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The Effect of Surface Tension in Polymer Flow during Reactive Rotational Molding

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Abstract

The Reactive Rotational Molding (RRM) is a manufacturing method for the production of one-piece hollow plastic part where the polymer synthesis and shaping of piece is carried simultaneously using heat and bi-axial rotation. The main drawback of RRM is poor control of the process due to the high number of influent parameters. In these conditions, the optimization of the process is quite complex. During RRM, it is very important to predict the fluid flow in order to be able to obtain a piece with homogeneous shape and with high quality. For this study, we have applied Smoothed Particles Hydrodynamics (SPH) to simulate the polymer flow during this process taking into account surface tension force. To implement force tension surface, the interface between polymer and air is tracked dynamically by seeking the particles constituting this border by algorithm developed by Barecasco, Terissa and NAA[1,2] in two and three dimensional. Then, we use Lagrangian interpolation or fitting circle to reconstruct the interface curve in two dimensions, and we apply the fitting sphere method in three dimensions to reconstruct the boundary surface. By using the basic method of SPH for fluid modeling, and a combination of 2D and 3D free curve or surface detection algorithm with interpolation method, we can simulate polymer flow phenomena during RRM with expected result.

Introduction

Reactive Rotational Molding (RRM) is shear-free and pressure-free used to create hollow. In this process, the polymer synthesis and piece shaping are carried simultaneously [3]. Modeling RRM is a challenge because a multiple parameters involved during this process like the rate of chemical reactions, viscosity variations during polymerization and fluid flow during crosslinking. These phenomena are complex and require detailed study to modeling the process. Previous work by our team permits the simulation of thermoset polyurethane in two and three dimensional configuration using Smoothed Particle Hydrodynamics [4]. In order to complete and enhance the solver's team because we have observed in the Team's model as it works can generate roughness or particle agglomerates on the internal surface. This phenomenon affects the flow of material and its adhesion process that can be slowed and even stopped. It will also consider this problem for example by integrating new model or criterion then seeing if taking into account the viscoelasticity of the material and / or surface tension, this phenomenon can be reduced. In this study, the surface tension force will be integrated in SPH solver in order to simulate the polymer flow during RRM.

Zhang [5] proposed a new surface tension method where free surface boundary can be tracked dynamically by using an algorithm developed by Dilts and Haque [6-7]. However, this method is quite difficult to implement it and particularly in three dimensions. Later, Marrone[8]presented an algorithm based in the properties renormalization matrix in the first step and the use of a scan cone around the expected normal vector of the fluid surface to make a further check if there is any particle covering the test particle. Recently, Barecasco and Al[1,2] developed simple algorithm which permit to track the interface using a sum of normalized relative position vectors from neighbouring particles to the test status of SPH particle.
Finally, the interface curve is reconstructed locally with Lagrangian interpolation and Fitting circle in 2D and fitting sphere has been used to reconstruct the surface curve in 3D configuration, respectively.

Numerical Model

The SPH is a fully Lagrangian, grid free method in which a smoothing kernel is introduced to approximate functions and their spatial derivatives originating from the interactions with neighboring particles and has been applied to a wide range of flow problems[8-10]. In SPH, the fundamental principle is to approximate any function A(r) by:

$$\mathrm{A(r)} = \int \mathrm{A(r')W(r-r',h)dr'} \qquad (1)$$

h is smoothing length and W is weighting or kernel function which has compact support.
In present simulation, the cubic spline kernel has been used:

$$W(r,h) = \alpha_D \begin{cases} 1 - \frac{3}{2}q^2 + \frac{3}{4}q^3 & 0 \le q \le 1 \\ \frac{1}{4}(2-q)^3 & 1 \le q \le 2 \\ 0 & q \ge 2 \end{cases} \qquad (2)$$

