Creeping–Flow Computational Modelling of Optical Quality Free–Surfaces formed by Slumping of Molten Glass

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1. Introduction

Thermal replication is an industrial process used in the manufacture of aspheric optical surfaces, as discussed by Smith et al. [12]. A glass workpiece is placed on a ceramic mould and this combination heated in a kiln so that the glass softens and "slumps" into the mould, so replicating the mould surface. This process is illustrated in Figure 1.

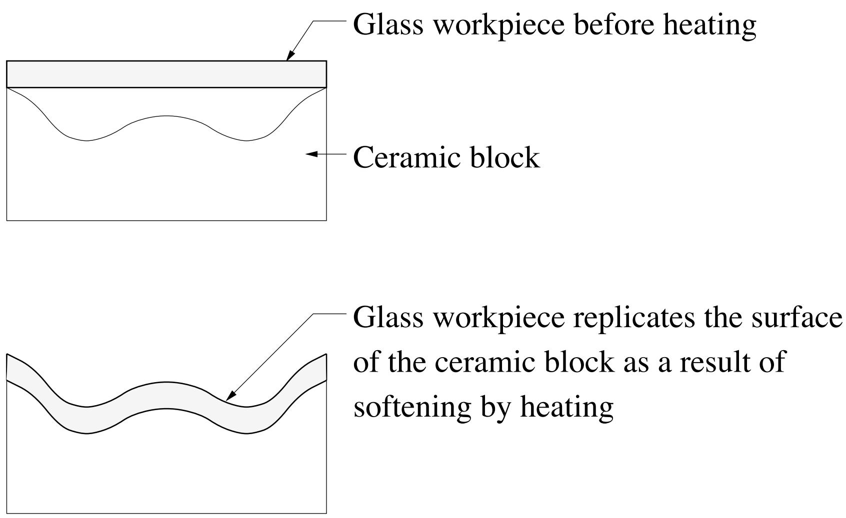

FIGURE 1. Thermal Replication (after Smith et al.)

The upper free–surface of the glass, that does not contact the mould, is the critical optical surface. It is very smooth and requires no polishing — a difficult process for complicated aspheric surfaces. However, this surface does not exactly replicate the mould surface, and an iterative process for correcting the mould in order to achieve the desired optical surface at the required accuracy, is necessary at the design stage. Here we investigate numerically modelling this slumping process, with the aim of greatly reducing, if not eliminating, the experimental iteration currently required.

Molten glass is a very viscous fluid having a viscosity of order 10^7 Pa·s and higher, at normal slumping temperatures. Thus, flow is very slow and can be modelled by the Stokes creeping–flow equations. We solve these using the finite–element method, which is the preferred numerical method for modelling of forming processes (see Preface of [9]), and is especially so where moving free–surface boundaries are involved.

The slumping of a bridge of very viscous fluid spanning the gap between two vertical no–slip walls, and involving no mould contact has been considered by Tuck et al. [14]. Similar to slumping, blow-moulding is a process where a layer of very viscous fluid is forced against a mould by creating a pressure drop across its thickness, and this has been the subject of considerable investigation with particular application to the manufacture of axisymmetric containers [3, 4, 6, 16]. In all of this work, slow-flow approximations have been made and finite–element methods employed. Asymptotic methods have also been used for pressure driven flows of thin viscous sheets without mould contact [8, 15], but are not easily extended to include mould contact.

2. Glass Properties

It is generally assumed that molten glass in the viscosity range at which moulding is done, is an incompressible fluid. While this is not strictly true, it is considered to be sufficiently accurate for practical purposes, and in any case, is an assumption made in all current methods for determining molten glass viscosities [7]. Furthermore, while a viscous isotropic Maxwell fluid model was used in some early glass modelling work [4, 16], it is now generally accepted that molten glasses, with but few exceptions, are Newtonian fluids [10], and this assumption has been adopted in more recent work [3, 6, 8, 14, 15]. Thus, we assume that slumping molten glass is an incompressible, Newtonian flow. The density of glass does not vary much with temperature so that we may reasonably assume this to be constant. We also ignore any surface tension effects, which we justify on the basis that the capillary number is large (see [14]).

Complex issues do however arise in the consideration of the relationship between temperature and viscosity, which must be the most important physical consideration in modelling of glass forming processes. Firstly, there is the phenomenon of relaxation and equilibrium viscosity, and secondly the viscosity of a molten glass is highly temperature sensitive.

