

PREDICTION OF FILLING TIMES OF POROUS CAVITIES

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SUMMARY

A recently proposed implicit scheme for tracking the filling front during liquid impregnation into porous moulds is extended to provide 'one-shot' predictions for the time to completely fill the mould and the location of the last point to fill. With general boundary conditions applied at the filling gates, it is shown that the time to fill and the location of the last point to fill can be predicted on solving, at most, two linear systems of equations (of size determined by the spatial discretization). This result is confirmed by numerical filling experiments that show, for a variety of mould cavities, that 'one-shot' solutions agree exactly with filling time and location predictions obtained with multi-time-step simulations.

KEY WORDS: flow in porous media; free surfaces; RTM

INTRODUCTION

A problem of interest in flow in porous media is the tracking of the filling of an initially empty porous cavity with a liquid; see Figure 1. A major industrial application is in polymer moulding, in particular resin transfer moulding (RTM), which involves the injection of polymer into moulds which contain reinforced fibre mats. A number of numerical approaches have been developed for tracking the filling front during an RTM process.^{1–4} For example, the approach used by Brusckhe and Advani¹ is based on a dual finite element/control volume (FE/CV) approach. In a given time step, for fixed location of the filling front, the pressure field is solved using a Galerkin finite element method; subsequently this field is used to update the fill fractions, $0 \leq F \leq 1$, of control volumes and update the front movement. The updating of the filling front is an explicit operation and restriction of the time step is required. In essence, at any given point in the calculations, the time step used has to be chosen so that no more than one control volume in the domain completes filling. Despite the time step restriction, the FE/CV scheme is very robust, is mass-conserving and its performance can be improved with the use of innovative solution strategies.⁵

Recently Voller and Peng⁶ and Voller *et al.*⁷ have proposed a finite volume approach that shares many similarities with the FE/CV approach.¹ The key differences are that (i) a single system of non-linear equations is solved for both the pressure P and fill fraction F and (ii) an implicit updating of the filling front location is employed, a feature that removes any stability restriction on the time step. In the testing of the method, Voller *et al.*⁷ have demonstrated that for a given space grid, under the assumptions of (i) negligible gravity force (a reasonable assumption for RTM where typically imposed gate pressures are large) and (ii) constant filling conditions (in an RTM context, isothermal

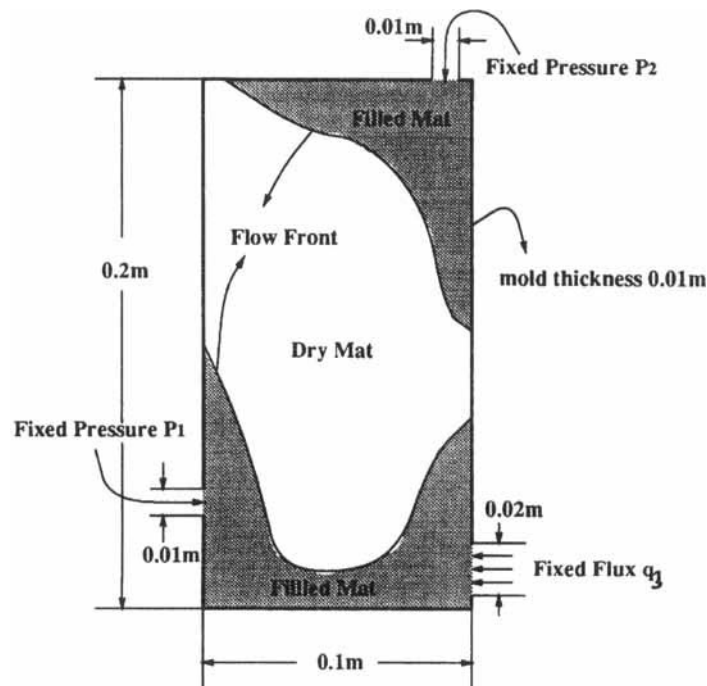


Figure 1. An RTM problem

filling with no curing), predictions of filling front location are independent of the choice of time step. That is, the front prediction at time t obtained with one large time step $\Delta t_{\text{large}} = t$ is, to within machine rounding, identical with the front position obtained using $n > 1$ time steps $\Delta t = t/n$.

