New Approaches to Accelerate Calculations and Improve Accuracy of Numerical Simulations in Liquid Composite Molding

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SUMMARY

Through-thickness flows occur typically in resin transfer molding in the case of thick parts of high fiber volume content containing multi-layer fibrous reinforcements or in thin parts when the mold is heated at a different temperature than the resin. In this latter case, viscosity changes through the thickness of the part. This results in irregular flows, usually faster in the skin when the mold is maintained at a higher temperature than the resin. Two new numerical approaches were devised to improve the accuracy of computer simulations of mold filling in Liquid Composite Molding (LCM). The motivation of this investigation is to avoid costly full 3D simulations and minimize the number of elements required to simulate mold filling. The first goal is achieved by using a mixed formulation based on a new prismatic non-conforming finite element. A mesh is extruded through the thickness of the composite in order to reflect accurately the detailed structure of the laminate and mold filling calculations are carried out on the extruded mesh. The second way to speed up calculations is to optimize the triangular in-plane mesh of the part. In order to evaluate the advantages of these new approaches in terms of accuracy and computer time, calculations performed with the new prismatic finite element are compared with finite element solutions obtained with 2D triangles and 3D tetrahedrons. The numerical performance of an optimized mesh is also assessed in terms of computer time and ability to conserve the resin mass during mold filling.

INTRODUCTION

Complex interactions caused by rheological, thermal, chemical and viscoelastic phenomena occur during composite processing. Several efforts have taken place to model these coupled phenomena. Different implementations using Taylor-Galerkin finite element (FE) formulation have been presented [1], but whenever the convective contribution to the total heat flux becomes important, temperature oscillations appear in the vicinity of the flow front.

An extension of these models using a stabilized Galerkin formulation coupled to a time Gear interpolation were shown to be unconditionally stable with no restriction on the time interval [2]. Unfortunately, for 3D simulations, much computer time is still required to solve these coupled systems. Extensive efforts through model simplification have consequently been made to decrease the computational time. Different approximations have been suggested typically based on mixed finite element and finite difference formulations [3, 4]. These methods are faster than a full 3D analysis, but neglect the through-thickness heat convection [3] and do not take into account the permeability and resin viscosity variations through the thickness of the part. Moreover, the finite difference formulation is not unconditionally stable and the grid usually needs to be refined as a function of Fourier's and Nusselt's numbers.

In order to solve the flow and heat problems in a novel way, a different way of combining finite elements (FE) and finite differences (FD) is proposed in this paper with different levels of coupling between the heat and flow equations. The fluid flow is solved with PAM-RTM [5]. Two numerical methods were implemented for the energy balance equation and resin cure. The first one is based on the new prismatic finite element, which approximates the heat exchange and resin cure in 3D parts. The second approach is a hybrid FE/FD formulation, in which the FE method is used to evaluate the in-plane heat exchange and the FD approximation solves the through-thickness heat flow.

The second way of speeding up calculations is based on constructing an optimum anisotropic mesh from the initial mesh of the mold cavity. On a fixed grid, the progression of the resin front is usually tracked by introducing a "level of resin saturation" inside each elementary volume of the mesh. The so-called "fill factor" [6] remains bounded between 0 and 1 (0 for an empty cell, and 1 for a fully saturated one). The new methodology is mainly based on the increase of the fill factor. The resulting mass accumulation in the "overfilled" elements is then redistributed to their immediate neighbors. This redistribution of resin results in newly filled elements without having to solve again the transport equations. However, resin redistribution on an isotropic mesh would very likely alter the real shape of the resin front, thus leading to inaccurate results. Therefore, in order to retain the maximum possible accuracy on the position of the flow front in time, the new proposed anisotropic refinement criterion will tend to stretch the mesh elements perpendicularly to the flow direction.

GOVERNING EQUATIONS

Based on volume averaging techniques, Darcy's law is often used to model the resin flow through porous media. It establishes a relationship between the average fluid velocity $\langle \vec{v}_r \rangle$ and the pressure gradient ∇P:

$$\langle \vec{v}_r \rangle = -\frac{[\mathbf{K}]}{\phi\, \mu_r} \langle \nabla P \rangle \tag{1}$$

where [**K**] is the permeability tensor, μ_r the resin viscosity and ϕ the porosity of the porous medium (fibrous reinforcement).

Assuming that the reinforcement is a not a deformable medium, the following equation of mass conservation may be considered:

$$div\left(\frac{[\mathbf{K}]}{\mu_r}\langle\nabla P\rangle\right) = 0 \tag{2}$$

Castro-Macosko [7] model is used to predict the viscosity variations due to resin conversion that may occur during impregnation.

