An Improved Method of Numerical Simulation of Resin Transfer Molding for Resin-Based Composite Materials Based on Unstructured Grid

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Abstract—The authors have a lot researches about numerical simulation of resin transfer molding for resin-based composite materials based on unstructured grid in the past. In these researches the authors found while the grid is orthogonal, the simulation is agreed with facts. But the grid is non-orthogonal, the energy equation has great error due to being simplified, and the results are wrong. The mesh distortion is larger, the deviations are bigger. Therefore, this paper conducted a study about the calculation methods of the energy equation, and validated through case reasonableness and accuracy of the calculation method. The results show the improvement is effective.

Keywords—numerical simulation; resin-based composite materials; unstructured grid; control volume / finite element method (CV/FEM)

I. INTRODUCTION

When simulating resin transfer molding of Resin-based composite materials using the control volume / finite element method (CV/FEM) in order to adapt to the different shape of parts, non-structured grids are often used, but calculated precision and grids has the very big relations due to diffusion of the energy equation. When the computational grid is the structured grid, the connection between the adjacent nodes and the common interface of control volume is orthogonal. So, the cross diffusion term of the energy equation is equal to zero. When grids are unstructured, the connection between the nodes and the boundary of the control volume is non-orthogonal, then cross diffusion is not zero, especially when the crossover is far from orthogonal, the cross diffusion has a great influence on the numerical results.

In most of the previous researches [1,2,3,4,5,6], the simulations were simplified by calculating the flow under the two-dimensional(2D) setting and assuming the heat diffusion to be only in the plane. Another previous researches [7,8,9]developed 2.5-dimentional (2.5D) non-isothermal models, which include the flow in plane and heat diffusion in the thickness for the thin parts based on the CV/FEM. In some other researches [10,11], the 3D simulation of filling was performed during the RTM using the CV/FEM based on regular structured mesh. There are also previous studies, say Refs. [12,13], focusing on applying the 3D Galerkin finite element methods to simulate the filling stage or the curing stage. Ref. [14] thinks that control volume method is no way to directly calculate the cross diffusion of common interface.

Therefore, the cross diffusion term is not directly calculated from the integral of the diffusion term on the common interface.

The author has done a lot of research on the numerical simulation of Resin-based composite materials [15-18]. In these studies, the numerical simulation can help the researches know and understand the RTM process. These studies contribute to find the relevant parameters affecting the process and optimize the way. In these researches, in order to improve the calculation accuracy, the structured hexahedral mesh was used and hence the flexibility of dealing with complicated shapes was not sufficient. Therefore.

II. CONTROL EQUATIONS

In this section, we present the basic control equations. For the non-isothermal RTM process under investigation, we make the following assumptions:

- (1) The resin is an uncompressed liquid and its viscosity is a function of the temperature and curing ratio.
- (2) The temperature of the resin and fiber is identical at each position.
- (3) There is no resin before the flow front and the control volume is fully saturated after the flow front.
- (4) There is a quasi-steady time window, in which the viscosity dissipation energy can be neglected.
- (5) Resin stops flow at the curing stage.

A. The Control Equation

1) The flow equation

At filling stage, Darcy's equation, which describes how the resin flows in the fiber, is still applicable. In the case, Darcy's law, which describes the flow within the mold, can be written as follows:

$$\vec{v} = -\frac{1}{\mu} [K] \nabla P \quad (1)$$

Where, $\vec{v}$ is the Darcy velocity vector, K is the permeability tensor, ∇P is pressure gradient, which is a

function of the resin temperature and degree of cure given below:

$$\mu(T, \alpha) = \mu_0 e^{\frac{E_\mu}{RT}} \left(\frac{\alpha_g}{\alpha_g - \alpha} \right)^{d_1 + d_2 \alpha}$$

Where, μ_0 is the initial degree of viscosity, E_μ is the activation energy of resin, α_g is the degree of cure of the resin gel point, d_1 and d_2 are two constants, R is the gas constant, and T and α are the temperature and the degree of cure, respectively.

Based on the quasi-steady state assumption, the mass balance equation at each node is given by:

$$\phi \frac{\partial \rho}{\partial t} = -\nabla \cdot \vec{v} \quad (2)$$

Where, ρ is the mass density, t is time.

