SciVerse ScienceDirect

Procedia Food Science 1 (2011) 1202 – 1208

Procedia Food Science

11th International Congress on Engineering and Food (ICEF11)

Modeling food process, quality and safety: Frameworks and practical aspects

Ashim Datta[a]*, Ashish Dhall[a]

[a] Cornell University, Ithaca, United States of America (akd1@cornell.edu)

Abstract

Physics-based models provide increased understanding and predictive capabilities that can increase efficiency in food product, process, and equipment design, and improve quality and safety. However, certain key food specific developments are needed to enable widespread use of simulation technology in the food sector. First and foremost need is the development of concise modeling frameworks (how to formulate various food processing situations into mathematical models) for various classes of processes, as opposed to a custom model for each process, as it mostly exists today. Deformable porous media with multiphase transport can provide such framework, as will be discussed through examples of various processes that have been modeled by many researchers. The next critical piece is to have easy access to properties needed to model. State of property prediction, starting from simple correlations to multiscale modeling, thermodynamics-based, and molecular dynamics, as being pursued by researchers around the world will be shared. Prediction beyond process, into quality and safety is the third topic where various approaches to modeling quality in diffusion-reaction modeling framework would be presented. For safety, a practical approach that groups various food products and thus provide an avenue to simulate safety for great many situations, will be shared. Finally, efforts to integrate the modeling components into a novel user-friendly software for increased use of modeling will be described.

Keywords: multiphase transport; porous media; deformation; texture; microbiology.

---

1. Introduction: Overview of Modeling Frameworks

Food materials, processes and equipment cover a very large set of scenarios. Modeling of food processes has also been approached in a number of ways, starting from completely empirical to completely physics-based. The question is can we develop a few general frameworks for modeling of food processes that can effectively handle a large number of practical situations and be implementable

---

* Corresponding author. Tel.: +1-607-255-2482 ; fax: +1-607-255-4449 .
E-mail address: akd1@cornell.edu .

doi:10.1016/j.profoo.2011.09.179

easily (preferably in a commercial software) for widespread use of computer-aided food process engineering. In other words, what is a methodical and the most effective approach in modeling a process?

2. Materials & Methods

Over the years, the author’s research group has modeled temperature and moisture transport in microwave heating, baking, deep frying, puffing and meat cooking [1]. These models are fundamentals based and it appears that this same general framework of multiphase transport in deformable/swellable porous media with rapid evaporation worked for this spectrum of processes. Survey of most of the existing models in food literature shows that of the fundamental physics-based approaches, this framework is broad, flexible in accommodating many different processes and easier to implement in commercial software. By looking at additional processes as transport + deformation + reaction kinetics, it was investigated as to how this same framework can include other processes and thus indeed be a general framework. Also investigated was auxiliary relationships (e.g., evaporation, deformation) would be needed for such framework and whether such information is available or can be available with reasonable effort. Finally, the frameworks were extended to quality and safety prediction.

3. Results & Discussion

The frameworks that can be used to model an arbitrary food process are summarized here. As shown in Figure 1, first all formulations are divided into three major categories—continuum formulation, porous media formulation and deformable porous media formulation. Each of these would be called a framework. The typical continuum formulation (Framework F1) will not be discussed here and neither will be the large pores formulation (Framework F2) that has been discussed elsewhere [2]. Here, we elaborate more on the small pore formulation and especially how to handle deformation. Thus, Figure 2 shows a schematic of various possibilities for dealing with mass transport, heat transport and deformation (Frameworks F3 and F4).