To model heat transfer, the whole system including the mold, resin and fibrous reinforcement is considered. The "lumped" approximation assumes that the fibers and the surrounding fluid are at an averaged temperature. Following this approach any averaged physical property may be estimated by the rule of mixture, based on the mass fractions of the lumped components. In the case of dominant convection, the heat balance equation includes a source term *f(T)* arising from the heat generated by resin polymerization. Therefore it is written in the following form:

$$\frac{\partial T}{\partial t} + \bar{v} \cdot \nabla T = f(T) \tag{3}$$

At the flow front, a Dirichlet boundary condition may be imposed based on the temperature of the dry fibrous reinforcement or a flux boundary condition is derived by a backwind approximation to estimate the heat transferred by the incoming resin. At the interface between the mold and the fluid, a heat transfer condition is usually imposed.

Neglecting species diffusion, the mass balance can be expressed as:

$$\phi\frac{\partial \alpha}{\partial t} + \bar{v} \cdot \nabla \alpha = \phi\,\dot{H} \tag{4}$$

where $\dot{H}$ is the rate of heat generated by resin polymerization. Reaction kinetics is usually described by Kamal-Sorour [8] model.

FINITE ELEMENT / FINITE DIFFERENCE FORMULATION

To solve the flow and heat problems, a new approach is proposed by combining finite elements (FE) and finite differences (FD) with different levels of coupling between the heat and flow equations. The fluid flow is solved with PAM-RTM [5]. Two numerical methods were implemented for the energy balance equation and resin cure. The first one is based on a new prismatic finite element, which approximates the heat exchange and resin cure in 3D parts. The second approach is a hybrid FE/FD formulation, in which the FE method is used to evaluate the in-plane heat exchange in the part and the FD approximation solves the through-thickness heat flow.

The numerical solution is obtained by the standard Galerkin method as implemented by Bohr [2]. In order to avoid spurious oscillations, a Lesaint-Raviart formulation with discontinuous FE is used to solve the transport problem.

Using the Galerkin formulation, the weak form of equation (3) is expressed as:

$$\int_{\Omega} w\left(\frac{\partial T}{\partial t}+\bar{v}\cdot\nabla T\right)d\Omega=\int_{\Omega} w\, f\, d\Omega+\int_{\Gamma_d}\left|T^{+}-T^{-}\right|(\hat{n}\cdot\bar{v})\,d\Gamma_d \tag{5}$$

for any test function w belonging to the space $F(\Omega)$, where T^{+} and T^{-} are the temperature values on the two sides of the boundary Γ_d. The finite element solution of equation (5) is obtained by an iterative process. Beginning with the elements adjacent to the injection gate, the temperature field is calculated explicitly by an upwind scheme. The heat convection is finally solved using a Gear implicit scheme for the time derivative formulated as:

$$\int_{\Omega} w\left(\frac{1.5T^{n}-2T^{n-1}+0.5T^{n-2}}{\Delta t}+\bar{v}\cdot\nabla T^{n}\right)d\Omega=\int_{\Omega} w\, f\, d\Omega+\int_{\Gamma_d}\left|T^{n^{+}}-T^{n^{-}}\right|(\hat{n}\cdot\bar{v})\,d\Gamma_d \tag{6}$$

where indices *n*, *n*-1 and *n*-2 account for the current and previous time steps respectively.

To evaluate the temperature field, a classical predictor-corrector method is used. The temperature is predicted by the diffusion equation and corrected by the convection solution. The iterative procedure consists of advancing half a time step in conduction and the other half in convection. Conforming shape functions are used in order to insure temperature continuity at the finite element nodes. Similarly, a 4th order Runge-Kutta method is used to predict the evolution of the polymerization reaction. The degree of cure obtained is transported on the geometrical domain by a Lesaint-Raviart integral formulation like temperature in equation (6).

The crossing time F_t at each mesh node was obtained from a first filling simulation on a coarse mesh from which the anisotropic remeshing algorithm can be initiated. Mesh anisotropy is achieved by constructing the anisotropic size map that will indicate how stretched the elements will be [9]. At any point X in a triangulated domain Ω, a metric tensor M is known and is represented by a d x d positive symmetric matrix (d = dimension of Ω). In 2D this matrix can be written as:

$$M(X)=\begin{bmatrix} a(X) & b(X) \\ b(X) & c(X)\end{bmatrix} \tag{7}$$

with $a(X)>0$, $c(X)>0$ and $a(X)c(X)-b(X)^2>0$. The distance between two points A and B belonging to the geometric domain Ω is redefined as:

$$dist(AB)=\int_0^1\sqrt{\left(\frac{\partial s(t)}{\partial t}\right)\cdot M(s(t))\cdot\left(\frac{\partial s(t)}{\partial t}\right)}\cdot dt \tag{8}$$

where $s(t)$ is a parametric representation of the path connecting A and B.

