Thermal Replication: A Comparison of Numerical and Experimental Results

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1 Introduction

A mathematical model of an industrial processes is invariably based on numerous simplifying assumptions that render the problem more tractable, and indeed solvable using current knowledge. Often, much useful insight into and understanding of the process can be gained from a simple model that involves only its most important aspects. Additional complexity can then be added, and tests conducted to determine the effects this might have. During this model-development procedure, validation against experimental data is necessary, to ensure that the model gives results that are consistent with reality. Such validation may also indicate a need to include in the mathematical formulation, features of the process previously neglected.

The industrial process that we consider is thermal replication, whereby a glass workpiece and ceramic mould combination are heated so that the glass slumps into and (approximately) replicates the mould, as illustrated in Figure 1. This process

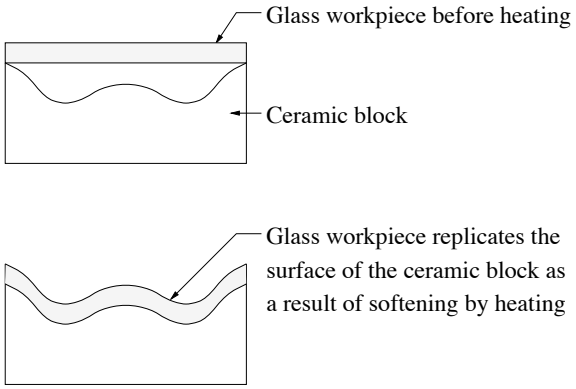

FIGURE 1. Thermal replication (after Smith et al.).

is used in the manufacture of aspheric optical components [4], for which accurate surface curvatures on the upper free surface are critical. Because this surface does not exactly replicate the mould surface, it is currently necessary to go through an iterative experimental process of slumping and mould modification, to determine the exact mould shape needed to yield the required optical surface. A numerical simulation of the process, that can be used as a predictive tool, would therefore be of great benefit.

We have developed a creeping-flow finite-element formulation of thermal replication, which is described in [5]. As discussed in [5], the viscosity of molten glass is highly sensitive to temperature, and with the tight tolerances required on the quality of optical surfaces, it is possible that spatial temperature variations within the glass, arising from oven non-uniformity, glass-mould contact and other things, may significantly affect its flow behaviour and hence the final product. On the other hand, because glass and mould are heated together from room temperature, there is reason to believe that spatial temperature variations will be less important in thermal replication than in other glass-forming process such as blow moulding, in which hot glass contacts a cold mould and a coupled heat and fluid flow model should be used [1]. Thus, for thermal replication, an initial assumption of isothermal slumping conditions is both reasonable and simplest as a first approximation. Temporal temperature changes are easily accomodated with this model as discussed in [5].

While we do not attempt to model heat transfer in the thermal replication process, our finite-element formulation does permit us to impose an arbitrary viscosity distribution in the glass, which can be equated with a temperature distribution via the Vogel-Fulcher-Tammann (VFT) equation [3]. Thus we are able to compare experimental slumping results with numerical simulations under both isothermal and selected non-isothermal conditions. By this means we seek to determine whether spatial temperature variations are sufficiently important, to warrant addressing the very difficult task of developing a model that couples heat transfer and fluid flow.

2 The Experiment

The particular test case that we use for current validation purposes, consists of a glass disc with small initial spherical curvature, supported on a circular concave mould with larger spherical curvature. This arrangement is shown in Figure 2, with all dimensions scaled by the mould radius R. In practice we have $R = 45$mm.

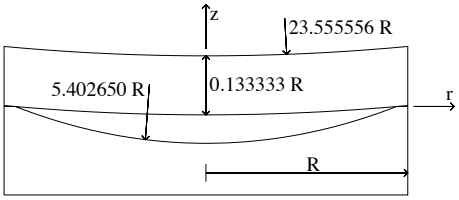

FIGURE 2. Test case geometry.

The glass disc and mould combination is placed in an oven and heated from room temperature at 4°C/minute to a temperature of 700°C. The temperature is then held at this value for a period of time known as the "soak", before the oven is turned off and the system allowed to cool naturally.

