Some Numerical Schemes for the Numerical Treatment of the Advection Equation in Liquid Composites Molding Processes

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SUMMARY: Liquid Composites Molding (LCM) processes simulation involves an efficient treatment of the advection equation governing the evolution of different process variables (volume of fluid, heat transfer, incubation time, etc). In a previous work [1], a second-order scheme with flux limiters has been developed for the integration of the advection equation, which governs the volume fraction evolution. Due to the fact that other properties, like the incubation time, are not defined in the empty part of the mold, some numerical difficulties are found during the process updating [2]. Then the scheme described in [1] must be modified to solve the extra difficulty introduced by the advection equation governing the evolution of the incubation time. This paper describes a new flux limiter technique, based on TVD schemes [3], for the calculation of the incubation time and the fluid fraction in mold filling simulation in thin cavities with replaced fiber mats using a fixed mesh.

KEYWORDS: Fixed Mesh Resolution, Incubation Time, RTM, Liquid Composite Molding, Advection Equation.

INTRODUCTION

In LCM (Liquid Composite Molding) processes several properties must be transported by the flow: curing reaction, temperature, incubation time, fluid fraction, etc. In this work different schemes for the numerical treatment of the advection equation that governs the evolution of a generic fluid property are proposed. The application of the integration of the fluid presence function and the incubation time is achieved by using a new flux limiter strategy that allows to obtain accurate results in bidimensional LCM simulations.

In order to analyze the accuracy of the different techniques proposed in this work, we consider the resolution of the advection equation that governs the evolution of a generic fluid property J :

$$\frac{dJ}{dt}=\frac{\partial J}{\partial t}+\underline{v}\cdot\nabla J=S \tag{1}$$

An appropriate technique for the discretization of eq.(1) consists in applying the Leisant-Raviart technique (discontinuous finite element method). We can write the conservative form of the eq.(1) as

$$\int_{\Omega^e}\left(\frac{\partial J}{\partial t}+Div\left(J\underline{v}\right)-J\ Div\ \underline{v}\right)d\Omega=\int_{\Omega^e}S\,d\Omega \tag{2}$$

where Ω^e represents an element of a finite element mesh of the fluid domain $\Omega_f(t)$. From eq.(2), using the divergence theorem and taking into account the fluid incompressibility, results

$$\int_{\Omega^e}\frac{\partial J}{\partial t}d\Omega+\int_{\partial\Omega^{e+}}J\underline{v}\underline{n}ds+\int_{\partial\Omega^{e-}}J\underline{v}\underline{n}ds=\int_{\Omega^e}Sd\Omega \tag{3}$$

where $\partial\Omega^{e+}$ denotes the outflow boundary and $\partial\Omega^{e-}$ the inflow boundary of the element Ω^e, respectively.

One of the main difficulties related to eq.(3) is that the function J associated to the fluid is not defined in the element boundaries along which are applied the boundary integrals. If we consider a constant value in the element, the discontinuous finite element method assumes that on the outflow boundary the function J is equal to the existing value inside the element Ω^e, i.e. $J(\underline{x}\in\partial\Omega^{e+})=J^e$ and that on the inflow boundary the function J is given by its value in the upstream element, i.e. $J(\underline{x}\in\partial\Omega^{e-})=J^{e-}$. Thus, eq.(3) can be rewritten in the equivalent form:

$$\frac{\partial J^e}{\partial t}\left|\Omega^e\right|=-J^e\int_{\partial\Omega^{e+}}\underline{v}\underline{n}ds-J^{e-}\int_{\partial\Omega^{e-}}\underline{v}\underline{n}ds+S^e\left|\Omega^e\right| \tag{4}$$

where $\left|\Omega^e\right|$ denotes the volume of Ω^e. Considering a first order explicit approximation of the time derivative, we can write (4) as

$$J_e^{n+1}=J_e^n-J_e^n\frac{\Omega^+}{\left|\Omega^e\right|}+J_{e-}^n\frac{\Omega^-}{\left|\Omega^e\right|}+S_e\Delta t \tag{5}$$

where we define the inflow and outflow fluid volumes as $\Omega^-=q^-\Delta t$ and $\Omega^+=q^+\Delta t$, being q^+ and q^- the outflow and inflow flow rates, respectively. In the above equation, the subscript for the property J, denotes the considered element and the superscript indicates the time step.

