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COUPLED DPM AND VOF MODEL FOR ANALYSES OF GAS STIRRED LADLES AT HIGHER GAS RATES

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ABSTRACT

Modelling of gas stirred ladles is often carried out under the assumption of a flat liquid surface with a degassing boundary condition. At higher gas rates the liquid surface is deformed and we may experience sloshing and swirling. The dynamic behaviour of the surface will potentially influence the mixing performance of the ladle process. Under these conditions it is important to capture the surface behaviour, and the assumption of a flat surface may not be applicable. The modelling approach therefore needs to account for a dynamic liquid surface and the rising bubble plume. In this paper an Eulerian-Eulerian-Lagrangian method which treats the bubbles as Lagrangian particles and the liquid and the top gas as Eulerian phases with a sharp interface is described. The method applies a *volume of fluid* (VOF) model for the liquid and top gas which interacts with Lagrangian bubbles implemented with a *discrete phase method* (DPM). The coupled DPM and VOF model is applied to gas stirred ladles with bottom injection and validated against experiments. It is shown that the assumption of a flat surface is acceptable if the purpose is to obtain velocity profiles at different elevations in the ladle. If mixing time is the purpose of the investigation, the flat surface assumptions is not valid. The model is also applied to prove that the lift force is not significant at higher gas rates.

NOMENCLATURE

C_D	drag coefficient
C_L	lift coefficient
d	bubble diameter
e	specific energy rate
Eo	Eotvos Number
F	force / mass
g	gravitational constant
H	ladle height
k	turbulent kinetic energy
M	ladle mass
p	pressure
Q	volumetric gas rate at STP conditions
Re	Reynolds number
T	temperature
u	velocity
V	volume
α	volume fraction
ε	turbulent energy dissipation
μ	viscosity
ρ	density
σ	surface tension

Subindexes

0	ambient conditions
b	bubbles
eq	equilibrium
g	gas
l	liquid
t	turbulence

INTRODUCTION

Ladle refining is a metallurgical process in which mixing is a key issue. Due to the non-transparent property of most metals, it is practically impossible to observe the hydrodynamics in the ladle. Thus modelling of ladle hydrodynamics is of general interest to the metallurgical industry. The subject has been addressed by several authors like Johansen & Boysan (1988), Deen *et.al.* (2001) and Mazumdar & Guthrie (1995). The modelling approaches often assume a flat liquid surface with a degassing boundary condition. This has been successfully applied to gas stirred ladles at low and medium gas rates. Many metal refining processes are conducted at medium and high gas rates. For these gas rates the assumption of a flat surface becomes questionable and it might is be necessary to include the effect of a dynamic free surface. A comparison of modelling results with a flat surface and a dynamic surface will therefore yield insight on when the assumption of a flat free surface is valid.

Modelling of ladle hydrodynamics with a dynamic free surface is more challenging since it requires the combined multiphase aspects of both dispersed phases and a large scale interface at the liquid surface. This can be accomplished by different modelling techniques. A combined Eulerian and Lagrangian method has successfully been applied to both ladle refining and subsea gas release (Cloete *et.al*., 2009a, Cloete *et.al*., 2009b). The method uses a volume of fluid model to capture the free surface behaviour and a discrete particle model to track the gas in the bubble plume.

The modelling of bubble plumes accounts for such forces as buoyancy and drag. Also the lift force tends to be included. The lift coefficient is well known for a single bubble, but for bubbles in a turbulent plume little is known. Some authors set the coefficient to zero and some use it as a tuning parameter. Whether the lift force is significant or not is still open for debate. The effect of lift is therefore considered in the following study.

MODEL DESCRIPTION

To study the hydrodynamics of a ladle, one need to account for the behaviour of the liquid in the ladle, the gas above the liquid and the bubbles in the liquid. Sometimes the ladle may contain secondary liquid phases or the top

gas may be ignored and a degassing boundary condition applied. The coupled Volume of Fluid (VOF) and Discrete Phase Model (DPM) applies the VOF model to describe the fluid behaviour of the liquid in a ladle, the continuos gas phase above the liquid and the interface between them. Since the VOF model can not resolve the bubbles with an affordable grid resolution, a Lagrangian method, DPM, is used to track the bubbles. The Lagrangian bubbles are connected to the Eulerian phases with a two-way coupling through interchange terms such as the drag force in the respective momentum equations.