In order to find the point at which full contact between the lower glass surface and the mould is achieved, a number of experiments with different soak times have been conducted. Full contact is deemed to have occurred if the slumped glass component shows marking over the whole of its lower surface. This is not easy to see, and it is possible that full contact occurs at an earlier time than we identify.

In Figure 3 we show the curvature (K) profile (multiplied by the mould radius R) on the upper glass surface for a 40 minute soak after which it appears that the glass may not have made full contact with the mould, and for a 50 minute soak after which it is more certain that full contact has been made. Curvature is calculated in the manner described in [5], from vertical sag measurements made across a diameter of the glass component using a profilometer. Two data sets of (r, z) coordinates across two perpendicular diameters intersecting at $r = 0$ are obtained, to give two curvature profiles for each of the two slump cases.

Since the slumping geometry is axisymmetric (or at least nearly so), we expect all of these curves to be symmetrical about the vertical axis and the two curves for a particular soak time to be identical. Neither of these expectations are realised in Figure 3 and there are a number of possible reasons for this. In considering these, it must be borne in mind that quite significant changes in curvature can arise from even small variations in the surface profile of the glass. The wiggly character of the left portion of the curves compared with the right portion, strongly indicates imperfections in the experimental components and/or setup. The way in which the central peaks of the curves are offset either side of the vertical axis for the 0° and 90° diameters, initially suggests that the glass components were not quite centrally positioned on the profilometer, so that the intersection of these 'diameters' identified with the disc centre is in fact offset from the true centre. However, examination of the raw profilometer sag data shows the size of the offset (less than 0.1 mm in both horizontal directions) to be much less than that required to rectify this problem, so that it too is probably mostly due to imperfections in the experimental components and/or setup. There is also evidence of small inaccuracies in the sag measurements themselves, although this should have a uniform effect over all data sets and cannot explain the magnitude of asymmetry that we are seeing.

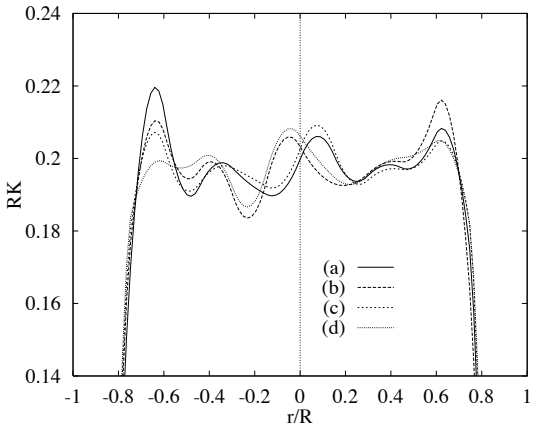

FIGURE 3. Top surface curvature for (a) 0° diameter, 40 min. soak, (b) 90° diameter, 40 min. soak, (c) 0° diameter, 50 min. soak and (d) 90° diameter, 50 min. soak.

On combining the 0° and 90° data sets for a slump case and calculating curvature from points $(|r|, z)$, we obtain indicative (axisymmetric) profiles for 40 and 50 minute soak times as shown in Figure 4. We use these in comparisons with our numerical simulations.

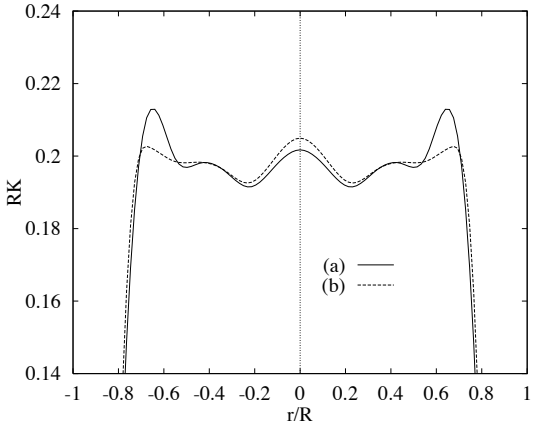

FIGURE 4. Top surface curvature for (a) 40 min. soak, and (b) 50 min. soak.

3 Isothermal Numerical Simulation

Our first numerical simulation is for isothermal conditions, that is, the temperature throughout the glass is uniform at any point in time, although that temperature varies with time. By measuring the sag of glass components after slumping

with one hour soaks at temperatures from 450 to 650°C, it has been found that, for the glass in use, slumping will only occur if the temperature is at least 600°C. Thus it is necessary to model only that portion of time during which the temperature is 600°C or higher.

