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A first-principles model for plant cell rupture in microwave-assisted extraction of bioactive compounds

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ABSTRACT

A first-ever theoretical model describing the cell rupture mechanism for microwave-assisted extraction (MAE) of bioactive compounds from plant samples is presented. This model incorporates the microwave heating of intracellular moisture within the plant cells using Lambert's law. It then calculates the heating time and the intrinsic energy required to pressurize and stretch the plant cells until rupture using thermodynamic relations. The attainment of cell rupture is determined from elasticity theory for solids. The simulation requires the inputs of the effective shear modulus of the plant cell wall and the incident microwave irradiation flux entering the extraction mixture. The predicted cell rupture time by the intrinsic energy validated excellently against the optimum extraction time found in experiments. This model is generally applicable over a wide extraction parameters and microwave systems.

1. Introduction

Microwave-assisted extraction (MAE) is among the efficient techniques to extract bioactive compounds from plants. It employs microwave to enhance the heating of the extraction solvent containing the plant materials. Generally, it requires shorter extraction time and lower volume of solvent compared to those use conventional heating such as Soxhlet extraction (Chan et al., 2011; Wang and Weller, 2006). Despite its superior performance, MAE is widely adopted only in the laboratory scale because the technique is difficult to scale up and its optimum operating condition is hard to gauge using different configurations. As such, the optimum operating conditions for MAE reported in the literature are applicable only for specific systems and on a restricted scale. These issues, which arise from a lack of fundamental understanding of the underlying physico-chemical processes, should be resolved before MAE can be fruitfully commercialized.

To this end, various optimization and modeling methods had been developed for optimization and scaling up of MAE. The modeling of MAE has been conventionally based on two-parametric empirical models such as film theory (Stankovic et al., 1994) and chemical kinetic equation (Rakotondramasy-Rabesiaka et al., 2007) to describe the dynamics in the washing and the diffusion steps of the extraction (Chan et al., 2014). The constants of the models rely heavily on experimental data, making them only useful in comparative studies such as to indicate the extraction kinetics at different operating conditions. Response surface methodology (RSM) and artificial neural network (ANN) models had also been applied to simulate and optimize the operating parameters of MAE (Sinha et al., 2012, 2013). These models are able to simulate and optimize MAE using less experimental data compared to the two-parametric empirical models. However, screening of suitable range of operating parameters is needed to achieve reliable optimization results. Further, it is not obvious what those parameters should be on scale-up. Besides these efforts, modeling of MAE had been attempted using Maxwell's equations for electromagnetism, energy and species balance equations via COMSOL Multiphysics™ software in the work (Chumnanpaisont et al., 2014). On top of simulating the extraction profile using empirical parameters, the model is able to capture the spatial distribution of electromagnetic wave and temperature profile in the MAE system. Recently, a few predictive mass transfer models (Chan et al., 2013, 2015a, 2015b) had been derived from two-parametric empirical model with the incorporation of energy-based parameters, namely the absorbed power density and the absorbed energy density. The energy-based models is able to predict the optimum extraction time and extraction profile at various microwave powers, extraction scales,

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microwave system and heating modes (e.g. constant-power, intermittent-power and constant temperature). Despite the apparent success of the later developments, all parameters from the above-mentioned models have no physical meanings thus they are not suitable to be used for equipment design, process optimization and scale up. Hence, to complete the picture, theoretical modeling of MAE should consider the mechanism of rupturing plant cell as had been suggested by various works (Gujar et al., 2010; Yan et al., 2010; Zhang et al., 2013). To the best of our knowledge, there was no literature available on this topic.

For the first time the cell rupture mechanism of MAE is described using fundamental principles in this work. The ultimate goal is to investigate the intrinsic energy to rupture plant cells and to predict the optimum extraction time from the temporal-evolutions of the intracellular thermodynamics during MAE. This work presents the theoretical framework of the model in Section 2. Following that, a case study is elucidated in Section 3, followed by the results validated over a broad range of MAE conditions. Finally, conclusions to this study are given in Section 5.