Eulerian Phases

In the coupled DPM and VOF model we treat the ladle liquid and the continuous gas on top of the liquid as Eulerian phases. They are modelled with a continuity equation and a single set of momentum equations for the mixture of the two phases. A procedure to sharpen the interface between the liquid and the gas above is applied. There is no slip between the phases. This constitutes the basis of a VOF model. In addition a standard k-ε model is applied to capture the effect of turbulence on the flow. The model is modified to account for bubble induced turbulence (Sato & Sekoguchi, 1975) by adjusting the turbulence viscosity μ_t

$$\mu_t = \rho_l C_\mu \frac{k^2}{\varepsilon} + \rho_l C_{\mu B} \alpha_b d_b \left| \mathbf{u}_b - \mathbf{u}_l \right| \qquad (1)$$

The second term is the bubble induced turbulence where u_b-u_l is the slip velocity between liquid and bubbles. The model constants are $C_\mu = 0.09$ and $C_{\mu B} = 0.6$. The standard k-ε turbulence model does not adjust for the presence of a liquid-gas interface which in reality reduces turbulence in its proximity (Johansen & Boysan, 1988). A more sophisticated turbulence model may be applied in the future.

Lagrangian Bubble Phase

The bubbles are modelled as discrete particles without particle-particle interaction. This is carried out with a *Discrete Particle Model* (DPM) which tracks the bubbles with a Lagrangian momentum equation:

$$\frac{d\mathbf{u}_b}{dt} = \frac{\mathbf{g}\left(\rho_b - \rho\right)}{\rho_b} + \mathbf{F}_D\left(u - u_b\right) + \mathbf{F}_{VM} + \mathbf{F}_L \qquad (2)$$

Five forces are accounted for: buoyancy, drag, lift, virtual mass and turbulent dispersion. The first term on the right hand side is the buoyancy force and the second is the drag force (in force per mass). The drag force also includes the effect of turbulent dispersion as mentioned below. F_D is

$$F_D = \frac{18\mu}{\rho_b d_b^2} \frac{C_D \,\mathrm{Re}}{24} \qquad (3)$$

The drag coefficient for bubbles in a plume is not necessarily the same as the coefficient for a single bubble. We use the expression of Xia *et.al*. (2001) which represents the behaviour of a bubble plume:

$$C_D = \frac{2}{3}\left(\frac{\mathrm{Eo}}{3}\right)^{0.5} \qquad (4)$$

The drag coefficient is a function of the Eotvos number

$$\mathrm{Eo} = \frac{\left(\rho_l - \rho_g\right) g d_b^2}{\sigma} \qquad (5)$$

which makes it dependent upon size and shape. The force required to accelerate the fluid surrounding the particle is known as the *virtual mass force*. It can be written as

$$\mathbf{F}_{VM} = \frac{1}{2}\frac{\rho}{\rho_b}\left(\frac{\partial \mathbf{u}}{\partial t} - \frac{\partial \mathbf{u}_b}{\partial t}\right) \qquad (6)$$

The lift force on the bubbles is included as

$$\mathbf{F}_L = C_L \rho_l V_b \left(\mathbf{u}_l - \mathbf{u}_g\right) \times \left(\nabla \times \mathbf{u}_l\right) \qquad (7)$$

where C_L is the lift coefficient. For turbulent bubble plumes, little is known about the lift coefficient. For dilute bubble plumes and single bubbles, the lift coefficient is known to vary with bubble size and shape. Small bubbles tend to move towards the edge of a plume and larger bubbles tend to move towards the centre of a plume. Tomiyama (2004) published an expression for the lift coefficient which captures this. The lift coefficient of Tomiyama C_{LT}

$$C_{LT} = C_{LT}(\mathrm{Eo}) \qquad (8)$$

is a function of the Eotvos number which accounts for particle size and shape. The lift coefficient of Tomiyama is valid for single bubbles or dilute plumes. To accurately model dense plumes, a lift coefficient accounting for higher void fractions is necessary. Behzadi *et.al.* (2004) published a model for the lift coefficient which accounts for higher void fractions. Unfortunately this model does not account for bubble size and shape. We use a combination of the Tomiyama lift coefficient and the Behzadi lift coefficient:

$$C_L = \begin{cases} C_{LT} & \alpha_g \le 0.007 \\ 0.0026 \cdot C_{LT} \alpha_g^{-1.2} & \text{else} \end{cases} \qquad (9)$$

The expression of Behzadi *et.al.* has been normalized such that the Tomiyama lift coefficient is used for void fractions below 0.7% and a combined coefficient is used for higher void fractions.

