Multiscale modelling of transport and deformation during food processing

Zachary Welsh[a] and M. A. Karim*[a]
[a] Chemistry, Physics and Mechanical Engineering, Queensland University of Technology, Brisbane, Australia
Corresponding author: Azharul Karim, Queensland University of Technology
2 George Street, QLD 4000 Australia,

azharul.karim@qut.edu.au

Abstract

Fruits and vegetables demand special attention as these are considered important sources of essential nutrition for humanity. Horticultural crops are highly perishable and a lack of proper processing causes considerable damage and wastage of approximately 40% across the food cycle. Moreover, their seasonal production pattern results in frequent market overabundances and wastages. Drying is one of the major processes in food industry and a key post-harvest preservation technique. However, food industry suffers from some major drawbacks: food processing is very energy-intensive and time-consuming process and considerable quality deterioration takes place during processing. These problems could not be properly resolved as fundamental understanding of complex cell to bulk level heat and mass transport, and associated deformation during food processing is not well understood. Modelling of transport and deformation in heterogeneous porous media like plant-based food is a challenging problem due to the multiscale nature of the food structure. Development of a novel multiscale modelling framework will enable accurate prediction of micro and macro level transport process and deformation in plant-based food material during drying.

1. Introduction

Drying is a simultaneous heat and mass transfer process aiming to remove water in order to extend the shelf life of food. However, this process is very energy intensive, time consuming and results in quality deterioration during processing. Most fruits and vegetables contain about 80-95% water and therefore highly susceptible to microorganism growth. Removing this excess water by appropriate drying technique can extend the shelf life unto 25 years. Drying is one of the major processes in most food industries, and a key post-harvest preservation technique. However, traditional drying process is very energy-intensive, time-consuming and affect food quality considerably.

Heterogeneous microstructure of food materials dictates the characteristics of water migration and resulting deformation during drying. In particular, the migration of bound water to its surrounding environments cause uneven volume reductions, called anisotropic shrinkage [1]. This shrinkage can have many effects on food material, in particular, quality deterioration [2, 3]. The current modelling approach fails to incorporate heterogeneous structure of food materials, and the transportation of bound water. Multiscale modelling approach has the ability to address these concerns and model the simultaneous transport and deformation during food drying [4, 5]. This paper aims to review multiscale modelling for the application of food drying. The reminder paper will present; 2. multiscale nature of food and current modelling approach of food drying, 3. multiscale approaches for food drying, 4. recent advancements, 5. challenges and future directions and 6. conclusions.

2. Food materials multiscale nature and current modelling approach

Plant-based food materials have heterogeneous hygroscopic microstructure, which undergoes anisotropic deformation because of heat, mass and momentum transport during thermal processing. Their structure is complex and multiscale in nature, composing of polymers, air, minerals and a large portion of water [6]. Water within fruits and vegetables is found within three locations, intracellular spaces (loosely bound water), intercellular spaces (free water) and within cell walls (strongly bound water) as can be seen in Figure 1. Free water is easily transported during thermal processing. However, the migration of Loosely Bound Water (LBW) is a major concern. The LBW has ability to migrate through three possible pathways: cell to cell, cell to pore or through progressive cell rupturing, and has significant influence on deformation. Further details can be found in authors' previous works [1, 7].

The resulting deformation is anisotropic and complex, and its fundamental understanding across length scales is not well understood yet.