The possible boundary conditions are:

- (a) $p = p_0$ for constant pressure injection or $u = u_0$ for constant velocity injection at the inlet;
- (b) $p = 0$ at the flow front;
- (c) $\partial p / \partial n = 0$ at the mold wall

2) The energy equation

At the same time, it is supposed that the heat convection of the resin and fiber occurs and the temperature is equal at resin and fiber everywhere. So the energy equation is written as :

$$\begin{aligned} & \left[\phi \rho_r c_{pr} + (1 - \phi) \rho_f c_{pf} \right] \frac{\partial T}{\partial t} + \rho_r c_{pr} \left(u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} + w \frac{\partial T}{\partial z} \right) \\ & = k_{lx} \frac{\partial^2 T}{\partial x^2} + k_{ly} \frac{\partial^2 T}{\partial y^2} + k_{lz} \frac{\partial^2 T}{\partial z^2} + \phi \dot{s} \end{aligned} \quad (3)$$

Where, ϕ is the porosity, ρ_r and ρ_f are the resin density and the fiber density, respectively, c_{pr} and c_{pf} are the resin specific heat and the fiber specific heat, respectively, u , v , w is the velocity in x, y, z directions, k_{lx} , k_{ly} , k_{lz} is the whole heat conductivity of fiber and resin, which can be expressed as:

$$k_{lx} = \frac{k_{rx} k_{fx}}{k_{rx} W_f + k_{fx} W_r}$$

$$W_r = \frac{\frac{\phi}{\rho_r}}{\frac{\phi}{\rho_r} + \frac{1 - \phi}{\rho_f}}, \quad W_f = 1 - W_r$$

The boundary conditions are given as:

- ① $T = T_0$ at the inlet gate
- ② $k_L \frac{\partial T}{\partial n} \big|_n = (1 - \phi) \rho_f c_{pf} u_n (T_f - T)$ at the flow front;
- ③ $T = T_m$ at the mold wall.

3) The chemical equation

While resin is curing, the resin chemical reaction follows the chemical equation and that is written as :

$$\phi \frac{\partial \alpha}{\partial t} + u \frac{\partial \alpha}{\partial x} + v \frac{\partial \alpha}{\partial y} + w \frac{\partial \alpha}{\partial z} = \phi f(\alpha, T_r) \quad (4)$$

The boundary conditions are given by

- (a) $\alpha = \alpha_0$ at the inlet;
- (b) $\frac{d}{dt}(\omega \alpha) = \omega f(\alpha, T_r)$ at the flow front,

B. The Numerical Formulation

Before the control equations are used to simulate the RTM process, it must be integrated in the control volume. At the past, the structure mesh is good for part of rule shape. The calculation accuracy is ensured, also. While the part is not rule, the structure mesh is unfit for simulating. So, the unstructured mesh has wide adaptability for shapes of part. While the calculation accuracy is closed related with the grid. The unstructured mesh can lead to the error of calculation results. The main reason is the cross diffusion term of energy equation exists. The size of the value has closely related with the orthogonal relation between the element nodes and the cell boundary. If the orthogonal is existence, the cross diffusion needs not considered. But it can not be ignored for the non-orthogonal grid. Especially when the cross is far away from the orthogonal, the cross diffusion has a great influence on the numerical results, which can not be zero.

Literature [14] shows that the control volume method is not a direct and accurate calculation of the cross diffusion on the common interface. Therefore, this paper does not directly calculate the cross diffusion term in the public interface from the integral of the diffusion term.

The whole derivation process is based on the orthogonal grid. By introducing the non orthogonal quantity, the improved discrete scheme is derived.

As shown in Figure 1, the P control volume (CV) and the adjacent E CV public interface has two, namely: FN and NM edge.

FIGURE 1. THE P CV AND THE ADJACENT E CV

For the discretization of the energy equation, each part separately carries on the numerical integration, and finally all are carried on the combination assembly to obtain the final control equation the discrete format.