Turbulent dispersion is an additional drag force due to the velocity fluctuations. The standard drag force only accounts for drag due to the average velocity field. Turbulent dispersion creates a random addition to the liquid velocity of the drag force in Eq.(2). The random velocity is accounted for by a *random walk model* (Cloete *et.al*., 2009a). It results in a wider plume.

The DPM is coupled with the Eulerian phases through the momentum equation. The presence of a DPM particle in a volume cell does not affect the content of that cell since

there is no coupling in the continuity equation. Thus the DPM model becomes less accurate at higher void fractions and is not recommended for use at void fractions above 0.12.

Bubble Size Model

The bubble size is essential for many closure laws like drag, lift and heat and mass transfer. The local mean bubble size d_b is modelled by a Lagrangian transport equation

$$\frac{\partial(\rho_b d_b)}{\partial t} = \rho_b \frac{d_b^{eq} - d_b}{\tau_{rel}} \tag{10}$$

Here τ_{rel} is the relaxation time and d_b^{eq} is the mean equilibrium diameter. The equilibrium diameter is the diameter a bubble will achieve if it resides sufficiently long at the same flow conditions. The term on the right hand side forces the mean bubble diameter towards its equilibrium diameter d_b^{eq} during a timeframe given by the relaxation time. The relaxation time is given by the turbulence dissipation rate and kinetic energy. The equilibrium diameter is calculated as follows

$$d_b^{eq} = C_1 \alpha_b^{0.5} \frac{\left(\sigma/\rho\right)^{0.6}}{\varepsilon^{0.4}} \left(\frac{\mu_b}{\mu}\right)^{0.25} + C_2 \tag{11}$$

The coefficients C_1 and C_2 are tuning parameters. C_2 is often taken as the smallest possible bubble size, while C_1 is the more significant of the two parameters for which most of the tuning procedure evolves around. For air-water systems the following is often used: C_1=4.0 and C_2=100μm. More details of the bubble size model are given by Laux and Johansen (1999). The model gives good predictions of bubble size compared with experiments (Cloete *et.al*. 2009b).

Model Implementation and Numerical Methods

The model is implemented in Fluent 6.3 with specially programmed user defined functions for drag, lift and turbulent viscosity. The bubble size model is also implemented with a user defined function.

The model is run with higher order discretization schemes and a PISO scheme for pressure-velocity coupling. The interface sharpening routine applied for the VOF model is Geo-reconstruct. The bubbles are tracked as a group of particles, known as parcels, containing a specific mass and a specific number of bubbles. Since bubbles are not tracked individually, the method is affordable in terms of CPU. Together with the rapid convergence due to the PISO coupling, the coupled DPM and VOF model is an efficient method. The calculation of the Lagrangian bubble dynamics (DPM) is fully coupled with the Eulerian dynamics of the other phases. There is one DPM iteration per Eulerian time-step.

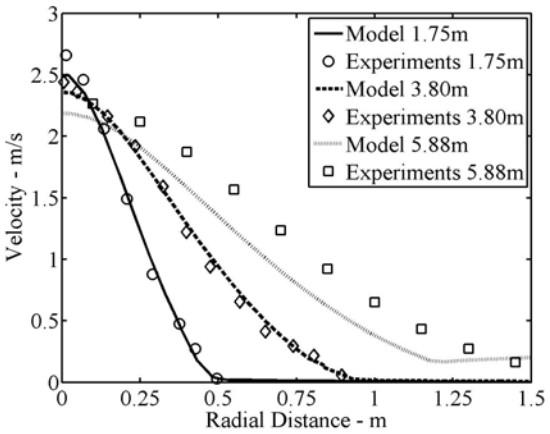

Figure 1: Modelling results of velocity profiles of the liquid phase at different heights above gas release point compared with experiments at a gas rate of 170 Nl/s.

