Perspectives of 3D viscoelastic simulations in process design and optimization

Natalie Germann

Fluid Dynamics of Complex Biosystems, School of Life Sciences Weihenstephan,
Technical University of Munich, 85354 Freising, Germany

ABSTRACT

With the recent advances in software tools and computers, it has become possible to perform large-scale simulations of real processing applications. Still today, it is standard practice to employ generalized Newtonian models to account for the deformation-rate dependency of the viscosity. However, important effects related to the elasticity of the material, e.g., the rod-climbing of bread dough during kneading, are not captured. Computational fluid dynamics researchers are encouraged to make more frequent use of viscoelastic constitutive models in process simulations. Whereas the computational costs involved in viscoelastic simulations are higher, the numerical predictions can be significantly closer to reality and provide useful insight that could otherwise not be obtained.

MOTIVATION

Most materials encountered in industrial processing belong to the class of viscoelastic materials. Such materials exhibit both liquid- and solid-like properties, including a deformation-rate dependent viscosity or normal stress effects in simple shearing flows. The theory of viscoelastic fluids flourished in the second half of the last century with the development of viscoelastic constitutive equations, including the Giesekus, Phan-Thien-Tanner, and White-Metzner models. Still today, these constitutive equations are most often used in benchmark simulations as they have simple mathematical structures and can qualitatively capture many viscoelastic features, including the Weissenberg or rod-climbing effect, the die swell phenomenon, elastic turbulence, among others. By utilizing a set of multiple relaxation times, even quantitative agreement with experimental data can be obtained in many cases. For a review of the various standard viscoelastic models, there are various books available.[1–3] The numerical solution of these viscoelastic constitutive equations has revealed many challenges when coupled with mass and momentum transfer. Within the last decades, several groups have been intensively working on these challenges and proposed viable solutions to the most important ones, including the spatial discretization of the convective stress term and the pressure-velocity-stress coupling. Many of these developments have been implemented in open-source and commercial computational fluid dynamics software packages, allowing non-specialists to perform large-scale viscoelastic simulations.[4–6] Even on today's workstations, it is now possible to perform three-dimensional viscoelastic simulations of real industrial applications. Despite the availability of advanced software packages, viscoelastic simulations have not yet been established in process design and optimization. In this article, I want to emphasize the importance of taking into account the viscoelasticity of the material using the example of the bread kneading process. Further, I want to encourage engineers to take advantage of these new opportunities.

EXAMPLE: BREAD KNEADING

Bread has 8000 years of history and is among the primary food products in the world. The production of bread dough starts with mixing the raw ingredients, including flour, water, salt, and leavening agents such as yeast.

After hydration with water, the dough is intensively kneaded to develop the gluten network and to bring air into the dough. As the dough is a solid-like viscoelastic material, the elastic forces can easily become much larger than the centrifugal and gravitational ones. A well known viscoelastic phenomenon that can be observed during kneading is the climbing of the material along the rotating rod. To obtain the desired bread quality, the kneading process must be stopped at the right time. Underkneading is undesired as it decreases the gas retention capacity. In contrast, over-kneading leads to a dense and tight dough and, consequently, impairs the dough's ability to rise.[7]

Bread making is a complex multi-step process that has been developed over centuries by trial and error. Even in the 21st century of industrial digitalization and automatization, many aspects are not fully understood from a scientific perspective. However, a thorough understanding is essential in today's highly competitive and global market as it can effectively support new developments. Computational simulations can give valuable insight into the geometrical configuration of the kneading machine, the impact of the kneading speed as well as other process variables on the mixing performance, amongst others. Apart from a realistic computational kneading geometry, a viscoelastic model is required to obtain physically reliable predictions.

Several researchers have performed dough kneading simulations during the past two decades. Dough kneading has been one of the key research topics of Webster and his coworkers. For their computational research, they utilized simplified three-dimensional cylindrical geometries and generalized Newtonian fluid models.[8–10] To the author's knowledge, only one single three-dimensional spiral kneader simulation has been reported in the literature so far.[11] A limiting aspect of this work is that the dough properties were approximated using the Newtonian constitutive equation. Recently, we utilized a differential multimode version of Tanner's viscoelastic damage model[12] to study the kneading of bread dough in a two-dimensional eccentric cylinder.[13] Whereas this advanced model can give valuable insight into the local microstructural development during kneading, it needs a spectrum of relaxation times to realistically describe the memory behavior of the material. The numerical calculation of the total extra stress from a large set of constitutive equations makes it an unfeasible candidate for three-dimensional processing simulations.

