typical Characteristics of Physical Processes in Food Processing

Following are some of the unique aspects of food processing problems (see *Engineering Properties of Foods)*:

- In addition to temperature changes during a heating or cooling process, there are biochemical (nutrient, color, flavor, etc.) or microbial changes that are important to know.

- The moisture in food is constantly undergoing either loss (due to evaporation, especially when heated) or gain (from humid surroundings).

- The properties of foods, such as density, thermal and electrical conductivity, specific heat, viscosity, permeability, and effective moisture diffusivity are often a function of composition, temperature and moisture content, and therefore keep changing during the process. The system is also quite non-homogenous. Such detailed input data are not available.

- The hygroscopicity of food materials can cause the food to shrink upon significant loss of moisture or swell when gaining moisture.

- Often irregular shapes are present.

- Processes such as temperature, moisture and mechanical changes are often coupled.

To make a realistic physics-based numerical model, these characteristics should be included as much as possible.

4.3. Typical steps in Numerical Modeling

The numerical computation or modeling process typically consists of three steps: Pre-processing, Processing and Post-processing. Pre-processing typically defines the geometry, computational grids, governing equations, boundary conditions, properties, and methods used for solving. In the processing step, the computer solves the problem. In the post-processing step, the solution is visualized by the user, using shaded contours, movies, etc.

4.3.1. Governing Equations and Boundary Conditions

In this the most important pre-processing step, mathematical analogues (equations) of the physical process, are developed in terms of a set of equations called the governing equations and the boundary conditions. The mathematical description is often an intelligent simplification, especially in the initial stages. This step is often the most important and most difficult. The goal is to keep as many details of the process as possible, without creating unnecessary complexities. Modeling software is typically able to solve a very general set of governing equations and boundary conditions, covering a wide range of processes. In choosing a software program, availability of necessary governing equations is only one of many factors. Each package has its strengths and weaknesses, i.e., it can be more efficient in solving a specific type of problem.

4.3.2. Mesh Generation

In this pre-processing step, after the geometry has been defined, the geometry needs to be broken down into smaller pieces for a numerical solution. The more the geometry is broken down, the more accurate the final solution, but the computation time can increase (sometimes dramatically) and eventually make it unrealistic to compute. Thus, this step is a careful balance between providing enough elements (or nodes) such that all the essential physics are captured (but not too many).

4.3.3. Material Property Data

A very important step in simulation-based engineering is to use accurate material property data. However, this is where food processes are also at a slight disadvantage, compared to processes not using natural materials. For example, properties of steel are more easily available and perhaps have a lot less variability than chicken soup. Data on food properties can be obtained from measurements, computerized databases, handbooks and prediction formulas. In simulation-based design, it is possible to relax the restrictions on requiring very accurate data. By varying the property data around their expected value in the computer model, one can bracket the properties and predict the effect of a range of properties on the process. Sometimes this is more useful than having the model predict output for a single property value since, in reality, food properties often vary from batch to batch due to differences in formulations, etc. This concept of bracketing can be extended to other input parameters, such as geometry, and is generally referred to as the sensitivity analysis of the model. Such sensitivity analysis can provide important insight into the model, as in which parameters are the most critical. Being able to perform easy sensitivity analysis is one of the greatest advantages of modeling.

4.3.4. Solution Technique

Once the equations and properties are defined, the next step is to select a solution method (choice of time discretization, matrix solution method, etc.) that provides the most efficient solution to the set of equations describing the food process. Today, there is a large quantity of software available in any given area, such as mechanics or heat transfer. For example, over 75 commercial computational fluid dynamics (CFD) software packages are currently available. The advantages of using available software are that often one can choose a solution method without having to be very knowledgeable about the details of such methods. Once the solution methods are specified, the computer takes over the solution procedure. This is the processing step. The equations are discretized and large linear systems of algebraic equations (matrices) are formed and solved using well-known procedures.

4.3.5. Post-Processing

Post-processing is the important step of visualizing the results and making further computations from raw data generated by the solution. Most commercial CFD packages are able to show nice contour, history, vector, and other plots. These spatial or temporal profiles in whole 3-D region can provide insight and understanding of the process, which is not possible using experimentation. For example, the spatial distribution of moisture or oil during a drying or a deep-frying process (see *Frying*) can be obtained computationally, however it requires elaborate and expensive experimentation using the MRI. Such visualization is one of the greatest advantages of modeling.

4.3.6. Trusting Computational Results

Computational results should never be trusted blindly and the software should never be used as a blackbox. However, it is also important to accept that there is no foolproof way to confirm the computational results. Several steps can be taken to minimize the chances of obtaining a wrong solution. Some of these include checking for mesh convergence, checking input file for accuracy of problem definition, using common sense about the process physics, comparing the experimental data, and checking against the results of a simpler problem.

4.4. Application Examples

Application of numerical modeling in food processing can include computational fluid dynamics (CFD) and heat transfer to solve flow/heating/cooling problems, computational mechanics to solve rheological and stress related problems, computational electromagnetics to solve microwave and other heating problems, and so on. Examples of some food applications are provided below.

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Websites

http://www.cfd-online.com/ For over 75 commercial computational fluid dynamics (CFD) software packages that are available.

Biographical Sketches

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Ashim K. Datta is Professor in the Department of Biological and Environmental Engineering, Cornell University, Ithaca, New York. His research and teaching interests are generally in fluid flow, heat transfer, and mass transfer in biological systems, particularly food processing systems. In teaching, he has developed a fundamental course covering these areas of biological transport processes. He also teaches how physics-based computer models in these areas can be used in both research and design of biomedical and food processes. The goal is often to obtain better insight into biological processes and to reduce prototype development. In his research, his groups goal is to develop computer models to understand complex food processes such as baking, microwave heating, and rapid freezing in engineering terms so that they can be optimized. Dr. Datta is a member of the American Society of Agricultural Engineers, the Institute of Biological Engineering, and the American Institute of Chemical Engineers, among others. He received a B. Tech. degree (1979) from the Indian Institute of Technology, Kharagpur, India, an M.S. degree (1982) from the University of Illinois at Urbana-Champaign, and a Ph.D. degree (1985) in Agricultural Engineering from the University of Florida, Gainesville.