



## Multiphysics pore-scale model for the rehydration of porous foods



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### ARTICLE INFO

#### Article history:

Received 25 July 2013

Accepted 17 November 2013

Available online 23 November 2013

Editor Received Date 16 December 2013

#### Keywords:

Multiphysics

Rehydration

Multiscale simulation

Freeze-drying

### ABSTRACT

In this paper we present a pore-scale model describing the multiphysics occurring during the rehydration of freeze-dried vegetables. This pore-scale model is part of a multiscale simulation model, which should explain the effect of microstructure and pre-treatments on the rehydration rate. Simulation results are compared to experimental data, obtained by MRI and XRT. Time scale estimates based on the pore-scale model formulation agree with the experimental observations. Furthermore, the pore-scale simulation model provides a plausible explanation for the strongly increased rehydration rate, induced by the blanching pre-treatment.

*Industrial relevance:* The increased insight in the physical processes governing the rehydration of porous or freeze-dried foods gives more rationale for optimizing all processing steps. Industry is seeking for means to give dried fruits and vegetables more convenience, but also higher quality concerning health and texture. This study shows that blanching pretreatment prior to freeze-drying strongly enhances the rehydration, while the loss of nutrients is hardly affected.

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### 1. Introduction

We are involved in a research programme focusing on the influence of food microstructure on their rehydration (Datta, van der Smán, Gulati, & Warning, 2012; van der Smán, Voda, van Dalen, & Duijster, 2013; Vergeldt et al., 2013; Vergeldt et al., submitted for publication; Voda et al.). Current approaches to understand this aspect on the rehydration of (freeze-)dried food products are rather empirical (Deep Singh, Sharma, Bawa, & Saxena, 2008; Krokida & Marinos-Kouris, 2003; Sagar & Suresh Kumar, 2010). A prerequisite for more rational approaches is modelling rehydration behaviour of porous food materials based on physical principles (Sam Saguy, Marabi, & Wallach, 2005). To this date, most physical modelling approaches make simplifications to the physics (Troygot, Saguy, & Wallach, 2011; Tze Lee, Farid, & Kiong Nguang, 2006; Wallach, Troygot, & Saguy, 2011) and even more regarding the multi-scale structure of food (Ho et al., 2013; Kelemu Mebatsion, Verboven, Tri Ho, Verlinden, & Nicolai, 2008; Ubbink, Burbidge, & Mezzenga, 2008; van der Smán, 2012a; van der Smán & Van der Goot, 2009). The majority of the few number of these physical models are based on Fick's law with an effective diffusivity (Cunningham, McMinn, Magee, & Richardson, 2007; Maldonado, Arnau, & Bertuzzi, 2010), which lumps most of the more involving physics like capillary suction and swelling, and the intricacy of the food microstructure (Datta, 2007; Zhu, Mukherjee, & Dhall, 2011). Saguy and coworkers have indicated correctly the importance of capillary suction (Sam

Saguy et al., 2005). However, swelling of cell wall materials has been ignored. Swelling of the food matrix has been considered only in a study on the rehydration of a non-porous food (Zhu et al., 2011).

We tackle the rehydration problem with experiments and physical modelling, with both approaches investigating all relevant physical phenomena at multiple length scales. The microstructure of the investigated rehydrated vegetables is created via freeze-drying. After subsequent storage under dry conditions, the dried foods are rehydrated via contacting them with liquid water – held at constant temperature. During freeze-drying pores are formed via sublimation of ice crystals. The pores have a size of 10 – 100 μm, which is several orders of magnitude smaller than the product size. This makes the rehydration of freeze-dried foods a multiscale problem (Ho et al., 2013).

For the problem of rehydration of freeze-dried vegetables we distinguish three length scales: 1) the microscale of molecules, 2) the meso-scale of pores, and 3) the macroscale of the product. The multiscale modelling approach is being developed bottom-up, starting from the molecular level. For each level a specific model will be developed, which will use relations that are derived from the model at the lower scale.

At the microscale water interacts with the molecules, which constitute the food. This interaction determines the driving force and kinetics for the moisture transport. Recently, we have developed predictive theories for them (Jin, van der Smán, & van Boxtel, 2011; van der Smán, 2012b; van der Smán, 2013a; van der Smán & Meinders, 2011; van der Smán & Meinders, 2013; van der Smán, Voda, Khalloufi, & Paudel, 2013). Predictions can be made, if the composition of the food is given in amounts of polysaccharides, proteins, disaccharides, monosaccharides,

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salts and water. The predictive theories account for effects of hydrogen bonding and free volume. For full details of these theories we refer the reader to the above cited papers. In the theoretical section we will shortly indicate for which quantities we have used these predictive theories. For the food system under investigation, freeze-dried carrots, all required relations at the molecular microscale are known now. In this paper we will focus on the multiphysics at the mesoscale.

At the mesoscale we describe the simultaneous transport of water and solutes via the food matrix and the pore space. While moisture transport in the solid food matrix is governed by diffusion and swelling, the moisture transport in the pore space is governed by capillary transport. One can state that food rehydration is a true multiphysics problem.

The capillary moisture transport in complex pore geometries can be investigated using Lattice Boltzmann, a mesoscopic simulation method (Pan, Hilpert, & Miller, 2004; Porter, Schaap, & Wildenschild, 2009; van der Sman, 2013b). Despite its huge versatility, simultaneous simulation of the matrix swelling and capillary transport is still beyond the capabilities of this mesoscale simulation method. Just recently, we have set the first steps in the modelling of swelling and diffusion via a one-dimensional Lattice Boltzmann model (van der Sman, 2014). We will employ Lattice Boltzmann only for the investigation of 1) capillary suction in complex geometries, and 2) swelling of the dried food-matrix at the length scale of the lamella in between the pores (van der Sman, 2014).

