An energy transport based evolving rheology in high-shear rotor-stator mixers

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Abstract

Rotor-Stator mixers such as the inline Silverson are widely used by the process industry. Existing literature on experimental and computational investigations of these devices focus on characterising the power draw and turbulent mixing of Newtonian fluids and non-Newtonian fluids such as emulsions. The current knowledge on the performance of these mixers in blending and mixing fluids with an underlying complex structure is limited. Modelling and simulation of such structured liquids has traditionally been challenging due to the complexity of the constitutive governing equations which are to be solved for the prediction of rheology. In this paper a novel approach to model evolving rheology is proposed. This approach incorporates important physical phenomenon such as the strain rate history effects in the generalised Newtonian fluid model. The new approach is used to model mixing in a pilot scale inline Silverson mixer via Computational Fluid Dynamics (CFD) simulations. A sliding mesh algorithm coupled to eddy viscosity turbulence closure is used. Experiments have been performed with the inline Silverson mixer placed in a recirculation loop for two different rotor speeds, and rheological measurements have been performed on the samples taken at the outlet of the mixer. Computational results are compared with the viscosity measurements and it is found that the model predictions for the evolution of viscosity are in reasonable agreement with the experimental data.

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1. Introduction

The mixing process plays a significant role in improving the homogeneity and quality of a wide range of products in the process industries. Inline rotor-stator mixers are widely used in processing due to their high efficiency and their capacity to accelerate the mixing process by providing a focussed delivery of energy [1]. However, the high energy dissipation rates and short residence times within the mixer limit current understanding of the fluid dynamics within these devices and consequently their relationship to overall mixer performance and product quality [2].

Rotor-stator mixers consist of high speed rotors surrounded by close fitting stator screens. The typical tip speeds during operation range from 10 – 50m/s, and the gaps between the rotor and stator range between 100 – 3000µm [3], generating high shear rates in the rotor-stator gap ranging from 20,000s$^{-1}$ – 100,000s$^{-1}$ [2]. The high kinetic energy imparted to the fluid by the rotating blades is mainly dissipated local to the stator screen; the high rate of energy dissipation makes such devices advantageous for physical processes such as mixing, dispersion, dissolution, emulsification and de-agglomeration [4]. The high energy dissipation rates and shear rates found in rotor stator mixers lend themselves to production of ever finer structures such as emulsions [5] and dispersion of powders [6].

Modelling of mixing in a pilot scale Silverson rotor-stator mixer has been the subject of several recent investigations. Baldyga et al. [7, 8] and Jasińska et al. [1, 9] have carried out CFD simulations of an inline Silverson 150/250 MS in-line mixer focussing on estimating the product yield during chemical reaction, distribution of particle aggregates and droplet size distributions. Recently Baldyga et al. [10] and Michael et al. [11] have modelled the drop dispersion and evolving rheology of dense emulsions in this mixer. The Reynolds Averaged Navier-Stokes (RANS) method along with sliding mesh is used to simulate the
Rotor-stator interaction.

This paper uses the CFD methodology of Michael et al [11] to model the turbulent flow dynamics within the Silverson mixer but with specific developments to characterise and model the evolving rheology of liquids containing wood and other plant fibres. These systems are frequently processed by high pressure homogenisers, microfluidisation, ball mills and grinding where scale up is carried out on the basis of pressure drop (i.e. energy) and frequently requires multiple passes [12, 13]. As the fibres are processed their size is reduced and the viscosity increases [12] and thus this system behaves in an interesting manner where the viscosity of the fluid and the efficiency of the mixer are coupled. In this paper we choose to use the Silverson mixer because of our previous experience in characterising its performance and availability.

The modelling of polymeric liquids is challenging owing to the complexity of the underlying constitutive equations [15]. The total stress tensor \( \sigma \) is decomposed into an isotropic and deviatoric part as \( \sigma = -pI + \tau \) with \( p \) being the pressure and \( \tau \) the stress tensor. Transport equations of varying complexity for the stress tensor have been proposed in literature [16]. This approach is however computationally challenging especially for highly inertial flow conditions such as that occurring in industrial high-shear mixing applications. A phenomenological model is thus the highly favoured approach in such situations wherein the nonlinear flow behaviour is cast in the form \( \tau = \alpha + \beta |\dot{\gamma}|^n \), where \( |\dot{\gamma}| \) is proportional to the square root of the second invariant of the strain rate tensor \( |\dot{\gamma}| \).