At large viscosity, a change in temperature takes a finite time to be reflected in the corresponding change in viscosity, with this time increasing as viscosity increases (and temperature decreases). This is known as relaxation, and the final viscosity reached is called the equilibrium viscosity. With viscosity (μ) measured in decipascal seconds (or poise), Scholze and Kreidl [10] give $L = \log(\mu) = 10$ as the point at which viscosity lags by some seconds behind a fast cooling rate, and $13 \leq L \leq 14.5$ as the glass transition in which lag time varies from around 15 minutes to 4 hours and properties are most definitely time dependent. In the numerical modelling of slumping, we are concerned with the change in glass viscosity as it is heated at the commencement of the slumping process, when viscosity is potentially higher than equilibrium. From our experience slumping will occur, given sufficient time, at viscosities as high as $L = 11$, which is just on the fringes of the time-dependent property region given in [10]. Practically however, very little slumping would occur at such high viscosities, since oven temperatures are quickly increased to bring the viscosity down into the region $7 \leq L \leq 8$ where slumping occurs at a faster and more acceptable rate, and any lag will only serve to further prevent slumping at this stage. Thus we assume that relaxation will not significantly affect slumping, and that computation based on equilibrium viscosities will be adequate. In any case any time lag in the viscosity can be easily corrected by adjusting the time scale as we will show.

The sensitivity of viscosity to temperature is an issue that is less easily dismissed. With viscosity varying by more than an order of magnitude over the slumping temperature range, there is a clear possibility that spatial variation of temperature throughout the molten glass may significantly affect its flow behaviour. Certainly for some processes such as blow-moulding, where a parison must first be formed and the mould is cold, spatial temperature variations are likely to be quite important, and thermal modelling should be coupled with fluid–flow modelling [3, 4, 16]. In slumping however, both mould and glass are heated together from room temperature so that spatial temperature variations will be considerably less than for blow-moulding. On the other hand, the tolerances on the quality of optical surfaces formed by slumping are necessarily very much tighter than tolerances on container wall thickness and surface finish, so that such spatial variations as do exist might still be of importance. Thus, while an isothermal model might be adequate, there is a need to investigate spatial temperature variation.

At this point however, we are presented with considerable difficulties. We can use the commonly adopted Vogel-Fulcher-Tammann (VFT) empirically derived equation to approximate the viscosity–temperature relationship of the glass [10, 11], but this relies on being able to determine the temperature within the glass. This is by no means trivial given a general lack of information on glass thermal properties and how these vary with temperature, plus very ill-defined issues of glass–mould contact and non-uniformity of kiln temperatures. As a result, in other work very approximate and simple thermal models have been assumed [3, 4, 16] or the isothermal case alone has been solved [6, 15], in order to get some qualitative idea of the flow behaviour.

From this discussion, it is apparent that sensitivity studies of this problem would be of considerable value, and for this purpose we develop a finite element formulation and program that enables us to impose any temperature/viscosity distribution that we might like to investigate. However, in this paper we assume isothermal slumping conditions to be reasonable, and focus on our computation methods. It is worth commenting that any temporal temperature profiles are easily accommodated with an isothermal model, as we will see.

3. A Stokes–Flow Model

The very large viscosity of molten glass and the consequent small slumping velocity scale ($\sim 1/\mu$) and Reynolds number ($\sim 1/\mu^2$) permit a quasi-steady formulation of the problem, obtained by simplifying the full Navier-Stokes flow equations to the creeping flow or Stokes equations [2, p.216 *ff*]. These are solved for the (steady) flow applicable over a small time interval. The fluid geometry is then updated to reflect the small changes brought about by this flow, and the process repeated.

For a fluid of density ρ and viscosity μ, in a gravity field of strength g acting in the $-x_3$ direction, the equations to be solved are (in tensor notation)

$$\frac{\partial p}{\partial x_i} = \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] - \rho g \delta_{3i} \tag{3.1}$$

together with the continuity equation for incompressible flow

$$\frac{\partial u_i}{\partial x_i} = 0. \tag{3.2}$$

At boundaries that are in contact with the mould we must satisfy the no–slip condition

$$u_i = 0 \tag{3.3}$$

and on all other boundaries, the no-stress free–surface conditions apply

$$-pn_i + \mu n_j\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) = 0, \tag{3.4}$$

where n_i is the unit normal. In all equations, indices i and j have range from 1 to 3 for three dimensions.

We solve equations (3.1) and (3.2) subject to the prescribed boundary conditions (3.3) and (3.4) for velocity u_i and pressure p, using the finite–element method with a mesh of 6-node triangles over the flow domain. As is usual, we use linear basis functions for pressure and quadratic basis functions for velocity.

