CASA-Report 09-13
March 2009

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glass parison shapes

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ISSN: 0926-4507

PVP2009-77946

**NUMERICAL OPTIMISATION OF BLOWING GLASS PARISON
SHAPES**

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ABSTRACT

Industrial glass blowing is an essential stage of manufacturing glass containers, i.e. bottles or jars. An initial glass preform is brought into a mould and subsequently blown into the mould shape. Over the last few decades, a wide range of numerical models for forward glass blow process simulation have been developed. A considerable challenge is the inverse problem: to determine an optimal preform from the desired container shape. A simulation model for blowing glass containers based on finite element methods has previously been developed [6, 7]. This model uses level set methods to track the glass-air interfaces. In previous work of the authors [8] a numerical method was introduced for optimising the

shape of the preform. The optimisation method aims at minimising the error in the level set representing the inner container surface. The objective of this paper is to perform an in-depth study of the optimisation method previously introduced and to improve its performance. In particular an initial guess of the preform for the iterative optimisation algorithm is constructed by means of an analytical approximation of the flow problem. The emphasis in this paper is on the analysis of the inverse problem and the development of the optimisation method in consideration of the application to containers of industrial relevance.

KEY WORDS: optimisation, inverse problems, level set methods, glass forming

NOMENCLATURE

c_p	[J kg ⁻¹ K ⁻¹]	specific heat
g	[m s ⁻¹]	gravitational acceleration
k_c	[W m ⁻¹ K ⁻¹]	effective conductivity
N	[-]	number of control points minus two
p	[Pa]	pressure
T	[K]	temperature
t	[s]	time
u	[m s ⁻¹]	flow velocity
R	[m]	spherical radius
r	[m]	cylindrical radius
z	[m]	height
Γ_i	[m ²]	inner container surface
Γ_m	[m ²]	mould surface
θ	[-]	level set function
μ	[kg m ⁻¹ s ⁻¹]	dynamic viscosity
ρ	[kg m ⁻³]	density
ϑ	[-]	angle of glass-air-mould contact point
φ	[-]	angle

INTRODUCTION

Industrial glass blowing is an essential stage of manufacturing glass containers, i.e. bottles or jars. A so-called preform or parison is constructed, usually by either a press stage or a blow stage. The preform is carried by a robotic arm to a mould for the final blow stage (Fig. 1). During this blow stage the preform is first left to sag under the influence of gravity and then pressurised air is blown into the mould to force the glass into the mould shape. This paper is concerned with the process of blowing the mould shape in the final blow stage.

Figure 1. SCHEMATIC DRAWING OF THE FINAL BLOW STAGE

Computer simulation models have played an important role in gaining more insight in and optimisation of glass forming processes over the last few decades. Since measurements are usually complicated, e.g. because of high temperatures, and trial-and-error methods with glass forming equipment are relatively expensive and time consuming, simulation models offer a good alternative. Moreover, simulations can be used for comparison of results.

Through the years numerous computer simulation models for glass blowing have been developed [3, 5, 6, 10, 16]. In general glass blow simulation models compute the final container from a given preform.

In practice usually a certain glass distribution over the mould wall is desired. Then the corresponding initial conditions, such as the shape of the preform and the initial temperature distribution, are sought in order to obtain a container with this glass distribution. Therefore, it is interesting to consider the inverse problem, to determine the initial conditions, given the glass distribution of the final container.

A numerical optimisation method to find an optimal preform from the desired container shape has been previously developed [8]. The method uses a modified Levenberg-Marquardt algorithm combined with a secant method. The 2D axial-symmetrical simulation model presented in [6, 7] is applied to compute the shape of the glass container. The simulation model is based on finite element methods and uses a level set method to track the glass-air interfaces. The optimisation method has been successfully applied to find an optimal preform for a jar.

This paper performs an in-depth study of the optimisation method to improve its performance. In particular, an analytic approximation of the flow problem is derived. On the basis of a.o. this approximation the optimisation strategy is revised and adapted to make it more efficient. Furthermore, an approximate preform is obtained, which is used as an initial guess for iterative optimisation. Finally, the approximation is used to gain an insight in the inverse problem.

PROBLEM FORMULATION

The forward and inverse problem for blowing glass parison shapes are formulated. The forward problem considered is to locate the glass surfaces during a glass blow process. The inverse problem is to find the shape of the preform, given the final container shape.