This form is the Herschel-Bulkley equation and such models are classed as Generalised Newtonian Fluids (GNF): \( \tau = \mu(|\dot{\gamma}|)|\dot{\gamma}| \). Such a formulation allows one to retain the tensorial structure of the Newtonian constitutive model whilst still being able to predict thixotropic effects such as time dependent shear-thinning and yield stress. However owing to the simple proportionality between the stress tensor and the instantaneous strain rate tensor the effect of the history of deformation on the stress is discarded in these models. Yet it is well known that the rheological behaviour of polymeric liquids is affected by flow history [17].

We propose the introduction of a damage parameter to track the evolution
of the microstructure. Taking a cue from the first law of thermodynamics, the work done on the microstructure by the fluid is equated to an energy like variable (denoted here by $E$ and referred to as the *mechanical* energy). The transport of mechanical energy is assumed to be governed by \( \frac{DE}{DT} = \nabla \cdot (\tau \cdot \mathbf{u}) - \mathbf{u} \cdot \nabla p \).

The second term on the right hand side is reversible and does not contribute to the microstructure evolution. The first term on the right hand side contains a strictly positive component which is taken to represent the irreversible growth of damage. The zero shear viscosity is modelled as a function of this damage. In this paper we solve this transport equation for mechanical energy of the fluid system to capture the effect of the fluid flow on the evolution of rheology in the mixer. In order to close this problem a precise form for the empirical parameters $\alpha$ and $\beta$ of the Herschel-Bulkley model need to be specified. These parameters of the Herschel-Bulkley model are taken to be the yield stress $\tau_0$ and the consistency index $k$ of the fluid. The power draw of the mixer is an experimentally measurable quantity and its product with process time gives the total mechanical energy. A functional relationship between this mechanical energy $E$ and the viscosity $\mu$ is experimentally determined and adopted in this paper. This allows $\tau_0$, $k$ and $n$ to be determined as a function of energy ($E$).

In Section 2 we present the mathematical formulation of the new energy based evolving rheology model giving further details on how viscosity may be related to energy. In Section 3 we briefly describe the test configuration investigated, and outline the experimental procedure. Section 4 outlines the numerical procedure. Results are then presented and discussed in Section 5 with the conclusions summarised in the last section.

2. **Mathematical formulation of the new model**

The mathematical details of the new energy based model that incorporates the flow history into the rheology are presented. A switch to Einstein index notation is made henceforth. The rheology evolution is modelled via a modified
energy transport equation:

\[
\frac{\partial \rho E}{\partial t} + \rho u_k \frac{\partial E}{\partial x_k} = -u_k \frac{\partial p}{\partial x_k} + \frac{\partial \tau_{km}}{\partial x_k},
\]

(1)

where \( p \) is the pressure and \( \tau_{km} \) is the viscous stress tensor for an incompressible fluid:

\[
\tau_{km} = \mu \left( \frac{\partial u_k}{\partial u_m} + \frac{\partial u_m}{\partial x_k} \right),
\]

(2)

The development of the rheology is considered as irreversible. The standard Herschel-Bulkley formulation is used to account for shear thinning of the fluid:

\[
\mu = \begin{cases} 
\mu_0 & \text{if } |\dot{\gamma}| \leq \dot{\gamma}_0 \\
 k |\dot{\gamma}|^{n-1} + \tau_0 |\dot{\gamma}|^{-1} & \text{if } |\dot{\gamma}| \geq \dot{\gamma}_0
\end{cases},
\]

(3)

where \( \dot{\gamma} \) is the shear rate, \( \tau_0 \) is the yield stress and \( \mu_0 \) is the limiting viscosity.

The new approach couples \( \mu_0 \) to the mechanical energy equation via:

\[
\mu_0 = A \left( 1 - \exp \left( -BE \right) \right),
\]

(4)

where \( A \) and \( B \) are model constants and can be calculated for a given fluid through experimental trials. Furthermore, note that the yield stress and \( k \) in Eq. (3) can be expressed as \( \tau_0 = \tau_0(E) \) and \( k = k(E) \) which is explored further in Section 5. According to this method the development of rheology is considered as irreversible and provides the strain rate history effects required for accurate modelling of rheology.

