Modelling of Polyurethane Foaming with Finite Pointset Method

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Abstract — The foaming process of polyurethane is numerically simulated with the Finite Pointset Method (FPM) which belongs to SPH techniques (Smoothed Particle Hydrodynamics). The present three dimensional model allows the investigation of the foaming process including the transient free surface flow and the strong coupling of the material properties with the chemical reactions. The potential of the FPM method to solve problems with free surfaces and complex boundary conditions is illustrated by means of a mould filling of an automotive underlay carpet cavity.

Key words — polyurethane foaming, finite pointset method, expansion

1. Introduction

Polyurethane foams are used in several fields such as automotive, aeronautic and buildings. These materials offer many opportunities thanks to their wide range of stiffness, densities and other physical properties. During the foaming process a number of defects (air entrapment, weld lines, unfilled regions in the mould…) may occur and can affect the quality of the final product. Thus, the modelling and the numerical simulation of the foaming process are very important during the mould design process in order to define suitable injection points and air vents to avoid the potential defects.

Foaming processes are complex due to the transient free surface nature of the process and the strong nonlinear coupling of the material properties with the chemical reactions. Consequently, the production of polyurethane foams is still based on trial and error method.

In this study, the foam is considered as Newonian fluid. The flow equations, energy equation, polymerization and blowing (creation of CO2) reaction kinetics are coupled during mould filling. These equations are solved in 3D with a meshless finite pointset method using NOGRID-points software.

2. Physical model

2.1. Model of reactive foam expansion

Polyurethane is formed by reacting a polyol with a diisocyanate in the presence of suitable catalysts and additives. The two primary reactions are the curing reaction which leads to the formation of polyurethane and the expansion reaction producing polyurea and carbon dioxide [1]. The curing (Eq. 1) and the gas generation (Eq. 2) reactions are governed by chemical kinetics:

\[
\frac{d\alpha}{dt} = \frac{1}{\tau_\alpha} \alpha^{2-n_\alpha} (1 - \alpha)^{n_\alpha}
\]
\[
\frac{d\beta}{dt} = \frac{1}{\tau_\beta} \beta^{2-n_\beta} (1-\beta)^{n_\beta}
\]  

where \( \alpha \) is the chemical conversion rate of CO\(_2\) generation, \( \beta \) is the chemical conversion rate of the gelling reaction, \( \tau_\alpha \) and \( \tau_\beta \) are the characteristic time of the reactions, and \( n_\alpha \) and \( n_\beta \) are the exponents of the reaction.

### 2.2. Viscosity model

The foam is considered as a Newtonian fluid whose viscosity depends on the temperature \( (T) \), the chemical conversion rate of the gelling reaction \( (\beta) \) and the porosity of the foam:

\[
\eta(T,\phi,\beta) = \eta_0(T)f(\phi)g(\beta)
\]

where the function \( f \) and \( g \) may take different forms [1-2].

### 2.3. Flow governing equations

The general governing equations for compressible Newtonian fluid with Stokes’ hypothesis include the continuity equation, momentum equation, and the energy equation:

\[
\nabla \cdot \mathbf{v} = \phi \left[ \frac{1}{\alpha} \frac{d\alpha}{dt} - \frac{1}{p} \frac{dp}{dt} \right]
\]

\[
\frac{d(\rho \mathbf{v})}{dt} = -\nabla p + \nabla \cdot \mathbf{s} + \rho \mathbf{g}
\]

\[
(\rho C_p) \frac{dT}{dt} = \nabla \cdot (k \nabla T) + \nabla \cdot (\mathbf{s} \cdot \mathbf{v}) - (\nabla \cdot \mathbf{s}) \cdot \mathbf{v} + p \cdot (\nabla \cdot \mathbf{v}) + \Delta H_\alpha \frac{d\alpha}{dt} + \Delta H_\beta \frac{d\beta}{dt}
\]

where \( \mathbf{v} \) is the velocity field, \( p \) is the pressure, \( \mathbf{s} = \eta(T,\phi,\beta) \left[ (\nabla \mathbf{v}) + (\nabla \mathbf{v})^T \right] \) is the deviator stress tensor, \( \rho \) is the foam density, \( C_p \) is the foam thermal capacity, \( k \) is the foam thermal conductivity, \( \Delta H_\alpha \) is the enthalpy of the reaction of isocyanate with water, and \( \Delta H_\beta \) is the enthalpy of the gelling reaction.

### 3. Numerical implementation

We have implemented the above foaming model in the NoGrid-points software. We have to solve a set of differential equations defined by (Eqs 1-6) with appropriate boundary conditions. This system is strongly non-linear with highly coupled physical variables. Thus, a splitting technique is used to decrease the degree of complexity. At a time step, knowing \( \alpha, \beta \) and \( T \), the velocity and pressure fields are determined through a least-squares particle method; then the obtained velocity is used to compute temperature, gas expansion and gelling rates.

The pressure-velocity equations are solved by applying an implicit projection method, which is based on the least-squares particle method called finite pointset method (FPM) [3]. FPM is a meshfree and fully Lagrangian particle method. The fluid domain is represented by a finite number of particles and can be arbitrarily distributed. The list of neighbor points is determined for each point at each time
step in order to construct afterwards a proper interpolation function using a Moving Least Square (MLS) method. A smoothing length is attached to each particle and may be defined as a function of time and space. The particles move with fluid velocity and carry with them all fluid information like density, viscosity, velocity, temperature and so on.

4. Results

The mould filling of an automotive underlay carpet is simulated numerically. Unexpanded foam is injected in the mould cavity through an injection gate with a fixed mass flow of 320 g/s and a closing time of 3 s. It is assumed that the cavity has isothermal boundary \( T = 60^\circ C \) and the gravity is acting in negative z direction. The model parameters are determined by an inverse analysis method described in a previous work [2].

Figure 1 shows the flow front progress at four different times. In the beginning of mould filling unexpanded foam flows due to the gravity. After a while, the foam flows and expands to fill the cavity.

Figure 2 shows a comparison between short shot foams obtained experimentally and by our simulations for injection times of 0.8 s and 1.2 s. The front positions are almost similar indicating a very good agreement between the experimental and the calculated results.

Figure 1 – Flow front positions in the underlay carpet mould cavity.
Figure 2 – Comparison between experimental and numerical short shot foams for the automotive underlay carpet.

5. Conclusions

Polyurethane foaming process has been modelled by considering the expansion of a compressible quasi-homogeneous continuous mixture. The computational domain is described by the finite pointset method (FPM). A splitting technique is used to decouple the velocity-pressure computation from the temperature and the evolution equations. The validation of the developed model has been achieved through the comparison between experimental and numerical short shot foams results for the foaming process in an automotive underlay carpet.

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6. References