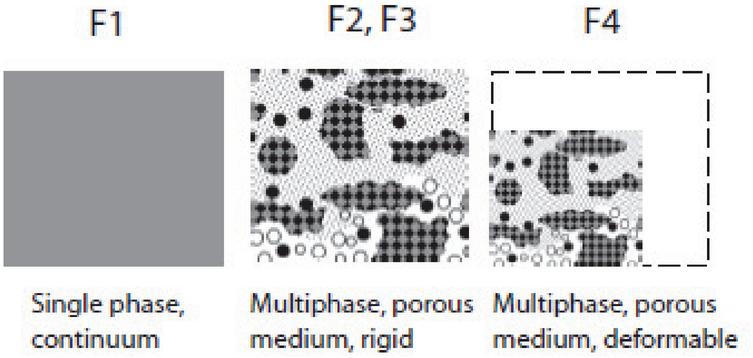

Fig. 1. Schematic showing three major classes of problems that are referred to as three formulations, F1, F2, F3 and F4

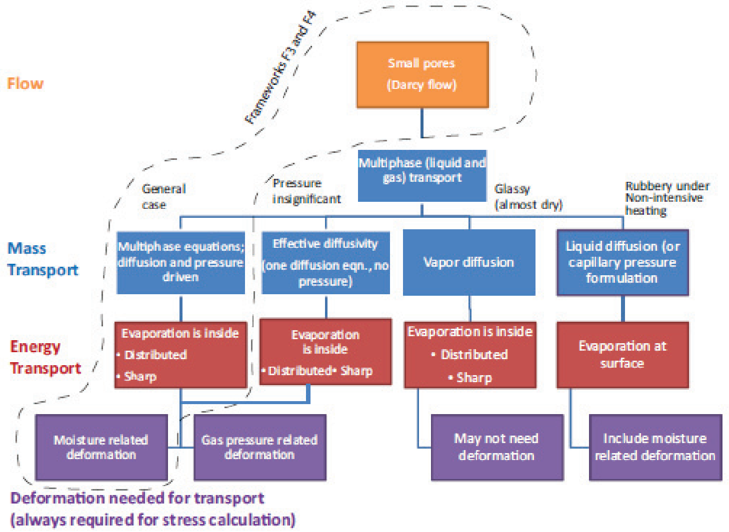

Fig. 2. Various formulations for food process modeling and their interrelations. For isothermal problems, energy equation is ignored. While deformation is always required for stress calculations, it may or may not be needed for transport

Framework F1: Single and multi-phase continuum equations

The most common set of transport equations are for single-phase transport equations, as available in any standard textbook on transport processes. Examples of processes that can be modeled using single and multi-phase continuum equations are shown in Table 1.

Framework F2: Large pores: Multiphase transport with Navier-Stokes equivalent of Darcy equation

Example of problem formulation in large pores is cooling of stacked bulk produce such as potato, chicory roots and Pears. The NavierStokes (N-S) analog of the Darcy equation, together with species transport and energy equations, are used in these studies. This is discussed in [2] in more detail.

Summary framework F3: Multiphase, rigid porous media continuum equations

An enormous range of food processes can be viewed as involving transport of heat and mass through porous media. Examples include drying, frying, microwave heating, meat roasting, puffing, and rehydration of solids. Most solid food materials can be treated as hygroscopic and capillary-porous. A porous media formulation homogenizes the real porous material and treats it as a continuum where the pore scale information is no longer available. Since this framework can cover a large range of situations and can be simplified to various levels, the general set of equations are presented first, followed by various adaptations that are the simplified versions.

In the most general version (for rigid porous media), individual phases of water, vapor, air, and energy are tracked using their conservation equations.

$$\text{Water} \qquad \frac{\partial c_w}{\partial t} + \nabla \cdot (\vec{n}_w) = -\dot{I} \tag{1}$$

$$\text{Vapor} \qquad \frac{\partial c_v}{\partial t} + \nabla \cdot (\vec{n}_v) = \dot{I} \tag{2}$$

$$\text{Air} \qquad \frac{\partial c_a}{\partial t} + \nabla \cdot (\vec{n}_a) = 0 \tag{3}$$

$$\text{Energy} \qquad (\rho c_p)_{eff} \frac{\partial T}{\partial t} + \left(c_{pv}\vec{n}_v + c_{pa}\vec{n}_a + c_{pw}\vec{n}_w\right) \cdot \nabla T = \nabla(k_{eff}\nabla T) - \lambda \dot{I} + \dot{Q} \tag{4}$$