The Forward Problem

In the mathematical model used for the forward problem, the glass melt is modelled as an incompressible, Newtonian fluid. Since viscous forces dominate, the flow of glass can be described by a Stokes flow problem:

$$\begin{cases} \nabla \cdot (\mu \nabla u) - \nabla p + \rho g = 0, \\ \nabla \cdot u = 0. \end{cases} \quad (1)$$

Because of the strong temperature dependency of the glass viscosity, the flow problem is coupled to an energy problem involving the heat equation:

$$\rho c_p \left(\frac{\partial T}{\partial t} + u \cdot \nabla T \right) - \nabla \cdot (k_c \nabla T) = 0. \quad (2)$$

Glass and air are distinguished by the sign of a level set function θ . The level set function is a solution of the evolution equation

$$\frac{\partial \theta}{\partial t} + u \cdot \nabla \theta = 0. \quad (3)$$

So, the glass-air interfaces at time t are implicitly given by $\theta(x, t) = 0$ [1, 4, 14, 15].

Together (1)-(3) form a fully coupled system of partial differential equations that describe the glass flow during a blow process. Boundary conditions include:

- an inflow pressure at the mould entrance,
- free-stress conditions for air and no-slip conditions for glass on the mould wall,
- 2D axial symmetry conditions on the symmetry axis.

Further details and analysis regarding the problem formulation of the glass blow simulation model are given in [6, 7].

The Inverse Problem

The inverse problem in [8] is formulated as follows: find the location of the initial glass surfaces, given the surfaces at time $t = t^*$. In terms of the level set formulation, the inverse problem is to find the initial condition $\theta(x, 0) = \theta_0(x)$, such that

$$\begin{cases} \frac{\partial \theta}{\partial t} + u \cdot \nabla \theta = 0, \\ \theta(x, t^*) = \theta^*(x), \end{cases} \quad (4)$$

where $\theta^*(x)$ is the level set function corresponding to the desired container. Furthermore, in [8] the constraint is added that the bottom of the preform at the symmetry axis is located at $z = -h$ with respect to the mould entrance.

In this paper it is explicitly prescribed that the outer container surface should be on the mould surface, that is, $\theta^* = 0$ on Γ_m , with Γ_m the mould surface. This condition implies that the outer interface will not change for different preforms. Consequently, the container has only one free surface, whereas the preform in problem (4) has two free surfaces. This indicates that inverse problem (4) is under-determined; either one of the surfaces of the preform should be given. This matter is discussed further on.

Note that since in the problem formulation no slip of glass is allowed on the mould wall, the inner glass surface will not change once the outer surface is in contact with the mould. This induces that there is an immediate relation between the preform interfaces and the container interfaces; time does not play any role in the inverse problem.

AN ANALYTICAL APPROXIMATION

An analytical approximation of the Stokes flow problem is derived. This approximation is used as an initial guess for iterative optimisation of the preform shape and for analysis of the inverse problem.

The approximation is based on two criteria. Firstly, the viscosity of glass is assumed to be constant in both space and time. Although this assumption seems to be rather crude at first sight, it can be validated by means of a dimensional analysis of (2). In [9, 11, 12] it is stated that if the Péclet number of glass is sufficiently large, the glass temperature can be assumed to be constant along streamlines, hence for uniform initial glass temperature the viscosity will remain constant. Typical

values for the following physical quantities glass are

$$\begin{aligned}\rho_g &= 2.5 \cdot 10^3 \text{ kg m}^{-3}, & V &= 10^{-2} \text{ m s}^{-1}, & L &= 10^{-2} \text{ m}, \\ c_p &= 1.5 \cdot 10^3 \text{ J kg}^{-1} \text{ K}^{-1}, & k_c &= 3 \text{ W m}^{-1} \text{ K}^{-1},\end{aligned}\tag{5}$$

where V and L are the characteristic flow velocity and length scale of the preform, respectively. As a result, the Péclet number of glass is

$$\text{Pe} = \frac{\rho \bar{c}_p V L}{\bar{\lambda}} \sim 10^2.\tag{6}$$

This number may not be considered large enough to assume that the viscosity of glass is constant in general, but it is considered sufficiently large for the approximation. Also note that close to the mould wall extreme temperature variations occur over a small length scale, which violates the assumption of constant viscosity. On the other hand, the approximation of the flow problem is mainly interesting in the glass area that is not (yet) in contact with the mould. Secondly, the glass tends to flow in perpendicular direction to the glass layer, except for the region where the glass is close to the mould. This can be seen in Fig. 2, where the flow velocity field is depicted for a (nearly) spherical preform and an ellipsoidal mould. This phenomenon can be reasoned as follows. Firstly, because of the pressure difference between the two glass surfaces the glass tends to flow in normal direction from one glass surface to the other. Secondly, the high viscosity causes a laminar behaviour of the glass flow. Furthermore, it is assumed that the glass surfaces and the mould surface are concave around the origin, which is usually located at the centre of the mould entrance. Then it is reasonable to assume that the glass surfaces evolve strictly outward from the origin in radial direction. This gives the following assumption:

$$\frac{dR}{dt} = u_R,\tag{7}$$

$$R \frac{d\phi}{dt} = u_\phi \approx 0,\tag{8}$$

where (R, ϕ) are 2D axial-symmetrical spherical coordinates. This assumption is useful in respect that for analysis purposes one is primarily interested in the outward evolution of the glass surfaces towards the mould wall. Note that the radial velocity component is mainly responsible for dilatation of the glass layer, while the azimuthal velocity component is mainly responsible for deformation and rotation. In summary, the following assumption is made:

Assumption 1.

