A NUMERICAL METHODOLOGY FOR PERMEABILITY DETERMINATION OF REINFORCEMENTS FOR POLYMERIC COMPOSITES

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Abstract. *This work focus on developing a numerical methodology for the determination of permeability of RTM reinforcements. The method allows the calculation of the three permeability components (K_{xx}, K_{yy} and K_{zz}) from a set of time dependent flow front coordinates data; one coordinate for each permeability component. An initial guess is set for the permeabilities and the difference between numerical and experimental values of flow front position at a specific time is minimized with the solution of an algebraic system of equations. Newton-Raphson method was used to solve the non-linear system of equations. The results presented in this paper were obtained for a rectilinear (1D) and a radial 2D problem, both with analytical solutions for the flow front position as a function of time. For the 1D comparison between the numerically calculated K_{xx} and the analytical value agreed within 1.7% and, for the 2D radial problem, numerical and analytical values of K_{xx} and K_{yy} agreed within 1.3%.*

Keywords: *RTM, permeability, Numerical modeling*

1. INTRODUCTION

Resin Transfer Molding (RTM) is a process that comprises the infusion of resin into a closed mold filled with a porous fibrous reinforcement. RTM is widely used in the production of polymeric composites with a variety of geometries and sizes. Polymer composites have reached a very important level of usage in the current context of engineering materials in various industries such as maritime, aeronautical, automotive and energy (wind turbines) (Breard et al., 2005). The main production centers in Brazil are located in São Paulo-SP, Belo Horizonte-MG, Caxias do Sul-RS and Joinville-SC.

The numerical modeling plays an important role in the RTM study. With the numerical simulation of the RTM process, it is possible to determine the flow advance inside the mold cavity, the appearance of empty regions (actually air bubbles) and predict possible structural problems in the final produced part. It is also possible to determine the correct position for the inlet and outlet sections, thus making the infusion process faster and more efficient and thereby minimizing costs related to mold design and part manufacturing. However, to obtain realistic results with the numerical simulation, accurate information about the physical properties of the resin and the reinforcement are necessary.

Most of the numerical models use Darcy's Law to correlate resin velocity with pressure drop inside the mold. Thus it becomes necessary the prior knowledge of the permeability of the medium and the viscosity of the resin. In addition , depending on the model used, it is also necessary to inform other resin properties such as density and specific heat (models in which energy equation is included) and medium porosity.

The quality of the obtained results is closely associated with the precise measurement of all above discussed properties. According to Sharma and Siginer (2008), there is a large number of studies in the literature that discuss the experimental determination of RTM reinforcement permeability. Most of them concentrate on planar permeability (K_{xx} and K_{yy}) and only a few focus on determining the transverse permeability (K_{zz}). Due to this, in the present work, a numerical methodology to determine medium permeability in all three directions from experimental data is proposed. The methodology is generic proposed for *n* dimensions and validated for the 1D and 2D cases. The 3D case will be investigated in a future work. Medium porosity, resin viscosity and density and flow position as a function of time are obtained experimentally and used to feed a computational model that calculates the unknown permeabilities. The computational model consists of a CFD (Computational Fluid Dynamics) application to solve the RTM resin infiltration problem combined with Newton-Raphson method to solve a non-linear system of equations and to calculate the desired permeabilities.

2. PROBLEM DESCRIPTION

Consider the simplified two dimensional (2D) geometry presented in Fig. 1. In this example, resin is entering into the mold through a central injection nozzle of radius *r*. The grey area represents the mold area filled with resin at time *t*. Consider also two points at the flow front line of coordinates (x_1, y_1) and (x_2, y_2). Reinforcement porosity (ε), resin viscosity (μ) and resin density (ρ) are considered known and constants.