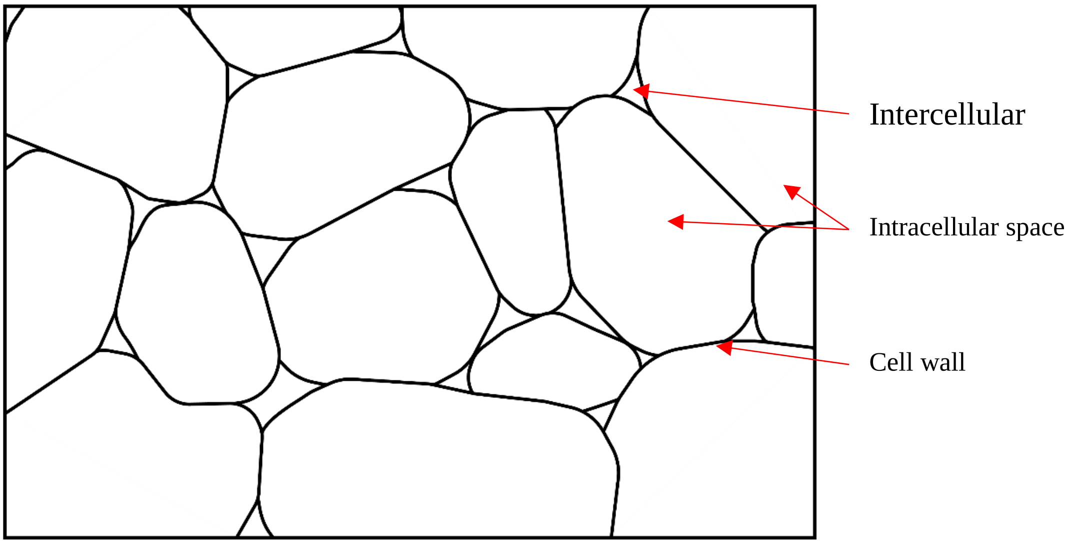

Figure 1. Heterogenous cellular structure of fruits and vegetables [4].

The existing macroscale continuum approach fails to incorporate heterogeneous structure of fruits and vegetables, rather treats the material as homogeneous and utilising empirical relationships to approximate its effects. This creates a dramatic demand in physical and mechanical characterisation of each sample being investigated [8]. Whitakers theory [9] forms the foundation of porous media modeling with two of his key assumptions being a rigid structure and the absence of LBW [10]. The work utilises a representative elementary volume (REV) to volume average the microscale conservation transport equations to a macroscale. The difference between the REV and real food material can be seen in Figure 2. Although many models based on Whitaker assumptions reported good agreement with experimental results, this is only because the main driving factor, the diffusivity, has been determined experimentally. Therefore, the diffusivity of every product sample and every drying condition needs to be determined. In addition, these curve fitting techniques often consider a perfect geometry with no deformation often causing the predictive model and experimental data to significantly deviate in the latter stages of drying [11].

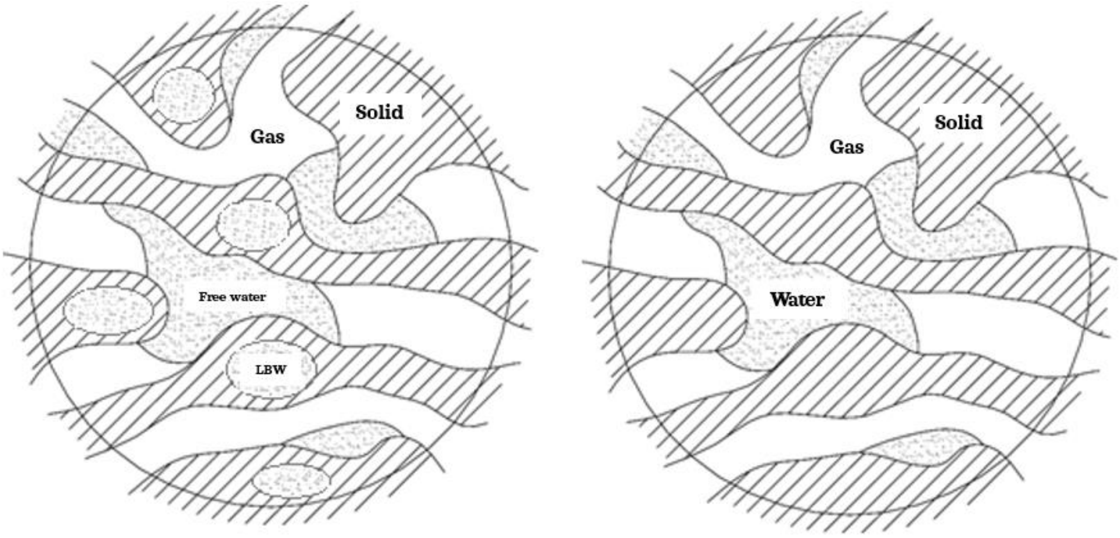

Figure 2. Distribution of cellular water, (a) Real structure including LBW and free, (b) REV approach only considering water as ‘free’.

