Computational Fluid Dynamic Modelling of the Rotational Viscometer

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ABSTRACT: The use of fillers in a bituminous binder satisfies two main criteria: the improvement of the system's mechanical properties and the utilisation of waste products with the associated environmental benefit. An increasing number of filler materials are being used, all with different gradations and specific gravities. It is important to the asphalt technologist to understand the effect the fillers have on the viscosity of the hot bitumen and to ensure even distribution of the filler particles within the mix. One of the instruments used to quantify the behaviour of hot bitumen and bitumen-filler mixtures is the rotational viscometer. Previous research has identified substantial changes in the viscosity with time of both the pure bitumen and the bitumen-filler mixture when measured by the rotational viscometer.

This study uses Computational Fluid Dynamics (CFD) to model behaviour of the bitumen and bitumen-filler in the viscometer. By means of complex rheological models, the pseudoplastic and thixotropic nature of the bitumen is identified and successfully modelled. In addition, the effect of filler drift is identified and modelled, indicating that the steady state equations used to calculate viscosity in the viscometer are invalid for such systems.

KEY WORDS: computational fluid dynamics, filler, rheology, bitumen.

1 INTRODUCTION

The high temperature rheology of bitumen and bitumen-filler systems is of importance to the asphalt technologist for two principal reasons. Firstly, it helps determine the optimum mixing temperatures to mitigate against filler drop out. Secondly, and more importantly, it may be used as a performance predictor of its in-service life. Accurate and reproducible measurement of the rheology is therefore of utmost importance and is often measured using a rotational viscometer. Previous research by Airey and Westwood (2004) identified a shear thinning effect in the high temperature behaviour of pure bitumen and bitumen-filler systems when measured in this way. The apparent viscosity was seen to decrease during the period of the test, sometimes by an order of magnitude.

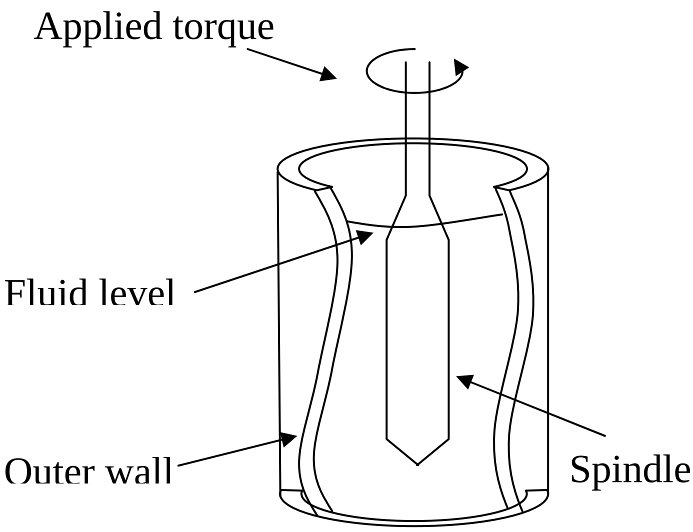
Shear thinning is a coverall term for two, often confused, effects: pseudoplastic flow where viscosity decreases as the shear rate increases; and thixotropic flow where the viscosity decreases with continued shear over a period of time. Often both effects coexist in fluids and are hence difficult to distinguish between. Aside from the shear thinning phenomena, there is also concern as to whether the steady state viscosity equations conventionally used for the rotational viscometer are still valid for bitumen-filler systems heavily loaded with high levels of fillers.

This paper aims to address both these concerns using Computational Fluid Dynamics (CFD) modelling. By bringing this powerful numerical technique to bear on the viscometer, the various effects seen in the tests will be explained in physical terms. No numerical technique, however, can exist in isolation and so an experimental testing programme utilising a Rheologica International rotational viscometer was used to measure the viscosities of pure bitumen and bitumen-filler mixtures as they vary with time. After a description of the experimental campaign, the results from it are presented. There then follows an introduction to CFD modelling, a description of the extra rheological models required for this application, and a comparison of both the empirical and numerical results. Finally a discussion of the findings is presented.