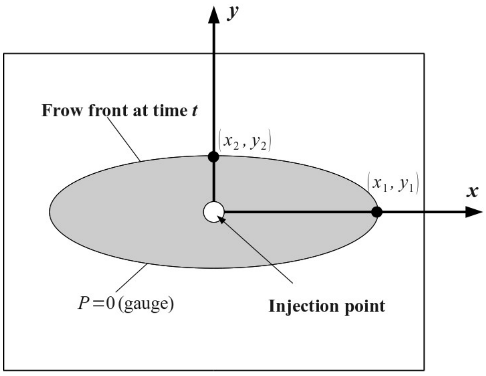

Fig. 1 - Schematic representation of the problem

Assuming that for time *t,* (x_1, y_1) and (x_2, y_2) were experimentally determined, and that $x_{1,n}$ and $y_{2,n}$ are the resin flow position calculated numerically, it is possible to write an equation for the residual such as

$$\begin{cases} f_1(K_{xx}, K_{yy}, t) = x_{1,n} - x_1 = 0 \\ f_2(K_{xx}, K_{yy}, t) = y_{2,n} - y_2 = 0 \end{cases} \tag{1}$$

In Eq. (1), K_{xx} and K_{yy} are the unknowns. Variables $x_{1,n}$ and $y_{2,n}$ can be numerically calculated with a Control Volume/Finite Element – CV/FE (Shojaei, 2006; Simacek and Advani, 2003) or the Volume of Fluid - VOF (Luoma and Voller, 2000; Yang et al., 2010) method. In this work, the VOF method was used within the OpenFOAM software to solve the problem.

Using the Newton-Raphson method (Kincaid and Cheney, 2001), the system given by Eq. (1) can be solved by

$$\vec{K}^{n+1} = \vec{K}^n - \frac{\vec{f}}{\bar{\bar{J}}} \tag{2}$$

where $\vec{K} = [K_{xx}, K_{yy}]^T$, $\vec{f} = [f_1, f_2]^T$, *n* the iteration and $\bar{\bar{J}}$ is the Jacobian matrix given by

$$\bar{\bar{J}} = \begin{bmatrix} \frac{\partial f_1}{\partial K_{xx}} & \frac{\partial f_1}{\partial K_{yy}} \\ \frac{\partial f_2}{\partial K_{xx}} & \frac{\partial f_2}{\partial K_{yy}} \end{bmatrix} \tag{3}$$

In Eq. (3), each derivative of the Jacobin matrix is numerically approximated by

$$\frac{\partial f_i(K_{ii})}{\partial K_{ii}} = \frac{f_i(K_{ii}+h) - f_i(K_{ii})}{h} \tag{4}$$

Solution of Eq. (2) results in the direct determination of the permeability components K_{xx} and K_{yy}.

The solution procedure has been presented for a 2D case, however it is easily extended to the 3D case. Actually, Eq. (2) has the same form regardless of the number of dimensions.

3. RECTILINEAR SOLUTION

The proposed methodology is first evaluated for a simple rectilinear problem to which algebraic solution can be obtained. Figure 2 shows the computational domain, the boundary conditions and the variables used in the current solution. The flow front position as a function of time can be analytically determined by (Rudd et al., 1997)

$$x = \sqrt{\frac{2 K_{xx} P_0}{\mu \epsilon} t} \tag{5}$$

where P_0 is the injection pressure.

For the analytical solution, K_{xx} was set equal to 3 x 10^{-10} m² and the calculated x value for t = 80 s was 0.239 m.

A grid with 2700 elements was used to discretize the computational domain. This grid was chosen to guarantee that a relative error smaller than 1% is obtained between numerical and analytical solutions when the right value of K_{xx} is used.

$$\text{error} = 100 \frac{K_{analytical} - K_{numerical}}{K_{analytical}} \tag{6}$$

The numerical procedure consists in guessing an initial value for K_{xx} (1 x 10^{-10} m²), using Eq. (1) (in this case the system has only one equation) to calculate K_{xx}.