Up until recently, the majority of food drying models have been developed at a bulk level (macroscale) [4]. However, recently, the authors have developed the first microscale transport model for food drying and investigated a heterogeneous microstructure during convective drying [12]. Additionally, investigations have been conducted on cellular water distribution in addition to the development of a realistic microstructure domain for apple tissue [1, 13, 14]. Some researchers attempted to model soft matter for deformation and water dehydration at a microscale [15-17]. Further studies are required to incorporate fruit and vegetables heterogeneous structure for food drying to better understand the multiscale nature of the anisotropic deformation and structure dependent transportation which occurs.

3. Multiscale approaches for food drying

Multiscale modelling is a considered to be a series of submodels spread across multiple length scales, allowing large amount of physics to be modelled. It has the ability to incorporate a material heterogenous structure with reasonable computational cost. Multiscale modelling has been applied to numerous fields over the years, but new to food drying. Literature has been published for multiscale timber drying [8, 18, 19] as well multiscale/microscale food dehydration during natural storage [15, 20]. Under an external heat source, fruits and vegetables deform in a unique way making it difficult model appropriately. Recently, some researchers have shown their immense interest in multiscale food drying modelling and provided some general background into the modelling [4, 5, 21, 22]. In a multiscale model, information is exchanged between two or more submodels. This can be achieved through two approaches, a one-way coupling technique; the submodels are kept independent and the information is fed from one scale to another (upscaling/downscaling), or a two way or concurrent coupling technique; data is exchanged and solved continuously. Homogenisation (one way coupling technique) and the heterogeneous multiscale method (concurrent technique) are discussed.

3.1 Homogenisation

Homogenisation is a traditional mathematical method which allows differential equations to be upscaled [23]. It considers the heterogeneity through a microscale model with an associated governing equation. In traditional homogenization approaches, the upscaling operation occurs once as a pre-processing technique. One property, which could benefit from applying homogenisation to food drying modelling, is diffusion. Currently, diffusion is defined through experiments and curve fitting techniques, approximating its heterogenous structure lumping together all the water transport mechanism. Effective diffusivity by applying homogenisation in a 2D geometry would result in a tensor, defined as,

$$D_{eff} = \begin{bmatrix} \frac{1}{A}\int_{x_o}^{x_L}\int_{y_o}^{y_L} D(x,y)\nabla(u_1(x,y)+e_1)\,dx\,dy & \frac{1}{A}\int_{x_o}^{x_L}\int_{y_o}^{y_L} D(x,y)\nabla(u_2(x,y)+e_2)\,dx\,dy \\ \frac{1}{A}\int_{x_o}^{x_L}\int_{y_o}^{y_L} D(x,y)\nabla(u_1(x,y)+e_1)\,dx\,dy & \frac{1}{A}\int_{x_o}^{x_L}\int_{y_o}^{y_L} D(x,y)\nabla(u_2(x,y)+e_2)\,dx\,dy \end{bmatrix} \tag{1}$$

where, A is the area of the microscale geometry, D is the cellular diffusion, and u is the corrective factors calculated by considering the microscale domain as periodic and solving

$$\nabla\cdot(D\,\nabla(u_j+e_j)=0 \quad, j=1,2 \tag{2}$$

$$\frac{1}{A}\int_A u_j dA = 0 \tag{3}$$

The reader is directed to Perré [8] for further details of homogenization for application of drying. Homogenization is a pre-processing operation with the upscaling occurring only once. Therefore, it is unable to incorporate any microstructural changes which occurs throughout the drying process. A concurrent approach is required to capture these changes.

3.2 Heterogeneous Multiscale Method

The Heterogeneous Multiscale Method (HMM) is a general framework for constructing concurrent multiscale models and applying it to specific problems can be a highly complex and non-trivial task [24]. HMM is a top-down framework and its formulation is constructed around having an incomplete macroscale model, commonly represented as

$$\partial_t U = L(U; D) \tag{4}$$

where, U denotes a key variable (i.e., temperature or moisture), D denotes the data needed to complete the model (i.e., fluxes or diffusion). The coupled microscale model is defined as

$$\partial_t u = L(u; U) \tag{5}$$

where, U is the macroscale variable being transferred to the microscale model (through an assumption/interpolation). The HMM formulation results in the following