The White-Metzner (WM) model[14] is a generalization of the upper-convected Maxwell model in which the viscosity and relaxation time are allowed to depend on the deformation rate. By employing Bird-Carreau-type of expressions for these variables, the WM model nicely predicts the shear rheology of bread dough.[15,16] Further, if the parameter values are properly selected, there is no singular behavior in extension.[17,18] The simplicity of this model combined with the high predictive capability motivates to utilize this model in computationally intensive bread dough kneading simulations. Because of these advantages, we selected the WM model to predict the dough kneading process in a spiral kneader. In the next section, I present the results of our latest three-dimensional computational fluid dynamics (CFD) simulations.[19]

RESULTS AND DISCUSSION

The kneader geometry considered in this work corresponds to a real three-dimensional DIOSNA SP12 spiral kneader (Dierks & Söhne GmbH, Osnabrück, Germany). The geometry contains a fixed shaft in the middle around which the dough is transported. Further, the kneading arm rotates at a speed 6.5 times faster than that of the bowl. The rotation of the spiral arm induces a spiral motion and is responsible for the transport of the air from the top to the bottom. The outer rotation of the bowl transports the material tangentially around the inner shaft and promotes radial mixing.

Fig. 1 shows a computational representation of the spiral kneader with 173,298 unstructured tetrahedral cells. For the three-dimensional numerical simulations, the finite volume CFD

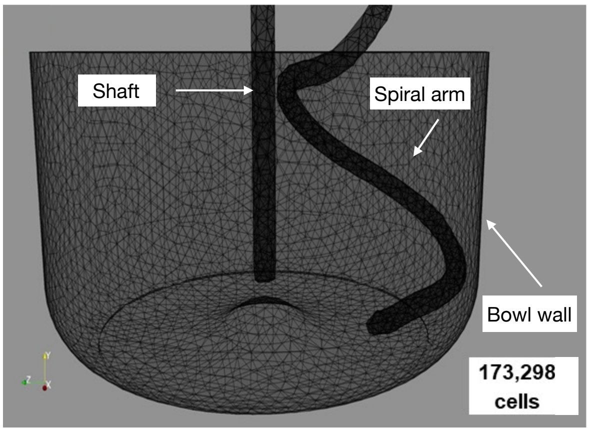

Fig. 1. Computational mesh of the spiral kneader geometry considered in this work.

software package OpenFOAM v4.0 along with the viscoelastic library Rheotool v2.0 was utilized. To simplify the numerical solution procedure, we did not use a moving mesh. Instead, the mesh was kept fixed, and the rotating WallVelocity boundary condition available in OpenFOAM was utilized to obtain the correct no-slip velocity values at the rotating parts. Although the real motion of the spiral arm is not captured, a first insight into the flow kinematics can still be obtained.

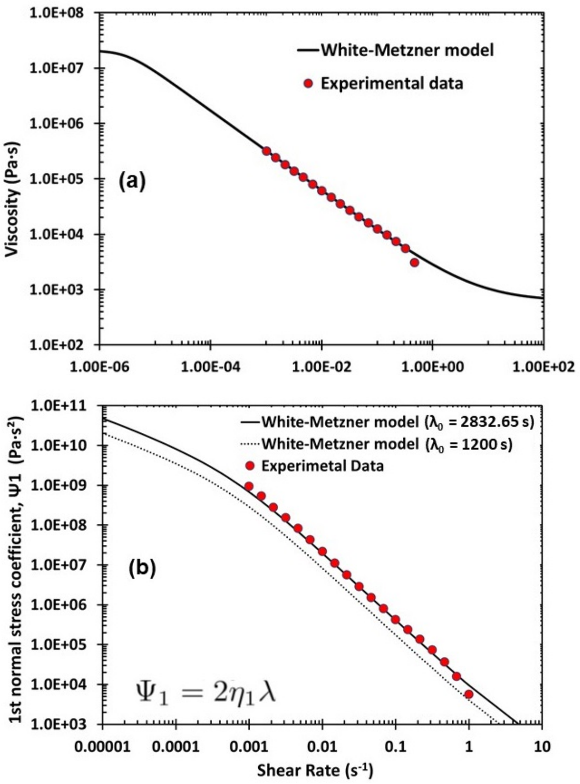

Fig. 2. (a) Shear viscosity and (b) first normal stress coefficient as a function of the shear rate. Comparison between the rheometric data and the analytical solution of the WM model.