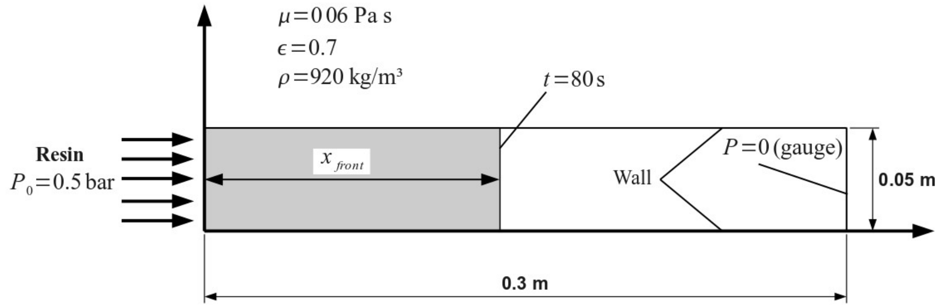

Fig. 2 - Computational domain for the rectilinear solution sumiu um "." de 0.06

Convergence history is shown in Tab. 1. It is recommended to have an initial guess of the same magnitude order of the real permeability, however this may not be a constraint to the proposed method. In this case, the initial guess is one third of the real K_{xx} value and a total of 13 iterations were necessary to reach a relative error of 0.01% between two successive K_{xx} values.

Table 1. Convergence for rectilinear problem

Iteration	K_{xx} (m²)	f(K_{xx})	Error (%)*
-	1.000 x 10^{-10}	0.1398540	-
1	1.991 x 10^{-10}	0.1966550	49.79
2	2.415 x 10^{-10}	0.2163499	17.53
3	2.858 x 10^{-10}	0.2351402	15.5
4	2.947 x 10^{-10}	0.2388119	3.02
5	2.986 x 10^{-10}	0.2403755	1.31
6	2.965 x 10^{-10}	0.2395431	-0.71
7	2.957 x 10^{-10}	0.2392256	-0.27
8	2.924 x 10^{-10}	0.2378732	-1.11
9	2.940 x 10^{-10}	0.2385506	0.54
10	2.954 x 10^{-10}	0.2391070	0.46
11	2.952 x 10^{-10}	0.2390474	-0.05
12	2.951 x 10^{-10}	0.2389880	-0.05
13	2.951 x 10^{-10}	0.2389960	0.01

* $\text{error} = \left(100\, K^{n+1} - K^{n}\right) / K^{n+1}$ where n is the iteration

The calculated K_{xx} value is 2.951 x 10^{-10} m² while the actual (analytically) value is 3 x 10^{-10} m². Thus, the final error in the K_{xx} calculation given by Eq. (1) is of 1.66%.

4. RADIAL SOLUTION

For the radial solution, assuming an orthotropic reinforcement medium, the unknowns of the problem are the permeabilities in the x and y directions. Here, the analytical solution for the 2D radial problem presented in Fig. 3 is used to test the proposed method in a 2D problem. Closed solution for 2D RTM problems are only available for isotropic media where $K_{xx} = K_{yy} = K$.

The radial flow front position, r, as a function of time for the condition shown in Fig. 3 can calculated by [Rudd et al., 1997]

$$t=\frac{\mu\epsilon}{2KP_0}\left[r^2\ln\left(\frac{r}{r_0}\right)-\frac{1}{2}\left(r^2-r_0^2\right)\right] \quad (7)$$

where r_0 is the injection radius.

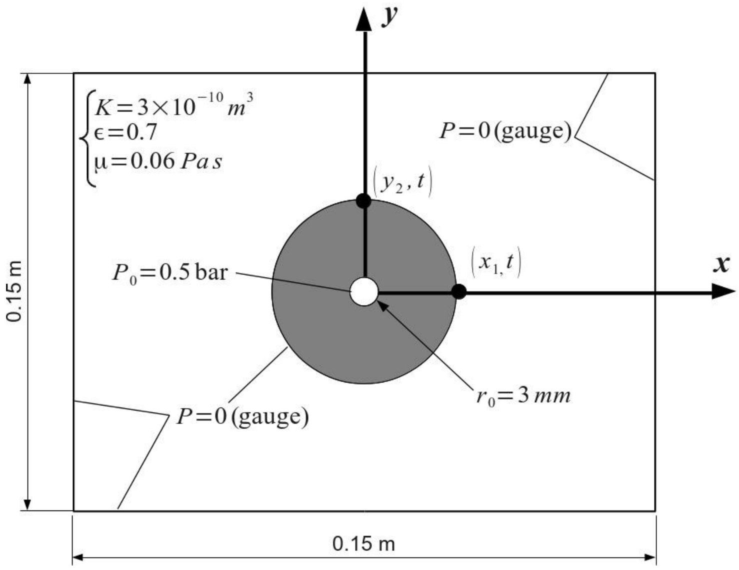

Fig. 3 - Computational domain for the radial 2D solution

Solving Eq. 7 for t = 1 s, the calculated flow front position is r = 0.0218561 m, thus in Fig. 3, $x_1 = y_2 = r$ = 0.0218561 m.

