Computational Fluid Dynamics of Viscoelastic Flows

Jozef L. Kokini

Department of Food Science and Center for Advanced Food Technology, Cook College, Rutgers, the State University of New Jersey, 65 Dudley Road, New Brunswick, NJ 08901.

Computational fluid dynamics (CFD) provide a very effective way to probe the dynamics of a process and learn about what goes on inside the material being processed non-intrusively (Puri and Anantheswaran, 1993). Numerical simulations have a wide range of applications in equipment design, optimization, scale up and scale down in many food processing operations. The geometrical complexities of process equipments and the non- linear viscoelastic properties of food materials makes it a necessity to invest in numerical simulation if appropriate progress is to be made in improving food operations (Connelly, 2004).

CFD offers a powerful design and investigative tool to process engineers. It assists in a better understanding of the complex physical mechanisms that govern the operations of food processes. CFD has only recently been applied to food processing applications. The advent of powerful computers and work stations has provided the opportunity to simulate various real-world processes. Food materials are subjected to mechanical and thermal effects during processing.

When simulating the processing of food products, it is necessary to take the rheological nature of a food into account as this will dictate its flow behavior. There are many CFD approaches to discretizing the equations of conservation of momentum, mass, and energy, together with the constitutive equation that defines the rheology of the fluid being modeled and the boundary and initial conditions that govern the flow behavior in particular geometries such as extruders and mixers (Connelly and Kokini, 2001 and 2004; Dhanasekaran and Kokini, 2003). The most important of these are finite difference (FDM), finite volume (FVM), and finite element (FEM) methods. Others CFD techniques can be listed as spectral schemes, boundary element methods, and cellular automata, but their use is limited to special classes of problems.

The use of the finite element method (FEM) as a numerical procedure for solving differential equations in physics and engineering has increased considerably. The finite-element method has various advantages contributing to this popularity: Spatial variations of material properties can be handled with relative ease; irregular regions can be modeled with greater accuracy; element size can be easily varied; it is better suited to non-linear problems; and mixed-boundary value problems are easier to handle (de Baerdemaeker *et al*., 1977). The major disadvantage of the method is that it is numerically intensive and can therefore take high CPU time and memory storage space.

In FEM there are three primary steps: The domain under consideration is divided into small elements of various shapes called finite elements. All elements are assumed to be connected at nodal points located along the boundaries and the collection of parts is called as the mesh. Over each part, the solution is approximated as a linear combination of nodal values and approximation functions, and algebraic relations are derived between physical quantities and the nodal values. Finally the parts are assembled to obtain the solution to the whole (Reddy, 1993).

Numerical simulation of processes is conducted by simultaneously solving continuum equations that describe the conservation laws of momentum and energy, with a rheological equation of state (constitutive models) of the food material to be processed, along with boundary/initial conditions.

Viscoelastic constitutive models in CFD

Constitutive models play a significant role in the accuracy of the predictions by numerical simulations. A proper choice of a constitutive model, either generalized Newtonian or viscoelastic, that describes the flow behavior of the material under investigation, is important.

Differential viscoelastic models have generally been more popular than integral models in numerical developments (Crochet, 1989). Nonlinear differential models are of particular interest in numerical simulations for process design, optimization and scale-up. This is because integral viscoelastic models are not well suited for use in numerical simulation of complex flows due to high computational costs involved in tracking the strain history, particularly in three-dimensional flows (Dhanasekaran, 2001).

Dhanasekaran *et al*. (1999, 2001, 2003) focused on the proper choice of constitutive models for wheat flow doughs for the design and scaling of extrusion by numerical simulation. The flow in an extruder is shear dominant, and therefore two groups of models which give a good prediction of shear properties of dough were tested: Generalized Newtonian models (Newtonian fluid, power-law fluid, Hershel-Bulkley fluid, and Morgan fluid) and differential viscoelastic models (Phan-Thien Thanner, White-Metzner and Giesekus-Leonov model).