In designing RTM processes, important pieces of information are the time required to fill the mould and the location of the last point to fill. Indeed, transient simulations of filling are often directed at obtaining predictions for these parameters. The objective of this paper is to utilize the independence of time step in the implicit filling scheme and develop a 'one-shot' prediction for the filling time and location.

In order to provide a complete and consistent presentation, the next section outlines the basic filling algorithm previously presented by Voller and co-workers (see References 6 and 7 for full details) and presents validation for the approach. This is followed by the presentation of a theoretical analysis that confirms the independence of time steps and the presentation and demonstration of a 'one-shot' filling prediction algorithm, which is seen as the major contribution of this work.

THE FILLING ALGORITHM

The problem

The test problem consists of a mould, containing a porous material, with impermeable walls. At time $t < 0$ the mould is empty of liquid. At time $t = 0$ flow enters the mould across a number of gates; see Figure 1. The objective of the analysis is to determine how long the mould takes to fill and the location of the last point to fill. The following key assumptions are made in this analysis.

1. The liquid is Newtonian and incompressible.
2. Darcy's law holds

3. The macroscopic front between the entering liquid and escaping gas is sharp, i.e. the saturated/unsaturated fringe is small.
4. Liquid and mould properties remain constant during filling (isothermal filling).
5. The pressure values required for filling are much larger than hydrostatic pressures and gravity terms can be neglected.

Additional assumptions to make the exposition of the approach clearer are as follows.

1. The domain is two-dimensional.
2. The porous material is isotropic.

It is stressed, however, that the development of the 'one-shot' filling approach does not depend on these two assumptions holding.

The governing equation

The domain in Figure 1 is covered by a grid of linear triangular finite elements (higher-order elements could also be used) defined by node points at their vertices. On this grid a mesh of control volumes is created by joining the midpoints of elements to the midpoints of elements sides. In this way each node point in the domain is associated with a control volume over which appropriate balances can be carried out; see Figure 2.

During the filling of the domain the balance of the liquid phase over a given control volume can be written as⁶

$$\epsilon A \frac{\partial F}{\partial t} + \epsilon \int_S \phi \mathbf{u} \cdot \mathbf{n} \, dS = 0, \tag{1}$$

where A is the area of the control volume, S is the surface of the volume, \mathbf{n} is the outward unit normal on S , \mathbf{u} (m s^{-1}) is the velocity of the liquid phase, ϕ is a microscopic phase marker (unity in a liquid-filled pore, zero in an empty pore), ϵ is the porosity and F is the macroscopic fraction of liquid in the control volume, defined as

$$F = \frac{1}{A_{\text{por}}} \int_{A_{\text{por}}} \phi \, dA, \tag{2}$$

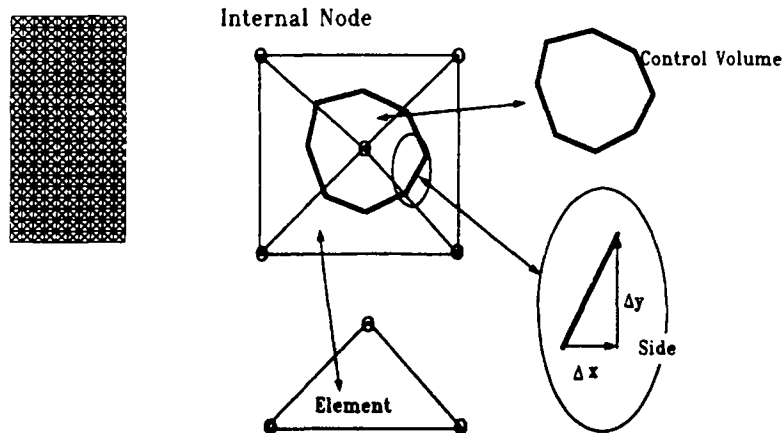


Figure 2. Components of finite element/control volume discretization

with A_{por} the area of the pores in the control volume. By Darcy's law the specific discharge ($\text{m}^3 \text{m}^{-2} \text{s}^{-1}$) is