We can proceed by computing the slumping of the glass at a temperature that is constant in time, and include temporal temperature and viscosity changes by post-processing via a time-varying time scale, as described in [5]. However, because we also wish to consider non-isothermal slumping, we rather keep the time scale constant (at $\mathcal{T} = \mu_0/(\rho g R)$ with $\mu_0 = 10^7\,\mathrm{Pa}\cdot\mathrm{s}$ and $\rho = 2500\,\mathrm{kg}/m^3$), and update the temperature and (relative) viscosity at each time step of the simulation. Thus, beginning with a temperature of 600°C for the first time step, the corresponding viscosity is determined from the VFT equation and the sag of the glass is computed. The temperature is then increased by an amount equal to the heating rate multiplied by the elapsed time, and the new glass viscosity computed. The sag of the glass is then computed for the next time step, and so on. Once the soak temperature is reached, the temperature and viscosity are held constant. A mesh of 889 6-node triangles is generated over the glass component, and we compute to a time of $0.3\mathcal{T}$ in 138 steps of size 0.005 or less. From this simulation, we identify the point at which full mould contact is achieved and compare this with the experimental results presented above. Thus we effectively assume that there is no glass flow once the oven has been turned off. This is not too unreasonable given that flow is very slow once full mould contact has been established and that the experimental results we are comparing with are for full mould contact.

Our numerical simulation gives full mould contact occuring at about $0.22\mathcal{T}$ to $0.23\mathcal{T}$, which in real terms is a total slumping time of 33 to 35 minutes. Since this includes the time for the temperature to rise from 600 to 700°C at a rate of 4°C/min., the soak time is only 8 to 10 minutes. This is considerably different from the 40 to 50 minute soak determined experimentally, and we will comment further on this later.

Figure 5 shows the upper-surface curvature profile obtained from the numerical data, compared with those obtained from the experimental data. The general behaviour of the numerical solution is in good agreement with the experiments. However, we would like the numerical prediction of the product RK to agree with the experimental results to within ± 0.001, since this is about equivalent to the manufacturing tolerance on curvature for ophthalmic lenses. With the present experimental data and processing methods, the maximum difference is about 0.008 for $|r/R| \le 0.6$, and considering that we see this magnitude of difference between experimental data sets that should be identical (see Figure 3), this is probably as good as can be expected. In the region $0.6 < |r/R| < 0.8$, the numerical simulation shows a larger peak than the experiments, particularly in relation to the 50 minute soak result. This could be due to using too coarse a grid when measuring sag with the profilometer, leading to an inability to properly capture what is happening in this region of rapid curvature change. Compared with the profilometer measurements, the numerical simulation gives about double the number points on the upper glass surface in this region, from which we calculate curvature. This is a matter that needs further investigation.

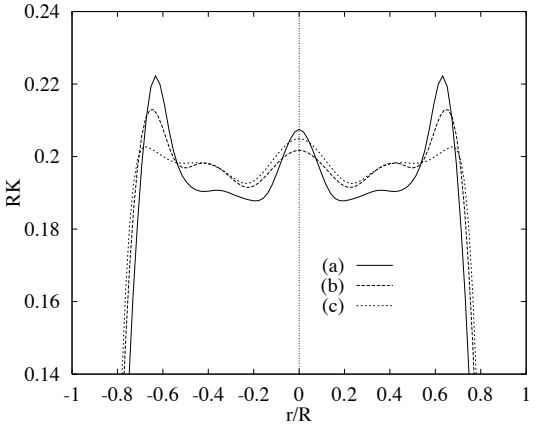

FIGURE 5. A comparison of upper-surface curvature given by (a) an isothermal numerical simulation, (b) experiment with a 40 min. soak, and (c) experiment with a 50 min. soak.

4 Non-isothermal Numerical Simulation

As discussed in [5], modelling of heat flow in slumping glass is extremely difficult, there being little knowledge of glass and ceramic thermal properties as well as very ill-defined issues of glass-mould contact and non-uniform oven temperatures. Nevertheless, it is interesting to consider the effects of some arbitrary spatial temperature/viscosity distributions in the glass. We here look at just two possibilities.