The time evolution of the flow geometry is given by solving the slumping dynamics equations

$$u_i = dx_i/dt \tag{3.5}$$

at each node using the known velocity field, to give the new node position x_i. The mesh is then adjusted by moving each node to its new position, to give a new geometry on which the procedure is repeated. As slumping progresses, the lower free–surface of the glass contacts the mould surface, and because of this we have chosen to use Euler's method to solve equation (3.5) for x_i at the $(n+1)$th time step

$$x_i^{n+1} = x_i^n + u_i^n \times \Delta t. \tag{3.6}$$

Then we can easily check that no node crosses the mould boundary, but at best just reaches it, and if necessary reduce the time step Δt to satisfy this criterion. We find this method gives good accuracy provided node displacements are sufficiently small. When a node reaches the mould boundary its boundary conditions are changed from free–surface to no–slip. This is exactly the method of handling mould contact described in [3, 6].

Rather than work with the dimensional equations given above, we solve the dimensionless equations obtained by setting ρ, g and μ to unity. Dimensional quantities are given by multiplying by the appropriate scales. Choosing the disc radius a as the length scale $\mathcal{L}$, the velocity, pressure and time scales $\mathcal{U}$, $\mathcal{P}$ and $\mathcal{T}$ are given by

$$\mathcal{U} = \frac{\rho g a^2}{\mu}, \qquad \mathcal{P} = \rho g a, \qquad \mathcal{T} = \frac{\mu}{\rho g a}. \tag{3.7}$$

From this we see that the Reynold's number ($\rho\mathcal{U}\mathcal{L}/\mu$) is like $1/\mu^2$ as claimed earlier.

An important consequence of the neglect of the time derivatives in the field equations (3.1), together with the isothermal assumption, is that temporal changes in viscosity may be accommodated by a time–varying time scale $\mathcal{T}(t)$. Then a time period of length t_f is in dimensionless terms given by

$$t_* = \int_0^{t_f} \mathcal{T}(t)^{-1} dt = \rho g a \int_0^{t_f} \mu(t)^{-1} dt. \tag{3.8}$$

Thus, given some initial geometry, the final product will be the same for different curves $\mu(t)$ and slumping periods t_f, provided that the value of t_* in each case is the same. In other words, the area under each curve of inverse viscosity must be equal (see Figure 2). This means that, if our assumption of isothermal conditions is shown to be valid, the dimensionless problem can be solved once and post-processing used to look at different viscosity profiles resulting from different temperature–time profiles.

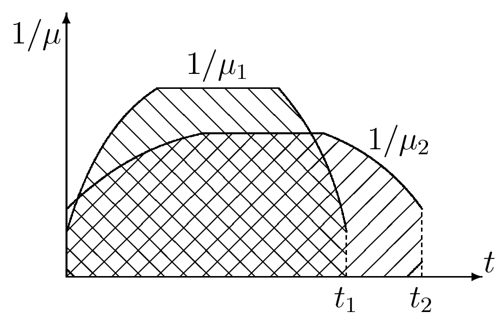

FIGURE 2. Equivalent Viscosity Curves

4. Numerical Slumping — An Example

To illustrate our methods, we take an axisymmetric arrangement of an initially flat glass disc supported on a concave mould as shown in Figure 3. For clarity the vertical scale is twice the horizontal scale. The mould surface may have an aspheric profile, though for our purposes we have chosen it to be spherical in order to more clearly show the differences that slumping produces in the top free–surface of the glass compared with the mould surface. While the axisymmetry of the problem certainly simplifies our computations, a fully three-dimensional case can be readily solved, once the more difficult tasks of mesh generation for both mould surface and glass have been accomplished.

Computation time for this example with a mesh of 1494 nodes, 695 triangular elements and 73 time steps of size 0.005 and less, was about 20 minutes using a single 167 MHz processor on a Sun Ultra Sparc 170 computer having 256MB of RAM.

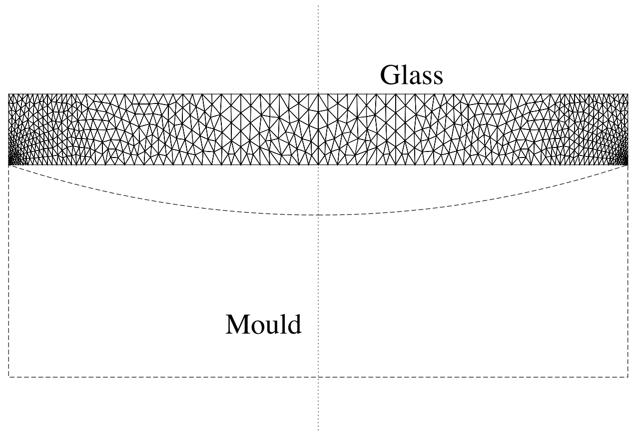

FIGURE 3. Geometry Prior to Slumping ($t = 0$)