The problem unknowns for the radial solution are K_{xx} and K_{yy}. For this specific case, Eq. (1) can be rewritten as

$$\begin{cases} f_1=x_{1,n}(K_{xx},K_{yy},t)-0.0218561=0 \\ f_2=y_{2,n}(K_{xx},K_{yy},t)-0.0218561=0 \end{cases} \quad (8)$$

Equation 8, which is a system of equations, is solved with the Newton Raphson method as suggested in Eq. (2). This equation set resembles a simple system of two algebraic equations with two unknowns, however it is important to notice that the flow front positions $x_{1,n}$ and $x_{2,n}$ are calculated with OpenFOAM by solving a multiphase (resin + air) fluid flow problem. Variables $x_{1,n}$ and $x_{2,n}$ need to be evaluated several times for every Newton iteration and, for this reason, the overall solution time will be considerably large if refined grids were used.

Convergence is stable and a good approximation for the permeabilities can be achieved with just a few Newton iterations (Tab. 2). It is only necessary to pay attention to the numerical approximation of the derivatives in Eq. 3. In this particular solution, the unknowns are very small (order of 10^{-10}) and, for this reason, the parameter h used to evaluate the derivatives (Eq. 4) must be a few orders smaller than K. In the solution presented in Tab. 2, it was used h = 1×10^{-15}.

Table 2. Convergence for 2D radial problem.

Iteration	K_{xx} (m²)	K_{yy} (m²)	residue*
-	1×10^{-10}	2×10^{-9}	-
1	3.30971×10^{-10}	3.92567×10^{-10}	0.0500893
2	3.50948×10^{-10}	2.82613×10^{-10}	0.00237166
3	2.98005×10^{-10}	3.03908×10^{-10}	0.000194801
4	2.96617×10^{-10}	2.97611×10^{-10}	8.11255×10^{-6}
5	2.96357×10^{-10}	2.97500×10^{-10}	5.52149×10^{-7}

$*$ residue $=f_1(K_{xx},K_{yy},t)+f_2(K_{xx},K_{yy},t)$

For the ortrotopic case, where $K_{xx} \neq K_{yy}$, positions x_1 and y_2 (Fig. 3) can not be analytically determined and for this reason this case has not been tested yet. This will be done in a future work of the group, however it is expect that the proposed algorithm will show the same performance (fast solution with a stable convergence curve).

5. CONCLUSIONS

A simple numerical methodology has been proposed for the permeability determination of porous reinforcements used in the RTM process. The method combines a numerical simulation for resin infiltration inside the porous media with the solution of a non-linear system of algebraic equations created by minimizing the residue between the numerical and experimental results for the time dependent flow front position. The method was first tested using two simple problems with analytical solution: rectilinear and radial injection in an isotropic medium.

Results showed that with only one sample of experimental data for each unknown permeability is needed to solve the problem. Moreover, once the flow advance inside the mold cavity can be numerically predicted with all its complexity, there is no need to ensure that the flow reaches a specific behavior in order to perform the experiment, i.e., in a rectilinear 1D permeability experiment, for example, there is no need to guarantee that the flow front become a strait line moving as and solid object. A single sample with x and t at any position inside the mold is sufficient to calculate the permeability with the proposed methodology. Other characteristics like the injection pressure dependence with time can also be accounted within the numerical solution, simplifying the experimental runs and improving the quality of the results (i.e. the determination of the permeability value).

The next step will be to run the simulation for a 3D geometry and to determine all three permeability components based on experimental information of three coordinates of the domain (x_1, t), (y_2, t) and (z_3, t).

6. ACKNOWLEDGMENTS

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