Journal of Food Engineering 145 (2015) 37–44

Contents lists available at ScienceDirect

Journal of Food Engineering

journal homepage: www.elsevier.com/locate/jfoodeng

# A soft condensed matter approach towards mathematical modelling of mass transport and swelling in food grains

M. Chapwanya [a], N.N. Misra [b,*]

[a] Department of Mathematics & Applied Mathematics, University of Pretoria, Pretoria 0002, South Africa
[b] School of Food Science & Environmental Health, Dublin Institute of Technology, Dublin 1, Ireland

ARTICLE INFO

*Article history:*
Received 3 July 2014
Received in revised form 11 August 2014
Accepted 13 August 2014
Available online 23 August 2014

*Keywords:*
Soft condensed matter
Hydration
Swelling
Flory–Huggins
Mass transfer
Navy bean

ABSTRACT

Soft condensed matter (SCM) physics has recently gained importance for a large class of engineering materials. The treatment of food materials from a soft matter perspective, however, is only at the surface and is gaining importance for understanding the complex phenomena and structure of foods. In this work, we present a theoretical treatment of navy beans from a SCM perspective to describe the hydration kinetics. We solve the transport equations within a porous matrix and employ the Flory–Huggin's equation for polymer–solvent mixture to balance the osmotic pressure. The swelling of the legume seed is modelled as a moving boundary with an explicit transient equation. The model exhibits a good agreement with the experimental observations and is capable of explaining the stages of hydration. Sensitivity analysis indicated that the degree of hydration is dependent on the bean size and is also sensitive to the selection of the intrinsic permeability of the bean.



## 1. Introduction

Soaking and hydration of legumes and cereals is an important unit operation in the grain processing industries. For example, legumes such as navy bean and kidney bean are often hydrated prior to canning operations. Hydration of beans decreases the cooking time, minimizes losses and improves the nutritional quality and protein digestibility of the cooked product (Wang et al., 1979; Abd El-Hady and Habiba, 2003). The problem of mass transfer during hydration of food grains has been treated both experimentally and theoretically, and in studies combining both approaches (Zanella-Díaz et al., 2014; Cozzolino et al., 2013; Ghafoor et al., 2014; Nicolin et al., 2012; Bello et al., 2010; Mohoric et al., 2004; Peleg, 1988; Hsu, 1983). Most of the mathematical descriptions reported in literature are either data driven regression models describing hydration kinetics or are based on simple Fickian diffusion. Diffusion in many legumes (and cereals) cannot be described adequately by a simple concentration dependent form of Fick's diffusion equation, especially when these undergo swelling (or large deformation in geometry). Such conventional approaches fail to capture the finer details of food structure and their dynamics. Because of the complexity of food systems, interdisciplinary scientific approaches are needed to enable demanding developments (Ubbink and Mezzenga, 2006; Ubbink et al., 2008).

Soft matter physics focusing on description of an increasingly important class of materials that encompasses polymers, liquid crystals, complex fluids, organic–inorganic hybrids, foams, gels and the whole area of colloidal science is a contemporary area of research with several opportunities. Soft matter science plays an important role in a wide variety of processes and applications, examples of which include polymer swelling, phase separation, transport and delivery of drugs, etc. The principles of soft matter physics are equally applicable to many food systems. Mezzenga et al. (2005) reviewed the nature of foods from a perspective of soft condensed matter physics. The details of structural changes at various scales in food systems often needs experimental and/or theoretical tools of soft matter physics, which are not fully adapted to food systems (Mezzenga, 2007; Mezzenga et al., 2005). An exposition of the potential of soft matter physics for explaining the complex food processes and structuring at various scales is also provided in van der Sman and van der Goot (2009) and van der Sman (2012).

About 60 years ago, Flory and Huggins independently proposed the lattice model to treat the mixing enthalpy and entropy of polymers in a very straightforward way (Huggins, 1942a,b; Flory, 1953). Although many other models have been developed to describe the thermodynamics of polymer systems, the original Flory–Huggins lattice theory always give a very clear and straightforward physical

* Corresponding author.
*E-mail address:* misra.nrusimhanath@dit.ie (N.N. Misra).

http://dx.doi.org/10.1016/j.jfoodeng.2014.08.010
0260-8774/

picture (Han and Akcasu, 2011). However, it is worthwhile noting that the Flory–Huggins theory also is based on some assumptions that are often not valid. This includes the assumption that volume changes are not incurred upon mixing the polymer and solvent. It is also supposed that the polymer chain can be modelled on a lattice, which excludes contributions to the entropy from chain flexibility, and specific solvent-polymer interactions are ruled-out (Hamley, 2007). In an early work, van der Sman (2007) deduced an excellent modelling framework based on soft condensed matter perspective to explain the heat and mass transport during cooking of meat. This was based on the Flory–Rehner theory for pressure driven mass-transport in swelling or shrinking gels.

The model that we present in this paper is an attempt at advancing the basis of the theoretical modelling of mass transport during hydration of porous foods with a soft matter perspective. The model described herein shares an integrated approach between the statistical thermodynamics based Flory–Huggins theory and the continuum mechanics of fluid transport in porous media. We take an example case of hydration of navy bean, which is modelled as a saturated porous media undergoing large deformation by swelling. We are including a comparison of the simulation results with experimental data as model validation and an illustration of the model application, while also reporting on the sensitivity of the model to selected parameters. By means of the latter, we attempt to both analyse the influence of the natural variability in food properties on model predictions as well as gauge the sensitivity of the model to potential errors in parameter estimation.