Consequently, the full multiphysics problem is investigated with a pore-scale model, which is reduced in complexity via integrating out the dimensions perpendicular to the capillary transport. In this paper, we present the mesoscale (pore scale) model for a single, straight square capillary, which solves the full multiphysics problem. The step-wise development of this pore scale model will be discussed in another paper, where we have shown that it follows the classical Lucas–Washburn solution of capillary suction in a rigid capillary. With the presented full model we will eventually derive relations, which will be fed to a pore network model describing the moisture transport at the macroscale level.

As will be shown, there is a strong interaction between various physical transport phenomena, as is typical in multiphysics problems. This strong interaction makes it difficult to predict beforehand, which phenomena are significant or not. This is also one of the goals for this coarse-grained model. A final goal of the model is to estimate the time scales for imbibition of real samples of freeze-dried carrots, which are compared to experimentally observed hydration rates. This is the basis for further model reduction and simplification.

Experimental data are obtained via an experimental multiscale approach, combining NMR, MRI and XRT, targeting the molecular scale, the pore scale, and the macroscopic product scale (Voda et al.; Vergeldt et al., 2013; Vergeldt et al., submitted for publication). Via NMR we have investigated the molecular mobility of water, via XRT we have imaged the freeze-dried samples, the swelling of lamella, and the filling of pores by water after rehydration, and via MRI we have imaged the ingress of water into the sample with time. More details on the experimental methods one finds in the accompanying paper in this issue (Vergeldt et al., submitted for publication).

The freeze-dried samples have been subject to different pre-treatments, which include blanching/non-blanching, and different freezing temperatures – which have created different microstructures and different pore sizes (van der Sman, Voda, van Dalen, & Duijster, 2013; Voda et al.). During rehydration the samples either remained floating on the air/water interface, or have been fully immersed in the water. During the first rehydration method, the water cannot ingress from the top of the sample – but air can easily escape via the top. In fully immersed samples, the escape of air is more difficult, because it has to pass the imbibing water, which moves in opposite direction. In porous literature these different modes of imbibition are denoted as co-current and counter-current imbibition (Unsal, Mason, Morrow, & Ruth, 2007; Unsal, Mason, Morrow, & Ruth, 2009). We expect different

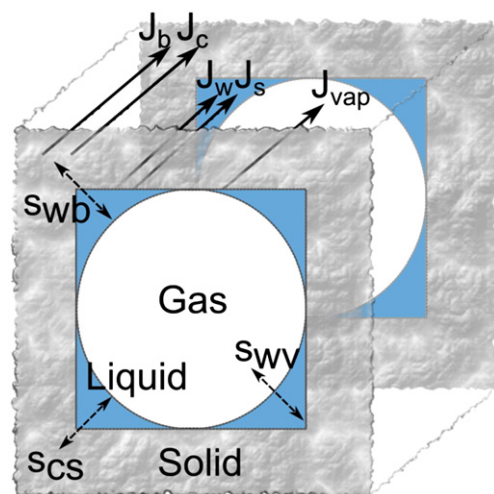
rehydration rates for the two different imbibition methods, and also more trapping of air during counter-current imbibition. Via simulations we will analyse the impact of the different pre-treatments, and the imbibition mode.

## 2. Multiphysics of mesoscale moisture transport

At the pore scale moisture can be present in three different phases, as is indicated in Fig. 1. Moisture can be absorbed in the solid phase of the food matrix, or it is present in the liquid phase as capillary water, or it is present as water vapour in the gas phase. The moisture absorbed by the food matrix is indicated as “bound water”, which does *not* have the same meaning as the frequently used, but ill-defined concept, of water in the first hydration shell – which is supposed to be strongly bonded (van der Sman, 2012b; van der Sman, Jin, & Meinders, 2013). Recent research has shown that this picture of strongly bonded hydration water is wrong (Ball, 2008), which opens the possibility to use “bound water” more appropriately to water “bound” to a food matrix – having a crosslinked biopolymer network.

The food matrix contains both biopolymers (mainly cell wall material) and solutes like sugars. Initially, the freeze-dried vegetable is at room temperature and dry, and in equilibrium with a low water activity. There is no liquid phase, and the pore space is only filled with air – with negligible amount of vapour. During imbibition the pore space can either be completely or partially filled with liquid. Such regions will be denoted as the saturated and unsaturated zones. In the unsaturated zone, liquid is present in the sharp corners of the pore space, also known as wetting layers. The boundary between the saturated and unsaturated zones is formed by the so-called main terminal meniscus (MTM). In the unsaturated zone, there is a meniscus between liquid phase and the gas phase, which is called the arc meniscus (AM). On occasion, we denote the combined gas and liquid phase as the fluid phase.

With respect to solutes, we consider two cases, 1) where the solute is immobilized, and remains in the solid phase, and 2) where the solutes are mobile, and can diffuse into the liquid phase. The first case we associate with non-blanched vegetables, while the second case is associated with blanched vegetables. In fresh vegetables, the solutes are compartmentalized in vacuoles, which are enclosed by a membrane that is impermeable to solutes. One can regard the fresh vegetable as a phase-separated system, with a solute-rich phase, and a biopolymer-



**Fig. 1.** Multiple phases present in the rehydrating freeze-dried vegetables: a) the solid phase containing the cell wall material with bound water and sugars, b) the liquid phase containing capillary water and possibly dissolved solutes, and c) the gas phase containing air and water vapour. There is interchange of components between phases, indicate with mass exchange  $s_{ij}$ . Convective/diffusive transport within one phase is indicated with  $j_i$ . Due to fast mass exchange between liquid and gas phase,  $s_{wv}$ , there is local equilibrium between gas and liquid phase.

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