MODEL VALIDATION AND INFLUENCE OF LIFT

In order to validate the model, modeling results have been compared to experimental results (Engebretsen *et.al*., 1997). A series of experiments were conducted in a rectangular basin with a depth of 6.9 m and a surface area of 6 x 9 m. The basin was filled with water and air was released at the bottom at gas rates of 83, 170 and 750 Nl/s (equivalent to 50, 100 and 450 l/s referred to the state at the inlet). The inlet was comprised of a release valve with a rapidly acting piston injecting gas vertically with arrangements in front of it to reduce the vertical momentum. Because of this momentum breaker, the fluctuations in the gas flow and the length of the inlet jet were minimized. Comparison without a lift force gave good agreement with experiments regarding velocity profiles, rise times and fountain height (Cloete *et.al*, 2009b). Some discrepancies were found for the highest gas rate and for the regions close to the water surface. The high void fractions resulting from the highest gas rate violate the assumption of the model as explained above.

Validation simulations for including the lift force have been conducted. The validation simulations used a grid of 508891 cells based on 2 refinements of an initially crude and uniform grid. The bubble size at the inlet was set to 5 mm and an adaptive time step was used which aimed at a Courant number of 0.7. The resulting velocity profiles are seen in Figure 1 with the corresponding experimental profiles. The profiles are sampled 20 seconds after initial gas release. Note that radial distance is the distance from the centre of the vessel. There is a near perfect match between model and experiments close to the bottom and in the middle of the vessel. Closer to the top surface there is some deviation, but the model still performs fairly well. The deviation may be explained by the simplistic turbulence model which does not account for the presence of the water surface. We also see from Table 1 that the time it takes for the first bubbles to reach the surface is well predicted by the model.

Gas Rate	83 Nl/s	170 Nl/s	750 Nl/s
Experimental	6.0 s	4.8 s	3.1 s
Modelled	6.6 s	5.2 s	3.2 s

Table 1: Experimental and theoretical bubble rise times.

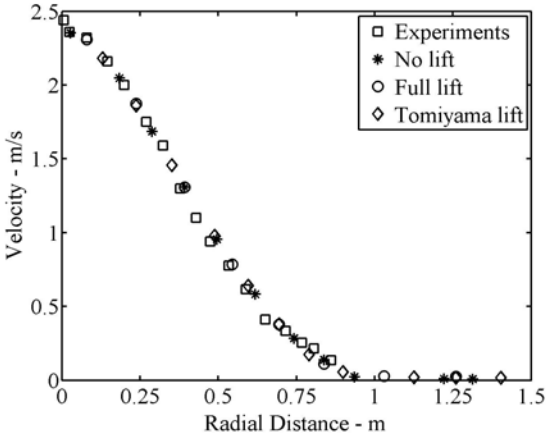

Figure 2: Modelling results of liquid velocity profile 3.8m above gas release point for different lift options compared with experiments at a gas rate of 170 Nl/s.

The effect of lift has been included in the model. For a gas rate of 170 Nl/s, several lift options have been applied. They include the full lift formulation described above, pure Tomiyama lift and no lift. The results of these numerical simulations are compared in Figure 2 where the velocity profiles are seen. The results indicate that there is no effect of the lift force. Even if there are doubts about what the real lift coefficient should be, these results show that two quite different lift formulations do not affect the results compared to a no-lift simulation. Note that at lower gas rates the lift may become important again. This has not been verified.

MIXING AND INFLUENCE OF FREE SURFACE

Many modelling approaches on ladle hydrodynamics assume a flat free surface. Whether this is a good assumption or not is open for debate. Johansen & Boysan (1988) were able to reproduce experimental velocity data very well when modelling with a flat surface assumption. They dealt with a low gas rate and it may be that the assumption is only good at low gas rates. Therefore results from simulations with a flat top surface and a dynamic surface have been compared at higher gas rates. In Figure 3 it is seen that the velocity profiles at different heights at a gas rate of 170 Nl/s are almost identical for the flat surface and dynamic surface simulations. Deen *et.al*. (2001) also got good results with a flat surface at higher gas rates. Based on this it might be tempting to conclude that the flat surface assumption is a good assumption for CFD analysis of ladle hydrodynamics. However, the issue is more complicated.