2 EXPERIMENTAL PROGRAMME

All tests were performed with a Rheologica International rotational viscometer, in conjunction with a Thermocell heating unit, using a SC4-27 spindle geometry as shown in Figure 1. A rotational viscometer measures the torque required to rotate the spindle surrounded by the testing medium for a given shear rate. If the dimensions of the bath and spindle are known then the shear rate across the spindle-bath gap may be calculated, assuming the shear rate is constant across the gap. From a knowledge of the torque, shear rate and test dimensions the viscosity of the testing medium may be calculated.

(a)



(b)

Figure 1: Photograph (a) and schematic (b) of the rotational viscometer.

The experimental programme was designed to investigate two main areas: the potential reasons for the decay in viscosity with time as the test progresses; and the effect of filler in the system and whether this invalidates the assumptions of constant viscosity across the spindle-outer wall gap. A straight run bitumen (100 penetration grade) and a bitumen filler mixture comprising bitumen mixed with steel slag of varying gravimetric proportions, were tested at two temperatures and varying shear rates as shown in Table 1. The range of shear rates at which testing can be undertaken are determined by the torque limits of the viscometer. For example, a high shear rate will not be possible when testing a bitumen filler system at a low temperature as the required torque will exceed the limits of the viscometer motor.

3 EXPERIMENTAL RESULTS & DISCUSSION

The results of the viscometer tests undertaken at 100°C are shown in Figure 2(a). One of the most noticeable features of the results is the time dependent decay of viscosity which occurs in both the bitumen and the filler. Interestingly, the bitumen tested at the lower shear rate of 1.36 s^{-1} experiences a greater reduction in viscosity when compared to the bitumen tested at the higher shear rate of 6.8 s^{-1}. However, both tests reach a stable value after approximately 15 minutes. The drop in viscosity for the bitumen tested at a shear rate of 1.36 s^{-1} is approximately 15 Pa.s, which is comparable to that seen in the bitumen-filler tested at the same shear rate. The stiffening effect of the steel slag filler is apparent – the bitumen-filler has an apparent viscosity of approximately 12 times that of the pure bitumen. The viscosity of the bitumen-filler system is still decreasing, albeit at a slow rate 60 minutes into the test – the reasons for this are discussed later.

Figure 2(b) shows the results of the viscometer tests undertaken at 150°C. The proportional decrease in viscosity with time at this temperature is greater than that observed for the 100°C tests for both bitumen and filler. In common with the previous test, the bitumen reaches steady state conditions in approximately 15 minutes, with the viscosity of the filler system still decreasing slowly at 60 minutes into the test. However, the effect of shear rate at the higher temperature of 150°C is different to that observed in the 100°C tests; for the case of the bitumen there is no significant difference in the viscosity behaviour for the two shear rates, and for the bitumen-filler system it is minimal with the higher shear rate test recording a slightly higher viscosity.

Testing was also undertaken on the pure bitumen at both temperatures over a range of shear rates, the results shown in Figure 2(c). In these tests the viscometer was started 20 minutes before a reading was taken to enable 'steady state' values to be obtained. As the viscosity appears to be independent of shear rate, the bitumen can be classified as a Newtonian fluid under steady state conditions.

Table 1: Experimental testing programme.

Mixture	Volume fraction (%)	Shear Rate (s^{-1})	Temperature (°C)	Density of bitumen (g/cm^3)	Density of steel slag (g/cm^3)
100 Pen bitumen	-	1.36, 6.8	100	1.05	2.7
Steel Slag Filler	30	1.36	100		
100 Pen Bitumen	-	51, 102	150		
Steel Slag Filler	10	51, 102	150		