Here $\vec{n}_w = -\rho_w(k_w/\mu_w)\nabla p_g - D_{w,c_w}\nabla c_w - D_{w,T}\nabla T$ is the flux of water due to gas pressure, moisture dependence of capillarity and temperature dependence of capillarity, respectively. Similarly, flux of vapor is given by $\vec{n}_v = -\rho_v(k_g/\mu_g)\nabla p_g - (c^2/\rho_g)M_v M_a D_{bin} p_v/p_g^2 \nabla p_g - D_{v,c_w}\nabla c_w - D_{v,T}\nabla T$, due to gradients in gas pressure and vapor pressure (decomposed into 3 separate effects representing the last 3 terms—binary diffusion, driven by liquid concentration and driven by temperature) [3]. There is no distinct flow equation as the Darcy's law is used in water, vapor and air transport equations is a replacement for the fluid flow or momentum equation. To complete the system, we need an additional equation. This additional information provides the rate of evaporation and can be formulated in one of two ways [1]:

$$p_v = p_{v,eq}(M, T) \tag{5}$$

$$\dot{I} = K(\rho_{v,eq} - \rho_v) S_g \varphi \tag{6}$$

Equation 5 is the equilibrium relation for the material relating the vapor pressure to moisture and temperature. Equation 6 is a non-equilibrium formulation that approaches Eqn. 5 for large values of K. A number of food processes (e.g., drying, baking, frying, microwave heating) have been modeled by several researchers using mostly Eqn. 5 but some with Eqn. 6.

Framework F3.1 Small pores: Effective diffusivity of the combined "moisture" phase

The liquid water and water vapor phases in the previous section can be combined into an effective "moisture" phase with the following equations that perhaps have been the most common of the formulations used in food.

$$\frac{\partial c_w}{\partial t} = \nabla \cdot (D_{c_w} \nabla c_w) \tag{7}$$

Here pressure gradient inside the food is ignored and transport of liquid or vapor due to temperature gradient are also ignored. The diffusivity Dcw_w is due to liquid and vapor diffusion from gradient in water content, $Dcw = Dw,cw + Dv,cw_w$, that includes capillary pressure dependence on moisture content in Dw,cw_w and vapor pressure dependence on moisture content in Dv,cw_w. Note that the rate of evaporation, $\dot{I}$ is not required if temperatures are not of concern. If temperatures are required, Eqn. 4 for energy will have convective terms contributed by the water and vapor.

Framework F3.2 Small pores: Transport of liquid phase only

Evaporation is considered only from the surface, thus ignoring evaporation inside the domain. This can happen for non-intensive heating of a very wet material. Energy equation will have the convective term due to water only:

$$\frac{\partial c_w}{\partial t} = \nabla \cdot (D_{w,c_w} \nabla c_w) \tag{8}$$

The liquid diffusivity, $D_{w,cw}$ includes parameters for Darcy flow and the swelling pressure estimated by linearized Flory-Rehner theory [5].

Framework F3.3 Small pores: Transport of vapor phase only

This is a special case when very little liquid moisture is present, as near the end of a drying process. Transport is dominated by that of vapor:

$$\frac{\partial c_w}{\partial t} = \nabla \cdot (D_{v,c_w} \nabla c_w) \tag{9}$$

Since there is not much liquid present, transport of liquid can be ignored, which then leads to the equation for $\dot{I} = -\partial c_w / \partial t$ which can be substituted in the energy equation.

Framework F4: Multiphase, deformable porous media continuum equations

A deforming (shrinking/swelling) porous medium is essentially handled by treating all the fluxes discussed earlier for a rigid porous media to be those relative to the solid skeleton, and combining this with a velocity of the solid skeleton that comes from deformation obtained from solid mechanical analysis. Since the solid has a finite velocity, $\vec{u}_{s,G}$, the mass flux of a species i with respect to stationary observer, $\vec{n}_{s,G}$, (used in Equations 12-15) can be written as sum of flux with respect to solid and flux due to movement of solid with respect to stationary observer:

$$\vec{n}_{i,G} = \vec{n}_{i,s} + c_i \vec{v}_{s,G} \tag{10}$$

Movement of solid, in turn, is obtained from stress-strain analysis. If $\vec{\sigma}'$ is the effective stress on the solid skeleton, it can be written as