Importance of viscoelasticity in mixing flows

The effects of viscoelasticity on mixing flows have been observed most dramatically in the secondary flows in mixers. This has been attributed to the complex interaction between the centrifugal forces caused by the primary tangential flow and inertia and the normal forces generated in elastic fluids (Connelly, 2004).

Viscoelasticity also affects power consumption, a key design parameter for mixers. In the laminar regime under creeping flow conditions, it has a negligible impact. At higher Reynolds numbers, a reduction in power consumption has been observed by some authors and is thought to be due to suppression of the inertia driven secondary flows. It has been suggested that as intermediate flow patterns develop, the opposing circulations would dissipate more energy and thus lead to increased power consumption. Other researchers found that elastically driven secondary flows are slower and require more energy to maintain than inertially driven flows, therefore increasing the power. They also suggested that increases in the stresses generated in elongational flow fields due to the much higher elongational velocity in viscoelastic fluids also play an important but undetermined role in increasing the torque requirements (Connelly, 2004).

FEM simulation techniques for viscoelastic fluid flows

The numerical simulation of various unit operations is conducted by simultaneously solving the continuum equations that describe the conservation laws of momentum and energy, with a rheological equation of state (constitutive models) of the food material to be processed, along with boundary and initial conditions.

For an incompressible fluid, the stress tensor (σ) is given as the sum of an isotropic pressure (*p*) component and an extra stress tensor (T).

$$\sigma = -pI + T$$

The conservation of linear momentum is then given by:

$$\nabla.\boldsymbol{\acute{o}} + \rho\mathbf{f} = \rho(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}.\nabla\mathbf{v})$$

where ρ is the fluid density and **f** is the external body force per unit mass. For incompressible fluids, conservation of mass yields the continuity equation:

$$\nabla.\mathbf{v} = 0$$

and the conservation of energy equation is given as:

$$\rho C(T).(\frac{\partial T}{\partial t} + \mathbf{v}.\nabla T) = \mathbf{T} : \nabla\mathbf{v} + r - \nabla.q$$

where $C(T)$ is the heat capacity as a function of temperature, r is the given volumetric heat source, q is the heat flux, and $\mathbf{T}:\nabla\mathbf{v}$ is the viscous heating term. These equations together with constitutive models form a complete set of governing equations. The solutions of these equations give velocity and temperature profiles for a particular problem. In most cases, the solution of these equations requires numerical methods, such as finite element method. An abundance of software tools are available in the market using finite elements methods to solve flow problems.

A variety of numerical methods based on finite element methodology are available. One of the formulations is the so called weak formulation. In this method, the momentum equation and the continuity equation are weighted with fields V and P and integrated over the domain Ω. The finite element formulations are given by

$$\int_{\Omega} - \nabla p + \nabla.\mathbf{T} + \mathbf{f}).\mathbf{u}d\Omega = 0, \ \forall \mathbf{u} \in V$$

$$\int_{\Omega} (\nabla.\mathbf{v})qd\Omega = 0 , \qquad \forall q \in P$$

where **T** is the extra stress tensor, V and P denote the velocity and pressure fields, respectively. The domain Ω, is discretized using finite elements covering a domain, Ω^h on which the velocity field and pressure fields are approximated using v^h and p^h. The superscript *h* refers to the discretized domain. The approximations are obtained using:

$$\mathbf{v}^h = \sum \mathbf{V}^i \psi_i , \qquad p^h = \sum p^i \pi_i$$

where V^i and p^i are nodal variables and ψ^i and π^i are shape functions. The unknowns V^i and p^i are calculated by solving the weak forms of equations of motion and the continuity equation, along with the formulations for the constitutive models, using two basic approaches.

The first approach also known as the coupled method is the mixed or stress-velocity-pressure formulation. The primary unknown, the stress tensor, is formulated using an approximation $\mathbf{T}^h$ with:

$$\mathbf{T}^h = \sum \mathbf{T}^i \phi_i$$

where T^i are nodal stresses while φ^i are shape functions. This procedure is normally used with differential models. The main disadvantage of this method is the large number of unknowns and hence high computational costs for typical flow problems.