A FIRST ORDER TECHNIQUE FOR THE CALCULATION OF THE FLUID PRESENCE AND INCUBATION TIME

The evolution of the volume fraction, I, and the incubation time, E, are given as a general linear advection eq. (1) where for the volume fraction, $J=I$, $S=0$, and for the incubation time $J=E$ and $S=1$, with the initial conditions:

$$I\left(\underline{x},t=0\right)=\begin{cases}1 & \underline{x}\in\Omega_f\left(t\right)\\ 0 & \underline{x}\notin\Omega_f\left(t\right)\end{cases};\qquad E\left(\underline{x},t=0\right)=\begin{cases}0 & \underline{x}\in\Omega_f\left(t\right)\\ \text{Not defined} & \underline{x}\notin\Omega_f\left(t\right)\end{cases}$$

Then the discretization form of the governing equation of the fluid fraction, *I*, is defined from eq.(5) considering *J=I* and *S=0:*

$$I_e^{n+1} = I_e^n - I_e^n \frac{\Omega^+}{\left|\Omega^e\right|} + I_{e-}^n \frac{\Omega^-}{\left|\Omega^e\right|} \tag{6}$$

On the other hand, the incubation time is defined as the elapsed time since the resin components were mixed just before the injection. The value of the incubation time *E* is then set to zero in the injection nozzle and varies throughout the filled part of the mold, but it is not defined on the empty one. The discretization form of the equation governing the evolution of the incubation time is obtained from eq.(5) considering *J=E* and *S=1:*

$$E_e^{n+1} = E_e^n - E_e^n \frac{\Omega^+}{\left|\Omega^e\right|} + E_{e-}^n \frac{\Omega^-}{\left|\Omega^e\right|} + \Delta t \tag{7}$$

A first problem appears if we consider the time t for which an element Ω^e starts its filling process from its upstream element Ω^{e^-}. To illustrate this limitation we consider the situation where the outflow volume is null, $\Omega^+ = 0$, then eq.(7) establishes that solution at t_{n+1} is dominated by solution existing in the element in the previous instant, even when this element is empty and *E* is then not defined. In order to solve, properly, the eq.(7) we use the method described in [2], by multiplying eq.(7) by the fluid fraction *I* and eq.(6) by the field *E* and sum both resulting equations, it results in solving eq.(1) for *J=EI* and *S=I* whose discretised form is given by

$$\left(EI\right)_e^{n+1} = \left(EI\right)_e^n - \left(EI\right)_e^n \frac{\Omega^+}{\left|\Omega^e\right|} + \left(EI\right)_{e-}^n \frac{\Omega^-}{\left|\Omega^e\right|} + S_e \Delta t \tag{8}$$

where taking *S* as *I* evaluated in the time *n+1* then $S^e = I_e^{n+1}$ and yields

$$E_e^{n+1} = \frac{\left(EI\right)_e^n}{I_e^{n+1}} - \frac{\left(EI\right)_e^n}{I_e^{n+1}} \frac{\Omega^+}{\left|\Omega^e\right|} + \frac{\left(EI\right)_{e-}^n}{I_e^{n+1}} \frac{\Omega^-}{\left|\Omega^e\right|} + \Delta t \tag{9}$$

It is important to notice that in order to obtain E_e^{n+1} will be necessary the previous resolution of I_e^{n+1}. Moreover we assume that only exists inflow volume in a given element when the upstream element is completely filled i.e. $\Omega^- \neq 0$ only if si $I^{e^-} = 1$, and exists outflow volume from a given element when it is completely filled, that is $\Omega^+ \neq 0$ only if $I^e = 1$. This condition is included in the formulation by means the parameter δ defined by

$$\delta_e = \begin{cases} 1 & if \quad I_e = 1 \\ 0 & if \quad I_e < 1 \end{cases} \qquad and \qquad \delta_{e-} = \begin{cases} 1 & if \quad I_{e-} = 1 \\ 0 & if \quad I_{e-} < 1 \end{cases} \tag{10}$$

If we include this condition in eq.(5), the discretization of the advection equation for a general variable can be rewriten as

$$J_e^{n+1} = J_e^n - \delta_e^n J_e^n \frac{\Omega^+}{\left|\Omega^e\right|} + \delta_{e-}^n J_{e-}^n \frac{\Omega^-}{\left|\Omega^e\right|} + S_e^{n+1} \Delta t \tag{11}$$