1. the viscosity is constant in time and space,
2. the azimuthal velocity component is zero: $u_\varphi = 0$.

Figure 2. INITIAL FLOW VELCOITY FOR BLOWING A GLASS PREFORM. THE FLOW OF GLASS SEEMS TO BE PERPENDICULAR TO THE SURFACES.

For a bottle the mould wall, hence the container surfaces, are partially convex at the neck part. Consequently, the glass layer is deformed to fit the mould during blowing. A resolution is to start at a point in time at which the neck part is already covered. Furthermore, the origin can be chosen at a position lower than the mould entrance, such that both the mould wall and the preform are concave with respect to the origin (see Fig. 3). The mould wall and the preform can still be slightly convex without excessively violating assumption 1.

By means of assumption 1 it is possible to find a direct relation between the preform and the container. Volume conservation of glass between glass surfaces $R_1(\varphi)$ and $R_2(\varphi)$ and between any two angles φ_1 and φ_2 in $[0, \frac{\pi}{2}]$ results in

$$\frac{d}{dt} \left(2\pi \int_{\varphi_1}^{\varphi_2} \int_{R_1(\varphi)}^{R_2(\varphi)} R^2 \sin \varphi \, dR d\varphi \right) = \frac{2}{3} \pi \frac{d}{dt} \left(\int_{\varphi_1}^{\varphi_2} \left(R_2^3(\varphi) - R_1^3(\varphi) \right) \sin \varphi \, d\varphi \right) = 0. \quad (9)$$

With assumption 1 it follows that

$$\frac{d}{dt} \left(\int_{\varphi_1}^{\varphi_2} \left(R_2^3(\varphi) - R_1^3(\varphi) \right) \sin \varphi \, d\varphi \right) = \int_{\varphi_1}^{\varphi_2} \frac{\partial}{\partial t} \left(R_2^3(\varphi) - R_1^3(\varphi) \right) \sin \varphi \, d\varphi. \quad (10)$$

Figure 3. DIFFERENT POSITIONS OF THE ORIGIN FOR A SPHERICAL COORDINATE SYSTEM ON THE SYMMETRY AXIS

Since this holds for any pair of angles φ_1, φ_2 , it can be concluded that

$$\frac{\partial}{\partial t} \left(R_2^3(\varphi) - R_1^3(\varphi) \right) = 0, \quad 0 \leq \varphi \leq \frac{\pi}{2}. \quad (11)$$

Furthermore, let $R_{0,1}(\varphi)$ and $R_{0,2}(\varphi)$ denote the surfaces of the preform, $R_i(\varphi)$ the inner surface of the container and $R_m(\varphi)$ the mould surface. Then

$$R_{0,2}^3(\varphi) - R_{0,1}^3(\varphi) = R_m^3(\varphi) - R_i^3(\varphi), \quad 0 \leq \varphi \leq \frac{\pi}{2}. \quad (12)$$

Thus under assumption 1, if either $R_{0,1}(\varphi)$ or $R_{0,2}(\varphi)$ is known, the other surface of the preform can be uniquely determined, provided that a container with the outer surface on the mould can be blown.

Next the evolution of the glass surfaces during blowing is studied. In view of assumption 1 the dimensionless Stokes flow equations for glass with constant viscosity in 2D axial-symmetrical,

spherical coordinates (R, φ) is considered, thereby neglecting u_φ :

$$\frac{\partial p}{\partial r} = \left(\frac{1}{R^2} \frac{\partial}{\partial R} (R^2 \frac{\partial u_R}{\partial R}) - \frac{2u_R}{R^2} + \frac{1}{R^2 \sin \varphi} \frac{\partial}{\partial \varphi} (\sin \varphi \frac{\partial u_R}{\partial \varphi}) \right) - \frac{\text{Re}}{\text{Fr}} \cos \varphi, \quad (13a)$$

$$\frac{1}{R} \frac{\partial p}{\partial \varphi} = \frac{2}{R^2} \frac{\partial u_R}{\partial \varphi} + \frac{\text{Re}}{\text{Fr}} \sin \varphi, \quad (13b)$$