Mixing is often the main purpose of the ladle process, and mixing quality depends on the liquid velocity in the more stagnant zones of the ladles. These velocities are not necessarily represented by the velocity profiles presented in Figure 3 (and in most other journal publications). Therefore it might be acceptable to apply a flat surface for model predictions of typical velocity profiles, but it might be a bad assumption when modelling the mixing time. Due to this suspicion, a series of simulations with and without the flat surface assumptions have been conducted to verify its influence on the prediction of mixing time. Mixing time is defined as the time it takes for an injected tracer element to be mixed such that the local minimum concentration is 95% of the average concentration.

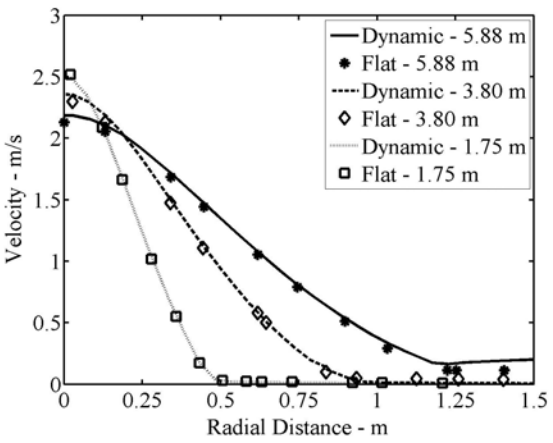

Figure 3: Liquid velocity profiles at different heights above gas release point at a gas rate of 170 Nl/s for simulations with flat free surface and dynamic free surface for a rectangular ladle.

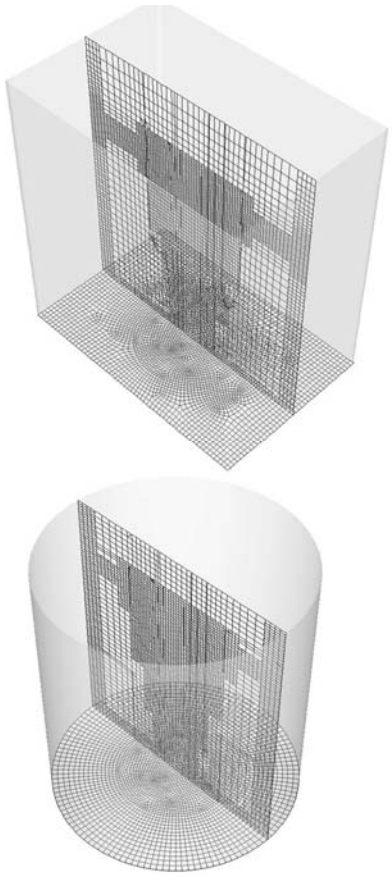

Figure 4: Geometries with grid for rectangular ladle (top) and cylindrical ladle.

A series of simulations have been carried out on two different geometries: cylindrical and rectangular. The rectangular geometry is the same as described above, and the cylindrical has the same height and same surface area (i.e. diameter of 8.3 m). 3D grids of the geometries were created from a uniform mesh with one level of refinement in the plume region and along the walls for the mixing studies. This gave grids of about 220000 cells for the geometries with dynamic surface and about 120000 cells for the geometries with flat surface. The larger amount of

cells in the dynamic surface simulations is due to the need to capture the movement of the liquid-gas interface. The geometries and grids are seen in Figure 4 for the dynamic surface conditions. Simulations were run until a quasi steady state solution was obtained. At that time, a tracer species was patched into a small region above the gas injection area. The tracer was then mixed by convection and turbulence. The minimum concentration was monitored as a function of time, and thus the mixing time was obtained for different geometries and gas rates for a dynamic top surface and a flat top surface.

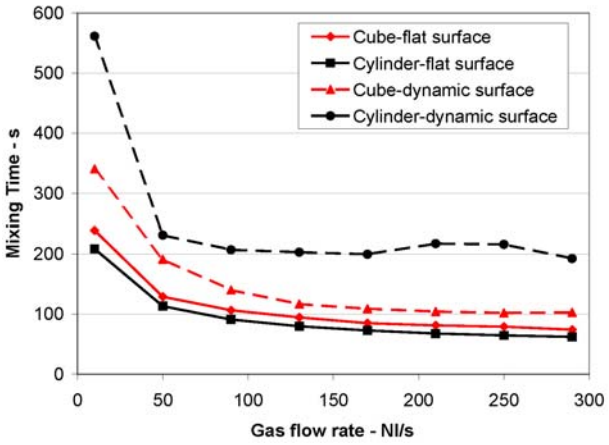

Figure 5: Mixing time as a function of gas rate and specific energy consumption for rectangular and cylindrical geometries with and without flat surface assumption.

