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Modelling surface tension with smoothed particle hydrodynamics in reactive rotational moulding

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ABSTRACT

Reactive Rotational Moulding (RRM) is the best process for producing large hollow plastic parts without weld lines. Constant quality in technical parts requires the process to be mastered by controlling on-line the main physical phenomena. However, 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. The aim of this work is to simulate the reactive fluid flow during RRM with Smoothed Particle Hydrodynamics (SPH) solver in two dimensions (2D) and three dimensions (3D) taking into account surface tension force. To implement this force, the interface is tracked explicitly using algorithm developed by Barecasco et al. (2013) and Terissa et al. (2013) and the reconstruction of curve or surface boundary by different interpolation or surface construction technique with Lagrangian interpolation and fitting circle methods in 2D and spherical regression in 3D, respectively.

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1. Introduction

Rotational moulding, known also as rotomoulding or rotocasting, is a process for manufacturing hollow plastic products with no weld lines, in virtually any shape, size, colour and configuration, using biaxial rotation and high temperature [3,4].

Rotational moulds are less expensive because it's not necessary to make them with higher performance materials. In this process the value of wasted materials are low, relatively, and excess material can be often reused, and it is very economically and environmentally viable manufacturing method. However, this process takes long times, about 20–40 min; typically, opposed to other processes such as injection moulding, which products can be made in a few seconds. The limited number of polymers only thermoplastics that can be charged for rotational moulding is also considered as disadvantage of this process. The various inconvenient of conventional rotomoulding have favored the emergence of Reactive Rotational Moulding (RRM) where the polymer synthesis and shaping are carried simultaneously. This kind of rotational moulding represents significant advantages compared to traditional rotational moulding: process cycle time is shorter; raw material is less expensive because polymerization occurs during processing and high performance polymers may be used such as thermosets or biobased polymer [5]. Modelling of this process is challenging because of the phenomena involved during this process like chemical reaction, viscosity variations during polymerization and the different hydrodynamics regimes of material flow during process material flow during are complex and requires detailed study in order to predict and simulate the process.

Previous work permits simulating thermoset polyurethane in two- and three-dimensional (2 and 3D) configurations using Smoothed Particle Hydrodynamics (SPH) [6–8] in order to complete our SPH solver, because we have observed that, as it works, it can generate roughness or particle agglomerates on the internal surface (Fig. 1). This phenomenon affects the fluid flow and the adhesion process which can be slowed and even stopped. It will also consider this problem, for example, by integrating a 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 the SPH solver in order to reduce the roughness and curvature in the final parts.

The surface tension plays an important role in Reactive rotational moulding process as regards the wetting of the internal surface of the mould during the first moments of the shaping of the piece where the fluid breaststroke this surface and permits to obtain a smooth internal surface. In addition, it is responsible for creating and layering polymer layers.

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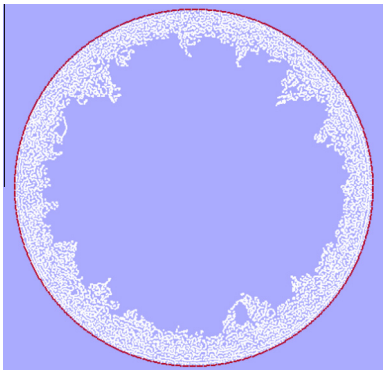

Fig. 1. Formation of particle agglomerates on the internal surface of the part.

The first approach is based on the model of Van der Walls and is to initiate an inter-particle interaction force in the equation of conservation of momentum. Nugent and Posch [9] were the first applied this approach to SPH method for the formation of a liquid drop from an initial regular shape. The cohesive pressure in the Van der Waals (VdW) equation of state is similar to the unbalanced molecular cohesive forces in which cohesive pressure works as surface tension.

Then, the VdW model is applied to simulate the oscillation of the deformed drop without tensile instability [10,11]. Later, Tartakovsky and Meakin applied the SPH method to the modelling of surface tension and contact angle [12,13]. The second approach to treat surface tension force in SPH method is based on the continuum surface force (CSF) model developed by Brackbill [14], where the interface curvature is calculated through a colour function [15]. The main disadvantage of this method is the estimation error of surface tension for large curvatures because the second derivative of a colour function is sensitive to particle disorder. Adami et al. [16] proposed a new surface tension model for multi-phase problems using a reproducing divergence approximation for getting accurate surface curvature without full support of kernel function.