$$\frac{1}{R^2} \frac{\partial}{\partial R} (R^2 u_R) = 0. \quad (13c)$$

From the continuity equation (13c) it follows that the the flow velocity has the following form,

$$u_R(R, \varphi) = v(\varphi) R^{-2}. \quad (14)$$

The resulting momentum equations are

$$\begin{cases} R^2 \frac{\partial}{\partial R} (p + \frac{\text{Re}}{\text{Fr}} R \cos \varphi) = (v'' + v' \cot \varphi) R^{-2}, \\ R \frac{\partial}{\partial \varphi} (p + \frac{\text{Re}}{\text{Fr}} R \cos \varphi) = 2v' R^{-2}, \end{cases} \quad (15)$$

Integration with respect to R and φ , respectively, yields

$$\begin{aligned} p(R, \varphi) &= -\frac{1}{3} (v''(\varphi) + v'(\varphi) \cot \varphi) R^{-3} - \frac{\text{Re}}{\text{Fr}} R \cos \varphi + Q_\varphi(\varphi), \\ &= 2v(\varphi) R^{-3} - \frac{\text{Re}}{\text{Fr}} R \cos \varphi + Q_R(R), \end{aligned} \quad (16)$$

where Q_φ and Q_R are integration constants with respect to the corresponding integration variable. It follows that

$$v'' + v' \cot \varphi + 6v = -\sigma^2 = \text{constant}. \quad (17)$$

This equation has solution

$$v(\varphi) = A (3 \cos^2 \varphi - 1) + 6B \cos \varphi + 2B (1 - 3 \cos^2 \varphi) \log |\csc \varphi + \cot \varphi| - \frac{\sigma^2}{6}. \quad (18)$$

To specify boundary conditions the part of the outer glass surface that is in contact with the mould

at time t must be determined. In the most simple case an angle $\varphi = \vartheta(t)$ can be found, such that the glass surface is in contact with the mould for $\varphi \geq \vartheta(t)$ and with air for $0 \leq \varphi < \vartheta(t)$. Here $\varphi = 0$ corresponds to the symmetry axis and $\varphi = \frac{\pi}{2}$ corresponds to the mould entrance. In this paper the angle ϑ is simply referred to as contact angle. For $\varphi \geq \vartheta(t)$ the flow velocity is zero; the surfaces do not evolve in time, but have already taken the final mould shape. Thus the domain of interest is bounded by $\varphi = 0$ and $\varphi = \vartheta(t)$. In this case the boundary conditions follow from axial-symmetry and no-slip:

$$v'(0) = 0, \quad v(\vartheta) = 0. \quad (19)$$

As a result

$$A = \frac{\sigma^2}{18 \cos^2 \vartheta - 6}, \quad B = 0. \quad (20)$$

The constant σ^2 can be found by imposing appropriate boundary conditions for the pressure. The more realistic case is more complicated. It presumes that the preform is first left to sag for a short period of time, before air is blown inside the mould. Consequently, part of the glass surface will touch the bottom of the mould before the entire mould wall is covered. In this case two contact angles $\vartheta_1(t)$ and $\vartheta_2(t)$ should be introduced. The resulting boundary conditions are

$$v(\vartheta_1) = 0, \quad v(\vartheta_2) = 0. \quad (21)$$

In this case A and B depend on ϑ_1 and ϑ_2 .

Figure 4. RADII OF GLASS SURFACES AND CONTACT ANGLE.

First consider the simple case with one contact angle. To solve evolution equations (7) the contact angle needs to be determined as a function of time. Let $R(t)$ be a glass surface with initial conditions $R(0; \varphi) = R_0(\varphi)$. Substitution of (14) into (7) yields

$$\frac{dR}{dt} = v R^{-2}. \quad (22)$$

Separation of variables gives

$$\int_0^t v(\varphi, \vartheta(\tau)) d\tau = \frac{1}{3} \left(R^3(t; \varphi) - R_0^3(\varphi) \right). \quad (23)$$

Note that the flow velocity only changes in time as a function of the contact angle. Therefore, it is convenient to define R as a function of φ and ϑ in the same way as v . Furthermore, $t \equiv t(\vartheta)$ can be seen as the time it takes for the glass to touch the mould at angle $\varphi = \vartheta$, i.e. t is the inverse of ϑ . For convenience, the integration variable is changed into ϑ , that is

$$- \int_{\vartheta}^{\vartheta_0} v(\varphi, \alpha) \frac{dt}{d\alpha} d\alpha = \frac{1}{3} \left(R^3(\varphi, \vartheta) - R_0^3(\varphi) \right). \quad (24)$$