$$q = \epsilon \mathbf{u} = -\frac{k}{\mu} \nabla P, \quad (3)$$

where k is the permeability, μ is the viscosity and P is the pressure. Substitution of the specific discharge into (1) results in the conserved governing equation

$$\epsilon A \frac{\partial F}{\partial t} = \int_S \phi \frac{k}{\mu} \nabla P \cdot \mathbf{n} dS, \quad (4)$$

with boundary conditions of prescribed liquid flux q on S_q ,

$$q = -\frac{k}{\mu} \nabla P \cdot \mathbf{n} \quad (5)$$

(note that $q = 0$ on the impermeable walls of the mould), and prescribed pressure ($P(x, y)$) on S_p , where $S = S_p + S_q$.

The numerical algorithm

On using a fully implicit time integration, the flow balance, represented by (4), on the control volume centred on node I becomes

$$\epsilon A_I F_I = \epsilon A_I F_I^{\text{old}} + \Delta t \sum_{j=1}^m \phi_j \left(\frac{k}{\mu} \frac{\partial P}{\partial x} \Delta y_j - \frac{k}{\mu} \frac{\partial P}{\partial y} \Delta x_j \right), \quad (6)$$

where Δt is the time step, the superscript 'old' refers to old time step values, the summation is over the control volume boundaries and Δx_j and Δy_j are the length components (measured in a counterclockwise sense around node I) along the j th boundary. Evaluations are made at the midpoints of the control volume boundaries and a fully discrete equation relating the nodal unknowns at node I to neighbouring nodal values is obtained on expanding in terms of the element shape functions. A considerable simplification can be obtained on noting that in the unfilled portions of the mould the pressure gradients are essentially zero. As such, the microscopic phase marker and pressure gradients in (6) are simultaneously zero and the phase marker can be dropped from the equation to arrive at

$$\epsilon A_I F_I = \epsilon A_I F_I^{\text{old}} + \Delta t \sum_{j=1}^m \left(\frac{k}{\mu} \frac{\partial P}{\partial x} \Delta y_j - \frac{k}{\mu} \frac{\partial P}{\partial y} \Delta x_j \right). \quad (7)$$

Subsequent use of the element shape functions to approximate the pressure gradients results in a set of non-linear equations in the nodal pressure and fill fraction fields characterized by the point equation

$$a_I P_I^{m+1} = \sum a_{nb} P_{nb}^{m+1} + \frac{1}{\Delta t} (F_I^{\text{old}} - F_I^m) + B_I, \quad (8)$$

where the a s are coefficients, the subscript nb refers to nodes that neighbour node I , the superscript m is an iteration counter and the term B_I includes contributions from the domain boundaries. Note that, owing to the incompressibility of the filling liquid and the underlying balance stated in (1), solutions of (8) will satisfy mass conservation.

Solution of the non-linear system defined by (8) hinges on noting that, assuming atmospheric conditions in the gas phase, the nodal pressure in empty and partially filled cells is $P_I = 0$. Iterative solution is then achieved as follows.

1. In a given time step and iteration at each node where $F_I^m < 1$, the nodal coefficient a_I is set to a large value (10^{16} is currently used).
2. Then, on solving (8) (currently an unstructured point iteration solver is used), a value of $P_I = 0$ is returned for nodal pressure in all the empty and partially filled cells. Furthermore, if the partially filled cells were correctly identified in step 1, the nodal pressures in all the filled cells will be consistent with the discrete balance represented in (7).
3. To account for the fact that the current iterative nodal fill fraction may be incorrect, after calculation of the nodal pressure field the fill fractions in filling cells are updated by⁶

$$F_I^{m+1} = F_I^{\text{old}} + \Delta t \sum a_{nb} P_{nb}. \quad (9)$$

This update is a reordering of the balance equation (8), applying the condition that the nodal pressure $P_I = 0$ in a filling cell, a condition imposed by the enhancement of the appropriate coefficient in step 1. For computational convenience the update in (9) is applied at every node with the under/overshoot correction

$$F_I = \text{MAX}[0, \text{MIN}(1, F_I)] \quad (10)$$

to account for fully filled/fully empty control volumes or control volumes that complete filling in the given time step.

