A review of dough rheological models used in numerical applications

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Abstract
The motivation for this work is to propose a first thorough review of dough rheological models used in numerical applications. Although many models have been developed to describe dough rheological characteristics, few of them are employed by researchers in numerical applications. This article reviews them in detail and attempts to provide new insight into the use of dough rheological models.

Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>$A'$</td>
<td>Relative increase in viscosity due to gelatinization, dimensionless</td>
</tr>
<tr>
<td>$b$</td>
<td>Index of moisture content effects on viscosity, dimensionless</td>
</tr>
<tr>
<td>$D$</td>
<td>Rate of deformation tensor</td>
</tr>
<tr>
<td>$k_a$</td>
<td>Reaction transmission coefficient, $^\circ K^{-1} sec^{-1}$</td>
</tr>
<tr>
<td>$MC$</td>
<td>Moisture content, dry basis, decimal</td>
</tr>
<tr>
<td>$MC_r$</td>
<td>Reference moisture content, dry basis, decimal</td>
</tr>
<tr>
<td>$m$</td>
<td>Fluid consistency coefficients, dimensionless</td>
</tr>
<tr>
<td>$n$</td>
<td>Flow behavior index, dimensionless</td>
</tr>
<tr>
<td>$R$</td>
<td>Universal gas constant, $1.987 \text{ cal/g mol \cdot K}$</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Index of molecular weight effects on viscosity, dimensionless</td>
</tr>
<tr>
<td>$\eta$</td>
<td>Apparent viscosity, $Pa.sec$</td>
</tr>
<tr>
<td>$\dot{\gamma}$</td>
<td>Shear rate, $sec^{-1}$</td>
</tr>
<tr>
<td>$\varphi$</td>
<td>Strain history, dimensionless</td>
</tr>
<tr>
<td>$\psi$</td>
<td>Time-temperature history, $K/sec$</td>
</tr>
<tr>
<td>$\Delta E_v$</td>
<td>Free energy of activation, cal/g mol</td>
</tr>
<tr>
<td>$\sigma_0$</td>
<td>Yield stress, $Pa$</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Velocity, $m/s$</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Stress tensor</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Stress, $Pa$</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Relaxation time, $sec$</td>
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1. Introduction

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Bread is the most important daily meal of people in the world. Furthermore, improving the quality of bread baked products and the development of relevant apparatuses completely depend upon a comprehensive knowledge of dough rheology. Therefore, it is essential to gain a deep knowledge of dough behavior and to ensure the accuracy of the measured rheological data. However, finding a constitutive model that has all accurate molecular and structural arguments to simulate the linear and non-linear properties of wheat flour dough is a tough challenge due to the complicated nature of wheat flour doughs. The challenge is due to the fact that once water, wheat flour dough and small amount of ingredients such as salt, yeast, preservatives, etc. are combined, a cohesive viscoelastic substance is produced called dough. All of these ingredients can considerably change the rheological properties of the dough during mixing, and make it rheologically complex. In fact, the combination of these ingredients produces a three dimensional network called gluten which has a crucial role in complex viscoelastic behavior of wheat flour dough.

Despite these complexities, the rheology of wheat flour dough has been an important of scientific researches topics. Over the years, several efforts have been made to experimentally and theoretically evaluate dough properties that affect its flow behavior. In this approach, Schofield and Scott Blair might be considered as pioneer researchers who studied the flow behavior of the wheat flour doughs. They also demonstrated that dough behaves both like a Hookean solid and also like a Newtonian liquid.

In order to provide information on the rheological properties of wheat flour dough, the measurement of dough material properties has been obtained using empirical instruments such as Farinograph, Alveograph, Extensigraph and Mixograph and capillary rheometry (shear and extensional viscosities for dough) and the Phan-Thien-Tanner model. In these studies they often employed the Brabender Farinograph to predict the measured rheological behavior of wheat flour dough at different moisture contents.

However, the limited application of their results and difficulties encountered in correlation between the quality of the baked products and values obtained from them complicate the task of characterizing the flow behavior of dough. In 1954, Cunningham and Hlynka tried to characterize the linear viscoelastic properties of dough using distribution of relaxation times. In order to characterize the viscoelastic properties of flour dough, Bagley and Christianson used the BKZ elastic fluid theory. Thereafter, the upper convected Maxwell model was used by Bagley et al. Till 1990, the aim of studies had been to simulate the rheological properties of wheat flour dough without considering its non-linear behavior. Dus and Kokini, therefore, tried to describe the steady state shear viscosity and oscillatory shear properties of hard flour dough using the five-parameter Bird-Carreau model. Bagley used of the upper-convected Maxwell model to explain the dough behavior in biaxial extension flow.

Before 1995, less attention was paid to the measurements of uniaxial and biaxial extensional rheological properties of wheat flour doughs in the strain rates region. Therefore, Wang and Kokini showed that one can profit by using the Wagner model to predict transient shear properties and uniaxial and biaxial extensional rheological properties of gluten doughs and also to simulate nonlinear shear properties. Dhanasekharan and Kokini used the Phan-Thien Tanner model as a more realistic model describing dough-like fluids for 3-D numerical modeling of viscoelastic flow in a single screw extrusion and then analyzed the effect of viscoelasticity considering a stationary screw and rotating barrel. Phan-Thien and Safari-Ardi derived relaxation spectra from both dynamic and relaxation data for Australian strong flour-water dough and reported dynamic oscillatory and stress relaxation data.
Till that time, most of the reported models simulating the rheological properties of wheat flour doughs or their protein components had been either linear differential viscoelastic models like the generalized Maxwell models or nonlinear integral viscoelastic models such as the Bird-Carreau and Wagner models [19].