A FLUX LIMITER TECHNIQUE FOR CALCULATION OF THE FLUID PRESENCE AND INCUBATION TIME

In order to extend the previously described first order schemes to second order with flux limiter ones for the resolution of the advection eq.(1), we change the notation and rewrite the eq.(11) as follows:

$$J_e^{n+1} = J_e^n - \frac{\Delta t}{A(e)} \underline{v}_e \sum_{j=1}^{3} l_{ej} \hat{\underline{f}}_{ej} \underline{n}_{ej} + \Delta t S_e^{n+1} \quad \text{with}$$
$$\hat{\underline{f}}_{ej} = \hat{\underline{f}}_{ej}^{UP} = \frac{1}{2}\left\{ \left(\delta_e J_e + \delta_j J_j\right) - \operatorname{sgn}\left(\underline{v}_e \cdot \underline{n}_{ej}\right)\left(\delta_j J_j + \delta_e J_e\right) \right\} \tag{12}$$

where $A(e)$ is the area of the element e, j represents a neighbour triangle element, $\underline{n}_{ej}$ is the outward unit vector on the common edge of the triangles e and j, l_{ej} is the length of that edge and the velocity vector of element e is $\underline{v}_e$, see Fig.1.

The extension of the above scheme to second order is described by eq.(12) replacing $\hat{\underline{f}}_{ej}$ by $\hat{\underline{f}}_{ej}^{SW}$ defined by:

$$\hat{\underline{f}}_{ej}^{SW} = \hat{\underline{f}}_{ej}^{UP} + \frac{1}{2}\chi\left(r_{ej}\right)\left(\operatorname{sgn}\left(\underline{v}_e \cdot \underline{n}_{ej}\right) - \frac{\Delta t}{d_{ej}} \underline{v}_{ej} \cdot \underline{n}_{ej} \right)\left(\delta_j J_j - \delta_e J_e\right) \tag{13}$$

where the average velocity between elements e and j is defined by v_{ej} and d_{ej} represents the distance between barycentres of the triangles e and j. The superscript UP denotes first order upwind scheme and SW second order with Sweby flux limiter (4). Note that we include again the use of the parameter δ defined by

$$\delta_k = \begin{cases} 1 & if \quad I_k = 1 \\ 0 & if \quad I_k < 1 \end{cases} \qquad \text{for} \qquad k = e, j \tag{14}$$

and r_{ej} is defined by

$$r_{ej} = \begin{cases} \min_{k \neq j, \cos\theta_{ek} < 0} \left\{ \dfrac{\delta_e J_e - \delta_k^e J_k^e}{\delta_j J_j - \delta_e J_e} \right\} & if \quad \cos\theta_{ej} > 0 \\ \min_{k \neq j, \cos\theta_{ek} < 0} \left\{ \dfrac{\delta_k^j J_k^j - \delta_j J_j}{\delta_j J_j - \delta_e J_e} \right\} & if \quad \cos\theta_{ej} < 0 \end{cases} \tag{15}$$

in which θ_{ej} (Fig.1) denotes the angle between $\underline{n}_{ej}$ and the velocity vector of element e, the definition of the Superbee flux limiter is then given by

$$\chi_{SB}(r) = \max\{\, 0, \min\{\, 2r, 1\}, \min\{\, r, 2 \,\}\} \tag{16}$$

For the integration of the fluid presence function I, we take $J=I$ and $S=0$ in eq.(12) and for the resolution of the incubation time, $J=EI$ and $S=I$. It is easy to note that if we take

$$\delta_k = 1 \qquad \text{if} \qquad I_k \leq 1 \qquad \text{for} \qquad k = e, j \tag{17}$$

the condition (17) means that neighbour elements can exchange fluid without complete its own filling previously.