Where
q = r/h, α_D is $10/(7\pi h^2)$ in 2D and $1/(\pi h^3)$ in 3D.
The equations governing the evolution of fluid quantities are expressed as summation interpolants using a kernel function W with smoothing length h, as:

$$\frac{d\rho_a}{dt} = \sum_b m_b(\vec{v}_a - \vec{v}_b)\vec{\nabla}W_{ab} \qquad (3)$$

Where: ρ_a,v_a are respectively the density and the velocity of particle a; m_a and v_b are the mass and the velocity of particle b.

$$\frac{d\vec{v_a}}{dt} = -\sum m_b\left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2}\right)\vec{\nabla}W_{ab}$$

$$\frac{d\vec{v_a}}{dt} = -\sum m_b\left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2}\right)\vec{\nabla}W_{ab} + \sum \frac{m_b(\eta_a+\eta_b)v_{ab}}{\rho_a\rho_b}\left(\frac{1}{r_{ab}}\frac{\partial W_{ab}}{\partial r_a}\right) + \vec{g} + \vec{f} \qquad (4)$$

Where: Pa, P_b,η_a, η_b are pressure and viscosity of particles a and b respectively and g represents the gravity.
And $\vec{f}$: surface tension surface and is given by :

$$\vec{f} = \sigma k\, \vec{n}\, \delta_s \qquad (5)$$

σ: coefficient of surface tension ;k : the curvature ;$\vec{n}$: normal vector of surface ;δ_s : surface delta function and it's equal to 1/ε where: ε represents particle spacing.

$$\frac{dE_a}{dt} = \sum_b \frac{4m_b}{\rho_a\rho_b}\frac{k_a k_b}{k_a + k_b}T_{ab}\frac{r_{ab}.\nabla_a W_{ab}}{{r_{ab}}^2 + \varepsilon^2} \qquad (6)$$

Where k_a and k_a are respectively the conductivity of particle a and b, T_{ab} is the difference between the temperatures of particles a and b.

To describe the thermodynamic behaviour of the fluid, we have associated to this system an equation of state:

$$P = P_0\left[\left(\frac{\rho}{\rho_0}\right)^{\gamma} - 1\right] \quad (7)$$

Where: P_0 is the magnitude of the pressure and ρ_0 is the reference density. P_0 is given by:

$$P_0 = \frac{c^2{}_s\rho_0}{\gamma} \quad (8)$$

With C_s: speed sound at the reference density and γ is a problem dependent parameter.

In our simulations, to prevent inner fluid particle from penetrating the wall, we employ an artificial repulsive force. Moreover, with repulsive forces, only one layer of particles is placed on the wall with identical mass and density to inner particles.

The boundary conditions adopted in our study produce no-slip conditions. In this configuration, the reactive fluid particles cannot adhere to the boundary particles. To simulate the adhesion of the RRM on the mold surface, Riviere[4] developed a model to fix the fluid particles when they reached a certain viscosity and when they are exposed to a certain distance from the mold (or the fixed material) during a certain time.

To make a faster calculation, we used a linked-list grid method to reduce the time of calculation. The method to get the position and velocity for each particle in a time step uses Newmark [11] integrator to advance in time, the variables are calculated according to:

$$v_i^{n+1} = v_i^n + \Delta t\left((1-\alpha)a_i^n + \alpha a_i^{n+1}\right) \quad (9)$$

$$x_i^{n+1} = x_i^n + \Delta t v_i^n + \Delta t^2\left((0.5-\beta)a_i^n + \beta a_i^{n+1}\right) \quad (10)$$

Where x and v represent position and velocity, respectively. Moreover $\alpha = 0.5$ and $\beta = 0.25$. Temperature and density are updated according to (12) and time step Δt depends on the Courant Friedrichs Lewy (CFL) condition [12].

Surface Tension

Generally, surface tension forces are caused by the unbalanced molecular dynamic forces at the free surface, in the region between two different immiscible fluids (polymer-air). In these regions the polymer molecules are forced to shift in the direction of the normal surface towards the liquid itself causing a minimization of the liquid's curvature at the surface.

Obviously, the surface tension force act only in the border polymer-air, so first of all, we must detect dynamically all the particles belonging to the interface.