Integration by parts leads to

$$-t(\vartheta)v(\varphi, \vartheta) + \int_{\vartheta}^{\vartheta_0} t(\alpha) \frac{\partial}{\partial \alpha} v(\varphi, \alpha) d\alpha = \frac{1}{3} \left(R^3(\varphi, \vartheta) - R_0^3(\varphi) \right). \quad (25)$$

By choosing $\varphi = \vartheta$ the integral equations for $R = R_1, R_2$ become

$$\begin{aligned} \int_{\vartheta}^{\vartheta_0} t(\alpha) \frac{\partial}{\partial \alpha} v(\vartheta, \alpha) d\alpha &= \frac{1}{3} \left(R_i^3(\vartheta) - R_{0,1}^3(\vartheta) \right) \\ &= \frac{1}{3} \left(R_m^3(\vartheta) - R_{0,2}^3(\vartheta) \right). \end{aligned} \quad (26)$$

Note that the second relation is exactly (12). For one contact angle it is easy to find an explicit formulation for the time, since $\frac{\partial}{\partial \vartheta} v(\varphi, \vartheta)$ is separable. Recall that the flow velocity for one contact

angle is

$$v(\varphi) = -\frac{\sigma^2}{6} \left(1 - \frac{3 \cos^2 \varphi - 1}{3 \cos^2 \vartheta - 1} \right). \quad (27)$$

Thus the time can be obtained as a function of the contact angle by dividing the integral equation by $3 \cos^2 \vartheta - 1$ and differentiating with respect to ϑ :

$$t(\vartheta) = -\frac{2}{\sigma^2} \left(\left(R_m^3(\vartheta) - R_{0,2}^3(\vartheta) \right) + \frac{d}{d\vartheta} \left(R_m^3(\vartheta) - R_{0,2}^3(\vartheta) \right) \frac{3 \cos^2 \vartheta - 1}{6 \sin \vartheta \cos \vartheta} \right). \quad (28)$$

This expression induces a constraint, since obviously $t(\vartheta_0) = 0$ leads to

$$\left(R'_m(\vartheta_0) - R'_{0,2}(\vartheta_0) \right) \csc \vartheta_0 \sec \vartheta_0 = 0. \quad (29)$$

which means that the tangent of the surface at the contact angle should equal the tangent of the mould surface. If the constraint is not satisfied, it is not possible to blow a container with outer surface Γ_m . A constraint that should be satisfied in order that the container can be blown in finite time is that the last term in (28) is finite at $\vartheta = 0$, which holds because of axial-symmetry. As a final result the evolution of glass surface $R(\varphi, \vartheta)$ is given by

$$\begin{aligned} R(\varphi, \vartheta) &= \left(3t(\vartheta)v(\varphi, \vartheta) + \mathcal{P}(\varphi, \vartheta) + R_0^3(\varphi) \right)^{\frac{1}{3}} \\ &= \left(Q(\varphi, \vartheta) + R_m^3(\vartheta) - R_{0,2}^3(\vartheta) + R_0^3(\varphi) \right)^{\frac{1}{3}}, \end{aligned} \quad (30)$$

where

$$\begin{aligned} \mathcal{P}(\varphi, \vartheta) &= 3 \frac{3 \cos^2 \varphi - 1}{3 \cos^2 \vartheta - 1} \int_{\vartheta}^{\vartheta_0} t(\alpha) \frac{\partial}{\partial \alpha} v(\vartheta, \alpha) d\alpha \\ Q(\varphi, \vartheta) &= \frac{3 \cos^2 \vartheta - \cos^2 \varphi}{2 \sin \vartheta \cos \vartheta} \left(R_m^2(\vartheta) R'_m(\vartheta) - R_{0,2}^2(\vartheta) R'_{0,2}(\vartheta) \right) \end{aligned}$$

In the case of two contact angles, a similar relation to (25) can be derived with $\vartheta = \vartheta_1$ if $t(\vartheta_1) < t(\vartheta_2)$ and $\vartheta = \vartheta_2$ otherwise. However, $\frac{\partial}{\partial \vartheta} v(\varphi, \vartheta)$ is not separable, so that it is not straightforward to derive an explicit expression for the time from (25).