$$F(U, D) = 0 \tag{6}$$

$$f(u, d) = 0 \qquad ; \quad d = d(U) \tag{7}$$

where, d denotes the data required to initiate the microscale mode (i.e., heat, temperature, or moisture). The reader is directed to Welsh, Simpson [4] for an in depth look into HMM for the application of food drying. A HMM framework requires much more computational resources as the scaling operations occurs multiple times throughout the simulation. However, this does allow the approach to incorporate the microstructural changes which occur during drying [4]. This is a huge advantage over homogenization, therefore, holding great potential for multiscale research in food drying. It is well documented that a product's structure heavily affects its quality [25, 26]. However, the relationship between the microstructural changes and the properties of the sample is not clearly understood from the limited available literature [5].

4. Recent advancements

Although multiscale modelling to food drying is challenging and complex, recently some progresses have been made in the area.

4.1 Investigation of cellular water distribution during drying

The distribution of cellular water within food material has been investigated by Khan, Wellard [27] and reported the initial water distribution for eleven different plant-based food materials. The work utilised H NMR T_2 relaxometry to investigate the products, and concluded that the typical range of LBW to be 80-90%, free water to be 6-16% and strongly bound water to be 1-6% (see Figure 3).

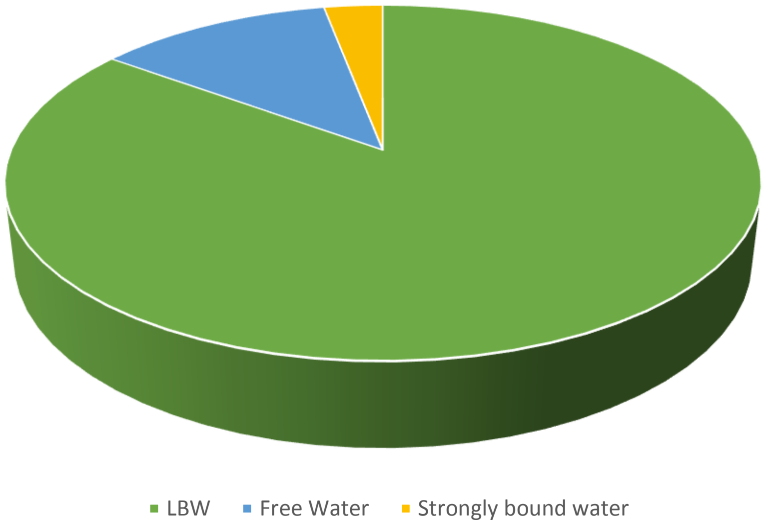

Figure 3. The percentage of different water type within plant-based food material [27].

Also, the distribution of cellular water during drying has been investigated for apple and potato tissue [13]. Three temperatures, (45°, 60° and 70°C), were investigated, and LBW and free water were tracked during convective drying. The work discovered that cell rupturing occurs progressively in relation to the drying temperature as demonstrated in Figure 4.