Tracking Free Surface Boundary Polymer-Air

The interface is detected dynamically by finding all boundary particles using algorithm developed by Barecasco and Al. In this method, the domain is representing by overlapping of spheres (s_i) where s_i represents a SPH particle centred at the particle's position x_i and r_i is sphere's radius. Then, we check if some part of segments of this sphere is or not covered. If there is some piece of it is not covered by the spheres of its neighbors, then it is a boundary particle. Otherwise, it's inner particle. Due to the non-uniform properties of SPH particles, we use a scan cone around the cover vector of the fluid surface which checks, if there is any covering particle.

The cover vector can be written as:

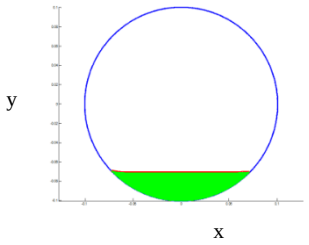
$$b_i = \sum_{j=0}^{n} \frac{x_i - x_j}{\|x_i - x_j\|} \quad (11)$$

The particle is boundary particle if:

$$arccos\left(\frac{x_j - x_i}{\|x_j - x_i\|}\frac{b_i}{\|b_i\|}\right) \le \frac{\theta_i}{2} \quad (12)$$

Where: θ_i, the angle of cone;

First, we used a mold with simple geometry; a cylinder rotating around its main axis (Figure 1.). The cylinder radius is 10 centimetres and the rotational speed is 7.5 revolutions per minute (rpm). The optimum angle $\theta_i = \pi/4$, permit to detect all the boundary particles.



Mold: 1502 particles
Fluid: 21069 particles

Figure 1. detection of boundary particle for a cylinder mold rotating around its main axis. The mold is shown in blue, the inner particle in green and boundary particle in red colour.

To test the efficiency of the algorithm to detect the border air-polymer in three dimensional configurations, we use cylinder as mold, as shown in the figure 3, containing the reactive fluid and the scan cone angle $\theta_i = \pi/4$.

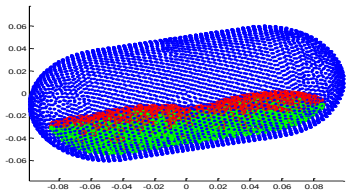


Figure 2. Detection of boundary particle in three dimensional configurations. The mold is shown in blue, the inner particle in green and boundary particle in red colour.

Reconstruction of the Curve Interface

Two Dimensional

Before reconstruction of the curve, the system coordinates are transformed into local coordinate system, in order to guarantee the interface curve will have one-valued in the local coordinate system.

The origin o' of the local coordinate system is given by:

$$x_{o'} = \frac{\sum_j x_j}{N_i} \quad (13)$$

$$y_{o'} = \sum_j y_j / N_i \quad (14)$$

Where j is the particle index of neighbors of boundary particle i and *Ni* is total number of neighbors of boundary particle i.

The relation between the local coordinate (x',y') and the coordinate system (x,y) is given by:

$$x = x'\cos\alpha - y'\sin\alpha \quad (15)$$

$$y = x'\sin\alpha + y'\cos\alpha \quad (16)$$

Where: α represents the angle between the angle between the two axis x and x'.

First, we use the fitting to reconstruct the boundary curve in the local coordinate system. A measure of the fit of the circle with the center being at the point $(x_{C_{i,j,k}}, y_{C_{i,j,k}})$ and the radius being "r" to the boundary particles points $P(x_i,y_i)$ is given by summing the squares of the distances from these points to the circle. The measure is formalized as follow:

$$S\left(x_{C_{i,j,k}}, y_{C_{i,j,k}}, r\right) = \sum_{i=1}^{n}\left(r - \sqrt{\left(x_i - x_{C_{i,j,k}}\right)^2 + (y_i - xy_{C_{i,j,k}})^2}\right)^2 \quad (17)$$

Where: the index i indicate the boundary particle.