NUMERICAL SIMULATIONS

In order to evaluate the accuracy of the different schemes described, we consider a saturated mold as depicted in Fig.2. In that case, the exact resolution of the pressure and velocity distribution are known and then they do not contribute to the numerical errors induced by the discretization of the advection equation. A comparison of the different fluid presence function integration schemes proposed is shown in Fig.3. It can be noticed that the use of the Superbee flux limiter allows to compute a more accurate solution in the neighbourhood of the discontinuity associated with the flow front. Moreover, as it was expected, the use of δ defined by eq.(14) instead of eq. (17) allows to avoid the diffusive flow front. Fig.4 shows the incubation time along a flow streamline in the elements comparing exact solution with the different ones given by eq.(12). Here once again the use of the Superbee flux limiter shows a more accurate solution. The convergence analysis shown in Fig.5 has been carried out for a complete mold filling. The error is defined by the L_2-norm at the solutions computed for different mesh sizes. The order of convergence is two times higher when the Superbee flux limiter is used instead of the first order upwinding scheme. Fig.6 depicts the incubation time distribution and the filling flow pattern of a U-Shaped mold of 500x260x10 *mm*. The constant flow rate is 4 cm^3/s. and the porosity is 0.5. It is interesting to note how the fluid located in the left upper part of the mold, even just closed to the injection nozzle, stops and gets 'older'.

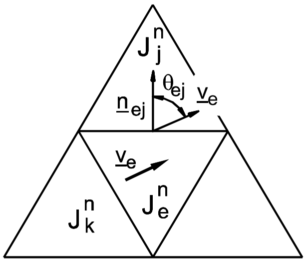

Fig.1. Discretization nomenclature

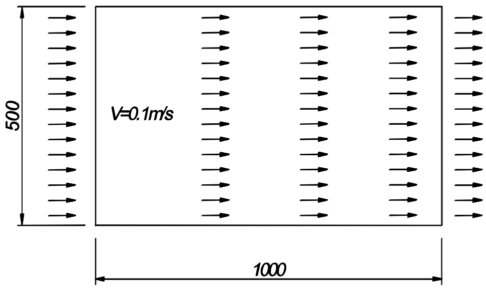

Fig.2. Saturated flow conditions

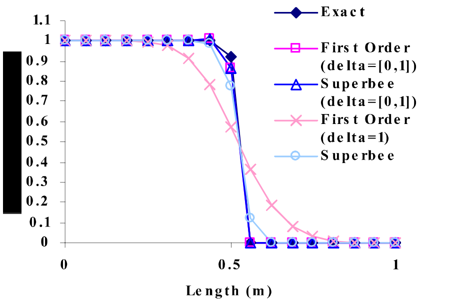

Fig.3. Schemes comparison used to compute *I*

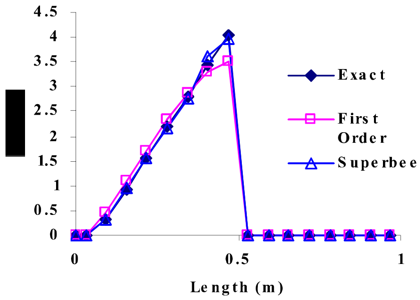

Fig.4. Schemes comparison used to compute *E*

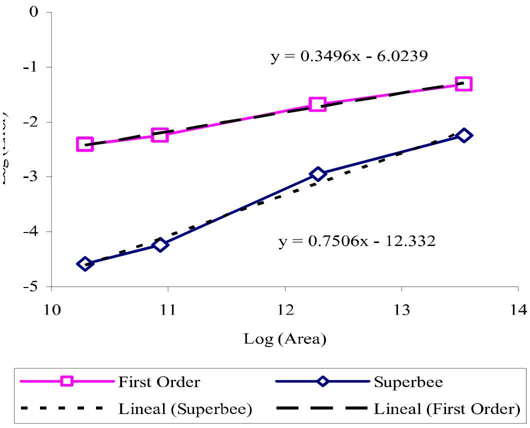

Fig.5. Convergence analysis

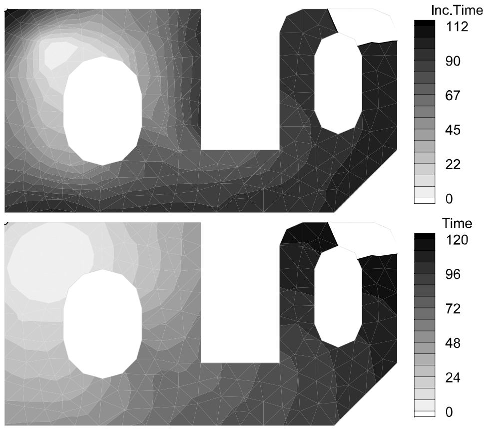

Fig.6. Incubation. time and flow pattern

CONCLUSIONS

A new approach to solve the advection equation of a general fluid variable using a second order flux limiter technique has been defined and tested. A fixed mesh numerical algorithm has been completed and improved for simulate both the bidimensional flow behavior and the incubation time in LCM process.

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