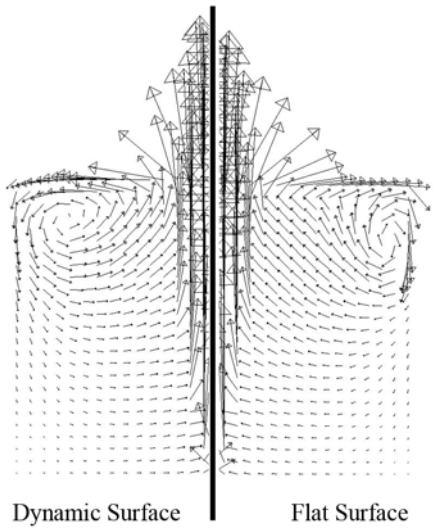

Figure 6: Comparison of velocity field for a dynamic surface simulation and a flat surface simulation at a gas rate of 170 Nl/s.

The results are seen Figure 5 in where we see that the flat surface assumption yields lower mixing times than the simulations with a dynamic surface for different gas rates and specific energy inputs. This can be explained by the increased viscous dissipation of mean flow energy in the dynamic free surface case. More energy is lost to viscous dissipation because the formation of a plume fountain requires the flow to go up into the fountain and then make a very sharp turn to go back down again. Naturally, stronger plumes will produce taller fountains which would require more acute flow turning angles and greater dissipation losses. When the surface is forced to be flat, however, the flows can simply perform a gentle right angle turn regardless of the plume strength. This flow situation is much less dissipative and the total momentum available for mixing can be severely over-predicted, especially when stronger plumes are employed. This is illustrated by Figure 6. It can also be seen in Figure 7 that the tracer moves faster downwards along the ladle walls with a flat surface assumption.

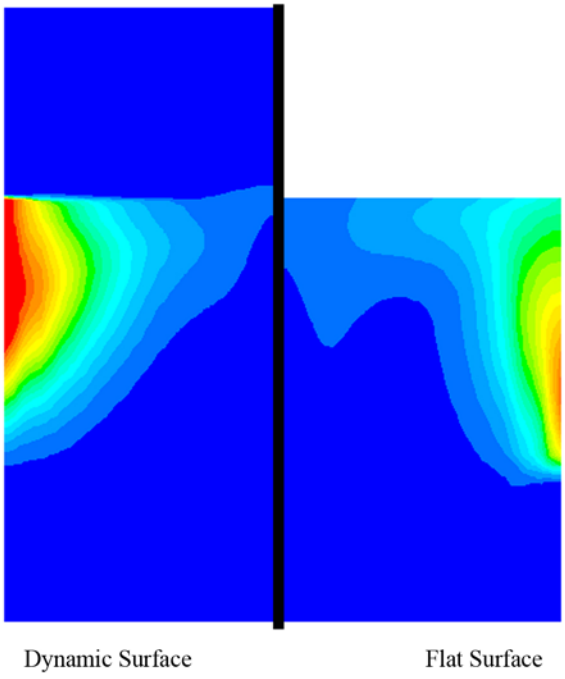

Figure 7: Comparison of tracer concentration 15 secs. after tracer release for a dynamic surface simulation and a flat surface simulation at a gas rate of 170 Nl/s. Blue= 0%, Red =1%.

CONCLUSION

An Eulerian-Eulerian-Lagrangian method for modelling ladle hydrodynamics has been presented. The method is a coupled DPM and VOF model which is numerically robust and efficient. By applying the method to gas stirred ladles with bottom injection, it has been shown that the lift force has no influence on the hydrodynamics for higher gas rates.

It has also been shown that the assumption of a flat surface is acceptable if the purpose is to obtain velocity profiles at different elevations in the ladle. We see no difference in results on the liquid velocity profiles. If mixing time is the purpose of the investigation, the flat surface assumptions is not valid. Then it is necessary to apply a modelling technique which captures the dynamic behaviour of the top surface.

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