Using the Phan-Thien Tanner, White-Metzner model and the Giesekus model applied by Dhanasekharan et al. [12] to study whole wheat flour doughs, Dhanasekharan et al. [10] compared the validity of these models to predict the steady shear and transient shear properties of gluten dough. Using the theory of rubber elasticity, Leonard et al. [19] studied the rheology of wheat flour doughs at large extensional strains and reported an intermediate behavior between rubber elasticity and plastic flow for dough.

In order to evaluate the constitutive equations introduced by Phan-Thien et al. [20], the large-strain oscillatory shear flow of flour dough was studied by Phan-Thien et al. [21]. Their results indicated that a model with a shear-rate dependent viscosity alone is inadequate to describe the response of flour dough since the material response is significantly non-linear which is mainly due to the strain softening behavior of the material. Furthermore, in order to be able to differentiate between different flour types, tests at large-strain deformations are required.

Although, the literature has explored numerous papers dealing with both theoretical and experimental methods of characterizing dough like materials, there are only a few scattered references devoted to evaluating the application of reported constitutive equations of wheat flour dough in numerical simulations. In characterizing dough behavior and its effects on different flow patterns, the most notable works belong to Kokini et al. [13, 22, 23, 24 and 26] and Phan-Thien et al. [18, 21, 25 and 26]. A numerical modeling of viscoelastic flow in a single screw extrusion conducted by Dhanasekharan and Kokini [13] can be considered as one of the earliest dough numerical simulations. Thereafter, Connelly and Kokini [23] conducted a simultaneous scale-up of mixing and heat transfer analysis of dough behavior in such a single screw extruder. In this study, in order to take into account the variations in the rheology of wheat flour dough, the Mackey and Ofoli viscosity model was applied. With regards to attempts to examine the mixing ability of single and double screw mixers, significantly Kokini et al. [23,24,26,27] examined the effects of shear thinning and differential viscoelasticity on dough mixing behavior.

For the first time, Binding et al. [28] examined the combination of numerical and experimental studies of dough kneading in a partially filled cylindrical mixer, with either one or two eccentric stirrers. The numerical procedure utilized a parallel numerical method based on a finite element semi implicit time-stepping Taylor-Galerkin/pressure-correction scheme. The same approach was then employed [29,30,31] to analyze the wetting and peeling of dough like material on solid surfaces considering the free surfaces, kinematics and stress fields produced by variations of stirrers’ speed and changing geometry mixer. For fluid rheology, Carreau-Yasuda, constant viscosity Oldroyd-B and two shear-thinning Phan-Thien/Tanner constitutive models were employed. Velocity profiles and relevant peeling stress were calculated using laser scatter technology, Laser Doppler Anemometry (LDA) and a video capture technique. Results revealed good agreements between the numerical and experimental studies.

It is not feasible here to even attempt to review many of efforts that have been made to explore both theoretical and experimental ways of characterizing and evaluating dough; however, Bagley [9], Kokini [19] and Phan-Thien et al. [21] have cited some useful references. Despite all these attempts, there is still a great need to understand the necessary constitutive equations to accurately describe wheat flour dough behavior. According to the author’s knowledge, there is no work in the literature that has reviewed the rheological models used in numerical applications of dough like materials. Therefore, this study aims to review the constitutive equations applied in numerical simulations of dough flow behavior during, approximately, the period 1987-2007. The
review represents all parameter values of these rheological models.

2. Dough rheological model

The characterization of a non-Newtonian, steady state, incompressible flow, is provided by the conservation of mass and momentum equations, respectively.

\[ \nabla \cdot \mathbf{u} = 0 \]  
(1)

\[ \nabla \cdot \sigma = 0 \]  
(2)

The stress tensor \( \sigma \) is defined by Eq. (3), where a constitutive equations or rheological model is required to define the deviatoric stress tensor \( \tau \). In constitutive models, the deviatoric stress tensor is described as the sum of the viscoelastic component \( \tau_1 \), and the purely Newtonian component \( \tau_2 \) (Eq. (4)).

\[ \sigma = -pI + \tau \]  
(3)

\[ \tau = \tau_1 + \tau_2 \]  
(4)

Where \( \tau_2 \) is given by Eq. (5) where \( D \) is the rate of deformation tensor.

\[ \tau_2 = 2\eta D \]  
(5)

Among all attempts that have been made to formulate the constitutive equations, those for viscoelastic materials have encountered difficulties due to their considerable nonlinearity [32]. In characterizing dough rheological behavior, more powerful models are linear differential viscoelastic models like the generalized Maxwell models, nonlinear integral viscoelastic models such as the Bird-Carreau and Wagner models and nonlinear differential models. The latter is of the particular interest in numerical simulations, which is used for process design, optimization and scale-up. [19] However, till 2000, due to high computational costs and lack of advanced software, there was a scarcity of work in viscoelastic flow analysis in extruder channels. However, nowadays, complicated calculations are possible using the current computational technology and available software tools [19].

Only a selection of the viscosity models applied in numerical applications is given here; more complete descriptions of such models and fundamental knowledge of non Newtonian models are available in many references [33-44].