The second approach, called as the decoupled scheme, uses an iterative method. The computation of the viscoelastic extra-stress is performed separately from that of flow kinematics. The stress field is calculated from flow kinetics. In this approach, the number of variables is much lower than in the mixed method, but the number of iterations is much larger.

A straightforward implementation of these two approaches gives an instability and divergence of the numerical algorithms for viscoelastic problems. FEM solvers use a variety of numerical methods to circumvent convergence problems for viscoelastic flows.

Viscoelastic fluids exhibits normal stress differences in simple shear flow. Early attempts to simulate viscoelastic flows numerically were restricted to very moderate Weissenberg numbers (i.e. a non-dimensional measure of fluid elasticity) as the solutions invariably became unstable at unrealistically low *Wi* values. This problem is called as the "high Weissenberg number problem" and it is mostly due to the hyperbolic part of the differential constitutive equations. Numerical methods were unable to handle flows at *Wi* values sufficiently high to make comparisons with the experimental results. Progress has been made by use of central numerical methods, such as central finite differences or Galerkin finite elements, by which small Weissenberg numbers are attainable. More insight in the type of the system of differential equations led to development of upwind schemes, such as the Streamline Upwind (SU) by Marchal and Crochet (1987) and streamline integration method by Luo and Tanner (1986a, 1986b). Furthermore, the Streamline Upwind/Petrov-Galerkin (SUPG) method was developed by rewriting the set of partial differential equations in the explicit elliptic momentum equation form. SUPG method is considered more accurate compared to SU method but it is only applicable to smooth geometries.

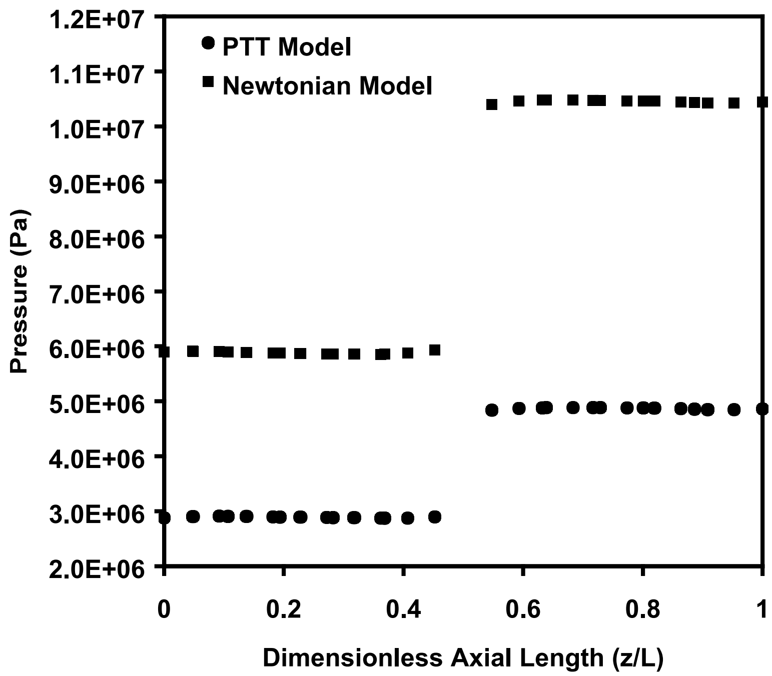
In order to ease the problems caused by the high stress gradients, viscoelastic extra-stress field interpolation techniques, which include biquadratic and bilinear subelements, are used. Marchal and Crochet (1987) introduced the use of 4x4 subelements for the stresses. These bilinear subelements smoothed the mixed method solution of the Newtonian stick-slip problem, as well as aided in the convergence of the viscoelastic problem. Perera and Walters (1977) introduced a method known as Elastic Viscous Stress Splitting (EVSS) by splitting the stress tensor into an elastic part and a viscous part, which stabilizes the behavior of the constitutive equations. EVSS is the only technique available for use in 3D or with multiple relaxation times.

