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A three dimensional simulation of a rubber curing process considering variable order of reaction

Mohammad-Reza Erfanian[a], Morteza Anbarsooz[b], Mohammad Moghiman[a,*]

[a] Mechanical Engineering Department, Ferdowsi University of Mashhad, Mashhad, Iran
[b] Mechanical Engineering Department, Quchan University of Advanced Technology, Quchan, Iran

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ABSTRACT

Calculating the optimum curing time for thick molded rubbery parts is an important challenge in the rubber industry. This presented work is focused on the development of a computational technique for numerical simulation of the rubber vulcanization process in injection molding machines that can be used as a method for determining the best curing time of the final product. The main innovation of the work is introducing a kinetics model with variable order of reaction which enhances the accuracy of the calculated optimum curing time, especially in three-dimensional complex rubber articles. The method is used for simulation of the injection molding process of an automotive rubber part, containing both the mold filling and the cure reaction processes. The numerical predictions of the mold filling time and the curing time are compared with those of experiments, which confirmed the accuracy and capability of the proposed model.

1. Introduction

Rubber is widely used in various applications, from tires to flexible tubing or absorbing systems, to mention just a few applications. They are favored when, in contrast to other engineering materials, their stronger attributes are needed and, at the same time, their highly deformable characteristics are desirable [1]. However, raw rubber is very soft with low mechanical properties. It must be cured in a mold which is called the vulcanization process. Following the vulcanization process, the compound which is made up of uncured rubber and curing agents, fills the mold cavity during the injection cycle and is heated up to a temperature at which the cure reaction starts. During the cure, an irreversible reaction takes place, leading to a three-dimensional molecular network, and as a result, the weak material is converted into a very strong elastic product [1]. Obviously, the curing process specifications such as the curing time and curing temperature have strong impacts on the quality and mechanical properties of the final product [2].

Using experimental techniques to determine the required curing time for a rubber article to reach certain mechanical properties, is a time-consuming and expensive procedure. As a result, numerical solutions have been widely used in the rubber industry, following the development of computers and CAE tools. A comprehensive review on the historical background of the development of these techniques are presented by Ghoreishy [2] and hence, they are not repeated here.

Various kinetic models have been used to describe the cure behavior of rubber. Generally, these models are divided into two main categories; mechanistic kinetic models and empirical models [3]. Mechanistic kinetic models attempt to quantify

* Corresponding author. Tel.: +985138805091; fax: +985138806055.
E-mail address: moghiman@um.ac.ir (M. Moghiman).

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the balance of chemical species involved in the curing reaction. Due to their complexity and the need to the knowledge of the underlying chemistry [4], these models have not been accepted as appropriate models for numerical simulations [3]. On the other hand, the empirical models or regression models ignore the chemical details of the cure system and fit the data to a mathematic functional form where the constants of the model are determined based on experimental procedures such as rheometry [4]. Some numerical studies that have applied empirical models in their simulations are reviewed below.

Ghoreishi and Naderi [5] developed a finite element model for the simulation of the rubber curing process in a mold. They used the kinetic model proposed by Kamal and Sourour [6] which has shown an acceptable agreement with the experimental data. Their investigations for a truck tire curing process also revealed that neglecting the heat transfer in one direction would produce significant errors in calculating the temperature fields and extends of the cure reaction [7]. Arillaga et al. [3] simulated the injection molding process for relatively simple geometries with uniform thickness using the Mold-Flow Software. This software has also been employed by Ramorino et al. [8] to perform a three-dimensional finite element simulation for the injection molding process of a rubber compound. Leroy et al. [9] presented a cure kinetic model predicting induction, main vulcanization and reversion stages and modeled the cure process for a sample test which had a uniform thickness. Rafei et al. [10] developed a numerical code to study the curing process of a simple rubber article in a mold using unstructured meshes. They also considered the thermal contact resistance between the rubber and the mold in their simulations. Their results demonstrated that the Kamal and Sourour [10] model fails to precisely describe the cure behavior especially at the early stages of the cure reaction and also at the non-isothermal conditions [10]. As a result, they introduced a modified version of that model which enhanced the accuracy of the results. They used the values of the state-of-cure at the initial and final stages of the reaction in their modified model.

The main motivation of the current study is to present a new modification to the Kamal and Sourour kinetic model. In the modified model, the model's order of reaction is no longer a constant, but it is a function of temperature. In order to verify the performance of the modified model, the injection molding process for an automotive rubber part, containing both the mold filling and the cure reaction processes, is studied numerically using the Fluent software. The new kinetic model is introduced into the Fluent 6.3.26 [11] software using a new User-Defined-Function (UDF) developed in C program. In order to determine the non-Newtonian fluid model constants, viscometry tests are performed. Rheometry tests are employed to determine the curing parameters of the kinetic model. Non-isothermal Differential Scanning Calorimetry (DSC) tests are also carried out at different temperatures to determine the temperature dependent specific heat of rubber. Mechanical compression tests are performed on the rubber component at different times of the curing process to determine the best curing time. The results of the numerical simulations with the Kamal kinetic model and the one modified in the current study are compared with the experimental results and the modified model has shown a better agreement with experimental data.

2. Mathematical modeling

2.1. Governing equations

Computational Fluid Dynamics (CFD) relies on solving conservation equations of mass, momentum and energy. These equations in a 3D Cartesian coordinate system are given below:

2.1.1. Continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho \vec{V}) = 0 \tag{1}$$

where ρ is the fluid density and $\vec{V}$ is the velocity vector.

2.1.2. Momentum conservation equation

$$\frac{\partial}{\partial t}(\rho \vec{V}) + \nabla.(\rho \vec{V}\vec{V}) = -\nabla p + \nabla.(\bar{\bar{\tau}}), \tag{2}$$

where p is the static pressure and τ is the viscous stress tensor. For a non-Newtonian fluid, the shear stress can be written as:

$$\bar{\bar{\tau}} = \mu(\nabla \vec{V} + \nabla \vec{V}^T), \tag{3}$$

where μ is the shear viscosity.

The non-Newtonian power law viscosity model, which has provided satisfactory predictions for rubber simulations, is applied in the present simulations. The model is given by Khor et al. [12]:

$$\mu = A(\dot{\gamma})^{B-1}\exp\left(\frac{T_0}{T}\right) \tag{4}$$

where A is a measure of the average viscosity of the fluid (the consistency index), $\dot{\gamma}$ is the shear rate, B is a measure of the fluid deviation from Newtonian (the power-law index), T is the temperature and T_0 is a reference temperature.

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