4. The iteration in steps 2 and 3 continues until the changes in the sum of the nodal fill fractions between interactions falls below a given small value (10^{-3} in the current work).
5. On convergence in a time step the position of the filling front is obtained by interpolating the fill fraction field for the contour corresponding to $F = 0.5$.

Validation

The above algorithm has been extensively validated by Voller and co-workers^{6,7} on both one- and two-dimensional problems. In this paper a single validation is presented. Consider the case of filling an initially empty, one-dimensional, porous, horizontal tube under a constant applied pressure P_0 at $x = 0$. In this case the boundary position $X(t)$ at any point in time is given by the analytical solution

$$X(t) = \sqrt{(2P^*t)}, \quad (11)$$

where $P^* = kP_0/\mu\epsilon$. Following Voller *et al.*,⁷ this problem is solved numerically with $P^* = 5 \times 10^5 \text{ m}^2 \text{ s}^{-1}$. The front position predictions on a mesh of size $\Delta x = 0.1$ are compared with the analytical solution in Figure 3. The predictions are highly accurate, matching the level of accuracy that has also been achieved in two-dimensional problems.^{6,7} Note the following.

1. In the results in Figure 3 a number of time steps have been used, i.e. $\Delta t = 2, 4$ and 8 s. As noted in the Introduction, it is observed that the accuracy of the front prediction is not affected by the choice of time step, a result that has been shown to hold in two-dimensional problems involving filling fronts with high degrees of morphology.^{6,7} This observation, with supporting analysis, is the underpinning for obtaining 'one-shot' solutions of the filling time and location of fill.
2. Another feature of the implicit filling scheme is its conserved nature. In problems based on well-constructed grids, mass imbalances are negligible (on the order of $10^{-6}\%$).

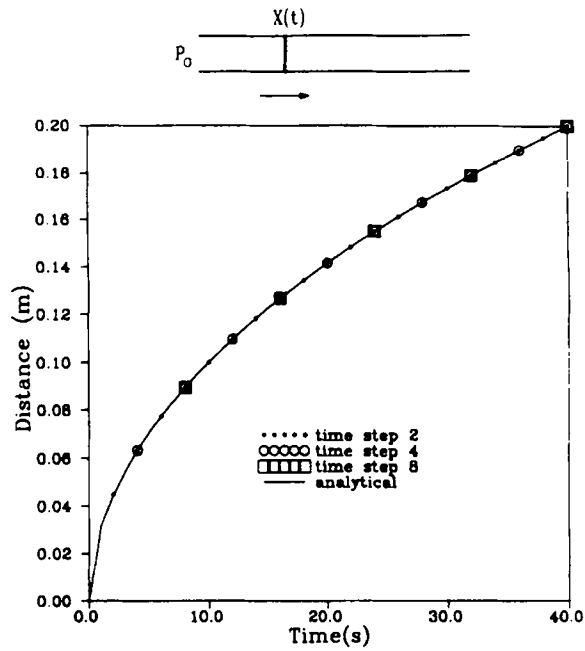


Figure 3. Movement of filling front in a porous, one-dimensional tube filled with a constant pressure gate

ANALYSIS

Before a method to predict the filling time and location of the last point to fill is presented, it is necessary to theoretically confirm that predictions obtained with the implicit filling algorithm are independent of the choice of time step. This is achieved by showing that the filling front position at time t predicted with a multi-time-step simulation $\Delta t = t/n$ ($n > 1$) is identical with the front position predicted with a single time step $\Delta t_{\text{large}} = t$. This essentially requires for a given time step an existence and uniqueness argument for the non-linear system defined by (8).