We note the solving (17) =0 for r yields to:

$$r = \sum_{i=1}^{n} \sqrt{\left(x_i - x_{C_{i,j,k}}\right)^2 - \left(y_i - x_{C_{i,j,k}}\right)^2} / n \qquad (18)$$

If we obtain $x_{C_{i,j,k}}$, $y_{C_{i,j,k}}$ by some other method, we can obtain good value of r by using the formula (21).

In this study, we use average of intersections method to fit circle to data points in order to obtain the coordinate of our circle [13]. The coordinates of the center of circle obtained by this method are given by:

$$\begin{cases} x_{C_{i,j,k}} = \dfrac{(y_k - y_i)(x_i^2 + y_i^2) + (y_i - y_k)(x_j^2 + y_j^2) + (y_j - y_i)(x_k^2 + y_k^2)}{2\Delta} \\ y_{C_{i,j,k}} = -\dfrac{(x_k - x_i)(x_i^2 + y_i^2) + (x_i - x_k)(x_j^2 + y_j^2) + (x_j - x_i)(x_k^2 + y_k^2)}{2\Delta} \end{cases} \qquad (19)$$

We use another method: Lagrangian interpolation to reconstruct the interface curve.

The Lagrange interpolation is formulated as follows:

$$P(x) = \sum_j P_j(x) \qquad (20)$$

Where:

$$P_j(x) = y_j \prod_{k \neq j} \frac{(x - x_k)}{(x_j - x_k)} \qquad (21)$$

j is particle index including boundary particle i and its neighbors on the boundary.

The curvature and the normal in local coordinate are obtained as:

$$k = \frac{|P''(x)|}{[1 + P'^2(x)]^{3/2}} \qquad (22)$$

$$\overrightarrow{n'} = \begin{cases} \langle P'(x), -1 \rangle & if\ P''(x) < 0 \\ \langle -P'(x), +1 \rangle & if\ P''(x) > 0 \end{cases} \qquad (23)$$

The coordinate of normal vector in the original system are given by:

$$\overrightarrow{n'} = \begin{cases} \langle P'(x)cos\alpha + sin\alpha, P'(x)sin\alpha - cos\alpha \rangle & if\ P''(x) < 0 \\ \langle -P'(x)cos\alpha - sin\alpha, -P'(x)sin\alpha + cos\alpha \rangle & if\ P''(x) > 0 \end{cases} \qquad (24)$$

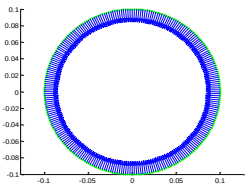


Figure 3.Particle position of 2D circle (radius=0.1m) with the normal vector on the surface.

The both methods give an accurate value of the normal (figure 3.). In the fitting circle method the value of the curvature is constant and it's equal to 10 which is the inverse of circle radius. On the other side, the value of curvature obtained by Lagrangian method is slight different from the 10 and the curvature value converges to 10 by increasing the number of the boundary particles and the relative errors for the 252,314, 628 and 1286 boundary particles are 0.084, 0.051, 0.013 and 0.00301% respectively.

Three Dimensional Configurations

The boundary surface is reconstructed using fitting sphere method. Before reconstruction of the curve, the system coordinates are transformed into local coordinate system, in order to guarantee the surface curve will have one-valued in the local coordinate system.

The origin o' of the local coordinate system is given by:

$$\vec{r}_{o'} = \sum_j \vec{r}_j / N_i \qquad (25)$$

Where j is the particle index of neighbours of boundary particle i and Ni is total number of neighbours of boundary particle i.