In Rheootool v2.0, the WM model and various other viscoelastic fluid models are available. The dough kneading process represents a two-phase problem with a purely viscous air phase and a viscoelastic matrix phase. The standard approach to deal with fluid-fluid interfaces with nontrivial surface tension is the volume-of-fluid method. The rheointerfoam solver provides the corresponding implementation for viscoelastic fluids. The total stress of the mixture is described as the sum of the viscous stress from the air and the viscoelastic stress from the dough matrix. The time evolution equation of the extra stress associated with the dough matrix is described according to the WM model as follows:

$$\boldsymbol{\tau} + \lambda\left(II_D\right)\overset{\nabla}{\boldsymbol{\tau}} = 2\eta_1\left(II_D\right)\mathbf{D}, \qquad (1)$$

where $\boldsymbol{\tau}$ represents the viscoelastic stress tensor associated with the dough matrix and $\mathbf{D} = [\boldsymbol{\nabla}\mathbf{v} + (\boldsymbol{\nabla}\mathbf{v})^T]/2$ is the rate-of-deformation tensor. The symbol $\bigtriangledown$ above the stress tensor indicates the upper-convected time derivative. The viscosity, $\eta_1\left(II_D\right)$, and the relaxation time, $\lambda\left(II_D\right)$, are not anymore constant as in the upper-convected Maxwell model. Utilizing the Bird-Carreau ansatz for the viscosity of the dough matrix yields

$$\eta_1\left(II_D\right) = \eta_\infty + A\left(1 + \left(\lambda_v\sqrt{2II_D}\right)^2\right)^{\frac{n_v-1}{2}}, \qquad (2)$$

where $A = \eta_0 - \eta_\infty$, $|\mathbf{D}| = \sqrt{2II_D}$ represents the magnitude of $\mathbf{D}$, n_v is the power index, λ_v is a characteristic time constant, η_0 and η_∞ are the lower and upper Newtonian plateau values, respectively. At small shear rates ($\dot{\gamma} \to 0$), the Bird-Carreau model assumes a plateau viscosity $\eta \simeq \eta_0$. The parameter λ_v controls the transition region and corresponds to the reciprocal shear rate at which the viscosity curve deviates from Newtonian to power-law behavior. At larger shear rates ($\lambda_v \dot{\gamma} \gg 1$), the Bird-Carreau model behaves like a power-law model with a fluid consistency $K \simeq \eta_0 \lambda_v^{n_v - 1}$ and a power-law index corresponding to n_v. As the shear-rate is further increased, we obtain $\eta_1 \to \eta_\infty$. For the relaxation time of the dough matrix, we utilized the simplified expression[17]

$$\lambda\left(II_D\right) = \frac{\lambda_0}{1 + \lambda_r \sqrt{2 II_D}}, \tag{3}$$

where λ_0 is the amplitude of the relaxation time and λ_r is a characteristic time constant. The model parameters appearing in the viscosity function, Eq. (2), were fitted to the viscosity curve and those appearing in the relaxation time, Eq. (3), were determined from first normal stress coefficient data using the analytical solution $\Psi = 2\eta_1\lambda$. For a reduced value of $\lambda_0 = 1200$ s, the WM model was found to nicely capture the steady rheometric shear data (Fig. 2) and to be free of any stress singularity in mixed flows.

Figs. 3a and b provide a comparison between dough surface visualized using isosurfaces of dough matrix fraction with screenshots recorded with a high-speed camera during the laboratory kneading experiment performed in a Diosna SP12 spiral kneader, respectively. From the comparison, it is evident that the basic features can be nicely captured. Overall, we find that the curvature of the free surface matches the experimental data well. The various kinematic phenomena, i.e., the gradual response of the viscoelastic dough to the imposed deformation, the convection of the dough mass around the inner shaft, the formation and breakup of the dough pockets by the action of the spiral kneader, as well as the inward movement of the dough accompanied with rod climbing, can be qualitatively captured.