The matrix form

A filling simulation based on the implicit algorithm outlined above involves at each time step the solution of the system

$$\mathbf{A}\mathbf{P}^j = \frac{1}{\Delta t_j}(\mathbf{F}^{j-1} - \mathbf{F}^j) + \mathbf{B}, \quad (12)$$

where, with reference to (8), \mathbf{A} is the matrix of coefficients, \mathbf{P} is the vector of nodal pressures, \mathbf{F} is the vector of nodal fill fractions, the vector \mathbf{B} includes contributions from the fixed pressure and fixed flux boundaries and $j = 1, \dots, n$ is the time step number ($j = 0$ corresponds to the initial condition). With known fill field \mathbf{F}^{j-1} a valid filling solution requires nodal fields \mathbf{P} and \mathbf{F}^j that satisfy (12) subject to the conditions

$$\begin{aligned} P_I &\geq 0 \quad \forall \text{ nodes } I, \\ P_I &= 0 \quad \text{at every node where } F_I^j < 1, \\ 0 &\leq F_I^j \leq 1 \quad \forall \text{ nodes } I. \end{aligned} \quad (13)$$

Since the matrix \mathbf{A} in (12) results from a conserved discretization of the Laplacian, it has two important properties.

1. It is positive definite.
2. in the context of the general linear equation $\mathbf{AP} = \mathbf{C}$,

$$\begin{aligned} \text{if } C_I \leq 0 \quad \forall I, \quad \text{then } P_I \leq 0 \quad \forall I, \\ \text{if } C_I \geq 0 \quad \forall I, \quad \text{then } P_I \geq 0 \quad \forall I. \end{aligned} \tag{14}$$

Note that in problems that only involve prescribed fluxes at the boundaries, the above properties can be retained by arbitrarily fixing a nodal value of P followed by, on solution, a rescaling with an additive constant if required.

Existence

Taking guidance from the explicit scheme,¹ one way of obtaining a valid solution of (12) is to enforce condition (13) based on the previous fill fraction field \mathbf{F}^{j-1} and solve using the smallest time step Δt^j that exactly fills at least one control volume in the domain. In this way a valid solution of (12) is always guaranteed. Further, choosing a single constant time step to be a common factor of the set of time steps Δt^j will also guarantee that control volumes never overflow and the existence of a solution to (12) at each step. After the multi-time-step simulation the contributions at each step can be combined into the single equation

$$\mathbf{AP} = -\frac{1}{t} \mathbf{F} + \mathbf{B}, \tag{15}$$

where $\mathbf{F} = \mathbf{F}^n$ and

$$\mathbf{P} = \frac{1}{n} \sum_{j=0}^n \mathbf{P}^j. \tag{16}$$

On noting that $\mathbf{F}^0 = 0$, equation (15) is recognized as the system that would be solved if a single time step $\Delta t_{\text{large}} = t$ had been chosen for the filling simulation. Further, the nodal fields \mathbf{P} and \mathbf{F} also satisfy the conditions given in (13). Hence, on combining the multi-step simulation results according to (16), a valid solution of the single-time-step simulation (15) can always be found. This solution will have the same fill fraction field as the multi-step simulation but a different pressure field; see equation (16).

Uniqueness

The result in the previous subsection shows that a valid filling solution for the single-time-step simulation can always be obtained on combining the solutions from the multi-step simulation. In order to completely show the equivalence between the multi-step and single-step predictions of filling, it is necessary to prove that the solution of (15) is unique, i.e. for a given value of t there is one and only one choice of nodal pressure field \mathbf{P} and one and only one choice of nodal fill fraction field \mathbf{F} that satisfy (15) subject to the conditions in (13).

As a first step towards showing uniqueness, it is noted that if the pressure field \mathbf{P} satisfies (15), it can be written as

$$\mathbf{P} = \alpha \mathbf{P}^F + \mathbf{P}^B, \tag{17}$$

where $\alpha = 1/t$,

$$\mathbf{A}\mathbf{P}^F = -\mathbf{F}, \tag{18}$$

with $P_I^F = 0$ at all fixed pressure gates, and

$$\mathbf{A}\mathbf{P}^B = \mathbf{B}. \tag{19}$$

Further, if filling is occurring, all entries in \mathbf{F} and \mathbf{B} are positive and the conditions on \mathbf{A} given in (14) imply that $P_I^F \geq 0$ and $P_I^B \leq 0$ for all nodes I in the domain.

Following a typical format for a uniqueness proof, the assertion is made that:

for a given value of α there exists at least two valid solutions of (15), the nodal fields $\mathbf{P}_1, \mathbf{F}_1$ and the nodal fields $\mathbf{P}_2, \mathbf{F}_2$.