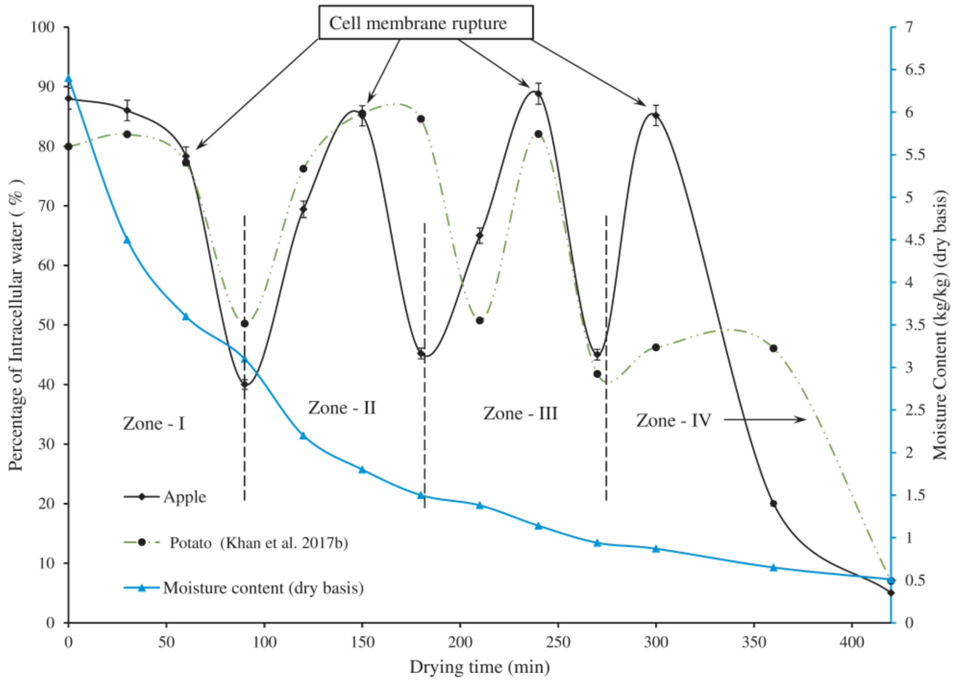

Figure 4. The change in percentage of intracellular water with drying time for convective drying at 60 degrees Celsius [7].

4.2 Development is a realistic microscale domain for modelling

A realistic microscale domain has now been constructed for plant-based food materials. Rahman, Gu [14] develop the virtual microstructure from a scanning electron microscope image with clear identification of the intracellular spaces and intercellular spaces for both granny smith and red delicious apples. The constructed microscale domain can be seen in Figure 5 (a). A new algorithm was developed based on the modified ellipse fitting method to generate the microstructure from the images. Linear discriminant analysis was used to identify the spaces and the proposed method was compared with the Voroni tessellation algorithm and direct ellipse fitting process. The new proposed method provided significantly better area distribution compared to the other methods.

4.3 The first microscale model for the field of food drying

The first microscale transport model for plant-based food materials during drying has been developed by the authors recently [12]. The work modelled the heterogeneous structure of food material to predict the cellular water transportation mechanism during drying. The model demonstrated that the moisture transport and distribution were significantly affected by the characteristics of the cell, intercellular space and cell walls, highlighting the necessity for a multiscale model for food drying. The model was validated using results from X-ray microtomography (μCT) images demonstrating good agreement with the model. The method of validation is detailed in Rahman, Joardder [28]. A summary of the results can be seen in Figure 5. The development of this microscale transport model is the first step toward applying multiscale modelling to food drying.