As an example an axial-symmetrical glass container with elliptical cross section is considered. For this example the origin for the spherical coordinate system can be chosen in the top centre of the mould. If the shape of the preform is strictly concave around the origin, the glass will have at most one continuous contact surface with the mould wall during blowing. Thus, this is a good example of the case of one contact angle. Let the mould surface be given by the ellipse

$$R_m(\varphi) = \gamma_m \left(1 - \frac{3}{4} \cos^2 \varphi\right)^{-\frac{1}{2}}, \quad (31)$$

with $\gamma_m = R_m(\frac{\pi}{2})$. Consider the forward problem. A preform with surfaces $R_{0,1}$ and $R_{0,2}$ is manufactured by either a blow stage or a press stage. Suppose the inner glass surface $R_{0,1}$ is essentially circular with a horizontal tangent at the symmetry axis. This makes it relatively easy to define the level set function corresponding to the inner surface as a signed distance function, which is required for the simulation. In cylindrical coordinates (r, z) it can be defined as:

$$\sqrt{\max(0, r - r_c)^2 + (z - z_c)^2} = \gamma_i, \quad (32)$$

for some constants r_c, z_c and γ_i . In spherical coordinates this expression reads

$$R_{0,1}(\varphi) = \begin{cases} (\gamma_i - z_c) \sec \varphi, & \text{if } \varphi \leq \varphi_c, \\ r_c \sin \varphi - z_c \cos \varphi + \sqrt{\gamma_i^2 - (R_c \cos \varphi + z_c \sin \varphi)^2}, & \text{otherwise,} \end{cases} \quad (33)$$

with

$$\begin{aligned} \varphi_c &= \arccos \left(\frac{\gamma_i - z_c}{\sqrt{(\gamma_i - z_c)^2 + r_c^2}} \right), \\ R_c &= \sqrt{r_c^2 + z_c^2}. \end{aligned}$$

The outer surface $R_{0,2}(\varphi)$ of the preform is given by the blank mould surface in the preceding

forming stage. It should satisfy the following constraints:

$$R_{0,2}(\vartheta_0) - R_m(\vartheta_0) = 0, \quad (34a)$$

$$\left(R'_{0,2}(\vartheta_0) - R'_m(\vartheta_0)\right) \csc \vartheta_0 \sec \vartheta_0 = 0, \quad (34b)$$

$$R'_{0,2}(0) = 0, \quad (34c)$$

$$R_{0,2}(\vartheta) < R_m(\vartheta), \quad \text{for } \vartheta < \vartheta_0. \quad (34d)$$

Considering the constraints let the derivative of the outer surface have the following form:

$$R'_{0,2}(\vartheta) = a \sin \vartheta \cos \vartheta + b \sin^2 \vartheta \cos \vartheta + c \sin \vartheta \cos^2 \vartheta. \quad (35)$$

Then integration yields

$$R_{0,2}(\vartheta) = \frac{a}{4} (\sin^2 \vartheta - \cos^2 \vartheta) + \frac{b}{3} \sin^3 \vartheta - \frac{c}{3} \cos^3 \vartheta + d. \quad (36)$$

Suppose $\vartheta_0 = \frac{\pi}{2}$. Then the second constraints implies $R''_{0,2}(\frac{\pi}{2}) = R''_m(\frac{\pi}{2})$. Therefore, to satisfy (34d) it is demanded that $R'''_{0,2}(\frac{\pi}{2}) \geq R'''_m(\frac{\pi}{2})$, which leads to $c \geq 0$. This constraint leaves some freedom to choose $R_{0,2}(0) = \gamma_m$. For this choice substitution of (35) in (34) gives $a = -\frac{3}{2}$, $b = \frac{3}{4}$, $c = \frac{3}{2}$, $d = \gamma_m + \frac{1}{8}$. Finally, the function Q in (30) for this example becomes

$$Q(\varphi, \vartheta) = 3 \left(\cos^2 \varphi - \cos^2 \vartheta \right) \left(\frac{1}{8} R_m(\vartheta)^5 + \frac{1}{6} R'_{0,2}(\vartheta) R_{0,2}^2(\vartheta) \csc \vartheta \sec \vartheta \right). \quad (37)$$

The simulation model presented in [6, 7] is used to compute the container using the given preform with $z_0 = \frac{1}{16}$ and $r_0 = \gamma_m + z_0 - \sqrt{(\gamma_m^2 - z_0^2)}$. For this example the values $\gamma_m = 1$ and $\gamma_i = \frac{3}{4}$ are chosen. Typical values for the simulation and further details are given in [8]. Figure 5 compares the results of the analytical approximation and the simulation for the forward problem. The purple area is the glass domain given by the level set functions in the simulation; the blue area is the air domain. The blue lines denote the glass surfaces given by the analytical approximation. Figure 5(a) shows the preform and Figure 5(b) shows the container. Figure 6 plots the signed distance between the inner container surfaces as a function of φ . Figure 7 plots the glass surfaces on the symmetry axis, i.e. $\varphi = 0$, as functions of the contact angle ϑ . By looking at Fig. 5(b) it can be observed that there is a slight deviation between the container surfaces. This is due to the fact that the approximation is based on assumption 1. The container obtained by the approximation is slightly thicker at the top and thinner at the bottom than the container obtained by the simulation, simply because the mass

Figure 5. GLASS SURFACES OF THE PREFORM AND THE CONTAINER. THE BLUE LINES ARE THE ANALYTICAL APPROXIMATIONS AND THE PURPLE AREA IS THE GLASS DOMAIN IN THE SIMULATIONS.