A detailed analysis of the flow patterns inside the kneader (Fig. 4) distinguishes between the spiral flow induced by the rotating arm and the tangential flow created by the rotation of the bowl. The results reflect the high impact of the

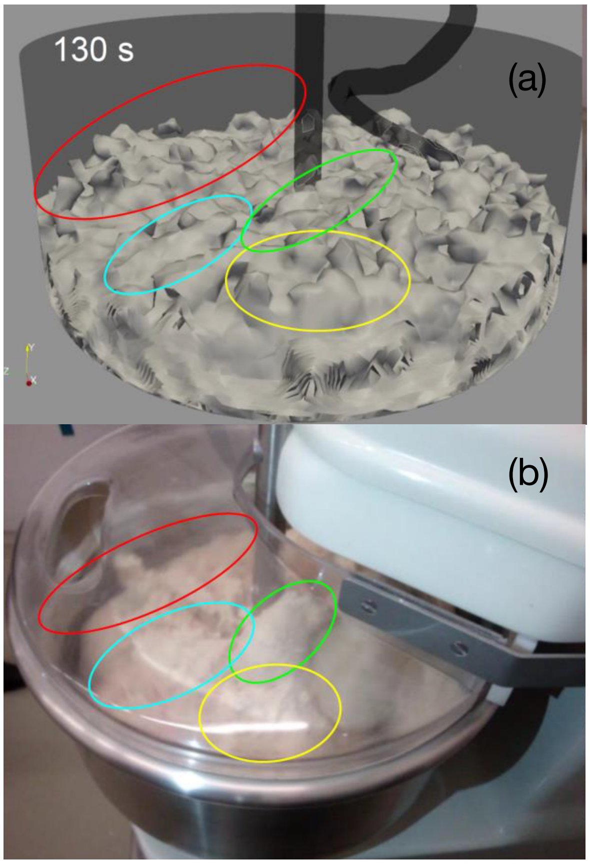

Fig. 3. Comparison of the dough surface visualized using the isosurfaces of the dough matrix fraction (top) with screenshots recorded with a high-speed camera during the laboratory kneading experiment performed in a Diosna SP12 spiral kneader (bottom) at a kneading time of 130 s.

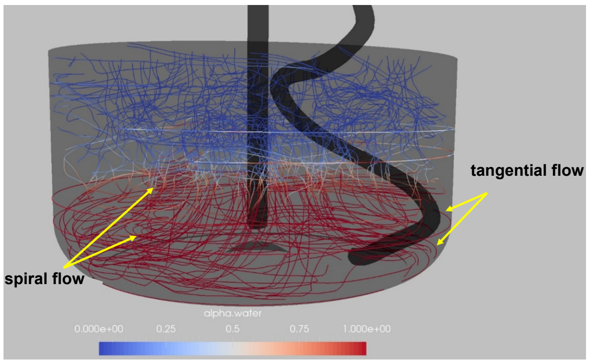

Fig. 4. Transient flow patterns in the flow domain at a kneading time of 10 s. The stream velocity tracers are colored with the dough matrix fraction to distinguish between the regions occupied by the dough and the air.

tangential flow near the outer wall and the pattern formation of the dough structure by the action of the spiral arm.

From a processing perspective, it is crucial to understand the mixing characteristics. The spatiotemporal profiles of the dough matrix fraction are presented in Fig. 5. In Fig. 5(b), we display the dough matrix fraction as a function of the axial position at x = 50 mm and z= 0 mm, corresponding to the yellow vertical line in the geometrical sketch provided in Fig. 5(a) for different kneading times. During the first 10 s of the kneading process, the dough matrix fraction sharply decreases near the dough surface (185 mm<y<210 mm) due to the incorporation of the air into the dough matrix. There is a gradual decrease for 100 s<t<350 s near the curvature of the kneader arm (135 mm<y<185 mm). The decrease near the bottom of the vessel is significantly smaller, indicating poor vertical mixing by the spiral kneader. The mixing may be further improved by using a more highly curved spiral arm or by replacing the stationary rod with an additional spiral kneader. In Fig. 5(c), we display the dough matrix fraction as a function of the radial position at x = 50 mm and y= 190 mm, corresponding to the green horizontal line in Fig. 5(a), for different kneading times. No significant effect of the radial position can be seen, indicating proper tangential mixing by the rotating parts.