2. 1. The power law (Ostwald de Waele) model

The relationship between shear stress and shear rate for a shear-thinning fluid can often be approximated by a straight line over a limited range of shear rate (or stress). For this part of the flow curve, an expression of the following form is applicable:

\[ \tau = m\dot{\gamma}^n \]  
(6)

Where \( m \) and \( n \) are the fluid consistency coefficient and the flow behavior index respectively. The apparent viscosity for the so-called power-law (or Ostwald de Waele) fluid is thus given by Eq. (7) [38].

\[ \mu = \tau_{xx}/\dot{\gamma}_{xy} = m(\dot{\gamma}_{xy})^{n-1} \]  
(7)

The power-law models are the preferred rheological model due to their ability to predict velocity and pressure distributions in uniform flows [19] and the simplest representation of shear thinning behavior [38]. However, their application in the process engineering encounters following shortcomings:

a. These models should be applied over only a limited range of shear rates and therefore the fitted values of \( m \) and \( n \) will depend on the range of shear rates [38].

b. They are not able to predict zero and infinite shear viscosities [38].

c. The dimensions of the flow consistency coefficient, \( m \), depend on the numerical value of \( n \) and therefore the \( m \) values must not be compared when the \( n \) values differ [38].

d. They are seldom able to provide accurate predictions of measurements of important operating parameters such as Specific Mechanical Energy (SME) and Residence Time Distribution (RTD) [19].
2. 2. Maxwell model

Certainly, the most striking feature connected with the deformation of a viscoelastic substance is its simultaneous display of 'fluid-like' and 'solid-like' characteristics [38]. Consequently, the idea of a linear combination of elastic and viscous properties by using mechanical analogues involving springs (elastic component) and dash pots (viscous action) has affected the early efforts in quantitative description of viscoelastic behavior [38].

Like other viscoelastic materials, dough was primarily characterized in terms of a simple Maxwell model [8]. As shown in Fig. 1, the Maxwell model can be represented by a purely elastic spring and a purely viscous damper connected in series, with the individual strain rates of \( \dot{\gamma}_1 \) and \( \dot{\gamma}_2 \) respectively. This model follows the following Eq. (8) [38].

\[
\dot{\gamma} = \dot{\gamma}_1 + \dot{\gamma}_2 = \frac{d\gamma_1}{dt} + \frac{d\gamma_2}{dt}
\]

Combining above equation with the Hooke's law of elasticity and Newton's law of viscosity, one can obtain:

\[
\tau + \lambda \dot{\tau} = \mu \dot{\gamma}
\]

In which \( \tau \) is the stress tensor, \( \dot{\gamma} \) total strain rate tensor, \( \dot{\lambda} \) is the time derivative of \( \tau \), \( \mu \) is the viscosity of the dashpot (viscose) fluid and \( \lambda (= \mu / G) \) is the relaxation time, which is a characteristic of the fluid. An important feature of the Maxwell model is its predominantly fluid-like response. A more solid-like behavior is obtained by considering the Voigt model which is represented by the parallel arrangement of a spring and a dashpot, as shown in Fig. 2.

Subsequent research showed that dough possesses complex viscoelastic properties that can only be represented by a generalized Maxwell model which includes a distribution of relaxation times (Fig. 3) [8, 14, 45, and 46].

The Upper Convected Maxwell model is a generalization of the Maxwell material for the case of large deformations using the Upper convected time derivative. The model was proposed by James G. Oldroyd [47] and is represented by Eq. (10).

\[
\tau + \lambda \dot{\tau} = 2\mu D
\]

\( \tau \) is the stress tensor; \( \lambda \) is the relaxation time; \( \nu \) is the upper convected time derivative of stress tensor; \( \mu \) is the material viscosity at steady simple shear and \( D \) is the tensor of the deformation rate.

The convected derivative \( \dot{\nu} \) and the rate of deformation tensor are defined by:

\[
\dot{\nu} = \frac{D\tau}{Dt} - [\nabla \dot{u} \tau] - [\tau, \nabla \dot{u}^T]
\]

\[
\tau = \frac{\partial \tau}{\partial t} + \nabla.(\mu \dot{u}) - (\nabla \dot{u})^T \tau - \tau.(\nabla \dot{u})
\]

\[
D = \frac{1}{2}[(\nabla \dot{u}) + (\nabla \dot{u})^T]
\]

Using the upper convected Maxwell model, Bagley et al. [16] tried to interpret the results of extensional deformation of viscoelastic dough. Their study showed that the upper convected Maxwell model is particularly convenient for an initial analysis of a constant crosshead speed experiment on dough, and the governing differential equations can be easily solved numerically [16].

2. 3. Oldroyd-B

Another form of viscoelastic model is Oldroyd-B model [32]:

\[
\tau_1 + \lambda_1 \tau_1 - 2\eta_1 (d + \lambda_2 d) = 0
\]

\( d \) is the rate of deformation tensor, \( \eta_0 \) is the shear viscosity, \( \lambda_1 \) is the relaxation time and \( \lambda_2 \) is the second relaxation parameter (retardation
time \[33\]). As it was previously (Eq. (11)) described \(\nabla\) is upper convected derivative.

1) \(\lambda_1 = 0\) the model simplifies to a second-order fluid with a vanishing second normal stress coefficient \[33\].

2) \(\lambda_2 = 0\) the model reduces to the convected Maxwell model \[33\].

3) \(\lambda_1 = \lambda_2\) the model reduces to a Newtonian fluid with viscosity \(\eta_1\) \[33\].

2. 4. Cross and Carreau model

The cross model \[48\] is a four parameter model which is written as \[34\]:

\[
\eta = \eta_\infty + \frac{\eta_0 - \eta_\infty}{1 + (\alpha_c \gamma)^m}
\]

(14)

\[
\eta = \eta_\infty + \frac{\eta_0 - \eta_\infty}{[1 + (\lambda_c \gamma)^2]^N}
\]

(15)

where \(\alpha_c\) and \(\lambda_c\) are time constants related to the relaxation times of the polymer in solution.

Since the magnitudes of 1700 of food polymer dispersions with concentrations of practical interest are usually very low in magnitude, they are difficult to determine experimentally. Therefore, to avoid consequent errors in estimation of the other rheological parameters in Eqs. (14) and (15), \(\eta_\infty\) is usually neglected \[49,50\].

\[
\tau = 2\eta_0(1+\lambda_1 \gamma)^{n-1}D
\]

(16)

In general, the model of Cross has been used in studies in Europe and that of Carreau in North America.