The gradient of the scalar variable F_t provides information about the flow direction and can be used as the reference variable for remeshing. Using linear functions to interpolate F_t, constant gradients are obtained inside each triangle of the mesh.

A local averaging is performed to derive the values G of the gradient at the element nodes. Using these values, equation (9) can be integrated over the total filling time in order to define a particle trajectory starting from any vector position X on a node of the mesh

$$\frac{dX}{dt} = \frac{G}{\|G\|} \tag{9}$$

Results and conclusion

The extrusion of the shell mesh of Fig. 1 into layers with different material properties led to 60,000 prismatic elements and 40,000 nodes. For a comparable accuracy to 3D simulations, a typical filling calculation based on this new approach required only 45 mn to run on an IBM IntelliStation M-Pro PC with a Pentium III (1.0 GHz) processor.

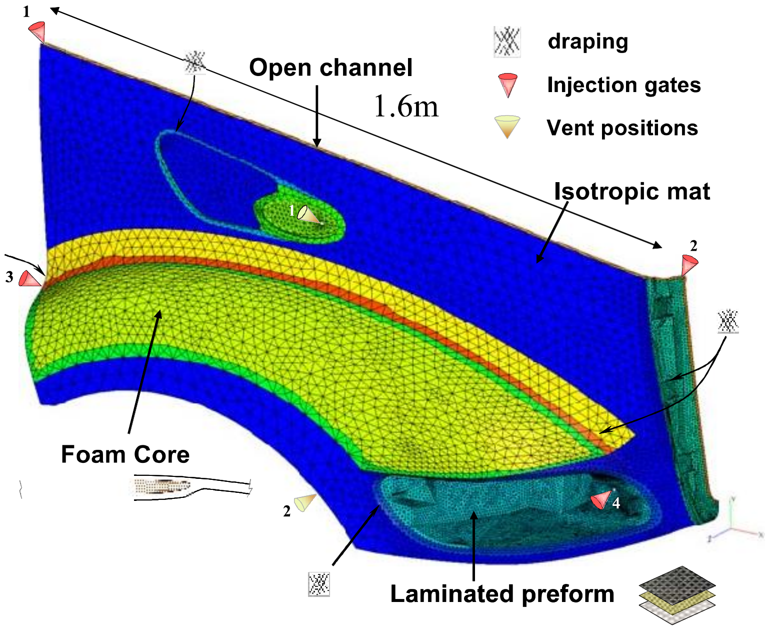

Fig.1 Mesh of an automotive fender

All possible coupling combinations have been tested for the automotive hood of Fig. 2. An example of mold filling simulation is shown in Fig. 3 (top), in which each colour corresponds to a different crossing time of the resin in the mold cavity. The degree of cure has also been predicted as shown in Figure 3 (bottom) at the end of the filling process. Figure 4 compares the performance of each type of coupling. For a comparable accuracy the time required to run a full 3D finite element analysis using tetrahedrons decreased from about 44h to 1h 40mn with the new prismatic element and 25mn for the hybrid formulation. The two new numerical schemes are stable, accurate and provide a solution at a relatively low computer cost.

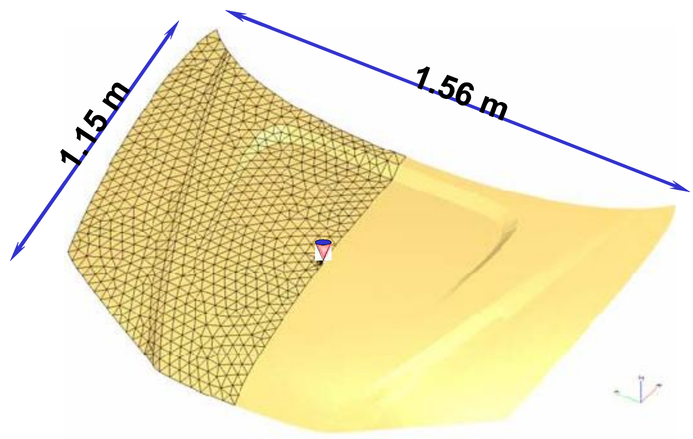

Fig. 2 Mesh of an automotive hood

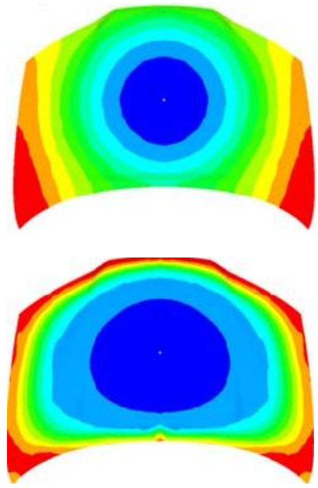

Fig. 3 Views of the hood showing mold filling in time (top) and degree of cure at the end of filling (bottom)