This work shows the potential of combining experiments with viscoelastic fluid flow simulations in process design and optimization. If the material is described by a reliable viscoelastic model, numerical simulations can give valuable spatiotemporal information that is experimentally not easily obtainable. For instance, in the case of this kneading simulation, we clearly showed that with the present geometry, vertical mixing is not as good. In the future, different setups could be pre-evaluated before constructing new prototypes. Numerical simulations not only make the development process more effective but also reduce the costs involved in prototype construction, experimentation, and scale-up.

CONCLUSIONS

The bread dough kneading simulations presented in this article show the importance of accounting for the viscoelasticity of the material in process design and optimization. Whereas the past decades have been spent on to formulate viscoelastic constitutive equations and to develop numerical tools for solving them in idealized benchmark cases, it is now time to make the transition to real simulations of industrial processes. The open-source software package Rheotool v2.0 has a variety of standard viscoelastic models available and is

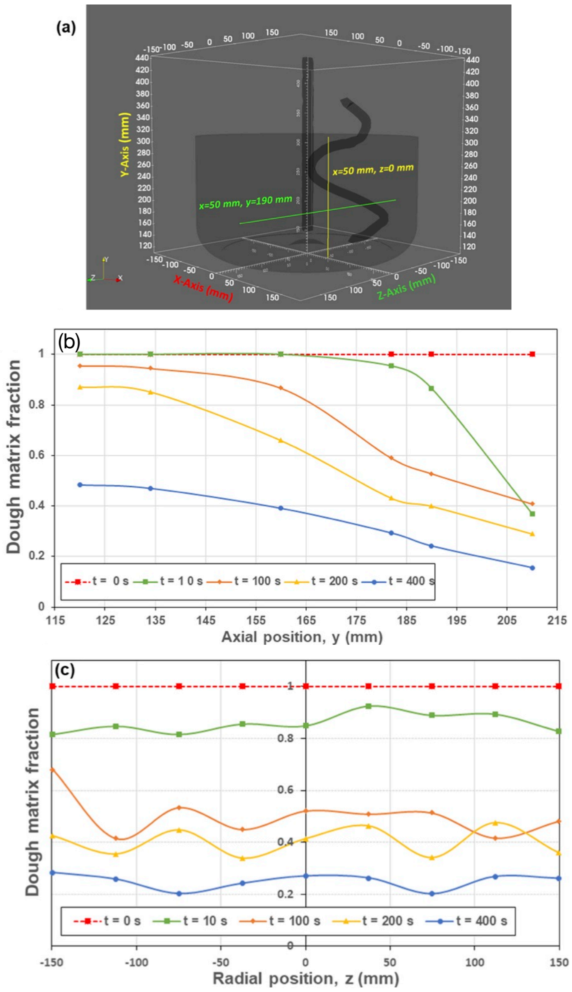

Fig. 5. Spatiotemporal profiles of the dough matrix fraction at kneading times of 0, 10, 100, 200, and 400 s. (a) Geometrical locations of the yellow axial line (x = 50 mm, z = 0 mm) and the green horizontal line (x = 50 mm, y = 190 mm), (b) axial profile of the dough matrix fraction, (c) radial profile of the dough matrix fraction.

a good starting point for viscoelastic simulations. Because of its ease of use, this toolbox is of interest to not only CFD experts but also application-oriented engineers.

ACKNOWLEDGEMENTS
This project of the Research Association of the German Food Industry (FEI) was supported by the German Federation of Industrial Research Associations (AiF) within the program for promoting the Industrial Collective Research (IGF) of the German Ministry of Economic Affairs and Energy (BMWi), based on a resolution of the German Parliament (project ID: 18960 N).