The local three-dimensional basis vectors were calculated, by equation 26:

$$\hat{Z}_{o'} = \frac{\vec{r} - \vec{r}_{o'}}{\|\vec{r} - \vec{r}_{o'}\|},\ \hat{X}_{o'} = \begin{cases} \frac{\hat{X} \times \hat{Z}_{o'}}{\|\hat{X} \times \hat{Z}_{o'}\|}, \hat{Y} \times \hat{Z}_{o'} = 0 \\ \frac{\hat{Y} \times \hat{Z}_{o'}}{\|\hat{Y} \times \hat{Z}_{o'}\|}, \hat{Y} \times \hat{Z}_{o'} \neq 0 \end{cases},\ \hat{Y}_{o'} = \frac{\hat{X} \times \hat{Z}_{o'}}{\|\hat{X} \times \hat{Z}_{o'}\|} \qquad (26)$$

To fit sphere from data points, we use method fitting sphere [14].The basic problem is to find a circle that best represents the data in some sense. With our sphere described by:

$$(x - a)^2 + (y - b)^2 + (z - c)^2 = R^2 \qquad (27)$$

Where: a,b,c and R are the coordinate of the center and the radius of sphere.

This relation can be written as:

$$x^2 + y^2 + z^2 + xA_1 + yA_2 + zA_3 + A_0 = R^2 \qquad (28)$$

Where

$A_0 = a^2 + b^2 + c^2 - R^2$; $A_1 = -2a$; $A_2 = -2b$; $A_3 = -2c$

Putting $\rho_k^2 = x_k^2 + y_k^2 + z_k^2$, the system to resolve is reduced to:

$$\begin{bmatrix} n & \sum x_k & \sum y_k & \sum z_k \\ \sum x_k & \sum x_k^2 & \sum x_k y_k & \sum x_k z_k \\ \sum y_k & \sum x_k y_k & \sum y_k^2 & \sum y_k z_k \\ \sum z_k & \sum x_k z_k & \sum y_k z_k & \sum z_k^2 \end{bmatrix} \begin{pmatrix} A_0 \\ A_1 \\ A_2 \\ A_3 \end{pmatrix} = - \begin{pmatrix} \sum \rho_k^2 \\ \sum \rho_k^2 x_k \\ \sum \rho_k^2 y_k \\ \sum \rho_k^2 z_k \end{pmatrix} \qquad (29)$$

The resolution gives A_0, A_1, A_2 and the coordinate of sphere:

$a = -\frac{A_1}{2}$; $b = -\frac{A_2}{2}$; $c = -\frac{A_3}{2}$;

To validate the current method for surface tension, the computations of normal vector and curvature of the interface on sphere is studied.

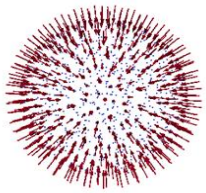


Figure 4. Particle position of 3D sphere (radius=0.1m) with the normal vector on the surface.

The reconstruction surface method used in our study give an accurate value of the normal and curvature. Indeed, the value of the curvature is constant and it's equal to 10 which is the inverse of circle radius (figure 4.).

Validation

We studied one benchmark, the two dimensional broken dam problems, to show the capability of our SPH solver to implement the effect of surface tension. The problem consists of a rectangular (H x L) column of fluid confined between a fixed wall and a temporary wall (dam) [15]. We compared our results with those obtained experimentally by Martin and Moyce [16] for the collapse of a water column. The computational domain has been discretised by 4344 particles and the fluid viscosity is set at 0.001 Pa.s (water at 20°C).

In figure 5., the non-dimensional surge front positions of the collapsing dam $X^* = x/a$ are plotted against the non-dimensional time $T^* = t\left(g/a\right)^{1/2}$ where a represents the width of the water column (m), t the time (s), and g the gravitational force.

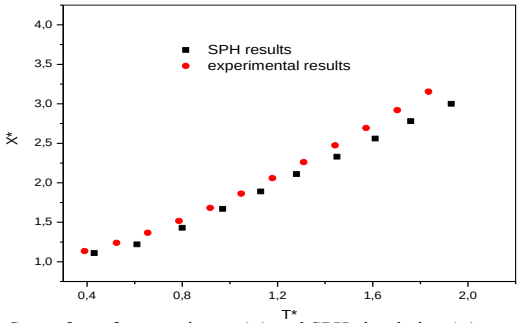


Figure 5. Surge front for experiment (●) and SPH simulation (■).