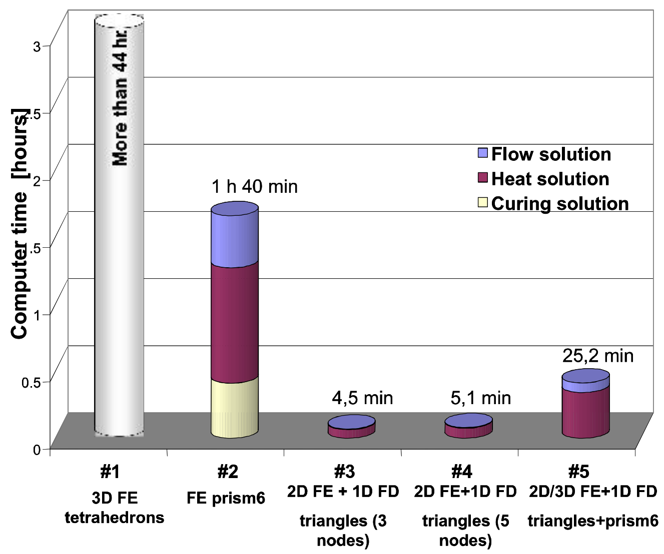

Figure 4 Comparison of computer times required for each model

A simple squared part is used as a test case to demonstrate the remeshing approach. As shown in Fig. 5, the part consists of 3 different zones. Zone 2 has a permeability two orders of magnitude higher that the two remaining ones. A filling simulation is performed by injecting at the left bottom corner of the squared part using the isotropic mesh (1000 triangles) shown in Fig. 6. The simulation took 46 seconds on an IBM 2.8 GHz Z Pro Intellistation with no overfilling of the elements during resin progression. The gradient of the resulting filling times was used to produce the anisotropic mesh (2000) elements shown on Fig. 2. The same filling simulation is again performed on the new mesh.

The total computational time including remeshing was 26 seconds on the same computer. It can be seen that the front progression is conserved and even smoother compared to the isotropic mesh.

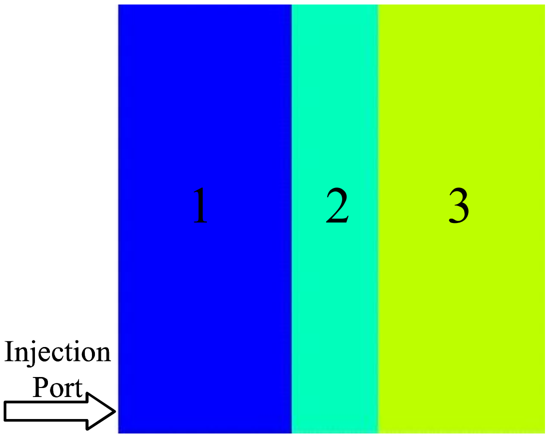

Fig. 5 Base case for the remeshing approach

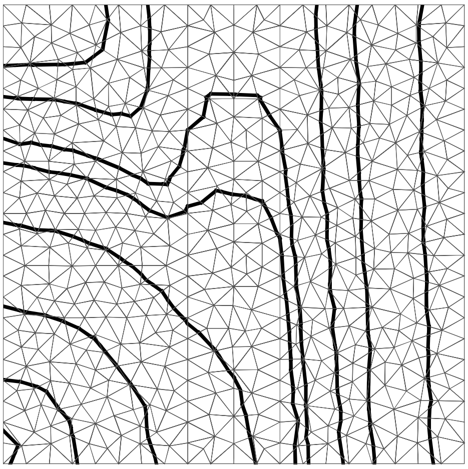

Fig.5 Resin front on isotropic mesh (No overfill)

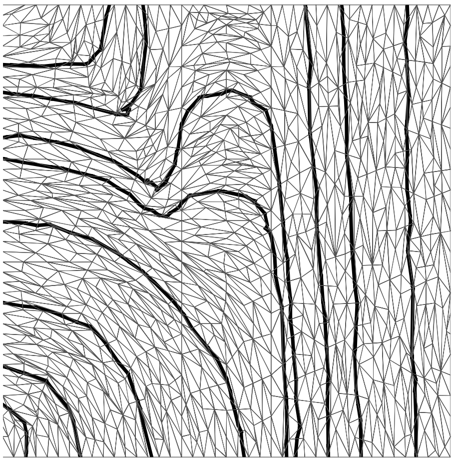

Fig. 6 Resin Front on Anisotropic mesh (Overfill factor of 2)

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