3. Test configuration and experimental methods

The Silverson double screen 150/250MS in-line mixer has been experimentally studied in several works [4, 18–21], measuring the power consumption and mixer performance at different operating speeds. The mixer has two rotors which rotate together within closely fitted stator screens. The rotors and stator screens of the mixer are shown in Figure 1 and further details can be found in [4, 19]. The mixer usually operates over a range of speeds varying from 3000 to 12000 rpm with the fluid flowing through the device at different flow rates.
Figure 1: Silverson 150/250MS mixer, (a) Rotor (b) Stator.

Figure 2 shows a piping and instrumentation diagram (P&ID) of the validation test configuration. A 50 L double-jacketed mixing vessel (R100) was used as the material holding tank. The vessel was also fitted with an anchor and a pitch blade turbine stirrer respectively to ensure that the material homogeneity inside the vessel was maintained all the time. Feed flowrate to the Silverson in-line mixer, which was also the recirculation flowrate of the loop, was regulated through the combination of a 1.5” lobe pump (J100) and a Coriolis meter (FT100). All the mechanical connections were made of 1.5” nominal size stainless steel pipes coupled with standard In Line Cleaning (ILC) or Swagelok fittings. A total of two tests were carried out, in which the test fluid containing the fibrous thickening agent was processed by the Silverson in-line mixer run-
ning at 6000 and 11000 rpm respectively. Each test started with 50 kg of a well
dispersed mixture containing 1 kg of fibre in water (i.e. 2% w/w) being manually
loaded into the 50 L mixing vessel. The mixture was then circulated within the
test loop by the lobe pump for 40 minutes. The Silverson in-line mixer was then
switched on at the target speed and samples were periodically taken (SP02)
over about 4 hours. Chilling water was allowed to circulate inside the double
jacket of the 50 L mixing vessel to maintain the mixture temperature below 25
°C. All the collected samples were stored in sealed plastic bottles for off-line
viscosity measurements. The torque was recorded [19] and used to calculate the
mechanical energy.

Rheological measurements were carried out at 25°C using Anton Paar DSR301
rheometer with a 12.5 mm diameter 4 vane geometry in a serrated cup. The
samples were conditioned for 10 mins at a stress of 1 Pa and then a controlled
stress sweep was carried out. The rheological quantity used to characterise the
experimental comparison is the value of viscosity at 200 s⁻¹.

4. Computational configuration and numerical methods

The simulations were performed using Code_Saturne, an open-source CFD
code developed by EDF [22] (see http://www.code-saturne.org). Code_Saturne
is an incompressible solver based on a collocated discretisation of the domain,
and is able to treat structured and unstructured meshes with different cell
shapes. It solves the Navier-Stokes equations with a fractional step method
based on a prediction-correction algorithm for pressure/velocity coupling (SIM-
PLEC), and Rhie and Chow interpolation to avoid pressure oscillations. The
code uses an implicit Euler scheme for time discretisation, and a second order
centred difference scheme is used for the spatial gradients. Rotating meshes are
handled via a turbo-machinery module, which solves the transport equations
for the initial geometry, updates the geometry and then corrects the pressure as
shown in Figure 3. The code has previously been validated in many industrial
and academic studies, ranging from simulations of incompressible flows (with
and without rotating meshes) [23,25] to low Mach number variable density reacting flows [26, 27].

A 2-D computational domain has been used in the current investigation as shown in Figure 4a; this provides a comparable basis to the 2-D MRF configuration adopted in earlier studies of Jasińska et al [1, 9]. The computational domain is meshed with 180000 cells and shown in Figure 4b. The mesh is refined in the regions near to the sliding interface located in the rotor-stator gaps (as shown in Figure 4c and Figure 4d). Grid sensitivity studies have been carried out and the grid size for mesh independent results is similar to that of Jasińska et al [1, 9]. Standard inflow conditions on the inlet faces and pressure outlet conditions on the outlet faces are specified. A no-slip condition is applied to the velocity at the walls along with the appropriate wall treatment through standard wall functions for turbulence and zero normal gradients for scalars. Symmetry conditions are used in the transverse direction. Similar boundary conditions have been used in the earlier study of Jasińska et al [1, 9] and Michael et al [11] for the same Silverson mixer.