1) Discrete of instantaneous term

The first item on the left of the differential equation. (3) is the integral of the instantaneous term by use differential method:

$$\int_{\Delta S} [\phi c_p + (1-\phi) \rho_c] \frac{\partial T}{\partial t} dS = \frac{[\phi c_p + (1-\phi) \rho_c] [T - T^0]}{\Delta t} \Delta S \quad (5)$$

Where, 0 is the result of the calculation of the previous time step, and ΔS is the area of the control section.

2) Integral of convection term

The convection term of the energy equation is integrated by the first order upwind scheme. As Fig 1 shown:

$$\begin{aligned} \int_{\Delta S} \rho_c c_p \left(u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right) dS &= \int_{\Delta S} \rho_c c_p T (\bar{v} \cdot \bar{l}) d\bar{l} \\ &= \rho_c c_p T (l_{12} \bar{v}_{12} \cdot \bar{l}_{12} + l_{23} \bar{v}_{23} \cdot \bar{l}_{23}) \end{aligned} \quad (6)$$

Where, $\bar{l}$ is the vector of the length of the outer normal unit of the control volume boundary, $\bar{v}$ is Darcy velocity vector of the resin that is expressed on the boundary.

So:

$$\int_{\Delta S} \rho_c c_p T (\bar{v} \cdot \bar{l}) d\bar{l} = \rho_c c_p T [(u n_x + v n_y)_{12} l_{12} + (u n_x + v n_y)_{23} l_{23}]_E \quad (7)$$

Where u is the component of Darcy velocity vector in the X direction, and v is the component of Darcy velocity vector in the y direction.

For all adjacent control volume of the control volume P, the integral of convection term in control volume can be obtained:

$$\int_{\Delta S} \rho_c c_p \left(u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right) dS = \sum_{E=1}^{N_s} \rho_c c_p T [(u n_x + v n_y)_{12} l_{12} + (u n_x + v n_y)_{23} l_{23}]_E \quad (8)$$

Where, N_s is the number of controls that are adjacent to the control volume.

Also,

$$\begin{cases} u = -\frac{k_x}{2A\mu} \sum_{i=1}^3 (b_i p_i) \\ v = -\frac{k_y}{2A\mu} \sum_{i=1}^3 (c_i p_i) \end{cases} \quad (9)$$

Formula (9) is introduced to formula (8), and gets:

$$\begin{aligned} \int_{\Delta S} \rho_c c_p \left(u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right) dS \\ = \rho_c c_p T \sum_{E=1}^{N_s} \left\{ -\frac{1}{2A_{PDE}\mu} (k_x \sum_{i=1}^3 (b_i p_i) n_x + k_y \sum_{i=1}^3 (c_i p_i) n_y)_{12} l_{12} \right. \\ \left. - \frac{1}{2A_{PCE}\mu} (k_x \sum_{i=1}^3 (b_i p_i) n_x + k_y \sum_{i=1}^3 (c_i p_i) n_y)_{23} l_{23} \right\}_E \end{aligned} \quad (10)$$

3) Integration of source terms

$$s_T = \phi \dot{s} = \phi \Delta H_f (\alpha, T_r) \quad (11)$$

By its linearization, it can be re written:

$$s_T = s_c + s_p T \quad (12)$$

Where, s_c and s_p Are constant, and $s_p \leq 0$.

Then the source terms are integral, and get:

$$\begin{aligned} \int_{\Delta V} \phi \dot{s} dV &= \int_{\Delta V} s_T dV \\ &= \int_{\Delta V} (s_c + s_p T) dV \\ &= s_c \Delta V + s_p T \Delta V \end{aligned} \quad (13)$$

4) Integration of diffusion terms

The first item on the left side of the equation is heat transfer by diffusion. According to Green Equation,,

$$\int_{\Delta S} (k_{1x} \frac{\partial^2 T}{\partial x^2} + k_{1y} \frac{\partial^2 T}{\partial y^2}) dS = \int_{\Delta S} k_{1x} \left(\frac{\partial T}{\partial x} \cdot \bar{l} \right) d\bar{l} \quad (14)$$