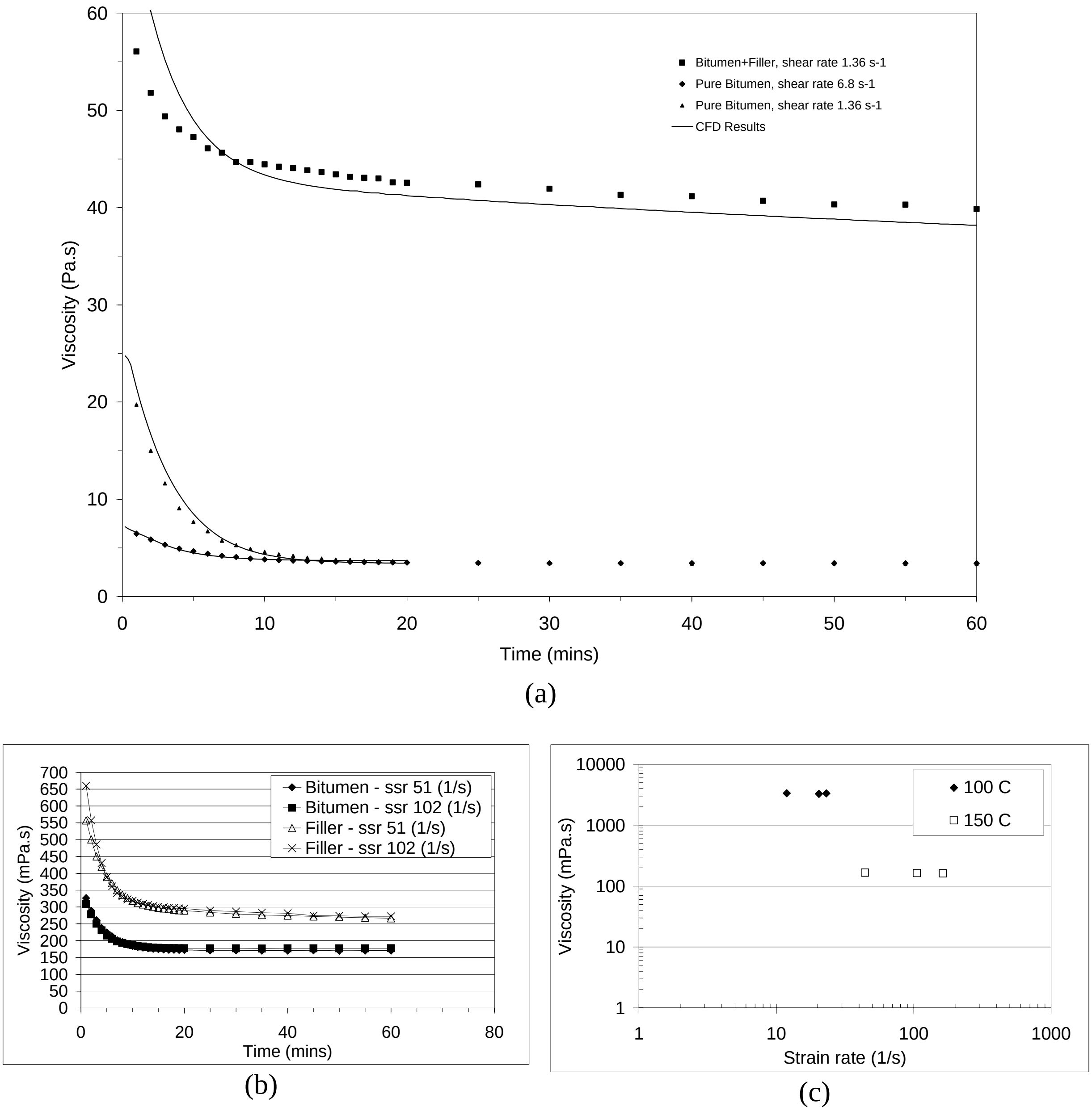


Figure 2: Experimental and CFD results of viscosity variation with time at (a) 100ºC; experimental only at (b) 150ºC and (c) steady state viscosity of pure bitumen.

4 CFD MODEL OF THE ROTATIONAL VISCOMETER

4.1 Introduction to CFD

The commercial CFD software FLUENT (Fluent Inc., 2003) was used in this work. The modelling involves the solution of the Navier-Stokes equations, which are based on the assumptions of conservation of mass and momentum within a moving fluid. In the absence of sources of mass and momentum, the conservation of mass is described by the differential equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \qquad (1)$$

where ρ is the density and $\mathbf{v}$ is the velocity of the fluid. The conservation of momentum is similarly described by the equation:

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v}\mathbf{v}) = -\nabla p + \nabla \cdot \overline{\overline{\tau}} \tag{2}$$

where p is the pressure and $\overline{\overline{\tau}}$ is the stress tensor. Equations 1 and 2 are presented for completeness only, the reader is referred to Ferziger and Peric (1997) for a detailed description of their derivation and solution using numerical techniques. The above equations are for Cartesian coordinates. Since the viscometer displays axial symmetry, it is possible to reduce the problem from 3D to 2D using appropriate techniques to capture the swirl (or circumferential) component of the velocity. Such a model is called a 2D axi-symmetric swirl model. The form of Equations 1 and 2 changes in this new coordinate system, and the reader should consult the FLUENT User's Manual (Fluent Inc., 2003) for further details. The shear stress, $\overline{\overline{\tau}}$, is given by,

$$\overline{\overline{\tau}} = \mu\left[\left(\nabla \mathbf{v} + \nabla \mathbf{v}^T\right) - \frac{2}{3}\nabla \cdot \mathbf{v}\mathbf{I}\right] \tag{3}$$

where μ is the dynamic viscosity, $\mathbf{I}$ is the unit tensor and the second term on the right-hand side above is due to volume dilation and is negligible in the present work. For incompressible Newtonian fluids, the shear stress is proportional to the rate of deformation tensor, $\mathbf{D}$,

$$\mathbf{D} = \nabla \mathbf{v} + \nabla \mathbf{v}^T \tag{4}$$

The shear rate, $\dot{\gamma}$, is defined as the second invariant of $\mathbf{D}$,

$$\dot{\gamma} = \sqrt{\mathbf{D} : \mathbf{D}} \tag{5}$$

Hence the often quoted fact that for a Newtonian fluid, the shear stress and shear rate are related as $\tau = \mu\dot{\gamma}$.

However, it is clear from the results of Section 3 that the bitumen and bitumen-filler mixture exhibit non-Newtonian behaviour, certainly during the decay phase. Before presenting the non-Newtonian models, the next sub-section describes the mesh and boundary conditions used, while the one after disregards several reasons for the initial decrease in apparent viscosity.

4.2 Grid and Boundary Conditions

Any CFD simulation requires the domain to be divided into a large number of small volumes or cells. In an axi-symmetry case, the cells are 2D faces and the grid used in the simulations in this work is shown in Figure 3 (with a zoomed region of the mesh shown on the right). Wall boundary conditions were applied to the inner, outer and bottom walls. The upper boundary was set as a symmetry plane, while the portion of the boundary lying below the spindle was set as an axis. The inner wall was given an angular velocity appropriate to the rotation of the spindle for a given shear rate.

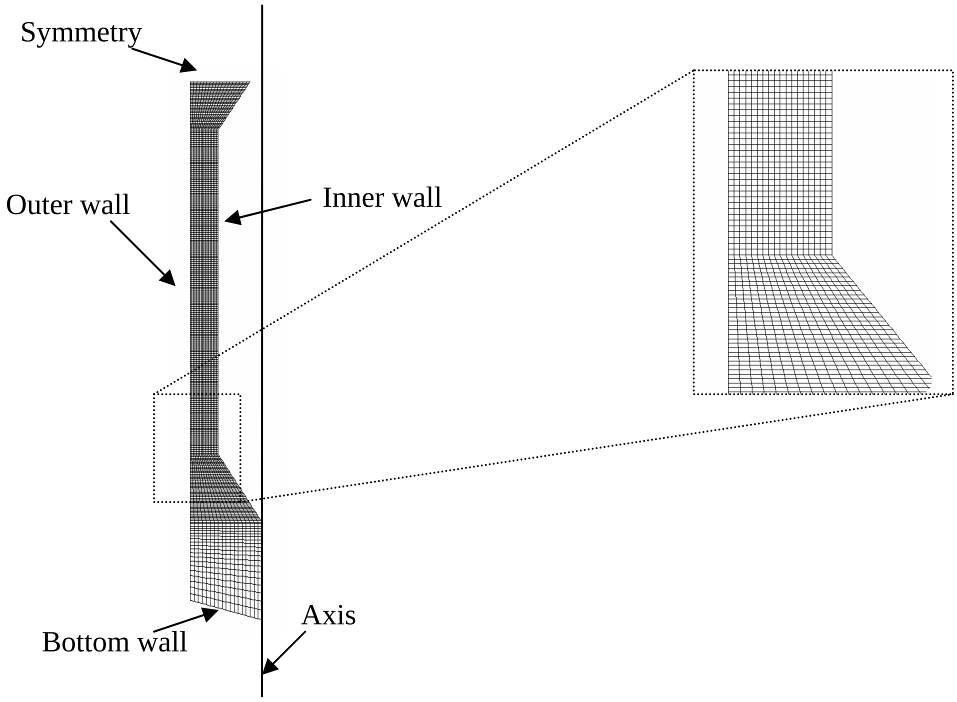


Figure 3: Grid and boundary conditions used in the CFD simulations.

