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Technical Paper

Three-dimension numerical simulation for vulcanization process based on unstructured tetrahedron mesh

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ABSTRACT

Numerical simulation of vulcanization process is very important for producing of rubber part. In the paper, the control equations are discretized in the control volume according to divergence theorem. In order to expand the use of numerical simulation, four-node unstructured tetrahedron element is applied for various parts. Finally, a case on known data is used to test and verify effectiveness of simulation. The validity of our method is established in the case where flexible meshes are used. The results show when the number of element and node is less, the numerical procedure using our method, tested on known data, provides numerically valid and reasonably accurate predictions.

1. Introduction

The technology for molding rubber products has attracted the attention of many researchers for many years. This is because the vulcanization process of rubber compound has an important influence on the quality of the final product. Some researchers [1,2] attempt to develop numerical model based on Finite Element Method (FEM) in order to predict the quality of rubber products. In Ref. [3], the authors investigate heating flowing in rubber products, obtain numerical model based on FEM and modeled the vulcanization process of rubber. But the vulcanization during the cooling when rubber is taken from vulcanizing machine isn't considered. In Ref. [4,5], simulation by using ABAQUS is done to discuss these probable problems which could be appeared in the vulcanizing process. The simulation uses more accurate models for the description of the variation of rubber thermal properties with temperature and state-of-cure. In some other studies [6–8], the Finite Difference Method is used to perform simulation. To improve results of simulation, the 3D Galerkin finite element method is applied in some issuers [9,10]. In above these researches, the discretion unit is structure mesh and hence it is difficultly to meet requirement of complex shape of part. In Ref. [11], in order to simulate heat transfer and fluid flow, the method is presented which is fit for varieties of shapes by using structure and unstructured mesh based on Control Volume (CV) and Finite Volume (FV). Hence, CV/FEM is applied in the study. Moreover, the unstructured mesh is used to discrete part, thus the simulation is effective on various shapes of parts. The latest research includes literature [12–14]. In Ref. [12], the heat transfer during molding of elastomer is studied. By means of quasi-exact and explicit finite difference algorithms, the experimental and the predicted temperatures were in good agreement throughout the entire examined temperature range between 20 °C and 200 °C. In Ref. [13], based on the mechanisms of cross-linking process reactions, a new theoretical kinetic model framework was developed incorporating blend morphology by the authors. The kinetic model was then applied to the cross-linking process reactions of various monomer moieties. The model demonstrated good agreement with experimentally measured data. In Ref. [14], the researchers investigate the Eyring equation reflecting the effect of the self-diffusion on reaction rate and integrate it into the classical Arrhenius equation for reaction rate constants. Using simulation, thermodynamic properties and diffusion coefficients can be predicted, but they are poorer agreement with the experimental results. In spite of various researches accomplished in the field of rubber vulcanization process, there are still some very precise points that have not been addressed for this topic in the literature. In these researches, the structured hexahedral element was used and hence the flexibility of dealing with complicated shapes was not sufficient. Therefore, they were limited to regular parts and simple flow fields. When calculating complicated shape parts, the results are usually not satisfactory.

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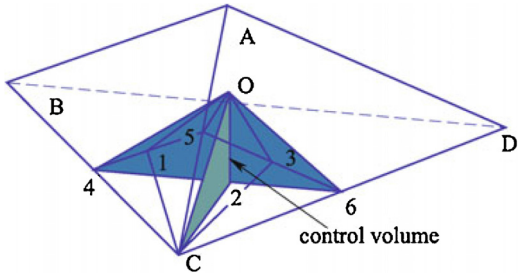

Fig. 1. The control volume composed of the tetrahedron element.

In the presented paper, by using the four-node unstructured tetrahedron mesh that fits complicated shapes and flow fields, we derive the discretization schemes of the heat conduction equation and the vulcanization equation based on upwind scheme in the three directions. Hence, our method can be widely applied to different kinds of parts and significantly improve the calculation precision.

2. Control equations

The control equations include the transient heat conduction equation and the vulcanization equation.

2.1. The heat conduction equation

In the section, the basic control equation is presented. Firstly, for the rubber vulcanization process, when the speed of heat transfer between the rubber and the mold is greater than flow of the rubber, the control equation of the transient heat conduction is simplified and is written as:

$$\rho c_p \frac{\partial T}{\partial t} = k_{Lx}\frac{\partial^2 T}{\partial x^2} + k_{Ly}\frac{\partial^2 T}{\partial y^2} + k_{Lz}\frac{\partial^2 T}{\partial z^2} + \dot{s} \tag{1}$$

where T denotes absolute temperature, c_p is heat capacity and ρ is density. k_{Lx}, k_{Ly}, k_{Lz} is the whole heat conductivity of rubber in the x, y and z direction, separately.