As Fig 1 shown:

$$\int_{\omega} k_{1x_i} \left(\frac{\partial T}{\partial x_i} \cdot l \right) dl$$

$$= \left[\left(k_{1x} \frac{\partial T}{\partial x} n_x + k_{1y} \frac{\partial T}{\partial y} n_y \right) l_{12} + \left(k_{1x} \frac{\partial T}{\partial x} n_x + k_{1y} \frac{\partial T}{\partial y} n_y \right) l_{23} \right]_E \quad (15)$$

a) When the connection between the nodes and the boundary of the control volume is orthogonal:

$$\begin{cases} \frac{\partial T}{\partial x} = \frac{T_E - T_P}{|PE|} n_x \\ \frac{\partial T}{\partial y} = \frac{T_E - T_P}{|PE|} n_y \end{cases} \quad (16)$$

So:

$$\int_{\omega} k_{1x_i} \left(\frac{\partial T}{\partial x_i} \cdot l \right) dl = \frac{T_E - T_P}{|PE|} \left[(k_{1x} n_x^2 + k_{1y} n_y^2) l_{12} + (k_{1x} n_x^2 + k_{1y} n_y^2) l_{23} \right]_E \quad (17)$$

b) When the connection between the nodes and the boundary of the control volume is non-orthogonal:

$$\int_{\omega} k_{1x_i} \left(\frac{\partial T}{\partial x_i} \cdot l \right) dl$$

$$= \frac{T_E - T_P}{|PE|} \left[(k_{1x} n_x^2 + k_{1y} n_y^2) l_{12} + (k_{1x} n_x^2 + k_{1y} n_y^2) l_{23} \right]_E + C_{diff} \quad (18)$$

Where, C_{diff} is cross diffusion term on a common interface.

By the formula (18), we can see that the diffusion term is mainly composed of two parts, namely, the main part and the cross diffusion C_{diff} on the common interface. The main part of the diffusion is direction ratio to temperature difference between adjacent control volumes, and inclined to the distance between the two controls. Therefore, the derivation of the cross diffusion term at the common interface can also be considered.

For the cross diffusion for 23-edge of a common interface, the cross diffusion term is proportional to the temperature gradient between the two adjacent control bodies. So:

$$C_{diff} \propto \frac{(T_E^0 - T_P^0)}{|PE|} \left[\sum k_{1x_i} n_i \right]_{23} l_{23} \quad (19)$$

Where, T_E^0 is the temperature of E at the end of a time step, and T_P^0 is the temperature of P at the end of a time step.

Secondly, basing on the derivation of the diffusion terms in the front, The size of the cross diffusion term is related to the

orthogonal relationship between the edge 23 and PE connections, and when the edge 23 and PE are connected with the orthogonal or close to the orthogonal, $C_{diff} = 0$. Or else, the cross diffusion term is greater. So:

$$C_{diff} \propto \frac{\overrightarrow{MN} \cdot \overrightarrow{PE}}{|\overrightarrow{MN}| |\overrightarrow{PE}|} \quad (20)$$

In the end, cross diffusion terms on the common interface can be expressed as follows:

$$C_{diff} = \frac{(T_E^0 - T_P^0)}{|\overrightarrow{PE}|^2} \left[\sum k_{1x_i} n_i \right]_{MN} l_{MN} \frac{\overrightarrow{MN} \cdot \overrightarrow{PE}}{|\overrightarrow{MN}|} \quad (21)$$

Formula (21) is write specific expressions, that is:

$$C_{diff} = \frac{(T_E^0 - T_P^0)}{|\overrightarrow{PE}|^2} (k_{1x} n_x + k_{1y} n_y)_{23} l_{23} \frac{[(X_2 - X_1)(X_E - X_P) + (Y_2 - Y_1)(Y_E - Y_P)]}{|23|} \quad (22)$$

Where, X and Y are the coordinates of each point, respectively.