2. 5. Bird-Carreau model

The Bird-Carreau model \[51\] is a nonlinear extension of the generalized Maxwell model. It uses four empirical constants \((\alpha_1, \lambda_1, \alpha_2\) and \(\lambda_2\)) and the zero shear rate viscosity, \(\eta_0\). Two constants, \(\alpha_1\) and \(\lambda_1\) are typically obtained from a logarithmic plot of \(\eta\) vs. \(\gamma\) and the

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![Fig. 1. Schematic of the Maxwell model.](image1)

![Fig. 2. Schematic of the Voigt model.](image2)

![Fig. 3. Schematic of the generalized Maxwell model.](image3)

and \(m\) and \(N\) are dimensionless exponents.
other two constants $\alpha_2$ and $\lambda_2$ are obtained from a logarithmic plot of $\eta$ vs. $\omega$ [52]. ($\eta$ is the viscosity function, $\eta'$ is the dynamic viscosity and $\omega$ is the frequency) [53]. The Bird-Carreau prediction for $\eta$ is [52, 53].

\[
\eta = \sum_{\rho=1}^{\infty} \frac{\eta_{\rho}}{1 + (\lambda_{1\rho} \gamma)^2}
\]  

(17)

At large shear rates the above equation is approximated by [53]:

\[
\eta = \frac{\pi \eta_0}{Z(\alpha_1) - 1} \cdot \frac{(2^{\alpha_1 \lambda_{2\rho} \gamma} (1 - \alpha_1) / \alpha_1)}{2 \alpha_1 \sin(1 + \alpha_1 / 2 \alpha_1 \pi)}
\]  

(18)

\[
\lambda_{1\rho} = \lambda_1 \cdot \left( \frac{2}{\rho + 1} \right)^{\beta_1}
\]  

(19)

\[
\eta_{\rho} = \eta_0 \cdot \lambda_{1\rho} \sum_{\rho=1}^{\infty} \lambda_{1\rho}
\]  

(20)

\[
Z(\alpha_1) = \sum_{\rho=1}^{\infty} k^{-\alpha_1}
\]  

(21)

The Bird-Carreau prediction for $\eta$ is [53]:

\[
\eta = \sum_{\rho=1}^{\infty} \frac{\eta_{\rho}}{1 + (\lambda_{2\rho} \gamma)^2}
\]  

(22)

and at high frequencies $\eta'$ is approximated by [53]:

\[
\eta' = \frac{2 \pi \eta_0}{Z(\alpha_1) - 1} \cdot \frac{(2^{\alpha_1 \lambda_{2\rho} \gamma} (1 - \alpha_1) / \alpha_1)}{2 \alpha_1 \sin(1 + 2 \alpha_2 - \alpha_1 / 2 \alpha_2 \pi)}
\]  

(23)

The Bird-Carreau model approximates the polymeric material as a loosely held structure where temporary network junctions are continuously formed and then destroyed during shear. This structural concept appears to be quite appropriate for wheat-flour dough since wheat gluten is a high molecular weight biological polymer whose components have been demonstrated to form entanglements [8]. These models are appropriate for liquid-like materials; they may yield the right behavior in a specific type of flow, but they are not appropriate in all types of deformations [21]. More complete description of this model is provided in many publications especially in [51] and [52].

The Bird-Carreau-Yasuda model is more complex and has the advantage of predicting both Newtonian and pseudo plastic behavior of polymers, as well as the transition region and contains five parameters. Mathematically the Bird-Carreau-Yasuda model can be expressed as follows [54]:

\[
\frac{\eta - \eta_{\infty}}{\eta_{0} - \eta_{\infty}} = [1 + (\lambda \gamma)^{\gamma}]^{n - (n - 1) a}
\]  

(24)

where $\eta$ is shear viscosity, $\eta_0$ is the zero-shear-rate viscosity, $\eta_{\infty}$ is the infinite-shear-rate viscosity, $\lambda$ is the time constant, $\gamma$ is the shear rate, and $n$ is the power law index. In the original Bird-Carreau model the constant $a$ equals to 2. In many cases the infinite-shear-rate viscosity is negligible, reducing Eq. (24) to a three parameter model [54].

Dus and Kokini [6] simulated the nonlinear viscoelastic properties of wheat-flour dough with the Bird-Carreau model. Although, this model showed significant deviation from primary normal stress coefficient data, it was adequate to predict steady shear viscosity and small amplitude oscillatory properties. Thereafter, Wang and Kokini [8] investigated the applicability of the Bird-Carreau model in predicting steady shear viscosity and primary normal stress coefficient data of gluten dough as a function of water content at two temperatures. The results reported that the small amplitude oscillatory shear properties could be successfully simulated using the Bird-Carreau constitutive model. However, the primary normal stress coefficient was overpredicted.

2. 6. Giesekus-Leonov model

Giesekus [55] proposed a constitutive model based on a concept of configuration-dependent
molecular mobility. According to this model, the viscoelastic component of the extra stress tensor is represented by Eq. (25) with four parameters $\eta_1, \eta_2, \lambda$ and $\alpha$. Due to the highly nonlinear nature of the model equations, all of the properties need to be obtained numerically [12].

$$I_{ij} + \alpha \frac{\lambda}{\eta_1} \tau^1_{ij} \tau^1_{ij} + \lambda \tau_{ij} = 2\eta_i \gamma_{ij}$$  \hspace{1cm} (25)

The parameter $\alpha$ is the dimensionless Giesekus model mobility factor and controls the extensional viscosity and the ratio of second normal stress difference to the first one. $\alpha > 0$ represents shear thinning behavior [12].