REFERENCES

1. A. N. Beris and B. J. Edwards. *Thermodynamics of Flowing Systems*. Oxford University Press, New York, 1994.

2. M. Deville and T. Gatski. *Mathematical Modeling for ComplexFluids and Flows*. Springer, New York, 2010.

3. R. Bird, C. F. Curtiss, R. C. Armstrong, and O. Hassager. *Dynamics of Polymeric Liquids: Fluid mechanics*, volume 1-2. Wiley, New York, 1987.

4. J. L. Favero, A. R. Secchi, N. S. M. Cardozo, and H. Jasak. Viscoelastic flow analysis using the software openfoam and differential constitutive equations. *J. Non-Newt. Fluid Mech.*, 165(23):1625 – 1636, 2010.

5. Pimenta J. F. and M. A. Alves. Stabilization of an open-source finite-volume solver for viscoelastic fluid flows. *J. Non-Newt. Fluid Mech.*, 239:85 – 104, 2017.

6. R. Comminal, F. Pimenta, J. H. Hattel, M. A. Alves, and J. Spangenberg. Numerical simulation of the planar extrudate swell of pseudoplastic and viscoelastic fluids with the streamfunction and the VOF methods fluids with the streamfunction and the vof methods. *J. Non-Newt. Fluid Mech.*, 252:1–18, 2018.

7. B. Schiedt, A. Baumann, B. Conde-Petit, and T. A. Vilgis. Short-and long-range interactions governing the viscoelastic properties during wheat dough and model dough development. *J. Texture Stud.*, 44(4):317–332, 2013.

8. K. S. Sujatha and M. F. Webster. Modelling three-dimensional rotating flows in cylindrical-shaped vessels. *Int. J. Numer. Methods Fluids*, 43(9):1067–1079, 2003.

9. D. M. Binding, M. A. Couch, K. S. Sujatha, and M. F. Webster. Experimental and numerical simulation of dough kneading in filled geometries. *J. Food Eng.*, 58(2):111–123, 2003.

10. K. S. Sujatha, M. F. Webster, D. M. Binding, and M. A. Couch. Modelling and experimental studies of rotating flows in part-filled vessels: wetting and peeling. *J. Food Eng.*, 57(1):67–79, 2003.

11. I. Litovchenko, M. Luchian, S. Stefanov, and C. Csatlos. Numerical modeling and simulation of bread dough mixing using concept of computational fluid dynamics (CFD). *Proceeding of 5th International Mechanical Engineering Forum, Prague, Czech Republic*, pages 584–590, 2012.

12. R. I. Tanner, F. Qi, and S. C. Dai. Bread dough rheology and recoil: I. Rheology. *J. Non-Newt. Fluid Mech.*, 148(1-3):33–40, 2008.

13. P. Šćepanović, Th. B. Goudoulas, and N. Germann. Numerical investigation of microstructural damage during kneading of wheat dough. *Food Struct.*, 16:8–16, 2018.

14. J. L. White and A. B. Metzner. Development of constitutive equations for polymeric melts and solutions. *J. Appl. Polym. Sci.*, 7(5):1867–1889, 1963.

15. M. Dhanasekharan, H. Huang, and J. L. Kokini. Comparison of observed rheological properties of hard wheat flour dough with predictions of the Giesekus-Leonov, White-Metzner and Phan-Thien Tanner models. *J. Texture Stud.*, 30(6):603–623, 1999.

16. M. Dhanasekharan, C. F. Wang, and J. L. Kokini. Use of nonlinear differential viscoelastic models to predict the rheological properties of gluten dough. *J. Food Process Eng.*, 24(3):193–216, 2001.

17. Y. Ide and J. L. White. Investigation of fail-

ure during elongational flow of polymer melts. *J. Non-Newt. Fluid Mech.*, 2(3):281–298, 1977.

18. H. A. Barnes and G. P. Roberts. A simple empirical model describing the steady-state shear and extensional viscosities of polymer melts. *J. Non-Newt. Fluid Mech.*, 44:113 – 126, 1992.

19. Laila Abu-Farah, Thomas B. Goudoulas, Soroush Hooshyar, and Natalie Germann. Numerical and experimental investigation of dough kneading in a three-dimensional spiral kneader. *Physics of Fluids*, 31(11):113104, 2019.