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Mathematical modeling of flow behavior and cell structure formation during extrusion of starchy melts

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ABSTRACT

The primary purpose of this research was to develop a mathematical model for flow behavior of starchy melts inside an extruder barrel and bubble growth dynamics after exiting the extruder using mass, heat and momentum transfer equations and obtain the physical characteristics of the product, such as expansion ratio and bubble radius, using input parameters such as feed rate, screw speed, water input in the extruder and pre-conditioner, etc. The model was written in Visual Basic and experimentally validated using pilot-scale twin screw extrusion for processing of cereal-based cellular products. Process and product data were measured at different in-barrel moisture contents (19–28% dry basis) and experimental screw speeds (250–330 rpm). Experimental process parameters such as die temperature (T_{die}) (120.7–170.6 °C) and pressure (P_{die}) (3160–7683 kPa) and product expansion ratio (ER) (3.3–16.9) and cell size (R) (435–655 μ) compared well with simulated results viz., T_{die}(116.8–176.1 °C), P_{die}(3478–6404 kPa), ER(4.6–19.4) and R(426–728 μ).

1. Introduction

Extrusion cooking is a widely used method in various food and non-food applications (Lai and Kokini, 1991; Tang and Alavi, 2012; Devi et al., 2013; Koppel et al., 2014; Lakshmi Devi et al., 2014). Cellular structure in extruded foods and the way they are processed affect their mechanical properties and texture (Agbisit et al., 2007; Babin et al., 2007). Cell structure also affects oil uptake during post-extrusion steps such as frying and hence is related to oil content in snack products (Bouchon et al., 2003). Studying flow behavior of the melt inside an extruder helps in understanding the cell structure formation during extrusion. This can be done by using theoretical tools such as mathematical modeling.

The concept of modeling the extrusion process started in the beginning of 1940's with the characterization of flow of polymers. The understanding of the behavior of plastics and other polymers is comparatively easier, because of the homogeneity in structure and well characterized physical and rheological properties (Tadmor and Gogos, 1979; Karwe and Jaluria, 1990; Gopalakrishna et al., 1992). Thus the polymers possess a predictable behavior upon carrying out mechanical interactions and thermal processing. The changes upon interactions between bio-molecules and extruder are more complex (Chiruvella et al., 1996). In food extrusion, the first model of a twin-screw corotating extruder was published by Yacu (1985). This model was too general and pointed out the need for better definition of geometry of twin-screw extruder and behavior of product. Tayeb et al. (1989) published a model computing the pressure profiles and filled length in the extruder where the product is a homogeneous melt. They validated the model using maize starch and a simple screw profile. This model also found good agreement between predicted and literature experimental residence time distributions.

The modeling of bubble growth surrounded by a polymeric fluid under a given pressure started many years ago. A large number of studies were made for polymer systems with different degrees of complication (Barlow and Langlois, 1962; Yang and Yeh, 1966; Street, 1968; Mikic et al., 1970; Street et al., 1971; Amon and Denson, 1984; Arefmanesh et al., 1990, 1992; Venerus and Yala. 1997, Venerus et al., 1998; Venerus, 2001; Pai and Favelukis, 2002). A detailed review of mathematical modeling of bubble growth in polymer systems is provided by Alavi et al. (2003a).

Several studies have also focused on modeling bubble growth or shrinkage in biopolymer systems including processes such as extrusion, baking and drying (Shimiya and Yano, 1987; Fan et al.,

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1994, 1999; Achanta et al., 1997; Shah et al., 1998; Mitchell et al., 1998; Huang and Kokini, 1999). Detailed models were provided by Schwartzberg et al. (1995) for bubble growth at the microscopic level in vapor induced puffing in popcorn, and Alavi et al. (2003a, 2003b) for supercritical fluid (CO_2) extrusion of starchy melts.

The formation of cell structure in expanded extrudates is dependent on the expansion and subsequent collapse of the cells in the melt. This is controlled by the complex balance between the forces which drive deformation and forces which resist deformation and extensibility of the melt (Alavi et al., 2011). However, there are no studies in the literature which integrate the flow inside the extruder and bubble dynamics models. This shortcoming was addressed in the current study. The goal of this study was to develop a mathematical model for the flow behavior and cell structure formation during extrusion and obtain the physical characteristics of the extruded product (output parameters) such as expansion ratio, bubble radius, open cell fraction etc using the independent variables (input parameters) such as feed rate, screw speed, water input in the extruder and pre-conditioner etc. This model was developed with the objective of eventually using in a stochastic simulation of the extrusion process, which is described elsewhere (Manepalli, 2014).