$$\nabla.\bar{\sigma}' = \nabla p_g - \nabla (S_w p_c) \tag{11}$$

where the first term on the right hand side is the gas pressure gradient (due to evaporation of water or gas release as for carbon dioxide in baking) and p_c in the second term on the right hand side represents not just capillary pressure but also other attractive forces between the solid and the liquid - it would be a function of the temperature and moisture content of the food material. In this equation, S_w is the water saturation. Kelvin's law can be used to estimate p_c from water activity. Flory-Rehner theory has also been used to estimate this pressure [5]. The food material can be treated as elastic or viscoelastic and the corresponding stress-strain relationship can be used with the appropriate solid momentum equation.

The transport equations in Framework F3 are generalized for this situation, using Eqn. 10 as:

$$\frac{\partial c_w}{\partial t} + \nabla.\left(\vec{n}_{w,G}\right) = -\dot{I} \tag{12}$$

$$\frac{\partial \left(c_g \omega_v\right)}{\partial t} + \nabla.\left(\vec{n}_{v,G}\right) = \dot{I} \tag{13}$$

$$\frac{\partial c_g}{\partial t} + \nabla.\left(\vec{n}_{g,G}\right) = \dot{I} \tag{14}$$

$$\left(\rho_{eff} c_{p,eff}\right) \frac{\partial T}{\partial t} + \sum_{i=w,v,g} \left(\vec{n}_{i,G}.\nabla\left(c_{p,i} T\right)\right) = \nabla.\left(k_{eff} \nabla T\right) - \lambda \dot{I} + Q \tag{15}$$

Here the air equation is replaced by gas (vapor plus air) equation (Eqn. 14), which is an equivalent form.

Framework for quality and safety modeling

Once the process modeling framework is developed, quality and safety models can be related to process models in somewhat straightforward way as long as the relationship between quality parameter and temperature/ moisture/ composition or their histories are available. Although there are missing areas, such relationships for kinetics of quality changes are available in a number of important areas [5]. A framework for eventual prediction of quality from temperature and moisture is shown in Figure 3a. We consider an effective quality attribute (texture, color) as a composite of a local (i.e., at a spatial location) quality attribute, obtained either by following relevant chemical reactions and transport, or, by following measured local properties. The local quality attribute, in turn, is predicted from local temperature and composition available from process models. The process and quality prediction models are thus coupled, closing the gap between process prediction and quality prediction for complex food processes. An application of this framework to modeling of texture in deep frying of potatoes is illustrated in Figure 3b. Here the temperature and moisture variations from process model are combined with relationship of Young's modulus to moisture obtained from thin sections of potatoes dried to various moisture contents to obtain a profile of Young's modulus throughout the cross-section of the fried potato. Using this varying Young's modulus, a small deformation mechanical analysis is performed to obtain the effective Young's modulus of the entire cross-section of the fried potato that correlates with texture.

In a very analogous way, safety prediction framework will couple microbiological (or chemical) kinetics to temperature, moisture and composition information obtained from the process model. The main issues in building such a framework included selection of predictive models, associations of different food types with pathogens (as determined from outbreak histories), and variability in data from different experiments [6]. More than 1000 data sets from published literature were analyzed and grouped according to microorganisms and food types. Final grouping of data consisted of the 8 most prevalent pathogens for 14 different food groups, covering all of the foods (> 7000) listed in the USDA National Nutrient Database. The primary advantage in obtaining group-specific kinetic data is the ability to extend microbiological growth and death simulation to a large array of product and process possibilities, while still being reasonably accurate. This integration has been included in a software to be publicly available [7].