There is a reasonably good agreement between the experimental results and SPH method. So, we can applied this solver to simulate the reactive fluid flow during RRM.

Some Numerical Results

2D Simulations

We performed 2D simulations of an increasing viscosity fluid in a mold and taking into account the tension surface force. To test the efficiency of the algorithm of implementation of surface tension force, we used a simple geometry. The cylinder radius is 10 centimeters and the rotational speed is 7.5 revolutions per minute (rpm) figure 6.The initial spacing particle is 5.10^{-4} meter. The mold is represented of approximately 1258 solid particles and its temperature is set at 80°C. The polymer which is a polyurethane is symbolized of approximately 17 000 fluid particles, the initial temperature is set at 25°C. With the initial amount of polymer, the final part wall thickness should be approximately of 5 millimeters. At the end of the simulation, around 10 particles should form the part thickness.
Once the reaction starts, the viscosity increases according to rheokinetik model[17]used in this study, which gives relationship between viscosity and rate of reaction. The parameters of adhesion models chosen are: η_{adhe}= 9Pa.s, t_{adhe}=3 s and Δ=1.5*dx. The coefficient of surface tension σ is set to 30mN.m^{-1}.

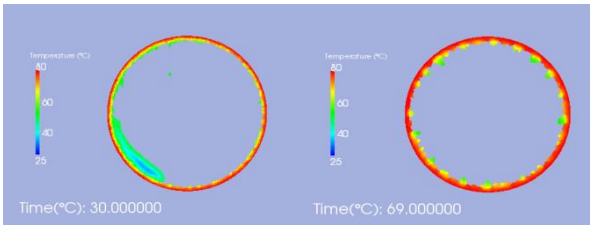


Figure 6. 2D cylinder (19000 particles).
In spite of, we have implemented the surface tension effects; the inner surface is not well smooth. To remedy to this problematic, we must incorporate new criterion in the artificial adhesion model in order to reduce the roughness and agglomerates particles.

3D Simulations

Like to the two dimensional simulations, we conducted the numerical study with simple mold geometry; cylindrical mold shape has a length of 20 cm and a diameter of 10 cm. The parameters of adhesion models chosen are: η_{adhe}=30Pa.s, t_{adhe}=1.25 s and Δ=2*dx. The coefficient of surface tension σ is set to 30mN.m-1.The initial spacing particle is 2 mm which corresponds to 4mm in final part. The mold is represented by 20000 solid particles and its temperature is set at 80°C. The polymer which is polyurethane is represented by 90000 of fluid particles; the initial temperature is set at 25°C (figure 7). The evolution of viscosity follows the same law which is used in two dimensional configurations.

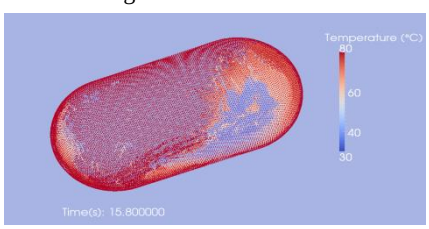


Figure 7. 3D cylinder (130000 particles).

Conclusion

The current method has been successfully applied to simulate RRM using SPH solver taking into account free surface tension force. Surface tension force is given explicitly in the current model. After detecting the boundary particles, the interface is fitted locally by using Lagrangian interpolation polynomial or fitting circle in 2D and by using fitting sphere in 3D, respectively.
The fitting sphere and fitting circle gives an accurate estimation and was validated in sphere domain and a represent an alternative method to moving least square in 3D and Lagrangian interpolation in 2D respectively. The advantage of these methods is a simple to implement mainly than MLS method in 3D.
Unfortunately, the implementation of surface tension effects did not remedy the problem of agglomerates particles in the inner surface of mold. To reduce the roughness and agglomerates particles, we would to take account of the non-Newtonian character of polymer using viscoelastic models describing the behavior of our material during the process.

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