Firstly, we consider that the temperature in the glass at time $t = 0$ is a linear function of radius only, decreasing from 600°C in the centre to 590°C at the edge (a drop of 10°C). For $t > 0$ the temperature at any point in the glass is then given by $T_i + 4°\mathrm{C/min.} \times t$, where T_i is the initial temperature at $t = 0$ and t is given in minutes. When the temperature at any point reaches 700°C it is not further increased. At any time t, the viscosity distribution can be obtained from the temperature distribution via the VFT equation.

Our second example is similar to the first, excepting that at $t = 0$ the temperature increases from 590°C at the centre to 600°C at the edge.

Both of these non-isothermal cases are extreme

in that we would not expect such a large temperature difference between the centre of the glass disc and its edge. However, they do give some indication of how spatial temperature variation influences the upper-surface curvature of the glass disc, and from this we can try to ascertain whether these are important in the slumping process.

Figure 6 compares the upper glass-surface curvature profiles after full mould contact for both of these non-isothermal cases, with the experimental results obtained with 40 and 50 minute soak times. The outcome with temperature decreasing from the disc centre to the edge, does not compare with the experiments nearly as well as did the isothermal case. The differences between experiment and the second case with temperature increasing from the disc centre to the edge, are about the same magnitude as with the isothermal simulation, but the overall shape of the curve in the central region is less in keeping with the experimental results. Thus it appears that the isothermal simulation gives the most satisfying comparison and that slumping is not subject to spatial temperature variations of sufficent magnitude to substantially change the outcome.

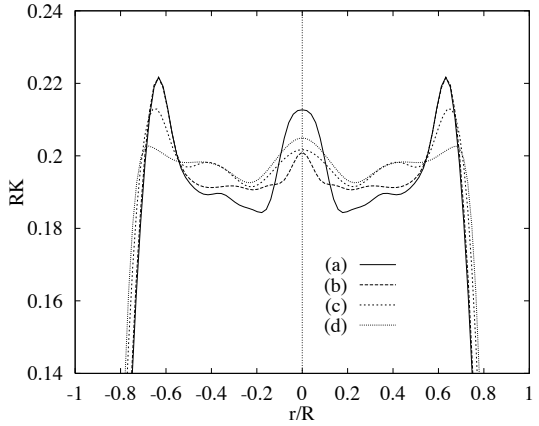

FIGURE 6. A comparison of upper-surface curvature given by (a) a numerical simulation with temperature decreasing linearly from the centre to the edge, (b) a numerical simulation with temperature increasing linearly from the centre to the edge (c) experiment with a 40 min. soak, and (d) experiment with a 50 min. soak.

The non-isothermal simulations show full mould contact occuring in only slightly longer times than the isothermal simulation ($0.23\mathcal{T}$ to $0.25\mathcal{T}$). Thus the time taken to achieve full mould contact, as determined by our numerical simulations, is not much affected by a 10°C radial temperature difference, and is significantly less than the time found by experiment to be required.

5 Discussion and Conclusion

We have compared isothermal and non-isothermal slumping simulations with experimental slumping data. The best agreement is obtained with an isothermal model, so that it does not seem necessary at this stage, to be concerned with coupling heat transfer to our fluid flow model. Rather we are encouraged to try to improve this agreement by refining our methods of collecting and processing both experimental and numerical data.

The most major difference between all the numerical simulations and the experimental work, that we have not yet attempted to explain, is in the time taken for the glass disc to achieve full contact with the mould. The experiments showed a soak time of 40 to 50 minutes to be necessary before full mould contact was achieved, while the numerical simulations give soak times of around 10 minutes. The most likely major cause of this is that the viscosities we are computing from the known temperature using the VFT equation, and which vary over several factors of 10, are in error. If we increase them by a factor of 2, then we double the time scale so that the numerical soak time is of the order of 45 minutes, which is in accord with the experiments. An error in the viscosity of this magnitude is quite possible, resulting from glass viscosity-determination methods and from computation using the VFT equation (see the discussion in [2]), and is not large relative to the applicable viscosity range and log scale.

Experimental validation of models of manufacturing processes such as this is often desirable or necessary, and problems such as we have discussed are typical. This work illustrates how useful information can be derived from comparison of numerical and experimental results, despite the difficulties encountered.

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