Let $f_1(x, y)$ define the location of the filling front based on the field \mathbf{F}_1 and let $f_2(x, y)$ define the location of the filling front based on the field \mathbf{F}_2 ; see Figure 4. With reference to this figure, consider the regions marked Ω_1 and Ω_2 . The region Ω_1 comprises the parts of the domain located between fronts f_1 and f_2 with f_1 ahead of f_2 , while the region Ω_2 comprises the parts of the domain located between fronts f_2 and f_1 with f_2 ahead of f_1 . Then in Ω_1

$$[P_2]_I = 0 \quad \text{and} \quad [P_1]_I \geq 0 \quad \forall I \in \Omega_1 \tag{20}$$

and it follows from (17) that if both candidate solutions are valid, then

$$[P_1^F]_I \geq [P_2^F]_I \quad \forall \text{ nodes } I \in \Omega_1. \tag{21}$$

Using similar arguments, it can be shown that

$$[P_2^F]_I \geq [P_1^F]_I \quad \forall \text{ nodes } I \in \Omega_2. \tag{22}$$

Now consider the linear equation

$$\mathbf{A}(\mathbf{P}_1^F - \mathbf{P}_2^F) = \Delta\mathbf{F}, \tag{23}$$

where $\Delta\mathbf{F} = \mathbf{F}_2 - \mathbf{F}_1$. In Ω_1 the term $\Delta\mathbf{F} \leq 0$, in Ω_2 $\Delta\mathbf{F} \geq 0$ and in the remainder of the domain $\Delta\mathbf{F} = 0$. Coupled with the positive definite property of \mathbf{A} , this implies that

$$\begin{aligned} [P_1^F]_I < [P_2^F]_I \quad \text{at, at least, one node } I \in \Omega_1 \\ \text{or} \\ [P_1^F]_I > [P_2^F]_I \quad \text{at, at least, one node } I \in \Omega_2. \end{aligned} \tag{24}$$

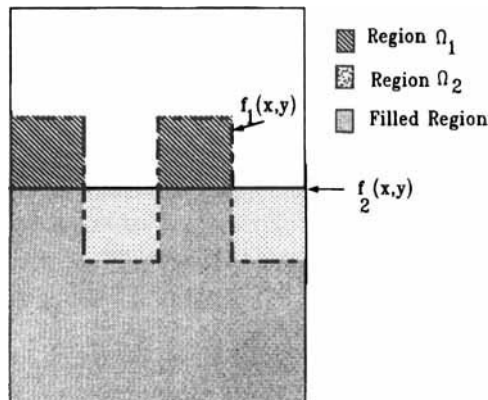


Figure 4. Assumption of two flow front predictions at time t

In any given case the condition in (24) will be in contradiction with the conditions in (21) or (22) and the assertion that two solutions of (15) are valid is not true. Hence, using the existence argument of the previous section, we have the following.

1. For a given value of α there is one and only one valid \mathbf{P} and \mathbf{F} field that satisfies (15).
2. The fill fraction field obtained with a multi-time-step simulation based on the implicit algorithm is identical with the fill fraction field obtained with a single-time-step solution, which is consistent with the results presented in Figure 3.

A 'ONE-SHOT' PREDICTION OF FILLING TIME AND LOCATION

The general case

Consider filling in the two-dimensional mould through three gates; see Figure 1. At gates 1 and 2 constant pressures P_1 and P_2 are applied and at gate 3 a constant flux $q_3 = 0.01 \text{ m}^3 \text{ m}^{-2} \text{ s}^{-1}$ is applied. Based on the proof of independence of time step presented above, the point of complete filling can be determined on solving

$$\mathbf{AP} = -\alpha \mathbf{1} + \mathbf{B}, \tag{25}$$

essentially equation (15) with \mathbf{F} set equal to $\mathbf{1}$. With reference to the condition in (13), a valid solution of the non-linear equation (25) involves finding the value of $\alpha (= 1/t_{\text{fill}})$ such that the resulting nodal pressure field $P_I \geq 0$ for all nodes I , with $P_I = 0$ at, at least, one node. An appropriate solution is