2.7. White-Metzner model

Modification of the viscosity and relaxation parameter as a function of the shear rate, $\dot{\gamma}$ leads to the White-Metzner model. This model exhibits shear thinning, not because of nonaffine motion, but because the relaxation is accelerated at high strain rates, where the relaxation is faster than any deformation [32]. The use of molecular considerations based on nonaffine Network Theories will result in the PTT model [32] which will be discussed in the next section.

In this model the viscoelastic component of the extra stress tensor is given by Eq. (26) [12].

$$\tau^1_{ij} + \lambda \tau^1_{ij} = 2\eta_i \gamma_{ij}$$ \hspace{1cm} (26)

The functions $\eta_1$ and $\lambda$ can be obtained from the experimental shear viscosity curve and the experimental first normal stress curve, respectively. Constant, Power law, and Bird-Carreau types can be considered for these two functions [12].

2.8. Phan-Thien-Tanner model

The literature describes many attempts to improve the Upper Convected Model [35]. In this approach, the model proposed by Phan Thien and Tanner [20,18,26] was claimed to correctly describe the nonlinear behavior of viscoelastic fluids, especially viscoelastic properties of wheat flour doughs [56]. The original Phan-Thien Tanner equations was written using both of the following modifications simultaneously: the Gordon Schowalter derivative and the segment kinetics term [35]. It employs specific forms for the creation and destruction rates of the network junctions in the network theory of Lodge and Yamamoto [56].

Although the Phan-Thien Tanner model overpredicts the shear viscosity at higher shear rates and the transient and extensional properties, it accurately predicts the zero shear viscosity $0$ and seems to be suitable for numerical simulations of wheat flour doughs. It is worth noting that, compared to the integral models such as the Bird-Carreau and Wagner models, the differential models such as the Phan-Thien Tanner model provide robust numerical algorithms [56] and exhibits good behavior in FEM simulations [23]. The interested reader is referred to [35] for more accurate comparison between the Wagner model (as integral model) and the PTT model.

In the PTT model, the extra stress tensor is considered as the sum of the viscoelastic component $\tau_1$, and the purely Newtonian component $\tau_2$ (Eq. (27)) [12].

$$\tau = \tau_1 + \tau_2$$ \hspace{1cm} (27)

In which $\tau_2$ is given by Eq. (28) where $D$ is the strain rate tensor.

$$\tau_2 = 2\eta_2 D$$ \hspace{1cm} (28)

The final form of the PTT model for the viscoelastic component $\tau_1$ is expressed by Eq. (29) [12].

$$\exp \left[ \frac{\lambda}{\eta} \tau_1 + \lambda \left( 1 - \frac{\xi}{2} \right) \tau_1 + \frac{\xi}{2} \right] = 2\eta D$$ \hspace{1cm} (29)
\[ \Delta = \frac{Dt}{\tau} + [\nabla u.\tau] + [\tau.\nabla u^T] \tag{30} \]

\( \varepsilon \) and \( \xi \) are the adjustable parameters and \( \lambda \)
and \( \eta \) are the partial viscosity and relaxation time respectively which can be measured from the equilibrium relaxation spectrum of the fluid [12]. The operators \( \nabla \) and \( \Delta \) are the upper convected derivative (Eq. (11)) and lower convected derivative (Eq. (30)), respectively. The Phan-Thien Tanner model can be solved using a single relaxation time or multiple relaxation times, similar to the Giesekus model [12].

2.9 Mackey & Ofoli model

Modifying the model of Morgan et al. [56], Mackey et al. [57] proposed a model for the viscosity of starch-based products related in Eq. (31).

\[
\eta = \left[ \left( \frac{\sigma_2}{\gamma} \right)^n_1 + \eta_\infty \dot{\gamma}^{n_2-n_1} \right]^{1/n_1}
\]

\[
\{ \exp[\left( \Delta E/v \right) + b(MC - MCPP)] \}
\]

\[
\{ 1 + A[1 - \exp(-k_2\psi)]^2(1 - \exp(-d\varphi)) \}
\]

\[
\tau_{(i)} = \frac{D\tau}{Dt} - [(\nabla u\cdot\tau) + \tau.\nabla u] \tag{33}
\]

Osswald and Hernández-Ortiz [33] provided a valuable general form of viscoelastic models represented in Eq. (32).

\[
Y_{\tau} + \lambda_{(i)} \tau_{(i)} + \omega_{(i)} \{ \gamma \cdot \tau + \tau \cdot \gamma \} = \eta_0 \{ \gamma + \lambda_{(i)} \gamma \}
\tag{32}
\]

where \( \tau_{(i)} \) is the first contravariant convected
time derivative of the deviatoric stress tensor and represents rates of change with respect to a convected coordinate system that moves and deforms with the fluid. All constants are defined in Table. 1 for various viscoelastic models commonly used to simulate dough like materials. The convected derivative of the deviatoric stress tensor is defined by Eq. (33).

This model provides accurate results for predicting the viscosity of relatively pure starches such as potato flour [57] and corn starch [7] and does not account for non starch components. However, Mackey and Ofoli [7] evaluated the viscosity of whole wheat flour doughs (which contains significant levels of non starch components) at low to intermediate moisture content. They incorporate the effects of shear rate, temperature, moisture content, time-temperature history, and strain history. Due to the presence of flour components such as bran, protein, and lipids, (which the model does not account for) the accuracy of rheological modeling for whole wheat flour was not nearly as good as had been observed in previous studies of corn starch and potato flour.

Similar summaries of viscoelastic models using general forms can be found in other references [36].