5. Results and discussion

The model proposed in Section 2 is first tested with different parameters and then compared against experimental data. The turbulence is treated via the standard \(k-\omega\) SST model proposed by Menter [28].
Figure 4: 2D computational domain and mesh for the Silverson 150/250MS mixer
<table>
<thead>
<tr>
<th></th>
<th>$k$</th>
<th>$\tau_0$</th>
<th>Number of fluid passes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case-A</td>
<td>fixed</td>
<td>fixed</td>
<td>1</td>
</tr>
<tr>
<td>Case-B</td>
<td>function of $E$</td>
<td>function of $E$</td>
<td>1</td>
</tr>
<tr>
<td>Case-C</td>
<td>function of $E$</td>
<td>function of $E$</td>
<td>Multiple</td>
</tr>
</tbody>
</table>

Table 1: List of different cases

<table>
<thead>
<tr>
<th></th>
<th>$k$</th>
<th>$n$</th>
<th>$\tau_0$</th>
<th>$\dot{\gamma}_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case-A</td>
<td>41.5</td>
<td>0.5526</td>
<td>0.8</td>
<td>$\tau_0/2\mu$</td>
</tr>
</tbody>
</table>

Table 2: Model parameters for Case-A

5.1. Initial simulations

Initially three different cases are considered as listed in Table 1. These simulations are run for 3 seconds at a rotation speed of 6000 RPM and an inflow rate of 680 kg/hr.

5.1.1. Case-A

This case is used as an initial calculation to test the implementation of the new model. The values used for yield stress, yield strain, $k$ and $n$ are given in Table 2. As this case is performed to test the methodology: the low shear behaviour incorporates the mechanical energy. The high shear limit behaviour is much less dependent on the viscosity build: consequently, for $\dot{\gamma} > \dot{\gamma}_0$, a simple (constant) inverse power law dependence has been assumed. The values for constants in Eq. (4) are $A = 3.3 \times 10^2$ and $B = 3 \times 10^{-3}$. Note that these are calculated by using data from multiple experiments at different mixer conditions (data fitting not reported here). Figure 5 shows the variation of energy and viscosity of the fluid in the Silverson mixer. It can be noticed that work done on the fluid by the mixer blades is converted into the energy contained in the fluid which results in increased viscosity.
5.1.2. Case-B

In this case the yield stress $\tau_0$ and yield strain are calculated as functions of mechanical energy calculated in Eq. (1):

$$\tau_0 = \frac{|\mu - C|}{D} \quad \text{and} \quad \dot{\gamma}_0 = \frac{\tau_0}{2\mu},$$

(5)

where $C = 8.2448 \text{Pa.s}$ is the viscosity of the fluid at $\tau_0 = 0$ and $D = 1.2064s$ is the inverse of the shear rate. Note that the expression for $\tau_0$ and the values for $C$ and $D$ in Eq. (5) are obtained by fitting a curve to the experimental data for yield stress and viscosity at different rotation speeds of the Silverson mixer (fitting of the data not shown here), while the expression for the yield strain in Eq. (5) is obtained by using the linear relation between the yield stress and yield strain as $\tau_0 = 2\mu|\dot{\gamma}_0|$. The continuity of the viscosity requires that in Eq. (4)

$$\mu_0 = k|\dot{\gamma}|^{n-1} + \tau_0|\dot{\gamma}|^{-1}$$

which leads to:

$$k = \frac{\mu_0 - \tau_0/|\dot{\gamma}_0|}{|\dot{\gamma}|^{n-1}}.$$  

(6)

Now substituting Eq. (6) into Eq. (4) yields:

$$\mu = \begin{cases} 
\mu_0 & |\dot{\gamma}| \leq \dot{\gamma}_0 \\
\mu_0 - \tau_0 \left(|\dot{\gamma}_0|^{n-1} - |\dot{\gamma}|^{-1}\right) & |\dot{\gamma}| \geq \dot{\gamma}_0
\end{cases}$$

(7)
Figure 6a and Figure 6b show the variation of viscosity and energy in the mixer when the modified \( \tau_0 \) and the expression in Eq. (7) are used. Note that the distribution of energy in the mixer is significantly different when compared with those of Case-A. These difference arise due to the modified definitions of \( k \) and \( \tau_0 \). Figure 6c shows the local variation of \( \tau_0 \) as predicted by using Eq. (5) and Eq. (7). It can be seen in Figure 6 that the local values of \( \tau_0 \) are higher than the ones used in Case-A. This implies that the local variation of energy control \( k \) and the yield stress and can consequently lead to variations in local viscosity in the fluid.