4.3 Disregarding Spin-up, Viscous Heating and Settling

It was thought that the initial reduction in the apparent viscosity of the fluid might be due to a spin-up effect. However, this was quickly discounted since the characteristic spin-up time in a flow dominated by viscous forces is given by,

$$t_{\text{spin-up}} \sim \frac{\rho H^2}{\mu} \tag{6}$$

where H is the height of the long side of the inner wall of the viscometer. In the present study, this spin-up time is approximately 0.36 ms for bitumen at 100°C and 10 ms at 170°C. Given that the decay in apparent viscosity occurs over a period of more than 10 minutes, then the spin-up of a Newtonian fluid can be discounted as a possible explanation. To test this assertion, a transient CFD simulation was carried out with a Newtonian bitumen with a dynamic viscosity of 3.026 Pa.s (the value for bitumen at 100ºC taken from Airey and Westwood, 2004). By using timesteps of 10^{-5}s, it was possible to capture the spin-up effect. Indeed, the CFD predicted that a steady-state was reached after approximately 2.0 ms, slightly longer than that predicted by Equation 6 but nonetheless it can be neglected as an effect.

Airey and Westwood suggested that localised heating effects could be responsible for the initial decrease in viscosity. Here it is assumed that the viscosity decreases with temperature alone. So, a thin region around the inner wall of the viscometer would pull the bitumen next to it, causing large local increases in the shear rate and thereby imparting heat into the bitumen, increasing its temperature above the ambient. Could this temporary, low viscosity region be responsible for the high apparent viscosity seen early in the experiments? Again a CFD model was used to prove this theory, the details of which are not included here. The results from the CFD simulation were conclusive – there is no significant heating effect seen. In a transient simulation of the first fraction of a second (the same period as used in the previous section on the spin-up effects), no temperature rise was seen, at least to the fourth decimal place. In a steady-state simulation, which represents the situation where everything is in equilibrium, a temperature rise next to the inner wall of 0.002^{o}C was seen. Such a rise is insufficient to compromise the Newtonian assumption.

For the bitumen-filler system, Airey and Westwood disregarded particle settling as an explanation for the decreasing viscosity.

4.4 Rheological Models

Billington (1960) stated “The thixotropic behaviour of wax containing oils is attributed to the individual wax crystallites which coalesce to form an internal structure of crystal aggregates…when the system is maintained free of stress…thus showing increased resistance when sheared again.” He went on to surmise that these aggregates sit in a background Newtonian fluid of un-aggregated crystals which break down under shearing. This can be compared with Read and Whiteoak (2003) who state that bitumen is regarded as a colloidal system consisting of asphaltene micelles dispersed in a oily medium of maltenes.

Here it is assumed that the high initial viscosity of the bitumen was due it being thixotropic, similar to the waxy oils described by Billington. A thixotropic model was added to Fluent using User-Defined Functions (UDFs), based on the work of Modigell and Koke (1999), who looked at the rheological behaviour of semi-solid alloys. Much of their work, however, is applicable to the present situation. To do this, a structural parameter, κ, is introduced which describes the level of aggregation within the bitumen. The kinetics of the structural parameter are modelled as a first-order reaction,

$$\frac{\partial}{\partial t}(\kappa) + \nabla \cdot (\mathbf{v}\kappa) = C \cdot (\kappa_e - \kappa) \tag{7}$$

where C is the reaction rate and κ_e specifies the equilibrium value of the structural parameter at a given shear rate. The reaction rate can be a function of the shear rate, but for the present study it is assumed to be a constant. To take into account the pseudoplastic behaviour of the bitumen, a power-law model for the viscosity is used,

$$\eta = k\dot{\gamma}^{n-1}\kappa \tag{8}$$

where k is the consistency index and n is an exponent whose value determines the nature of the fluid. For example, $n = 1$ indicates a Newtonian fluid and $n < 1$, a shear-thinning fluid. The structural parameter will decrease from an initial value, κ_0, and will tend to the equilibrium value as the simulation progresses. The equilibrium value is typically a function of the shear rate,

$$\kappa_e = (a\dot{\gamma})^m \tag{9}$$

where a is given the value of 1s and m is an exponent.