2. Model development

2.1. Modeling the flow behavior inside the extruder

Tayeb et al. (1989) and Yacu (1985) developed a basic model for a twin screw extruder, which were used to develop the basic model inside the extruder. Pressure profile was developed based on Tayeb et al. (1989) and temperature profile was developed based on Yacu (1985). They did not consider the effect of thickness of the screw flight. Hence, the equations were modified to incorporate the screw thickness effect as well based on Rossen and Miller (1973). There were two sections inside the extruder: Solid conveying section and melt pumping section. The actual length of the melt pumping section was the parameter which was affected by screw profile, screw speed, throughput, viscosity of the material and the overall flow resistance (Yacu, 1985). The temperature increases very quickly in the melt pumping section. Viscosity of the material was based on temperature and moisture content and hence it changes as well. Hence, initial length of the melt was assumed. The temperature and pressure profiles were developed along the barrel and final temperature and pressure at the end of the barrel were obtained.

The pressure drop across the die was calculated based on the final temperature obtained at the end of the barrel. If the pressure drop across the die was greater than the pressure at the end of the barrel, the actual length of the melt was increased. If the pressure drop across the die was lesser than the pressure at the end of the barrel; the actual length of the melt was decreased and the same pressure and temperature profiles were developed. This iterative evaluation was done till the pressure drop was almost same as the final pressure at the end of the barrel.

2.1.1. Temperature profile

The viscous heat dissipation in the conveying section was negligible as the screws were only partially full. The effect of thermal energy provided by the barrel on the temperature evolution inside the extruder was assumed as negligible. Hence, the temperature does not increase in the conveying section. The temperature profile along the barrel was developed based on the mechanical energy generated. The material flowing inside the extruder was considered to be homogeneous non-Newtonian fluid following the power law. The complex chemical reactions, degradation of starch components and phase transitions such as starch gelatinization, protein denaturation etc. were neglected due to difficulty in modeling such reactions. The amount of energy generated (ΔE) from an element of thickness Δx of screw (Yacu, 1985) is

$$\Delta \mathrm{E} = \frac{4\mu N^2 \Delta x \left(\pi D - \sqrt{2Dh}\right)}{h} \tag{1}$$

where μ is viscosity of the melt given by Eq. (2), N is screw speed, D is the diameter of the screw and h is screw channel depth.

$$\mu = K\gamma^{n-1} \tag{2}$$

$$K = 4.224 \times \exp\left(\frac{2650}{T} - 25\frac{X_w}{1+X_w}\right)\ \mathrm{Pa\ s^n} \tag{3}$$

$$\gamma = \frac{\pi DN}{h} \tag{4}$$

where n is flow behavior index and K is consistency coefficient of the melt at temperature T and moisture content X_w and was modeled based on a similar equation from Parker et al. (1989) and Padmanabhan and Bhattacharya (1993).

The increase in temperature (ΔT_E) inside the extruder due to the energy generated (ΔE) (Yacu, 1985) was given by

$$\Delta T_E = \frac{\Delta \mathrm{E}}{\left(m_f C_p\right)} \tag{5}$$

where m_f is mass flow rate of the product inside the barrel and C_p is specific heat.

Specific mechanical energy (SME) during the extrusion was calculated by

$$\mathrm{SME} = \frac{\sum \Delta E}{m_f} \tag{6}$$

2.1.2. Pressure profile

No pressure was developed in the solid conveying section as the screws were only partially full. Hence, the entire pressure was generated in the melt pumping section. The pressure developed was calculated using the flow rate equation. Leakage flow i.e. the material leaking past the screw in the small gap between screw and barrel was ignored. Hence, the flow rate consists of only two components: Drag flow along the direction of flow and pressure flow acting in opposite direction to the direction of flow due to the generation of pressure (Tayeb et al., 1989).

$$\begin{aligned}\frac{Q_v}{lv} = {} & F_D \frac{1}{4}\pi N D^2 \cos\Phi \left[1 - \left(\frac{D_i^2}{D^2 - D_i^2}\ln\left(\frac{D}{D_i}\right)^2\right)\right]\left(1 - \frac{n_f e}{t}\right) \\ & - F_P \frac{1}{32\mu}\frac{\Delta P_E}{\Delta\theta}\left(D^2 - D_i^2\right)\left[1 - \left(\frac{2DD_i}{D^2 - D_i^2}\ln\left(\frac{D}{D_i}\right)^2\right]\right. \\ & \times \left(1 - \frac{n_f e}{t}\right)\end{aligned} \tag{7}$$

where Q_v is the volumetric flow rate, lv is channel width, D_i is internal screw diameter and Φ is screw pitch angle. The term $\left(1 - \frac{n_f e}{t}\right)$ is incorporated to include the effect of screw thickness