$$\mathbf{P} = \alpha \mathbf{P}^E + \mathbf{P}^B, \tag{26}$$

where the pressure fields \mathbf{P}^E and \mathbf{P}^B are obtained on solving the two linear system

$$\mathbf{AP}^E = -\mathbf{1}, \tag{27}$$

with $P_I^E = 0$ on all constant pressure gates, and

$$\mathbf{AP}^B = \mathbf{B}. \tag{28}$$

Note that by (14), at all nodes I in the domain, $P_I^E \leq 0$ and, assuming at least one fixed pressure node on the boundary, $P_I^B > 0$. In this way there exists one and only one value of α for which $P_I \geq 0$ for all nodes I , with $P_I = 0$ at, at least, one node. This value of α is the inverse of the filling time and the node (or nodes) where $P_I = 0$ is the last point to fill. Hence for a given spatial discretization (effectively the coefficient matrix \mathbf{A}) the time to fill a cavity and the last point(s) to fill in that cavity can be predicted in 'one shot' on solving the two linear equations (27) and (28). The appropriate value of α and the last point to fill are determined on setting $P_I = 0$ in (26) and defining a nodal α field to be

$$\alpha_I = -\frac{P_I^B}{P_I^E}. \tag{29}$$

Then, on defining $\min(\alpha_I)$ to be the minimum nodal α , the filling time $t_{\text{fill}} = 1/\min(\alpha_I)$ and the corresponding node is the last point to fill.

Fixed Flux Gates

In problems that only have fixed flux gates, the above procedure is modified. Since the volume of the mould is known, with a fixed flux condition the time to fill, $t_{\text{fill}} = 1/\alpha$, can be readily calculated. The location of the final filling point is found by arbitrarily setting a single nodal pressure to $P_i = 0$ and solving the now linear system given by (25). The last point to fill then corresponds to the node with the minimum pressure.

RESULTS

Figure 5 shows a multi-time-step simulation of the filling of the three-gated mould in Figure 1, using the conditions $P_1 = 200$ kPa, $P_2 = 300$ kPa, $q_3 = 0.01 \text{ m}^3 \text{ m}^{-2} \text{ s}^{-1}$, $\mu = 10 \text{ N s m}^{-2}$, $k = 2 \times 10^{-9} \text{ m}^2$ and $\epsilon = 0.6$, with, in a 0.01 m layer adjacent to the wall, a 10-fold enhancement of the permeability (simulating the effects of poor fitting of the mat to the mould)⁶. With these data the 'one-shot' predictions, using the grid shown in Figure 2, for the time to fill is $t_{\text{fill}} = 28.6$ s and for the node location of the last point to fill is $x_{\text{fill}} = 0.03$ m, $y_{\text{fill}} = 0.13$ m, values that agree exactly with the multi-time-step solution. Figure 6 shows the contours of the P field obtained on solving (26)–(28). On comparison with the multi-time-step solution the last point to fill can be clearly identified in this figure.

Figure 7 shows the multi-time-step filling predictions of a mould with a constant flux gate. The conditions are almost identical with those of the previous problem, but in this case the fixed pressure locations, gates 1 and 2, are shut off during the simulation and only the fixed flux gate, gate 3, is