Table 2: Parameters used in the CFD simulations.

	Pure bitumen	Bitumen-filler
Consistency index, k	3.672	3.672
Exponent, n	0.814	0.814
Exponent, m	0.186	0.186
Structural parameter reaction rate, C	0.006 s^{-1}	0.006 s^{-1}
Initial structural parameter, κ_0	7.0	1.7
Initial volume fraction of filler, ϕ_0	0.0	0.3
Constant, B	-	8.5
Constant, K_c	-	1.0
Constant, K_η	-	1.0
Mean particle diameter, d	-	2.0×10^{-5} m

The significantly higher viscosity and longer decay time seen in the bitumen-filler system cannot be modelled using the model described above. Instead the effect of the filler particles must be included. According to Leighton and Acrivos (1987), a process called shear-induced diffusion is present in disperse solid suspensions in which the concentration of the particles can vary locally within the carrier fluid. There are two components to this cross-stream diffusion. The first is due to the particles moving away from regions of high concentration because they experience more collisions in such regions. In addition, the particles will move from regions of high shear to those of low shear. These two effects can be described by a flux of the form,

$$\mathbf{J}_c = -K_c d^2 \phi \nabla (\dot{\gamma}\phi) \tag{10}$$

where K_c is a constant, d is the mean particle diameter and ϕ is the particle volume fraction. The second component is due to particles moving from regions of high viscosity to low viscosity regions. This is described by a flux,

$$\mathbf{J}_\eta = -K_\eta d^2 \frac{\dot{\gamma}\phi^2}{\eta} \nabla \eta \tag{11}$$

where K_η is a constant. The transport equation for the particle volume fraction is,

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{v} + K_c d^2 \nabla \dot{\gamma})\phi + d^2 \nabla \cdot \left[K_c \phi \dot{\gamma} + K_\eta \frac{\dot{\gamma}\phi^2}{\eta} \frac{d\eta}{d\phi} \right] \nabla \phi = 0 \tag{12}$$

Equation (8) for the viscosity is updated to include the presence of the particulate phase,

$$\eta = k \dot{\gamma}^{n-1} \kappa \, e^{B\phi} \tag{13}$$

where B is a constant.

4.5 CFD Results

For the above model to fit the bitumen-only curves of Figure 2(a) at equilibrium, then $m = 1 - n$ to ensure that the final apparent viscosity is independent of shear rate. The other proviso is that the initial value, κ_0, is the same for both shear rates, since it is independent of the shear but only on the state of the sample before the test or simulation commences. The set of parameters used in both simulations is shown in Table 2. Figure 2(a) shows the results from the CFD simulations (in solid lines) superimposed on the first 20 minutes of the bitumen-only test results at 100^{o}C. As can be seen, the model agrees with the experimental data well for both shear rates.

In order for this model to then fit the observed data for the bitumen-filler from Figure 2(a), it was necessary to modify the initial value of the structural parameter, justifiable on the grounds that the presence of the steel slag particles disrupts the level of aggregation in the bitumen. In addition, the constant B was given a non-zero value to take into account the increased viscosity due to the presence of the particulate phase. A single, representative diameter of the particles (20 µm) was used in these simulations. Any number of particle sizes could have been used, but for the purposes of this demonstration it was limited to one. Again all values for this simulation can be seen in Table 2. The decay in the viscosity predicted by the CFD model does not fit the experimental data as impressively as before but it does capture the important effects. The initial rapid decrease over the first 10 minutes is due to the thixotropic nature of the bitumen carrier fluid, and the continued fall seen in the remainder of the simulation is due to particle migration. Since the latter process operates over much longer timescales, it is only seen after the thixotropic effects have ceased to play a role.

The particle migration has a marked effect on the viscosity in the gap between the inner and outer walls of the viscometer. A constant viscosity is one of the main assumptions made when testing such materials and, as can be seen from Figure 4(b), the viscosity is far from constant across the viscometer Also seen in the figure are (a) the particle volume fraction falls near the inner wall as the particles drift in the shear field. The swirl component of the flow (c) and the shear rate (d) are also shown in the figure.