3. Models and parameters used in numerical applications

Vergnes and Villemaire [58] investigated the effects of temperature, moisture content and intensity of the treatment on the rheological behavior of a molten maize starch in a low hydrated phase. In this approach, they applied a power law model with an exponential dependence on temperature, water content and mechanical energy provided to the product before measurement. Moreover, they introduced a dependence on temperature and water content for the pseudoplasticity index \( m \), which has been observed in different papers [59, 60] but never quantified. They have also summarized different expressions that had been reported before 1987 in the literature to describe the rheological behaviour of starchy products in three simplified expressions [58]:

\[
\eta = K\gamma^{m-1} \tag{34}
\]

\[
\eta = K_e \exp\left( \frac{E}{RT} \right) \exp[-\alpha MC]\gamma^{m-1} \tag{35}
\]

\[
\eta = K_e \exp(-bT) \exp[-\alpha MC]\gamma^{m-1} \tag{36}
\]
Table 1. Definition of constants in Eq. (32)[33].

<table>
<thead>
<tr>
<th>Constitutive Model</th>
<th>Parameters</th>
</tr>
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<tbody>
<tr>
<td>Model Parameters</td>
<td>$Y$</td>
</tr>
<tr>
<td>Generalized Newtonian</td>
<td>$\lambda_1$</td>
</tr>
<tr>
<td>Upper Convected Maxwell</td>
<td>$\lambda_1$</td>
</tr>
<tr>
<td>White-Metzner</td>
<td>$\lambda_1(Y)$</td>
</tr>
<tr>
<td>Pahn-Thien Tanner -1</td>
<td>$\exp(-\varepsilon(\lambda/\eta_0)\mu\tau)$ $\lambda$ $1/2 \xi \lambda$</td>
</tr>
<tr>
<td>Pahn-Thien Tanner -2</td>
<td>$1 - \varepsilon(\lambda/\eta_0)\mu\tau$ $\lambda$ $-1/2 \xi \lambda$</td>
</tr>
<tr>
<td>Giesekus</td>
<td>$1$</td>
</tr>
</tbody>
</table>

Eq. (35) has been used by Fletcher et al. [61] and Senouci et al. [62] to characterize maize grits, and by Cervone and Harper [60] in the case of pregelatinised maize flour. Eq. (36) particularly has been used by Yacu [59] on wheat starch [58]. Vergnes and Villemaire [58] showed that in comparing the results obtained, the main difficulty comes from the variety of products. Table 2 shows the scatter of the predicted parameters characterizing the viscosity over a wide range, even for equal products. Moreover, they claimed that their results are the first to take into account the influence of thermomechanical history on viscosity. Facilitating the progress achieved over the years, more researches have been carried out.

In order to summarize this paper and also to provide a useful and complete collection of models, their relevant parameters and applications which simplifies furthere access, a large number of constitutive equations employed for the simulation of dough like materials are summarized in Table 2.

4. Conclusions

Understanding the complex behavior of dough-like materials and interpreting it as one general equation require a vast knowledge of the characteristics and formation of this complex material. Since rheometers do not provide the necessary information for all important rheological properties, constitutive equations are ultimate tools for effective control of process.

The development of valuable models for complex dough behavior and the search for appropriate constitutive equations to describe this complex behavior have been a high priority of most scientific researches. However, understanding the mechanical behavior of wheat flour dough is a formidable challenge. Consequently, due to high computational costs, there has been a scarcity of work in numerical simulation of the flow behavior of the wheat flour dough, particularly in the numerical simulation of the viscoelastic flow analysis in the relevant dough preparation apparatuses.

Perhaps Vergnes and Villemaire’s [58] effort can be considered as the pioneer researches conducted in categorizing and comparing reported models for starchy products, generally, and for wheat dough, particularly. In this study, the authors try to provide a useful collection of models which simplifies further access of researchers. This approach can be developed in the near future by studying the rheological behavior of other starchy products.
References


Table 2. Rheological models and parameters used in different researches

<table>
<thead>
<tr>
<th>Researcher</th>
<th>Model Name</th>
<th>Products</th>
<th>Eq</th>
<th>Water content (dry basis) (wt. %)</th>
<th>Temperature (°C)</th>
<th>n</th>
<th>K0 (Pa.s)</th>
<th>E/R</th>
<th>α</th>
<th>β</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vergnes and Villenaire[38]</td>
<td>Power Law Model with influence of temperature and water content and thermomechanical treatment</td>
<td>Maize flour</td>
<td>34</td>
<td>47</td>
<td>88</td>
<td>0.34</td>
<td>17200</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Maize flour</td>
<td>34</td>
<td>28-54</td>
<td>90-150</td>
<td>0.356</td>
<td>36</td>
<td>4388</td>
<td>10.1 (a)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Maize grits</td>
<td>34</td>
<td>45</td>
<td>130</td>
<td>0.22</td>
<td>18700</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Maize grits</td>
<td>35</td>
<td>22-59</td>
<td>70-175</td>
<td>0.61</td>
<td>664</td>
<td>993</td>
<td>4.3 (a)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Maize grits</td>
<td>35</td>
<td>15.3-18.7</td>
<td>153-168</td>
<td>0.68</td>
<td>4.9</td>
<td>3966</td>
<td>3 (a)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Dehydrated potato</td>
<td>35</td>
<td>21.5-157</td>
<td>82-142</td>
<td>0.21</td>
<td>773</td>
<td>1507</td>
<td>2 (a)</td>
<td>-</td>
</tr>
<tr>
<td>For Maize starch and introducing a table of researches before (1987) for different starch products</td>
<td>Wheat starch</td>
<td>36</td>
<td>25</td>
<td>150-170</td>
<td>0.3-0.7</td>
<td>182600</td>
<td>7</td>
<td>0.005</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Maize starch</td>
<td>35</td>
<td>26-49</td>
<td>110-170</td>
<td>0.27-0.56</td>
<td>7.04 (c)</td>
<td>4250</td>
<td>10.6 (b)</td>
<td>-</td>
</tr>
</tbody>
</table>