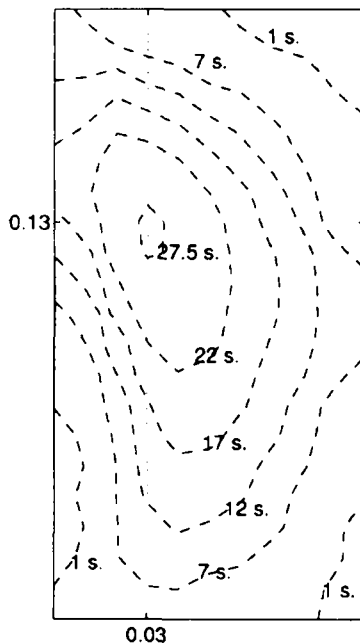


Figure 5. Filling of RTM cavity shown in Figure 1

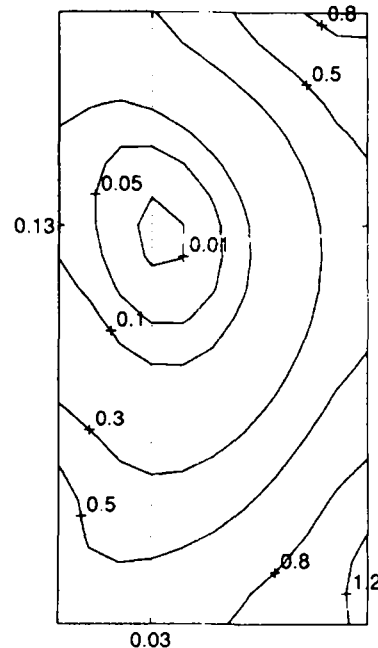


Figure 6. Pressure contours $P/3 \times 10^5$, P calculated with (26), for RTM cavity of Figure 5

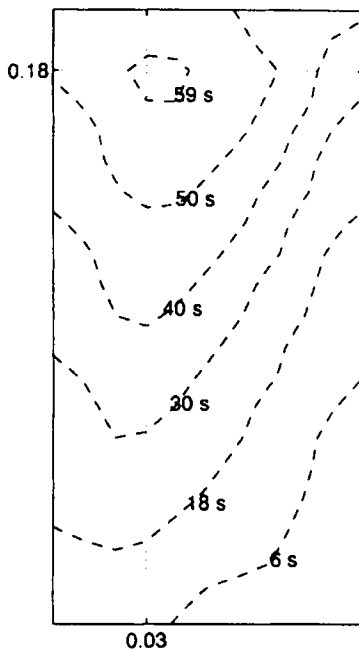


Figure 7. Filling of RTM cavity shown in Figure 1 with a fixed flux gate only

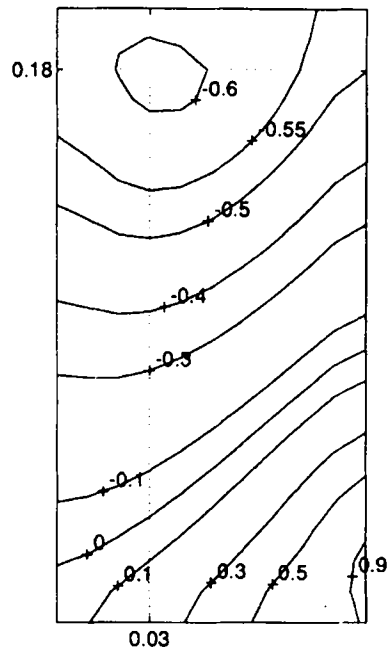


Figure 8. Pressure contours $P/3 \times 10^5$, P calculated with (26) for flux-filled RTM cavity of Figure 7

active. The value of $t_{\text{fill}} = 60$ s is readily obtained on dividing the mould volume by the gate area and prescribed flux. A plot of the P field obtained by solving (25) with the nodal pressure at $x = 0.045, y = 0.045$ set to zero is shown in Figure 8. The minimum value in the P field clearly corresponds to the last point to fill identified by the multi-time-step solution in Figure 7.

CONCLUSIONS

In polymer moulding, estimates of the last point to fill and the time taken to fill are important pieces of process information. The above algorithm provides a way, under the assumptions of constant conditions during filling, to predict the time to fill and the last point to fill on solving, at most, two linear sets of equations (with the size determined by the spatial discretization). This approach is seen as a significant advantage over the alternative of determining the filling pattern using a multi-time-step simulation, an approach that typically involves the solution of multiple non-linear systems of equations.

On reference to Figure 5 or 6 it is observed that the last point to fill is located in the interior of the mould. In the analysis we have assumed that the empty cavity is in vacuum or that the air, pushed by the incoming liquid, can easily escape through the mould boundaries. In reality the air could become trapped, the pressure build-up could prevent additional filling and a so-called dry spot could form. In polymer moulding operations the object of a filling simulation is to predict the possible location of dry spots so that vents can be located to allow the air to escape. Clearly the proposed algorithm is effective in determining the dry spots that occur at the end of filling. Dry spots, however, can also form during the early stages of the filling process, located at points not associated with the last point to fill. Further work is being directed at the 'one-shot' prediction of all possible sites for dry spots in complex RTM moulds.

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