CFD simulations of flow in an extruder

Dhanasekharan and Kokini (1999) characterized the 3D flow of whole flour wheat dough using three nonlinear differential viscoelastic models, Phan-Thien Tanner, the White-Metzner and the Giesekus models. The Phan-Thien-Tanner (PTT) model gave good predictions for transient shear and extensional properties of wheat flour dough. Based on the rheological studies using differential viscoelastic models, PTT model was concluded to be the most suitable for numerical simulations (Dhanasekharan *et al*., 1999).

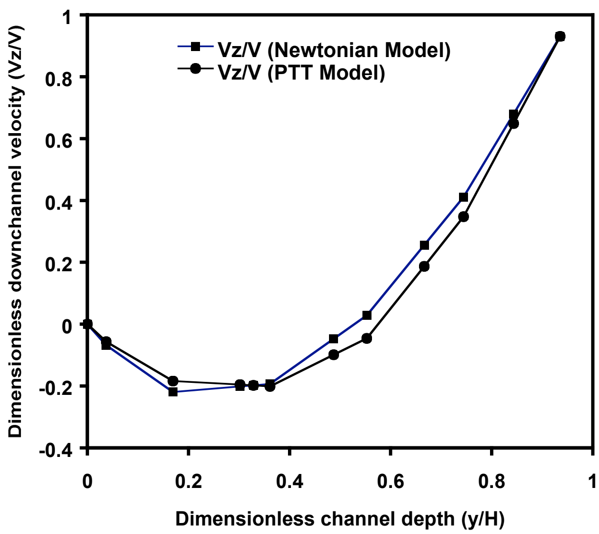
Dhanasekharan and Kokini (2000) modeled the 3D flow of a single mode PTT fluid in the metering zone of completely filled single-screw extruder. The modeling was done by means of a stationary screw and rotating barrel. The pressure buildup for the PTT model was found to be smaller than the Newtonian case (figure 1), which is explained by the shear-thinning nature incorporated into the differential viscoelastic model. The velocity profile generated using the viscoelastic model, however, was found to be very close to the Newtonian case (figure 2).

Figure 1. Comparison of pressure profile of PTT model prediction with the Newtonian model (Dhanasekharan, 2000).



A fundamental analysis was done using two important dimensionless numbers, Deborah number (De) and Weissenberg number (Wi). For the chosen flow conditions and the extruder geometry, Deborah and Weissenberg numbers were reported to be 0.001 and 5.22, respectively. De=0.001 explained the velocity profile predictions close to Newtonian case, as De → 0 indicates a viscous liquid behavior. When the relaxation processes are of the same order of magnitude of the residence time of flow (i.e. De ~ 1), the impact of viscoelasticity on the flow becomes significant. Wi=5.22 indicated "high Weissenberg number problem". In spite of the difficulties in convergence due to high Wi, these results provided a starting point for further simulations of viscoelastic flow using more realistic parameters.

Figure 2. Comparison of down channel velocity profile of PTT model prediction with the Newtonian model (Dhanasekharan, 2000).



CFD Simulations of Flow in Model Mixers

Classical geometries such as contraction flows, flow past a cylinder in a channel, flow past a sphere in a tube and flow between eccentrically rotating cylinders have been traditionally used as benchmark problems for testing new techniques and understanding fundamental effects involved in mixing. Studies involving simple model mixer geometries have been done to understand mixing phenomena in mixers with geometries closer to industrial mixers. Only recently mixing in complex geometries such as the twin-screw continuous mixers and batch Farinograph mixers has been addressed utilizing new advances in numerical simulation techniques and computational capabilities (Connelly and Kokini, 2004).