For the cross diffusion of the 12-edge, can be expressed as follows:

$$C_{diff} = \frac{(T_E^0 - T_P^0)}{|\overrightarrow{PE}|^2} (k_{1x} n_x + k_{1y} n_y)_{12} l_{12} \frac{[(X_2 - X_1)(X_E - X_P) + (Y_2 - Y_1)(Y_E - Y_P)]}{|12|} \quad (23)$$

Finally, the cross diffusion terms on the common interface between the P controller and the adjacent control volume E can be expressed as follows:

$$C_{diff} = \frac{(T_E^0 - T_P^0)}{|\overrightarrow{PE}|^2} \left\{ (k_{1x} n_x + k_{1y} n_y)_{23} l_{23} \frac{[(X_2 - X_1)(X_E - X_P) + (Y_2 - Y_1)(Y_E - Y_P)]}{|23|} \right.$$

$$\left. + (k_{1x} n_x + k_{1y} n_y)_{12} l_{12} \frac{[(X_2 - X_1)(X_E - X_P) + (Y_2 - Y_1)(Y_E - Y_P)]}{|12|} \right\} \quad (24)$$

The formula (22) is introduced into the numerical integration of the diffusion term, that is, the formula (18), which can be improved by the numerical model of the energy equation under non isothermal conditions. According to the improved numerical model, the calculation accuracy of the temperature field is improved.

Integrated formula (5), formula (8), formula (11) and formula (16), in the time of the full implicit time integration scheme, and finally get the energy equation in the unstructured grid of two-dimensional discrete format:

$$m_p T_p = \sum_{E=1}^{N_E} m_E T_E + m_R \quad (25)$$

$$\text{Where, } m_p = \sum_{E=1}^{N_E} m_E + \frac{[\phi \rho_i c_{pi} + (1-\phi) \rho_i c_{pf}] \Delta S}{\Delta t} - s_p \Delta S$$

$$m_R = \frac{[\phi \rho_i c_{pi} + (1-\phi) \rho_i c_{pf}] \Delta S}{\Delta t} + s_c \Delta S$$

Since the first-order upwind scheme is used, so:

$$m_E = D_E + \text{Max}(0, -F_E)$$

Where,

$$D_E = \left\{ \frac{1}{|PE|} \left[(k_{1x} n_x^2 + k_{1y} n_y^2) l_{12} + (k_{1x} n_x^2 + k_{1y} n_y^2) l_{23} \right] \right\}_E + C_{diff}$$

$$F_E = \rho_i c_{pi} \left\{ -\frac{1}{2A_{PDE} \mu} (k_x \sum_{i=1}^3 (b_i p_i) n_x + k_y \sum_{i=1}^3 (c_i p_i) n_y) l_{12} \right. \\ \left. - \frac{1}{2A_{PCE} \mu} (k_x \sum_{i=1}^3 (b_i p_i) n_x + k_y \sum_{i=1}^3 (c_i p_i) n_y) l_{23} \right\}_E$$

The chemical equation can be deduced like the aforementioned, and gets:

$$n_p \alpha_p = \sum_{E=1}^{N_E} n_E \alpha_E + n_R \quad (26)$$

$$\text{Where, } n_p = \sum_{E=1}^{N_E} n_E + \frac{\phi \Delta S}{\Delta t} - f_p \Delta S$$

$$n_R = \frac{\phi \Delta S}{\Delta t} + f_c \Delta S$$

$$n_E = \text{Max}(0, -F_E)$$

$$F_E = \left\{ -\frac{1}{2A_{PDE} \mu} [k_x \sum_{i=1}^3 (b_i p_i) n_x + k_y \sum_{i=1}^3 (c_i p_i) n_y] l_{12} \right. \\ \left. - \frac{1}{2A_{PCE} \mu} [k_x \sum_{i=1}^3 (b_i p_i) n_x + k_y \sum_{i=1}^3 (c_i p_i) n_y] l_{23} \right\}_E$$

III. CASE STUDY

The calculation flow chart is shown in Figure 2. Using the non isothermal model which was derived from the author's previous works, and the injection process and the material parameter are from literature [19], as Tab 1 shown, the

numerical simulation was carried out to verify the improved method above.

A. Modification of Non-isothermal Simulation of RTM Process

The case is provided by reference [19]. In the case, the part and position of resin inlet are shown in Fig 3. The improved calculation results are compared with the previous calculation results as shown in Figure 4.

