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Incorporating food microstructure and material characteristics for developing multiscale saturated and unsaturated transport models

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This communication discusses hybrid mixture theory and how it could be utilized for food science applications by presenting examples on drying, frying and expansion of biopolymers. Hybrid mixture theory, which has a continuum mechanics basis can be used to merge the quality changes in food biopolymers with processes such as transport of heat, water, vapors, oil, etc. in food systems. Once a developed model has been validated, obtaining the solution via numerical simulations yields a large amount of data on transport of fluids, heat, species, etc. in the food matrix and food's rheological and microstructural characteristics. Hybrid mixture theory and some other continuum mechanics based theories have advanced to a stage that they can be used to describe the fate of multiphases and multiconstituents in complex foods undergoing phase and state transitions during processing. The developed modeling equations also help to serve as a guide for designing parameter estimation experiments, and solution of the model helps to fill gaps in experimental knowledge on underlying physical mechanisms. The solution of developed model provides information on optimum processing conditions needed to improve the quality of food products and efficiency of processes.

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Introduction

Continuum mechanics involves treating the matter as continuous, and studying its motion and deformation as a function of internal or external forces. Continuum mechanics also utilizes the laws of thermodynamics by including energy balance and entropy inequality [1]. The field has helped to enhance our understanding of the behavior of materials, their interaction with the environment, design new materials, and improve their quality by predictably modifying the processing conditions. Continuum mechanics involves developing mathematical models describing material behavior during processing by utilizing the laws of conservation of mass, momentum and energy balance that are universal as they apply to all materials; including the nature of material via constitutive theory; and applying restrictions using the second law of thermodynamics. Using the framework of continuum mechanics, a large number of engineering models can be obtained via mathematical derivations. Examples include thermoviscous, thermoelastic and thermoviscoelastic relations, integro-differential viscoelasticity relations, generalized Fourier's law of heat transfer, Navier–Stokes equation, Fick's law, Darcy's Law, magnetoelasticity relations, etc. (see e.g. [2•]).

Field equations in continuum mechanics (conservation of mass, momentum and energy) apply to all types of materials when the hypothesis of continuum holds. However, there are more variables than the number of equations. This is expected because we know that different materials behave differently under deformation. The system of equations is closed by including additional relations by formulating the constitutive theory, which involves incorporating the nature of materials (e.g. elastic, viscoelastic, viscous, plastic, conductive, diffusive, etc.). Most relations available were obtained in pure fields of engineering for materials with simpler nature than foods. Foods are complex mixtures of biopolymers (e.g. carbohydrates, proteins, lipids), solutes (e.g. sodium) and fluids (water, vapors, oil, etc.); exhibit porous microstructure with scale hierarchy (e.g. pores in cell walls at microscale, cell cytoplasm at mesoscale and tissue at macroscale); undergo phase and state transitions; and transform their constitutive behavior, structure and composition during processing. Thus, when continuum mechanics based models are derived for food materials, more general and often novel relations are obtained [3,4–6,7••].

To include the hierarchical porous structure of materials and mixture of species (e.g. solutes and biopolymers), various theories have evolved within the framework of continuum mechanics (see [8•] for an overview). Examples of these theories are — volume averaging the smoothed transport equations with material coefficients from micro to macroscales [9] (see [10,11,12••] for the food science application); homogenizing the microscale differential equations describing transport processes