Good progress has been made in understanding the effects of rheology and geometry on the flow and mixing in batch and continuous mixers, as well as in identifying conditions necessary for efficient mixing (Connelly and Kokini, 2003 and 2004). Finite element method (FEM) was used for numerical simulations of the flow of dough-like fluids in model batch and continuous dough mixing geometries. Several FEM techniques, such as elastic viscous stress splitting (EVSS), Petrov-Galerkin (PG), 4x4 subelements, streamline upwind (SU) and Streamline Upwind/Petrov-Galerkin (SUPG) were used for differential viscoelastic models.

Connelly & Kokini (2004) explored the viscoelastic effects on mixing flows obtained with kneading paddles in a single screw, continuous mixer. A simple 2D representation of a single paddle in a fully filled, rotating cylindrical barrel with a rotating reference frame was used as a starting point to evaluate the FEM techniques. The single screw mixer was modeled by taking the kneading paddle as the point of reference, fixing the mesh in time. Here, either the paddle turns clockwise with a stationary wall in a reference frame or the wall moves counterclockwise in the rotating reference frame originating from the center of the paddle.

The single-mode, non-linear Phan-Thien Tanner differential viscoelastic model was used to simulate the mixing behavior of dough-like materials. Different numerical simulation techniques including EVSS SUPG, 4x4 SUPG, EVSS SU and 4x4 SU were compared for their ability to simulate viscoelastic flows and mixing. Mesh refinement and comparison between methods were also done based on the relaxation times at 1 rpm and the Deborah number (*De*) to find the appropriate mesh size and the best technique to reach the desired relaxation time of 1000 seconds. The limits of the *De* that were reachable in this geometry with the PTT model are listed in Table 1. The coarser meshes allowed convergence at higher *De* since the high gradients at the discontinuity are smoothed in the boundary layers.

Table 1. Limits of Deborah number reached by several methods used in viscoelastic simulations during mesh refinement at 1 rpm (Connelly and Kokini, 2003).

Mesh Size	**EVSS SUPG**		**4x4 SUPG**		**EVSS SU**		**4x4 SU**	
	λ(1 rpm)	**De**	**λ**(1 rpm)	**De**	**λ**(1 rpm)	**De**	**λ**(1 rpm)	**De**
360 elements	0.327	0.034	0.23	0.024	651.04	68.2	1000	104.7
600 elements	0.178	0.019	1.04	0.109	14.12	1.47	23.4	2.45
1480 elements	0.089	0.009	0.089	0.009	0.73	0.076	131.78	13.8
2080 elements	-	-	0.066	0.007	0.79	0.082	543.58	56.9
3360 elements	-	-	-	-	0.58	0.061	110.32	11.6

The SUPG technique and less computationally intensive EVSS technique were found to be not adequate for this geometry. Only the 4x4 SU techniques was able to reach *De* values representative of the level of viscoelasticity closer to dough viscoelasticity. Even this technique was unable to reach the desired relaxation time of 1000 seconds at low rpm values. High rpm values are more representative of the actual conditions found in this type of mixer. At high rpm levels the instabilities in the calculations were found to disappear.

The effect of shear thinning and viscoelastic flow behavior on mixing was systematically explored using the Newtonian, Bird-Carreau viscous, Oldroyd B and Phan-Thien Tanner models using single screw simulations with the rotating reference frame approach. For the application of these techniques the rheological data and non-linear viscoelastic models for wheat flour doughs previously studied by Dhanasekharan *et al*. (1999), Wang and Kokini (1995a and 1995b) were utilized. Comparison of the predictions by these viscoelastic models with experimental data showed that viscoelastic flow predictions differ significantly in shear and normal stress predictions resulting in a loss of symmetry in velocity (Figure 3) and pressure profiles (Figure 4) in the flow region. Introduction of shear thinning behavior resulted in a decrease in the magnitude of the pressure and stress and an increase the size of low velocity or plug flow regions.

Figure 3. Velocity magnitude distribution at 1 rpm of a) Newtonian (λ=0s), b) Oldroyd-B (λ=0.5s), c) Bird-Carreau Viscous (λ=60s) and d) PTT (λ=100s) where the units of velocity are cm/s (Connelly, 2004).