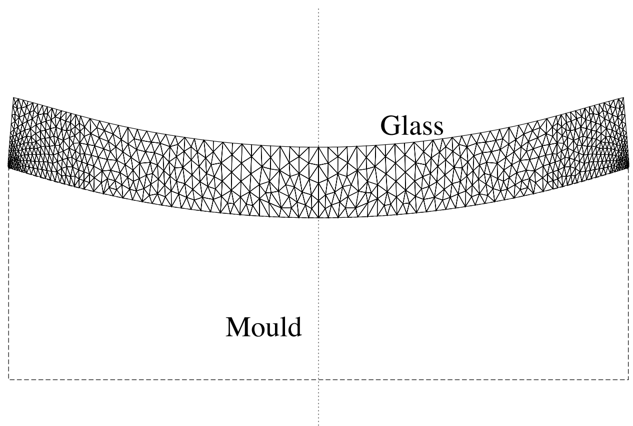

FIGURE 4. Full Mould Contact at $t = 0.075$

Figure 4 shows the slump after full mould contact has been attained. Prior to full mould contact, slumping proceeds quite rapidly, though in real terms this may take in excess of 1 hour. Mould contact greatly reduces the rate of flow, and after full mould contact, slumping effectively ceases with further flow taking many hours or even days.

Figure 4 does not show at optical accuracy, how well or poorly the mould surface has been replicated on the top glass surface. Hence we now look at determining surface curvature.

5. Surface Curvature

For optical surfaces, the design criterion is that the surface curvature meets the specification to within tolerance. For the axisymmetrical example under consideration, the top glass surface height z is a function of radius r only and curvature κ is given by

$$\kappa = \frac{z''}{(1 + z'^2)^{3/2}} \tag{5.1}$$

where primes denote differentiation with respect to r. As output from our finite–element program we obtain the coordinates (r,z) of nodes located on this boundary, and from this we want to obtain second derivatives to give curvature to within ± 0.001. The obviously difficult task of accurately differentiating non-exact data such as is obtained from any discretized computation process is an area of current research [1].

The method that we use is to fit a least squares B-spline series [5] to the surface node coordinates using about one fifth as many terms as nodes. Knots and nodes are not coincident (excepting at end points), and we use B-splines of high degree ($k \geq 4$), to ensure adequate continuity and smoothness. From this we can obtain first and second derivatives and so calculate the curvature along a radius of the glass disc. This method may also be extendible to three-dimensional surfaces (see [5]), though we have not yet progressed this far.

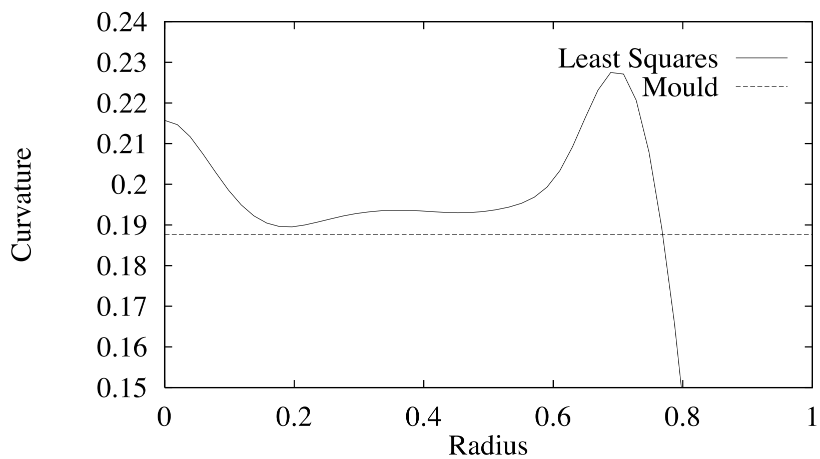

Figure 5. Surface Curvature

Figure 5 shows curvature from a degree 6 least squares B-spline series for our numerical slumping example (solid curve), as well as the constant mould curvature (dashed line). A comparison of curves obtained by varying the number of terms and the degree of the B-splines, leads us to believe that we are able to calculate curvature to an accuracy that is close to, if not actually, within tolerance, but further work is required to verify this. However, even allowing for error in curvature calculation greater than the desired tolerance, it is clear that the actual slumped profile differs from the mould curvature that we are attempting to replicate by amounts well outside the given optical tolerance, and we could proceed immediately to modify the mould surface so as to more nearly obtain the desired optical surface.

6. Conclusion

We have developed tools to numerically simulate the slumping of molten glass into an axisymmetric mould which may have an aspheric profile, and to compute the curvature of the resulting top free–surface. We have demonstrated their use for a flat glass disc slumping into a spherical mould, and shown that the mould surface is not replicated to optical accuracy. This work is in qualitative agreement with some initial experimental results [13]. We are now able to utilise these tools to investigate the importance of spatial temperature variations, and to iteratively determine the mould profile that will yield the required free–surface.

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