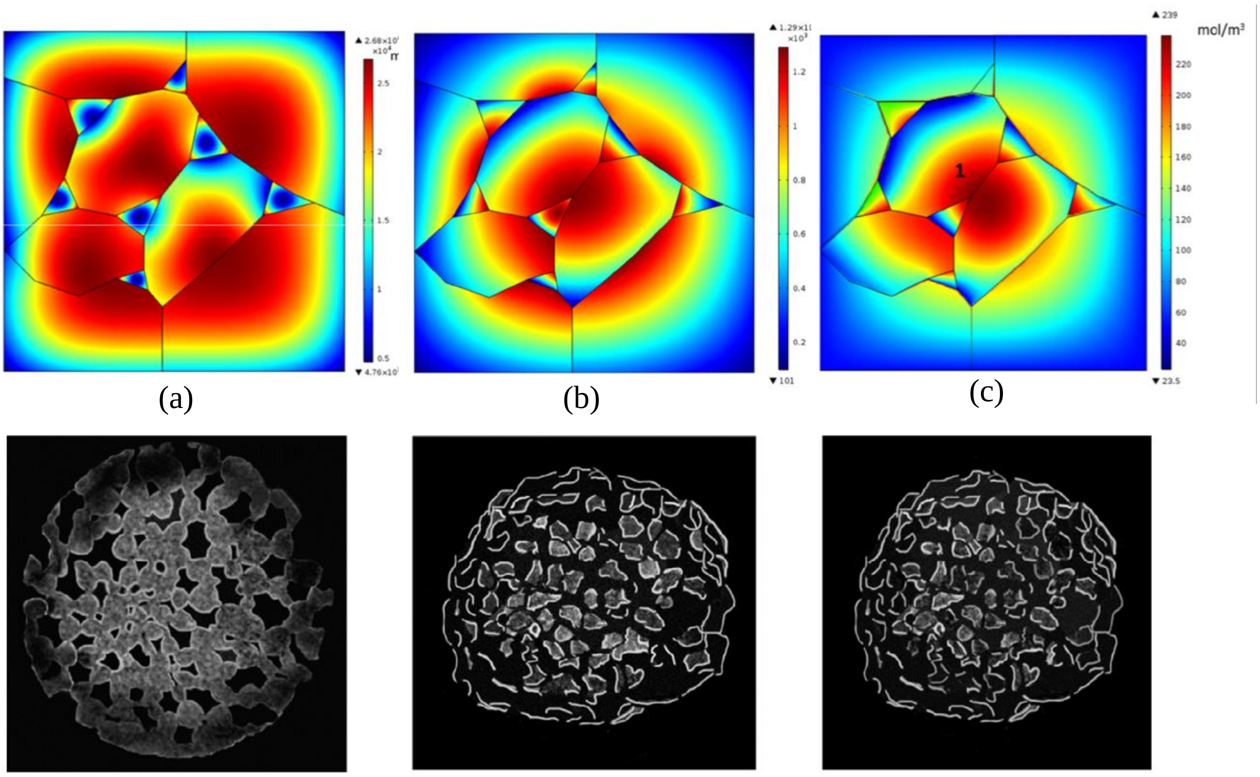

Figure 5. Microscale model predictions vs X-ray microtomography results, (a) 60 minutes of drying, (b) 200 minutes of drying, (c) 300 minutes of drying [12].

5. Challenges and future directions

Multiscale modelling for food drying is still in its infancy with knowledge at a cell level being limited. Even with the recent advancements, many cell level properties have not been investigated. These will be the key to investigate when applying multiscale modelling to food drying. Fruits and vegetables undergoes unique deformation under an external heat source restricting the applicability of many existing multiscale methods in food. Adopting a framework to formulate a multiscale model would be ideal [4]. Additionally, the spatial and temporal couplings are extremely important when considering the model formulation and solution technique. Most frameworks provide a guide but achieving an appropriate concurrent scheme for the large number of variables, which are required for theoretical food drying modelling, is a major concern. The development of such a scheme paired with a multiscale framework will aid to establish multiscale modelling for food drying [4].

The implementation of multiscale modelling for food drying will be the key to the next generation of food drying research. The construction of a homogenisation food drying model would allow the heterogeneous structure of fruits and vegetables to be incorporated for a reasonable computational cost. The limitation of this approach is that the scaling operation occurs only once and if the materials microstructure changes significantly during drying, this cannot be captured in this technique. A concurrent approach provides a platform to incorporate the microstructural changes within a model allowing the properties to be changed throughout the simulation. This style of model is much more computationally demanding and should only be considered if the deformation is large [4]. A concurrent model would be ideal for food drying, have higher degree of precision and more potential applications.

6. Conclusions

Multiscale modelling holds great potential for food drying with its ability to consider heterogeneous structure of food and associated transport and deformation in modelling. It could allow the migration of LBW to be modelled and better understood which would result in energy improvements and better-quality fruits and vegetables which existing models are unable to consider. Recent advancements within the field make applying multiscale modelling to food drying closer than ever. The cellular distribution of water and its migration during drying has now been investigated. A microscale domain representing the real food structure has been developed and the first microscale model has been established with the field. Applying a multiscale framework to develop the first multiscale food drying model is recommended, although it is a highly complex task. Additionally, fruit and vegetables experience unique deformation under an external heat source. The development of a novel concurrent multiscale modelling scheme will enable accurate predictions of micro and macro level transport processes and deformation in plant-based food material during drying.