(a) dry basis, (b) wet basis, (c) for a mechanical energy of 5 × 108 J/m3

\[
\eta = K_0 \exp(-bT) \exp[-\alpha \cdot MC]^{\gamma^*+1}
\]

\[
\eta = K_1 \exp\left(\frac{E}{RT}\right) \exp[-\alpha \cdot MC]^{\gamma^*+1}
\]

\[
\eta = K \gamma^{\alpha+1}
\]
<table>
<thead>
<tr>
<th>Researcher</th>
<th>Model Name</th>
<th>Model</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dhamasekharan et al. [12]</td>
<td>Phan-Thien Tanner Model</td>
<td>$\eta = \eta_\infty + (\eta_0 - \eta_\infty)(1 + \lambda_\gamma^\gamma \gamma^2)^{\beta_\gamma^{1/2}}$</td>
<td>$\eta_\infty$</td>
<td>$4\times10^6$</td>
</tr>
<tr>
<td></td>
<td>Giesekus-Leonov Model</td>
<td>$\lambda(\gamma) = \lambda_0(1 + \lambda_\gamma^\gamma \gamma^{2(\beta_\gamma^{1/2})})$</td>
<td>$\lambda_\gamma$</td>
<td>$1\times10^5$</td>
</tr>
<tr>
<td></td>
<td>White-Metzner Model</td>
<td>$\tau_2 = 2\eta_\gamma \gamma$</td>
<td>$\tau_2$</td>
<td>$0.35$</td>
</tr>
<tr>
<td></td>
<td>Hard Wheat Bread Dough</td>
<td>$\tau = \tau_1 + \tau_2$</td>
<td>$\tau$</td>
<td>$0.35$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\sigma = pI + \tau$</td>
<td>$\sigma$</td>
<td></td>
</tr>
<tr>
<td>Dhamasekharan &amp; Kokini [13]</td>
<td>Phan-Thien Tanner Model</td>
<td>$\exp\left[s\frac{2}{\eta}\tau_2(\tau_1)\right] + \lambda\left[\frac{3}{2}\tau_1 + \frac{3}{2}\tau_2\right] = 2\eta_\gamma D$</td>
<td>$\lambda(s)$</td>
<td>$1$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\tau_2 = 2\eta_\gamma \gamma$</td>
<td>$\tau_2$</td>
<td>$1\times10^5$</td>
</tr>
<tr>
<td></td>
<td>Hard Wheat Bread Dough</td>
<td>$\tau = \tau_1 + \tau_2$</td>
<td>$\tau$</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\sigma = pI + \tau$</td>
<td>$\sigma$</td>
<td></td>
</tr>
</tbody>
</table>
## Dough Parameters

<table>
<thead>
<tr>
<th>Researcher</th>
<th>Model Name</th>
<th>Model</th>
<th>Parameter &amp; Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conolly &amp; Kokini</td>
<td>Phan-Thien Tanner</td>
<td>Model</td>
<td>$\lambda(s)$ 888888.9</td>
</tr>
<tr>
<td></td>
<td>Model</td>
<td></td>
<td>$\eta_1 (Pa.s)$ 0.08</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\varepsilon$ 0.01</td>
</tr>
<tr>
<td>Breuillet et al.</td>
<td>Power Law Model</td>
<td></td>
<td>$\tau = K(\gamma)^n$ 818</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$n$ 0.57, $K$ 72</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\eta_0, \eta_m$ 818</td>
</tr>
<tr>
<td>Ding &amp; Webster</td>
<td>Carreau Yasuda</td>
<td>Model</td>
<td>$\eta_0 = 1.05 \text{ (Pa.s)}$, $\eta_m = 0.001 \text{ (Pa.s)}$, $\lambda = 0.083 \text{ (s)}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Baloch &amp; Webster</td>
<td>Newtonian</td>
<td></td>
<td>$\tau_s = 2\mu D$, $\eta/\eta_c = 0.001$, $\eta_c = 1.05, 105 \text{ (Pa.s)}$</td>
</tr>
</tbody>
</table>