Table 1. Frameworks for food process modeling discussed here

	Framework description	Examples of food processes	Governing equations to use
F1	Single and multi-phase	Simple heating of solids at lower temperatures, canning of solid, liquid and mixtures	Momemtum (N-S equation for fluid flow; species equations for each component; energy equation
F2	Multiphase, porous media (large pores)	Cooling of stacked produce such as potatoes/ strawberries in a cold room	N-S analog of Darcy equation; species equations; energy equation
F3	Multiphase, porous media (small pores), capillary pressure and/or gas pressure, rigid	Microwave heating, drying, frying, and other heating situations with significant moisture loss but where dimension changes can be ignored	Darcy equation replacing momentum equation; species equations; energy equation
F3.1	Effective diffusivity of combined liquid water and vapor for rigid or rubbery material	Ideally only for less intensive heating	Effective diffusivity for a combined (water + vapor) equation; energy equation
F3.2	Liquid diffusivity for rigid material or rubbery state	Less intensive heating or intensive heating of wet (rubbery) material where evaporation is only at surface (meat cooking)	Only capillary pressure (no gas pressure); species equation for liquid phase; energy equation
F3.3	Vapor diffusivity for rigid material or glassy state	Very little liquid moisture, e.g., last stages of drying	No liquid transport; species equation for combined (primarily liquid) phase with vapor diffusivity; energy equation
F4	Multiphase, porous media (small pores), with deformation	Bread baking, puffing, rehydration	Darcy equation replacing N-S equation; species equations; energy equation; solid mechanics equations for small or large deformation providing solid velocity

4. Conclusion

A deformable porous media framework can effectively model a large number of complex food processes. Such a generalized framework that is also easily implementable in existing software can go a long way toward enabling computer-aided food process engineering. Simplifications of this framework are possible that resembles commonly used formulations but starting from the most general equations makes it easier to see the assumptions that are involved in the simplified formulations. A synthesis is provided for frameworks for modeling the largest collection of food processes. Framework for process models can be included into an overall diffusion-reaction framework to predict quality and safety.

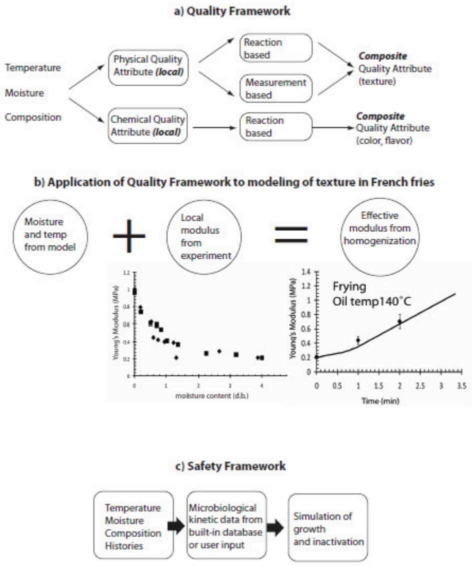

Fig. 3. a) Quality framework; b) Application of quality framework to texture prediction; c) Safety framework

References

[1] Halder, A., A. Dhall and A. K. Datta. 2011. Modeling transport in porous media with phase change: Applications to food processing. Journal of Heat Transfer, Transactions of the American Society of Mechanical Engineers. 133(3): 031010-1–031010-13

[2] Datta, A.K. 2007. Porous media approaches to studying simultaneous heat and mass transfer in food processes. I: Problem formulations. Journal of Food Engineering, 80: 80-95.

[3] Dhall, A. 2011. Multiphase transport in deformable phase-changing porous materials. PhD Dissertation, Cornell University.

[4] van der Sman, R.G.M. 2007. Soft condensed matter perspective on moisture transport in cooking meat. AIChE Journal, 53(11):2986-2995.

[5] van Boekel, M. A. J. S. 2009. Kinetic modeling of reactions in foods. CRC/Francis & Taylor, Boca Raton.

[6] Halder, A., D.G. Black, P.M. Davidson and A.K. Datta. 2010. Development of associations and kinetic models for microbiological data to be used in comprehensive food safety prediction software. Journal of Food Science, 75(6):R107-R120.

[7] Halder, A., Dhall, A., A. K. Datta, D. G. Black, P. M. Davidson, J. Li and S. Zivanovic. 2011. user-friendly general-purpose predictive software package for food safety. Journal of Food Engineering, 104:173-185.

Presented at ICEF11 (May 22-26, 2011 – Athens, Greece) as paper MCF1201.