5.1.3. Case-C

The mathematical formulation for this case is exactly the same as that used for case-B; the only difference being the fluid from the outlet of the mixer is reintroduced at the inlet of the mixer to check the influence of the history effects of energy contained in the fluid on the viscosity. Figure 7a and Figure 7b show the changes in viscosity and energy when the fluid is recycled from the outlet of the mixer to the inlet of the mixer. An increase in energy contained in the fluid can be seen when compared with case-B (see Figure 6 and Figure 7) which consequently leads to an increase in the viscosity of the fluid as shown in Figure 7a. Note that the values of \( \tau_0 \) are different from those reported in case-B (see Figure 6c). This variation in \( \tau_0 \) implies that the history effect of the work done on the fluid is contained in the fluid in the form of mechanical energy and leads to variations in yield stress and viscosity over time after multiple passes of the fluid. In this case when the fluid is recycled the value of the yield stress increases.

5.2. Comparison with experimental data

The simulation results are now compared with experimental measurements. In these simulations the flow rate is set to 300 kg/h and two different rotation speeds of 6000 RPM and 11000 RPM are used to match the experimental settings. The fluid from the mixer outlet is recycled into the inlet of the mixer as
Figure 6: Variation of viscosity, energy and yield stress in the Silverson 150/250MS mixer for Case-B
Figure 7: Variation of viscosity, energy and yield stress in the Silverson 150/250MS mixer for Case-C
done in the experiments. Figure 8 shows the viscosity and energy variation in
the mixer at the two different rotation speeds. It can be seen that the energy
contained in the fluid increases with an increase in the rotation speed. Some
differences in the evolution of viscosity can be seen in the wake of the mixer
blades at different rotation speeds as shown in Figure 8a and Figure 8c. These
variations in viscosity arise due to the differences in the energy transfer from
the mixer blades to the fluid at different rotation speeds.

Figure 9 shows the predicted viscosity compared with the rheological mea-
measurements of the outlet samples. Note that in the simulations the viscosity at
the exit plane is averaged on the exit surface area to increase the sample size
for averaging of viscosity. The power draw calculated in the experiments is
converted into mechanical energy as:

\[ E = \frac{Pt}{M}, \]  

where \( P \) is the power draw, \( t \) is the time and \( M \) is the total mass of the fluid in
the mixer. It can be seen in Figure 9 that the predicted viscosity is in reasonable
agreement with the experimental data and the model is able to capture the
correct qualitative trends in the viscosity variation with a change in energy. The
viscosity increases with an increase in \( E \), and this increase is directly related to
the rotation speed of the mixer as shown in Figure 8. Some differences in the
predicted viscosity and the experimental data can be seen in Figure 9. These
differences arise due to several reasons including the uncertainty regarding the
performance of the turbulence model used, and also due to the uncertainty in
the experimental measurements. The increase in viscosity in the experiments
occurs over multiple passes of the fluid in the full equipment which includes a
pump and a mixing vessel (shown in Figure 2), while no attempt is made to
include this equipment in the simulations. Furthermore, the energy from the
experiments is obtained via the total power draw of the mixer which includes
frictional and other mechanical losses in the mixer and these losses are not present
in the simulations.
Figure 8: Prediction of variation of viscosity and energy in the Silverson 150/250MS mixer for experimental conditions
Figure 9: Comparison of viscosity and energy with the experiments at different rotation speeds with an inflow rate of 300 kg/h
6. Summary and Conclusions

In this paper a new evolving rheology modelling approach based on mechanical energy ($E$) is proposed. This model incorporates the strain rate history effects into the Generalised Newtonian fluid (GNF) model. The new approach is coupled with the modified Herschel-Bulkley formulation. A pilot scale in-line Silverson mixer is chosen as the representative configuration to test the predictive capabilities of the new model. Experiments have been performed to determine the constants in the new modelling approach and also to validate the viscosity predictions from the new model.

Initial simulations with only one flow through of the fluid in the mixer have been carried out to determine the performance of the new modelling approach and it is found that the model is capable of predicting an increase in viscosity with an increase in the mechanical energy. Furthermore, the model is also capable of predicting an increase in the yield stress with an increase in the local viscosity in the mixer. In the case of recirculation of the fluid from the outlet of the mixer into the inlet of the mixer the new model is capable of retaining the history effects and is capable of predicting the change in viscosity. The viscosity predictions from the new model are in reasonable agreement with the experimental measurements at the rotation speeds and flow rates considered in this paper. Further assessment of the model performance for different flow conditions and the prediction of power draw forms part of the ongoing work.

References


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