FIGURE II. THE FLOW CHART

TABLE I. RESIN AND FIBER PARAMETERS ^[19]

parameters	Value
$\rho_f / (\text{kg} \cdot \text{m}^{-3})$	2560
$\rho_r / (\text{kg} \cdot \text{m}^{-3})$	1100
$k_f / (\text{W} \cdot (\text{m} \cdot \text{K})^{-1})$	0.0335
$k_r / (\text{W} \cdot (\text{m} \cdot \text{K})^{-1})$	0.168
$c_{pf} / (\text{J} \cdot (\text{kg} \cdot \text{K})^{-1})$	670
$c_{pr} / (\text{J} \cdot (\text{kg} \cdot \text{K})^{-1})$	1680
$k_x = k_y = k_z / \text{m}^2$	2×10^{-9}
ϕ	0.7
$\Delta H / (\text{J} \cdot \text{m}^{-3})$	1.54×10^8
m_1	0.3
$\mu_0 / (\text{Pa} \cdot \text{s})$	2.78×10^{-4}
$E_\mu / (\text{J} \cdot \text{mol}^{-1})$	18000
α_g	0.1
d_1	1.5
d_2	1.0
$A_1 / (\text{s}^{-1})$	3.7833×10^5
$A_2 / (\text{s}^{-1})$	6.7833×10^5
$E_1 / (\text{J} \cdot \text{mol}^{-1})$	54418
$E_2 / (\text{J} \cdot \text{mol}^{-1})$	50232
m_2	1.7

FIGURE III. THE PART AND POSITION OF RESIN INLET

FIGURE IV. TEMPERATURE HISTORY CURVE OF TWO POINTS IN FILLING STAGE

Fig 4 for the corresponding temperature history of different points. Considering the cross diffusion in the common interface, the accuracy of the temperature field compared with previous work ^[15] is effectively improved.

Fig 5 is the predicted temperature and cure degree of part at the end of filling. Based on the predicted data, This process can be better described and understood.

a: The temperature of part

b: The cure degree of part

FIGURE V. THE PREDICTED TEMPERATURE AND CURE DEGREE OF PART AT THE END OF FILLING.

B. Modification of Curing Process Simulation

Another case is provided by reference [20]. The material parameters are described using table 2 and table 3. The part is a flat with $15.24 \times 15.24 \times 25.4 \text{ mm}$. A comparison between

pervious works and current study was made with the temperature at the center of the plate, as Fig 6 shown.

TABLE II. MATERIAL PARAMETERS^[20]

	Resin	Fiber
$\rho/(\text{kg}\cdot\text{m}^{-3})$	1890	2540
$C_p/(\text{J}\cdot(\text{kg}\cdot\text{K})^{-1})$	1260	840
$k_z/(\text{W}\cdot(\text{m}\cdot\text{K})^{-1})$	0.2163	0.01
$k_x, k_y/(\text{W}\cdot(\text{m}\cdot\text{K})^{-1})$	0.4326	0.1, 0.01
$\Delta H/(\text{J}\cdot\text{kg}^{-1})$	77500	

TABLE III. CURING KINETIC PARAMETERS^[20]

parameters	Value
A_1/s^{-1}	0
A_2/s^{-1}	6.1667×10^{20}
$E_1/(\text{J}\cdot\text{mol}^{-1})$	0
$E_2/(\text{J}\cdot\text{mol}^{-1})$	1.674×10^5
M	0.524
N	1.476

FIGURE VI. TEMPERATURE HISTORY CURVE OF THE CENTER POINT OF THE FLAT PLATE

FIGURE VII. PARTIAL DETAIL FIGURE OF FIG 6

Considering revision, the predicted temperature peak is very close to experimental value, about 1°C error which is reduced by approximately 2 °C than the original prediction error, as shown in Figure 6. Therefore, it can be said that considering the cross diffusion item in the discrete equation, the calculation precision is improved under not changing the calculation conditions.

FIGURE VIII. THE TEMPERATURE AT THE END OF CURING

Fig.8 accurately reflects the temperature inside and outside the part. Based on the temperature distribution, Product quality can be predicted accurately.

IV. CONCLUSION

During the derivation of the diffusion term of the energy equation, the cross diffusion term appears on the common interface between control volumes when they are not orthogonal, but the calculation is usually ignored in the past. In this paper, an approximate calculation formula of the cross diffusion term between non-orthogonal control volumes is proposed in order to improve the accuracy of numerical calculation. In the end, two numerical examples show that the method can effectively improve the accuracy of numerical calculation of temperature field.

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