5 DISCUSSION

This paper shows that the rheology of high temperature bitumen in a rotational viscometer is a complex system. Once particles are introduced, the system becomes even more complex with many competing processes contributing to the behaviour of the mixture. By using CFD modelling, it has been shown that pure bitumen is shear thinning, but that this is a combination of pseudoplasticity and thixotropy that, in the steady-state, produce Newtonian behaviour. Before the steady state is reached, however, the two processes compete to make predictions of the transient variation of the viscosity difficult.

When filler is introduced, the presence of the particles disrupts the thixotropic process to some extent and clearly the drift of filler particles operates over longer timescales. Again quantifying these effects is possible using properly calibrated CFD models.

The CFD modelling was limited to the 100°C case, the 150°C case displayed behaviour that would necessitate the extension of the model described herein to include temperature effects. Since the two curves for different shear rates for pure bitumen in Figure 2(b) collapse onto each other, it would indicate that a temperature dependency should be introduced that would diminish the contribution from pseudoplasticity to the model. The advantage of CFD modelling is that the introduction and testing of such an extension to the model is greatly simplified and will form part of a future paper.

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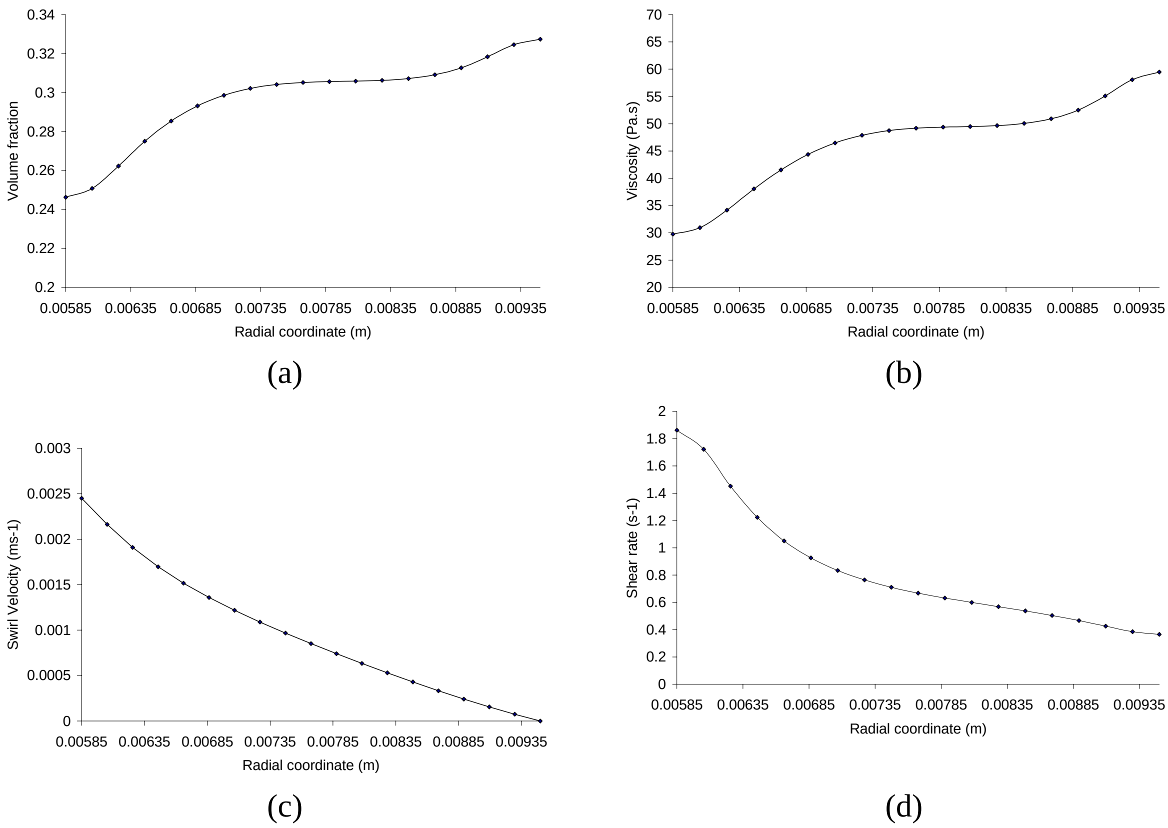

Figure 4: Variation across the viscometer gap of (a) particle volume fraction; (b) viscosity; (c) swirl component of velocity; and (d) shear rate.