## 2. Problem description

Fig. 1 provides a summary of the geometric domain of the bean under consideration. The geometry of the navy bean can be described as a porous scalene ellipsoid, which is capable of undergoing global deformation. For the present study, we also assume that the pores are ideally filled with water which simplifies the problem to a saturated porous media case. We assume that the complex structural elements of navy bean, mainly proteins and carbohydrates can be approximated as ideal polymers. When applying principles of soft condensed matter physics to foods, it may be noted that polysaccharides and proteins are to foods what polymers are to soft condensed matter (Mezzenga et al., 2005). Notably, navy beans are by large chemically comprised of starch (50–60%), protein (20–38%) and fibre (∼18%) (Kereliuk and Kozub, 1995; Berg et al., 2012). This gives sufficient reason to justify our soft condensed matter analogy for navy beans. To formulate a feasible model, we also assume that the outer pericarp/skin is very thin and has no influence on the moisture transport.

We now simplify the problem geometry, by assuming that bean is spherical in shape and the swelling gives an evolving radius, $R(t)$ which varies with time, $t$. While assuming a spherical geometry for simplicity, we account for the deviations from the ellipsoid solid by calculating the radius of the sphere whose volume is equal to that of the scalene ellipsoid (Fig. 1(b)). The following equation was employed for calculating the equivalent radius, $r$ (mm) (see Fig. 1(a) for notation):

$$r = \left(\frac{G_m + S_m + A_m}{6}\right). \tag{1}$$

Herein, $G_m = 2(abc)^{\frac{1}{3}}, A_m = \left(\frac{2a+2b+2c}{3}\right)$, and $S_m = \left(\frac{4ab+4bc+4ca}{3}\right)^{\frac{1}{3}}$ are the geometric mean diameter, arithmetic mean diameter, and square mean diameter, respectively (Mohsenin, 1986). In accordance with Ghafoor et al. (2014), we take the temperature to be constant (16 °C) throughout the duration of soaking and therefore, temperatures capable of causing gelatinisation are not encountered. Finally, we define the volume fraction of the solids in the bean to be $\phi$, and to satisfy the criteria of saturation, we have $(1-\phi)$ as the volume fraction of the liquid water.

## 3. Mathematical model

In this section a mathematical model based on the Flory–Huggins theory for hydration of navy bean is presented. Part of the modelling approach has been presented elsewhere in the literature in the context of biofilms (Winstanley et al., 2011). For completeness, we summarise the equations here. Mass conservation of the polymer is given by

$$(\rho_s\phi)_t + \nabla\cdot[\rho_s\phi\mathbf{v}] = 0, \tag{2}$$

where $\rho_s$ (kg m$^{-3}$) is the averaged phase density and $\mathbf{v}$ (m s$^{-1}$) is the protein velocity. Similarly, conservation of the liquid is given by

$$(\rho[1-\phi])_t + \nabla\cdot[\rho(1-\phi)\mathbf{w}] = 0, \tag{3}$$

where $\rho$ (kg m$^{-3}$) is the averaged water density and $\mathbf{w}$ (m s$^{-1}$) is the water velocity.

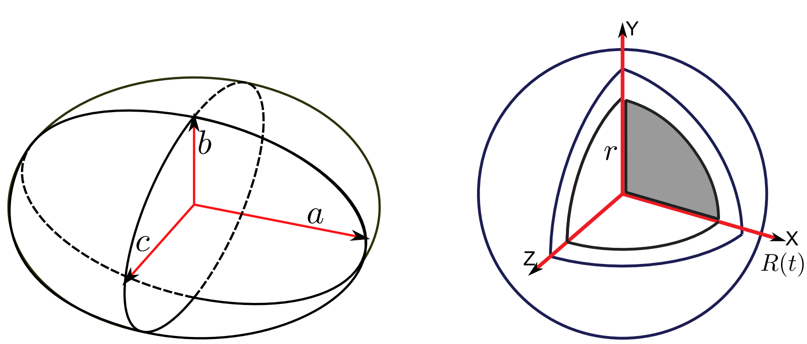
The bean is assumed to be a porous structure, hence the momentum equations as given by Darcy's law holds. We relate the liquid velocity to the liquid pressure, $p$ (Pa), via

$$-(1-\phi)\nabla p + \frac{\mu(1-\phi)^2}{k}(\mathbf{v}-\mathbf{w}) = 0, \tag{4}$$

where $\mu$ is the water viscosity, $k$ is the grain permeability. By analogy with (4), the momentum equation for the polymer takes the form

$$-\phi\nabla p_s - \frac{\mu(1-\phi)^2}{k}(\mathbf{v}-\mathbf{w}) = 0, \tag{5}$$

where $p_s$ (Pa), is the pressure of the polymer. Note that our approach in dropping the viscous stress for Eqs. (8) and (9) is consistent with the work of Winstanley et al. (2011), where the viscous




(a) Ellipsoid geometry of navy bean. (b) Equivalent geometry for the model.

**Fig. 1.** Schematic illustration of (a) the ellipsoid geometry of a navy bean grain and (b) the equivalent sphere concept with model boundaries.