Figure 6. THE SIGNED DISTANCE BETWEEN THE INNER SURFACES OF THE CONTAINERS FOR THE ANALYTICAL APPROXIMATION AND THE SIMULATION AS A FUNCTION OF THE ANGLE ϕ .

Figure 7. THE GLASS SURFACES ON THE SYMMETRY AXIS AS FUNCTIONS OF THE CONTACT ANGLE θ .

flow in azimuthal direction, which inclines towards the symmetry axis in the simulation, is lacking in the approximation. Nevertheless the approximation is close enough to be used as an initial guess

for iterative optimisation and to justify the analysis of the inverse problem based on assumption 1. The next step is to verify if the approximation is useful in finding a solution to the inverse problem, by using it as an initial guess for the optimisation method and to impose real physical restrictions on the preform shape.

Finally, Figure 8 shows the outer surface of the preform and the mould surface as functions of the angle ϕ . It can be verified that constraints (34a)-(34b) are met.

Figure 8. THE MOULD SURFACE AND THE OUTER PREFORM SURFACE AS FUNCTIONS OF ϕ .

OPTIMISATION STRATEGY

An optimisation strategy was previously described in [8]. The interfaces were discretised by parametric curves, e.g. splines or Bezier curves. The control points of the curves at the mould entrance were fixed. The remaining points could be adjusted in r and z -direction to control the shape of the preform, except for the points on the symmetry axis, which could only be adjusted in z -direction. The variable coordinates of the control points were the parameters in the optimisation method. Then the modified Levenberg-Marquardt method combined with a secant method was applied to find the optimal positions of the control points.

The optimisation strategy used in this paper is slightly different. First of all only one preform surface is optimised; the other surface can be given by any smooth curve within the constrained domain. Recall that the container has only one free surface, which does, moreover, not evolve in time, but merely depends on the preform shape. Furthermore, under assumption 1 it is shown that, if either surface is known, the other surface has a unique optimum, namely the solution of (12), provided that a container with the outer surface on the mould can be blown. This gives reason to believe that faster convergence of the optimisation method can be achieved by prescribing one of the preform interfaces.

In addition, the control points are adjusted in radial direction only (see Fig. 9). There are two main reasons to choose for this parametrisation. Firstly, for efficient optimisation the number of parameters should be kept to a minimum, while the number of control points should be sufficiently large to accurately represent the glass surface. Secondly, an arbitrary distribution of the control points over the constrained domain is avoided. In this way undesired curves, including those intersecting themselves, are prevented. Thus for N variable control points $P_1, \dots, P_N$ the vector $\mathbf{p}$ comprising the parameters to be optimised is defined by

$$\mathbf{p} = (R_{P_1}, \dots, R_{P_N})^T. \quad (38)$$

Figure 9. PARAMETRISATION OF A PREFORM SURFACE BY A CUBIC SPLINE WITH FIVE CONTROL POINTS. THE CONTROL POINTS VARY IN RADIAL DIRECTION.

To fit the inner interface of the approximate container to the inner interface of the model container an objective function is minimised. In this paper the L^2 -norm of the level set function on the interface is used:

$$\Phi(\theta) := \int_{\Gamma_i} \theta^2 d\Gamma, \quad (39)$$

where Γ_i denotes the inner interface of the model container and θ is the level set function corresponding to the inner container surface, which is maintained as a signed distance function during

the simulation. The integral is computed by applying a composite Gauss quadrature rule. The residuals are computed in the points for the quadrature rule.

Finally, in case the mould wall is covered with glass the blow process can be stopped because the glass form will not change anymore. Therefore after a certain time period (e.g. half times the expected end time) it is verified every few time steps if the mould wall is completely covered with glass. This can be a significant saving in computational time, particularly if it is difficult to estimate the end time. It is still advisable to state an end time, because the preform may break during a simulation, so that the mould wall will not be completely covered with glass.