7. References

1. Khan, M.I.H. and M.A. Karim, *Cellular water distribution, transport, and its investigation methods for plant-based food material.* Food Research International, 2017. **99**(Part 1): p. 1-14.
2. Mulet, A., et al., *Effect of shape on potato and cauliflower shrinkage during drying.* Drying Technology, 2000. **18**(6): p. 1201-1219.
3. Senadeera, W., et al., *Modeling dimensional shrinkage of shaped foods in fluidized bed drying.* Journal of food processing and preservation, 2005. **29**(2): p. 109-119.
4. Welsh, Z., et al., *Multiscale Modeling for Food Drying: State of the Art.* Comprehensive Reviews in Food Science and Food Safety, 2018. **17**(5): p. 1293-1308.
5. Rahman, M.M., et al., *Multi-scale model of food drying: Current status and challenges.* Critical Reviews in Food Science and Nutrition, 2018.
6. Khan, M.I.H., et al., *Determination of appropriate effective diffusivity for different food materials.* Drying Technology, 2017. **35**: p. 335-346.
7. Khan, M.I.H., S.A. Nagy, and M.A. Karim, *Transport of cellular water during drying: An understanding of cell rupturing mechanism in apple tissue.* Food Research International, 2018. **105**: p. 772-781.
8. Perré, P., *Multiscale aspects of heat and mass transfer during drying.* Transport in Porous Media, 2007. **66**: p. 59-76.
9. Whitaker, S., *Simultaneous heat, mass, and momentum transfer in porous media: a theory of drying*, in *Advances in heat transfer*. 1977, Elsevier. p. 119-203.
10. Wang, W., G. Chen, and A.S. Mujumdar, *Physical interpretation of solids drying: An overview on mathematical modeling research.* Drying Technology, 2007. **25**(4): p. 659-668.
11. Tzempelikos, D.A., et al., *Numerical modeling of heat and mass transfer during convective drying of cylindrical quince slices.* Journal of Food Engineering, 2015. **156**: p. 10-21.
12. Rahman, M.M., et al., *A micro-level transport model for plant-based food materials during drying.* Chemical Engineering Science, 2018. **187**: p. 1-15.

13. Khan, M.I.H., et al., *Fundamental Understanding of Cellular Water Transport Process in Bio-Food Material during Drying.* Scientific Reports, 2018. **8**(1): p. 15191.
14. Rahman, M.M., Y.T. Gu, and M.A. Karim, *Development of realistic food microstructure considering the structural heterogeneity of cells and intercellular space.* Food Structure, 2018. **15**: p. 9-16.
15. Aregawi, W.A., et al., *Prediction of water loss and viscoelastic deformation of apple tissue using a multiscale model.* Journal of Physics: Condensed Matter, 2014. **26**: p. 464111.
16. Fanta, S.W., et al., *Microscale modeling of coupled water transport and mechanical deformation of fruit tissue during dehydration.* Journal of Food Engineering, 2014. **124**: p. 86-96.
17. Fanta, S.W., et al., *Microscale modeling of water transport in fruit tissue.* Journal of Food Engineering, 2013. **118**(2): p. 229-237.
18. Carr, E.J., I.W. Turner, and P. Perré, *A dual-scale modeling approach for drying hygroscopic porous media.* Multiscale Modeling & Simulation, 2013. **11**: p. 362-384.
19. Perré, P., *Multiscale modeling of drying as a powerful extension of the macroscopic approach: Application to solid wood and biomass processing.* Drying Technology, 2010. **28**: p. 944-959.
20. Ho, Q.T., et al., *Multiscale modeling of transport phenomena in plant-based foods.* Dynamic Process Modeling, 2013.
21. Defraeye, T., *Advanced computational modelling for drying processes – A review.* Applied Energy, 2014. **131**: p. 323-344.
22. Ho, Q.T., et al., *Multiscale modeling in food engineering.* Journal of Food Engineering, 2013. **114**: p. 279-291.
23. Hornung, U., *Homogenization and porous media*. Vol. 6. 2012: Springer Science & Business Media.
24. Weinan, E., et al., *Heterogeneous multiscale methods: A review.* Communications in Computer Physics, 2007. **2**: p. 367-450.
25. Ko, S. and S. Gunasekaran, *Error correction of confocal microscopy images for in situ food microstructure evaluation.* Journal of Food Engineering, 2007. **79**(3): p. 935-944.
26. Witek, M., et al., *The structural and hydration properties of heat-treated rice studied at multiple length scales.* Food Chemistry, 2010. **120**(4): p. 1031-1040.
27. Khan, M.I.H., et al., *Investigation of bound and free water in plant-based food material using NMR T2 relaxometry.* Innovative Food Science & Emerging Technologies, 2016. **38**: p. 252-261.
28. Rahman, M.M., M.U.H. Joardder, and A. Karim, *Non-destructive investigation of cellular level moisture distribution and morphological changes during drying of a plant-based food material.* Biosystems Engineering, 2018. **169**: p. 126-138.