$\dot{s}$ is the quantity of the heat in the rubber vulcanization process which can be present: $\dot{s} = \Delta H G(\alpha, T)$, in where ΔH is the heat of reaction and the vulcanization kinetics equation $G(\alpha, T) = d\alpha/dt$ (based on Kamal's model [15–17]).

Secondly, the boundary conditions are given according to specified nodal temperature (the first-type boundary condition) and convection boundary (the third-type boundary condition). The first-type boundary has been better applied in many domains. While in other boundary domains the third-type boundary condition is given as following:

$$-\left(k_{Lx}\frac{\partial T}{\partial x}n_x + k_{Ly}\frac{\partial T}{\partial y}n_y + k_{Lz}\frac{\partial T}{\partial z}n_z\right) = h(T - T_\infty) \tag{2}$$

where n_x, n_y, n_z is components of the unit vector normal to the boundary, respectively. h is heat transfer coefficient. T_∞ is ambient temperature at boundary.

2.2. The vulcanization kinetics equation

Vulcanization of rubber is that temperature and reaction kinetics are dependent. According to relationship, they should be calculated simultaneously. For decreasing the risk of non convergence, they are calculated sequentially coupled in the present work. Vulcanization kinetic equation with the form of $d\alpha/dt$ is used:

$$d\alpha/dt = f(\alpha, T) \tag{3}$$

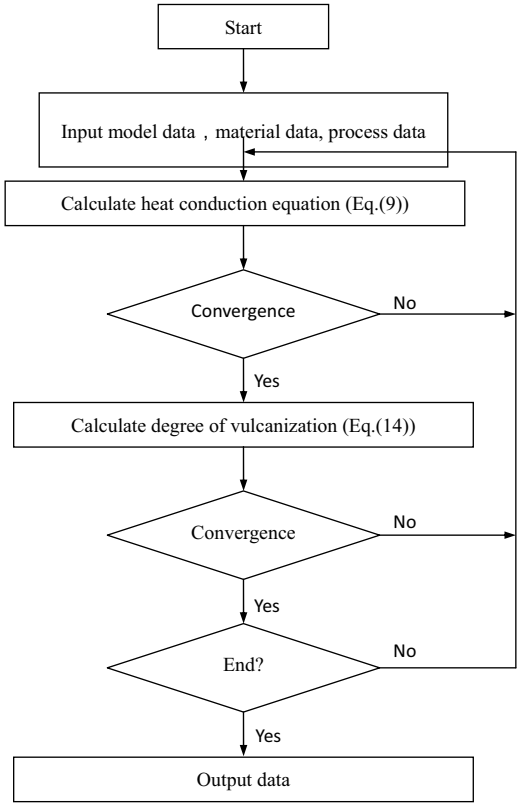

Fig. 2. The flow chart.

Table 1
Parameter of rubber used in simulation [10].

Parameter	Value	Parameter	Value
φ_0	1.4×10^{25}	E(J/gmol)	260622
m	2.91	T_0(K)	293
$\Delta H(J/m^3)$	4.54×10^6		

where, $f(\alpha, T)$ is expressed as (for Kamal and Sourour model):

$$f(\alpha, T) = m\varphi^{1/m}\alpha^{(m-1)/m}(1-\alpha)^{(m+1)/m}$$

where, α is degree of vulcanization, and m is constant. φ is a rate constant with an Arrhenius-type temperature dependence of the form:

$$\varphi = \varphi_0 \exp(-E/RT) \tag{4}$$

where φ_0 is constant, E is activation energy, and R is gas constant. As a result, the degree of vulcanization can be calculated based on Eq. (3). For solving this nonlinear equation, but, the initial conditions of Eq. (3) α is not equal to zero. Otherwise, a zero profile is gotten (initial condition).

3. Numerical formulation

For getting numerical formulation of control equations, firstly the volume of mold cavity is divided into a large number of small units which is same as four-node tetrahedron with good adaptability for complex shape, shown in Fig. 1 (Tet.ABCD). The sub-CV is constructed around node within the solution domain. Finally the CV mesh is established by assembling all of sub-CVs. The control equations are discretized based on CV/FEM within the CV mesh.