The single-mode Phan-Thien Tanner nonlinear, viscoelastic fluid model was used with parameters for a dough-like material [23].
<table>
<thead>
<tr>
<th>Researcher</th>
<th>Model Name</th>
<th>Model</th>
<th>Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baloch &amp; Webster [31]</td>
<td>Carreau</td>
<td>[ \tau_\text{c} = \frac{2 \eta \tau}{1 + (\lambda \tau)^m} ]</td>
<td>( \eta_c = 0.001, \quad \eta_c = 1.05, 105 \text{ (Pa.s)} )</td>
</tr>
<tr>
<td></td>
<td>Shear-Thinning</td>
<td>[ \eta = \frac{\eta_0 - \eta_m}{1 + (\lambda \tau)^m} + \eta_m ]</td>
<td>( \eta_0 = 1.05, 10.5, 105 \text{ (Pa.s)}, \quad \eta_m = 0.001 \text{ (Pa.s)} )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[ \tau_c = 2 \eta_2 D + \tau ]</td>
<td>( m = 0.62, \quad \lambda = 0.083 \text{ (s)} )</td>
</tr>
<tr>
<td>Dough and Dough like materials</td>
<td>Phan-Thien Tanner</td>
<td>[ \lambda \tau + f \tau = 2 \eta_2 D ]</td>
<td>( \varepsilon = 0.25, \quad \lambda_1 = 1 )</td>
</tr>
<tr>
<td></td>
<td>Viscoelastic fluids</td>
<td>[ f = \exp\left(\frac{\varepsilon}{\eta_1}\right) ]</td>
<td>( \eta_1 / \eta_c = 0.999, \quad \eta_2 / \eta_c = 0.001 )</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>( \eta_c = 1.05, 105 \text{ (Pa.s)} )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Researcher</th>
<th>Model Name</th>
<th>Model</th>
<th>Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dhanasekharan &amp; Kokini [22]</td>
<td>Mackey-Oofli Model</td>
<td>[ \eta \sim \left( \frac{\delta}{\gamma} \right)^n \eta_1 \eta_2 ]</td>
<td>( \sigma_0 = 93.8 \text{ kPa} )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[ \eta = \left( \frac{\delta}{\gamma} \right)^n + \eta_1 \eta_2 ]</td>
<td>( \eta_\infty = 1.05 \times 10^5 )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[ n_1 = 1.0 ]</td>
<td>( n_2 = 0.4 )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[ \Delta E_v = 5354.4 \text{ cal/g-mol} ]</td>
<td>( b = -7.91 )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[ A \sim \exp(-59.99 + 2.08 \times 10^4 \frac{1}{T} \Delta C) ]</td>
<td>( k_\infty = \begin{cases} 2.5 \text{ sec} &amp; 0.346 \text{ g/d,} \ 1.1 \text{ sec} &amp; 0.337 \text{ K at} 0.337 \text{ g/d,} \ 1.1 \text{ sec} &amp; 0.385 \text{ g/d,} \end{cases} )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[ k_\infty = \exp(-59.99 + 2.08 \times 10^4 \frac{1}{T} \Delta C) ]</td>
<td>Reference variables: ( T_r = 523.150 \text{K (500C),} ) ( \Delta C = 0.533 \text{ dry basis.} )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[ \Delta E_v = 5354.4 \text{ cal/g-mol} ]</td>
<td>( b = -7.91 )</td>
</tr>
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<td></td>
<td></td>
<td>[ A \sim \exp(-59.99 + 2.08 \times 10^4 \frac{1}{T} \Delta C) ]</td>
<td>( k_\infty = \begin{cases} 2.5 \text{ sec} &amp; 0.346 \text{ g/d,} \ 1.1 \text{ sec} &amp; 0.337 \text{ K at} 0.337 \text{ g/d,} \ 1.1 \text{ sec} &amp; 0.385 \text{ g/d,} \end{cases} )</td>
</tr>
</tbody>
</table>

Reference variables: \( T_r = 523.150 \text{K (500C),} \) \( \Delta C = 0.533 \text{ dry basis.} \)
<table>
<thead>
<tr>
<th>Researcher</th>
<th>Model Name</th>
<th>Model</th>
<th>$\eta_1$, $\eta_0$ (poise)</th>
<th>$\eta_\infty$, $\eta_0$ (poise)</th>
<th>$\lambda$, $\xi$</th>
<th>Other</th>
</tr>
</thead>
<tbody>
<tr>
<td>Connely &amp; Kokini [23]</td>
<td>Newtonian</td>
<td>$\tau_1 = 2\eta_1 D$</td>
<td>100000</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Bird-Carreau</td>
<td></td>
<td>$\tau_1 = 2\left[\eta_\infty + (\eta_0 - \eta_\infty)(1 + \lambda^2 \gamma^2)\gamma^{(n-1)/2}\right]D$</td>
<td>100000</td>
<td>11111.11</td>
<td>80</td>
<td>$n=0.2$</td>
</tr>
<tr>
<td>Oldroyd-B</td>
<td>$\tau_1 + \lambda \nabla \tau_1 = 2\eta_1 D$</td>
<td>8888.89</td>
<td>11111.11</td>
<td>0.5, 1.5</td>
<td>-</td>
<td>$\xi = 0.01$</td>
</tr>
<tr>
<td>Phan-Thien Tanner</td>
<td>exp $\left[\frac{\lambda}{\eta_1} tr(\tau_1)\right] \tau_1 + \lambda \left[(1-\frac{\gamma}{2})\tau_1 + \frac{\gamma}{2} \nabla \tau_1 \right] - 2\eta_1 D$</td>
<td>8888.89</td>
<td>11111.11</td>
<td>100</td>
<td></td>
<td>$\varepsilon = 0.08$</td>
</tr>
<tr>
<td>Researcher</td>
<td>Model Name</td>
<td>Model</td>
<td>Parameter &amp; Value</td>
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<td></td>
</tr>
<tr>
<td>Connely &amp; Kokini [24]</td>
<td>Newtonian (Corn syrup)</td>
<td>$\tau = \eta D$</td>
<td>$\eta = 54$ poise</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Viscous Newtonian and shear thinning fluids</td>
<td>Power Law (2% CMC solution)</td>
<td>$\tau = 2(K \gamma \dot{\gamma})D$</td>
<td>$n = 0.397$, $K = 157.4$ poise</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cross (0.11% Carbopol solution)</td>
<td>$\gamma = \sqrt{2(D_{11} - D_{22})}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Viscous Newtonian and shear thinning fluids</td>
<td>Bird Carreau Model</td>
<td>$\eta = \eta_\infty + (\eta_0 - \eta_\infty)(1 + \lambda^2 \gamma^2)\gamma^{(n-1)/2}$</td>
<td>$\lambda = 29.85$ s, $n = 0.1718$, $\eta_0 = 3214$ poise</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Researcher</td>
<td>Model Name</td>
<td>Parameter &amp; Value</td>
<td></td>
<td></td>
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<tr>
<td>------------</td>
<td>------------</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Connely &amp; Kokini [25]</td>
<td>Bird Carreau Model</td>
<td>$\eta_0 = 10^{10}$ Pa</td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>Dough</td>
<td></td>
<td>$\eta_0 = 100$ Pa</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>$\lambda = 10^3$ s</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\eta = 0.35$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>