RESULTS

Consider the example of the axial-symmetrical glass container with elliptical cross section. Suppose the inner container surface is given by

$$\Gamma_i : (r, z)(\alpha) = \left(\left(R_0 + \sqrt{\gamma_i^2 - Z_0^2} \right) \cos \alpha, -\left(\frac{8}{5}\gamma_m + \frac{2}{5}\gamma_i \right) \sin \alpha \right). \quad (40)$$

Figure 10 shows the container. Suppose that a blank mould for the preceding forming stage is to be constructed, which prescribes the outer surface of the preform, such that blowing the preform results in the container with surfaces Γ_i and Γ_m . The inner preform surface is given by (32). A cubic spline with six control points is used for the parametrisation of the outer preform surface, that is the control points are chosen as follows: first points are chosen on the intersection of the mould surface by substituting the following values of α in (40):

$$\alpha_j = \frac{j(2N + j - 3)}{6(N - 1)N}, \quad j = 1, \dots, N. \quad (41)$$

The reason for this choice is that the difference between consecutive angles $\alpha_j - \alpha_{j-1}$ increases with the ratio of the semimajor axis of the elliptical intersection of the mould to the semiminor axis. Then the angles of the control points of the parametric curve are the angles of the points on the intersection of the mould surface, i.e.

$$\phi_j = \text{atan2}(-z(\alpha_j), r(\alpha_j)), \quad j = 1, \dots, N. \quad (42)$$

The initial guess for $R_{0,2}$ required for the modified Levenberg-Marquardt method follows directly from (12). Figure 11 shows the initial guess of the preform and the container that results from the simulation with this preform. If the radius of the mould entrance were 5cm, the average distance

between the inner surfaces of desired container in Fig. 10 and the container in Fig. 11(b) would be approximately 3mm.

Figure 10. THE DESIRED CONTAINER.

(a) PREFORM

(b) RESULTING CONTAINER

Figure 11. INITIAL GUESS OF THE PREFORM.

The following constraints hold on the outer preform surface. Let $\eta = 0.1$ be a constant margin. Firstly, the variable control points should be located at some distance from the mould (constraint (34d)):

$$R_m(\phi_j) - R_{P_j} + \eta > 0, \quad j = 1, \dots, N. \quad (43)$$

Secondly, the preform should have a minimum thickness:

$$R_{p_j} - R_{0,1}(\phi_j) - \eta > 0, \quad j = 1, \dots, N. \quad (44)$$

These constraint are included in the modified Levenberg-Marquardt method as weighted penalty functions [2, 8, 13]. Furthermore, (34a) is automatically satisfied by fixing control point P_0 . Finally, constraint (34c) can be satisfied by defining the derivative of the cubic spline at end point P_5 . Constraint (34c) holds for assumption 1, but differs with the flow velocity. To deal with this constraint, for instance, the second derivative of the spline at P_0 can be fixed, that is $R''_{0,2}(\frac{\pi}{2}) = R''_m(\frac{\pi}{2}) = \frac{3}{4}$. It is left to the optimisation method to find a solution that satisfies the full constraint.

Figure 12. OPTIMAL PREFORM FOR THE DESIRED CONTAINER.

Figure 13. RELATIVE SIGNED DISTANCE TO THE RADIUS OF THE MOULD ENTRANCE BETWEEN THE DESIRED CONTAINER AND THE APPROXIMATE CONTAINER RESULTING FROM THE OPTIMAL PREFORM AS A FUNCTION OF THE ANGLE.

The optimisation method is applied to find the outer surface of the preform. Each iteration the control points are adjusted and the new glass container is computed from the corresponding preform. The difference between the inner glass surfaces of the obtained glass container and the model container in Fig. 10 is computed to determine the new value of the objective function. Figure 12 shows the final results of the optimisation method. Figure 12(a) shows the optimal preform for the desired container and Figure 12(b) shows the resulting container. It can be observed the container is a good approximation of the model container in Fig. 10. The tolerance for the average distance between the surfaces of the approximate and the desired container is one percent of the radius of the mould entrance, which is quite strict with respect to the discretisation error made. The number of iterations required for the simulation is 13. Figure 13 plots the relative signed distance to the radius of the mould entrance between the surfaces as a function of ϕ , i.e. the relative difference between the containers in Fig. 10 and Fig. 12(b). Compared to the previous results presented in [8] a smaller distance between the surfaces is achieved within fewer iterations. However, it should be noted that test results for the optimisation method presented in this paper are still limited.

CONCLUSIONS

An in-depth study of the optimisation method previously introduced in [8] has been performed. The optimisation method has been improved in several ways, in particular by reformulating the inverse problem and using an analytical approximation as an initial guess for iterative optimisation. This analytical approximation is also useful to gain an insight in the inverse problem, e.g. which conditions should be satisfied by the preform. A numerical example for the preform optimisation method presented is the blowing of a 2D axial-symmetrical ellipsoidal glass container. The results presented demonstrate the efficiency of the optimisation algorithm and the use of the analytical approximation. The next step of the development is the application of the method to more complex container shapes of industrial relevance.

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