Nomenclature

Latin symbols

D^{α}	coefficient of diffusivity of the phase α [m^2/s]
${}^{\beta}\dot{e}^{\alpha}$	net rate of mass transfer from the phase β to the phase α [$kg/(m^3\ s)$]
$\dot{E}^{s}_{KL}$	first order material time derivative of E^{s}_{KL} [s^{-1}]
$\overset{(m)}{E}{}^{s}_{KL}$	mth order material time derivative of E^{s}_{KL} [s^{-m}]
E	coefficient of elasticity of the biopolymeric matrix [Pa]
K^{α}	permeability of the α phase [m^2]
M	moisture content on mass dry basis [g/g solids]
$\mathcal{M}^{\alpha}$	$=M^{\alpha}/R^{\alpha}$, memory function in Darcy's law Eq. (2) [$m^5/(kg\ s)$]
M_g	glass transition moisture content [g/g solids]
p^{α}	physical pressure in the phase α [Pa]
p_c	capillary pressure [Pa]
REV	representative elementary volume [m^3]
T	temperature [K]
T_g	glass transition temperature [K]
M_g	glass transition moisture content [g/g solids]
v_l^{α}	velocity of the α phase [m/s]

Greek symbols

ε^{α}	volume fraction of the α phase (dimensionless)
ϕ	porosity of the biopolymeric matrix (dimensionless)
ρ^{α}	density of the phase α [kg/m^3]

Subscripts

k, l	indices for Eulerian coordinates
K, L	indices for Lagrangian coordinates

Superscripts

α	general representation of a phase
β	general representation of a phase
m	order of the material time derivative of E^{s}_{KL} that varies from 0 to p
s	solid phase
w	water phase
o	oil phase
g	gas phase

Special symbols

D^{α}/Dt	material time derivative with respect to velocity of the α phase particle [s^{-1}]
$v_l^{\alpha,s}$	velocity of the α phase relative to the solid phase ($=v_l^{\alpha}-v_l^{s}$) [m/s]
Dot (.)	$=D^{s}/Dt$, material time derivative with respect to velocity of the solid phase particle

using asymptotic methods [13]; and hybrid mixture theory that involves upscaling the microscale field equations to meso and macro scales, formulating the constitutive equations at macroscale to close the system and exploiting the entropy inequality to impose restrictions on the equations to make them physically viable [14••].

The focus of this communication will be on hybrid mixture theory (HMT) in, which the material properties in a system appear at the macroscale during the mathematical derivation process. This makes HMT specifically suitable for foods as it is difficult to measure their material properties at the micro and meso scales due to structural and compositional heterogeneity; tedious sample preparation of soft materials; and a wide contrast in properties and structure in different regions of a food (e.g. crystalline and amorphous regions in starch [15]).

Hybrid mixture theory (HMT)

Figure 1 shows three-scales in a porous material involving interactions between different phases at three scales. HMT allows including physical mechanisms at different scales in the developed models. It involves volume averaging the laws of mass, momentum, energy and entropy at the microscale to obtain equations at the meso and macro scales. First, microscale equations are averaged over the solid-vicinal fluid domain to obtain the mesoscale equations. At mesoscale, the equations are further averaged over the solid-fluid mixture and bulk phase to obtain equations at the macroscale. At macroscale, the constitutive equations are formulated by exploiting the entropy inequality using Coleman and Noll's [16•] method.

HMT was developed by Hassanizadeh and Gray [14••,17] to study the transport processes in soils. Achanta and Cushman [3], Bennethum and Cushman [18••] and Bennethum et al. [19] applied HMT to swelling and shrinking systems with dissolved species (solutes) and included interactions between phases and species. They treated the solid phase as elastic and the liquid phase as viscous. In earlier studies, HMT was used for either swelling clays [18••,19], or adapted for polymeric systems from clay systems [3] for which the assumption of elastic solid phase holds. The system depicted viscoelastic behavior with short-memory at the macroscale, which resulted from the interaction of the elastic solids with the viscous fluids at micoscale. Earlier HMT based studies ignored the microscale relaxation processes within the polymeric matrix, which occur due to conformational changes in the flexible thread-like polymers at the molecular scale [20]. These relaxation processes can cause a food material to exhibit viscoelastic behavior even in the absence of water or a plasticizing agent. These relaxation processes provide a force term, which affects liquid movement through the porous matrix [21,22•,23,24]. This force term plays a fundamental role when the time-scale of relaxation is of the same order as the time scale of the liquid movement, which occurs when the polymers are undergoing glass-transition.