2. Theoretical framework

This model was constructed based on the following premises. Plants samples contain a large number of parenchyma cells (Cutter, 1978) that store bioactive compounds. During MAE, microwave propagates within the extraction mixtures comprising of solvent and plant particles, the latter containing vacuoles with certain moisture content. Due to the favorable dielectric properties, the intracellular moisture of the plant particles absorbs a portion of the incident microwave energy, becomes heated and vaporized to generate internal pressure within the cell vacuoles. This causes the membrane surrounding the vacuoles to stretch and expand, eventually reaching the cell wall. Beyond that, the cell wall expands together. The membrane of the vacuole may or may not rupture, but this is immaterial as long as the cell wall remains intact. When the internal pressure exceeds the strength of the cell wall, the plant cell ruptures and the bioactive compounds are released into the surrounding solvent.

To account for the steps envisaged above, the cell rupture model needs to incorporate: (A) the pressure-volume relationship based on the mechanical properties of the parenchyma cell wall; (B) the average radiative heating power of intracellular moisture; and (C) the temporal-evolution of intracellular pressure, temperature and volume expansion, as summarized pictorially in Fig. 1. Details of each will be elaborated in the subsections below.

2.1. Pressure-volume relationship of plant cell wall

The first part of the model requires the pressure-volume relationship of the cell wall, modelled based on elasticity principles for a polymer-like substance (Wu et al., 1985). Approximating the shape of a parenchyma cell wall as a thin-shelled hollow sphere, its pressure-volume relationship can be described as follows (Wu et al., 1985):

$$P_{\text{int}} = P_{atm} + \gamma_0 \left[\left(\frac{V_c}{V_{c0}} \right)^{-1/3} - \left(\frac{V_c}{V_{c0}} \right)^{-7/3} \right] \tag{1}$$

where P_{int} is the intracellular pressure. Since the extraction vessel is not pressurized, the surrounding pressure or the intercellular pressure is at the atmospheric pressure. V-$_c$ and V_{c0} are respectively the expanded and the initial volume of the plant cell. The lumped parameter γ_0 is defined as:

$$\gamma_0 = \frac{2 t_{c0} G}{r_{c0}} \tag{2}$$

where t_{c0} and r_{c0} are the average thickness and radius of the cell wall in original condition, and G is the shear modulus. The parameter γ_0 which has the same units of but often a smaller magnitude than shear modulus, is known as the mechanical property constant of the plant cell wall. It can be interpreted as an effective shear modulus modified by the geometry.

The pressure-volume relationship is approximately linear at the beginning of the extension, by virtue of the form of the equation. The maximum of P_{int} occurs at $V_c/V_{co} = \sqrt{7}$ regardless of the value of γ_o. The maximum point is also known as yield point whereby extension beyond this point can be interpreted as the plastic-flow state of cell wall (Li et al., 2010). While the elasticity principle could not predict *a priori* whether the cell wall would rupture at, below or above this maximum pressure, for this pressure-volume model, the maximum pressure is assumed to be the cell rupture pressure. Upon rounding up, the cell rupture pressure is:

$$P_{rup} \approx P_{atm} + 0.62\gamma_0 \tag{3}$$

2.2. Microwave heating analysis

As illustrated in Fig. 1(B), the second part of the model incorporates the dissipation of microwave power within the extraction mixture in a cylindrical vessel. In reality, this heterogeneous mixture is non-uniform, with more solid particles (plant sample fragments) near the bottom of the container, and there could potentially be convective movements of the particles during the heating. The dielectric properties of the solvent, solid matrix and any moisture trapped within are also different, giving significantly different heating response under microwave irradiation. Hence a rigorous way to account for the microwave heating of this mixture is not obvious.

However, at low solvent to solid ratio, only a thin layer of the mixture is reasonably clear, while the rest of the mixture is quite densely packed with solid particles. Moreover, based on experimental observation, the particles do not churn around significantly because the temperature gradient of extraction solvent, which promotes movement of particle due to convection current, is not significant under the volumetric heating of microwaves. As such, it is first assumed that the solid particles are uniformly distributed within the extraction solvent, and second that there is no relative movement of particles throughout the process. With this simplification, the number of distributed solid particles aligned along the radial, r and the vertical, z directions are respectively n and m, related as below:

$$\pi n^2 m = V_s \rho_t \tag{4}$$

$$\frac{n}{m} = \frac{R}{Z} \tag{5}$$

where V_s is the volume of the solvent, R is the radius of the extraction vessel, Z is the level of solvent in the vessel and ρ_t is the total number of particles per unit volume of solvent, calculated as follows:

$$\rho_t = \frac{1}{SF} \times \frac{1}{V_p \rho_p} \tag{6}$$

where SF is the solvent to solid ratio, V_p is the average volume of a particle and ρ_p is the intrinsic density of the particle.