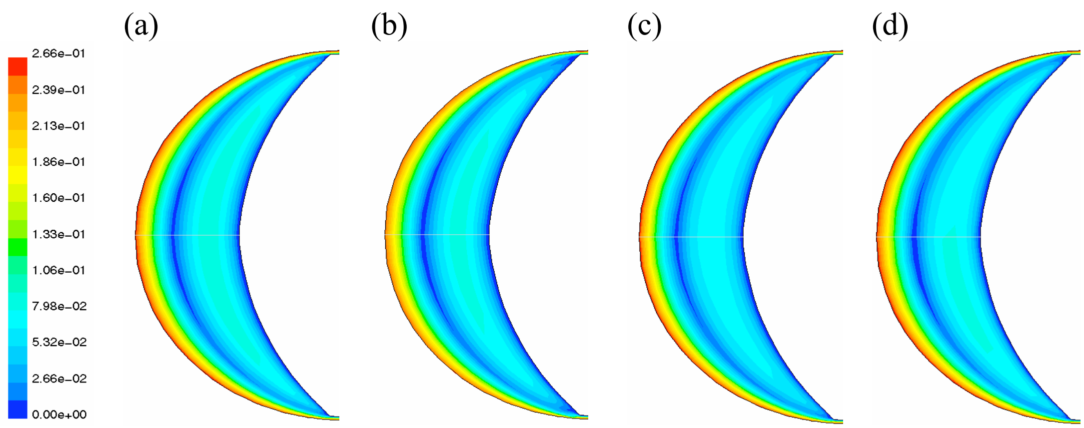
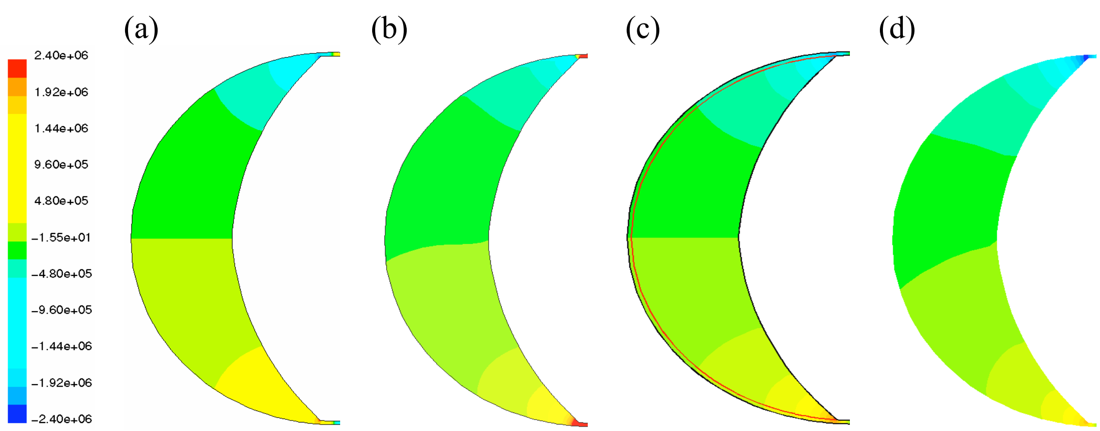


Figure 4. Pressure distributions at 1 rpm of a) Newtonian (λ=0s), b) Oldroyd-B (λ=0.5s), c) Bird-Carreau Viscous (λ=60s) and d) PTT (λ=100s) where the units of pressure are dyne/cm^2 (Connelly, 2004).



The studies mentioned above demonstrate the effectiveness of numerical simulation in studying the flow of materials with different rheological properties in different mixer and extruder geometries non-intrusively. Numerical simulations serve as valuable tools for process and design engineers to examine the flow behavior of materials of different rheological characteristics. CFD is also a very effective way to test new ideas to see if they will actually improve a specific food process application without having to build the process equipment in question.

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