The last class method for modelling surface tension in SPH method consists to track dynamically the interface between two immiscible fluids. The first work was carried out by this method are performed by Zhang [17] where the free-surface boundary can be dynamically tracked by using geometric algorithms [18,19]. But this method is quite difficult to implement it, particularly in 3D. However, Marrone et al. [20] presented a new method based on the properties renormalization matrix, defined by Randles and Libersky [21]. Recently, Barecasco et al. [1,2] developed a new method where the boundary particle in 2 and 3D configurations is detected by scanning the sphere around an SPH particle.

The aim of this work is to develop SPH surface tension model applied to reactive fluid flow during RRM and to meet the following requirements: implementing a simple algorithm to detect the air–polymer interface using the algorithm developed by Barecasco et al. constructing interface curve by fitting circle (2D) and the surface boundary using sphere (3D) using the geometrical algorithm and, finally, showing its capability to implement surface tension forces in the SPH solver and the effect of surface tension to enhance the quality of our simulations.

2. Method and material

The reactive fluid flow of liquid polymer during RRM will be simulated using the SPH method. The liquid reactive system is modelled as an incompressible viscous Newtonian fluid because the viscosity remains low until gelation and the shear force is ignored as the mould rotates very slowly (1–10 rpm). Also, the pressure into the mould remains constant during the process. The surface tension force is only applied for boundary particles. To undertake this study, we used reactive system composed from Isocyanate and a Polyol with functionality of more than two in order to produce thermoset polyurethane.

3. Numerical model

The study of fluid flow is governed by the Navier–Stokes equations that reflect the mass conservation, momentum and total energy. A state equation is combined in these equations in order to describe the thermodynamic behaviour of fluids. In Lagrangian formalism these equations can be written as [22]:

$$\nabla \vec{v} = 0 \tag{1}$$

$$\frac{\partial \vec{v}}{\partial t} = g + \frac{1}{\rho}\nabla \cdot \tau - \frac{1}{\rho}\nabla P + \frac{1}{\rho}\vec{f} \tag{2}$$

$$\rho \frac{dU}{dt} = \nabla \cdot (k \cdot \nabla T) \tag{3}$$

where g, P, v, U, k and ρ represent the gravitational acceleration, pressure, the velocity vector, thermal energy, conductivity and density, respectively, and $\vec{f}$ denotes the surface force which acts only at the interface.

Smoothed Particle Hydrodynamics (SPH) is a simple and efficient numerical method that can be used to solve a variety of difficult problems in computational mechanics [23,24]. In this method, the fluids are represents by a set of particles. Furthermore, SPH allows computing the value of any variable, such as density, at arbitrary density positions in the fluid by smoothing over the set of all nearby particles.

In SPH, the fundamental principle is to approximate any function $A(r)$ by:

$$A(r) = \int A(r')W(r - r', h)dr' \tag{4}$$

where h is smoothing length.

The continuous integral in SPH formalism can be converted to discretised form. Therefore, at a particle a the following equation is used:

$$A(r) = \sum_b \frac{m_b}{\rho_b} A_b W_{ab} \tag{5}$$

where a, b represent the SPH particles; m_b and ρ_b are the mass and density of particle b, respectively.

The summation is over all the particles within the region of the compact support of the kernel function determined by the kernel function W_{ab}.

In the present simulation, the cubic spline kernel has been used:

$$W(r,h) = \alpha_D \begin{cases} 1 - \frac{3}{2}q^2 + \frac{3}{4}q^3 & 0 \leqslant q \leqslant 1 \\ \frac{1}{4}(2-q)^3 & 1 \leqslant q \leqslant 2 \\ 0 & q \geqslant 2 \end{cases} \tag{6}$$

where

$q = r/h$, r is the distance between particle a and b.
α_D is $10/(7\pi h^2)$ in 2D and $1/(\pi h^3)$ in 3D.

The Navier stokes equations, the continuity equation (6), momentum equation (7) and thermal energy (9), governing the evolution of fluid quantities are expressed as summation interplants using a kernel function W with smoothing length h, as:

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