MATCHING CYLINDRICAL DOMAINS IN THE FINITE DIFFERENCE METHOD: APPLICATION TO VULCANIZATION

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RESUMEN

Se estudia un procedimiento simple para obtener el empalme de dominios cilíndricos por el método de diferencias finitas. Se realizan transformaciones de coordenadas en cada dominio para conseguir normalizaciones apropiadas y se desarrolla un algoritmo para empalmar perfiles de temperatura y flujos calóricos en las interfaces. Este procedimiento se aplica a una cámara de reacción cilíndrica para evaluar el grado de vulcanización de compuestos de caucho en función del tiempo de reacción.

ABSTRACT

A simple procedure to obtain the matching of cylindrical domains in the finite difference method is studied. Coordinate transformations are carried out in each domain to get appropriate normalizations and an algorithm to match temperature profiles and heat fluxes at interfaces is developed. This procedure is applied to a cylindrical reaction chamber to evaluate the degree of vulcanization of rubber compounds as function of reaction time.

INTRODUCTION

Heat transfer coupled to chemical reaction is an important phenomenon in tire vulcanization. This process occurs in two stages: first, there exists an induction time where the curing reaction does not take place, and then, the chemical reaction starts and proceeds with a rate that varies in time. Now, it is well recognized that an appropriate description of the state of cure in a rubber compound requires the consideration of both, induction time due to thermal history and non-isothermal vulcanization kinetics [1]. With this purpose, one dimensional models are frequently used with simplified boundary conditions [1], [2].

The present work is devoted to generate a simple numerical algorithm through finite differences to describe the process of curing in the reaction chamber shown in Figure 1, which was designed by researches of FATE S.A.I.C.I. for quality testing procedures.

The reaction chamber is composed of a cylindrical rubber sample that receives heat from the mold (upper and lower disks and wall). The disks are in direct contact with heat sources, at constant temperature. Other parts of the mold exchange heat with ambient air.

One should note that the green sample, initially at ambient temperature, receives heat from the mold, and since the rubber has a very low heat conductivity, temperature profiles varies in space and time.

A numerical algorithm describing this problem must be simple enough (short computational time) so that it can be used in microcomputers to generate rapid feed-back informations for the control of variables in the production line. Therefore, we show here a procedure to match in discrete form cylindrical domains of the chamber, allowing one to formulate the numerical algorithm in simple finite differences.

This work only presents the formulation of the mathematical model and also the procedure for matching the cylindrical domains. Temperature profiles and degree of vulcanization are also presented in a figure. However, the validation of this algorithm through comparisons with experimental results was carried out with researchers of FATE S.A.I.C.I. in an unpublished technical report.

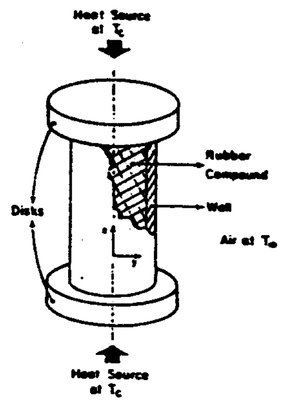

Figure 1: Curing chamber.

MATHEMATICAL MODEL

Since there is not momentum transfer in the chamber, the balance of thermal energy in cylindrical coordinates r and z can be simplified as follows,

$$\rho_i c_i \frac{\partial T_i}{\partial t} = k_i \{ \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial T_i}{\partial r} \right) + \frac{\partial^2 T_i}{\partial z^2} \} + \frac{\partial Q}{\partial t} \tag{1}$$

and it must be satisfied in the rubber compound , the disks and the wall. In equation (1), T_i is the temperature, ρ_i is the density, k_i is the thermal conductivity and c_i is the heat capacity. The subindex i takes values 1, 2 and 3 to indicate rubber, wall and disks, respectively. The term $\frac{\partial Q}{\partial t}$ is the rate of heat generation due to the curing reaction and can be expressed,

$$\frac{1}{Q_\infty} \frac{\partial Q}{\partial t} = k_o(T)\,(1 - \frac{Q}{Q_\infty})^n \tag{2}$$

$$k_o(T) = k_\infty \, exp(-\frac{E}{RT}) \tag{3}$$

$$\tau_i = \int_0^{t(T_1)} \frac{dt}{t_o \, exp(T_o/T_1)} \tag{4}$$

where $k_o(T)$ is a rate constant with an Arrhenius type temperature dependence and Q_∞ is the total heat of reaction. Also, E, k_∞, T_o and t_o are kinetic constants independent of temperature and $\frac{Q}{Q_\infty}$ is the degree of vulcanization that depends on time and position.

When dimensionless time τ_i reaches unity in equation (4), the upper limit t in the integral corresponds to the onset of vulcanization. Further physical aspects of this problem are discussed in [1].

The next step consists in writting equation (1) to (4) for each domain of the chamber in dimensionless form by using sçales defined in Figure 2. In this figure we show the computational domains obtained through considerations of symmetry.

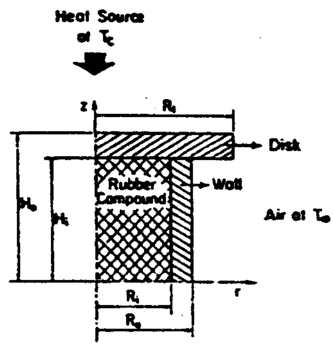

Figure 2: Computational domains.

* *Heat Balance in the Rubber*

We propose the following definitions,

$$\theta_1 = \frac{T_1}{T_{10}} \quad , \quad R = \frac{r}{R_i} \quad , \quad Z = \frac{z}{H_i}$$

$$f = \frac{Q}{Q_\infty} \quad , \quad \Lambda = \frac{R_i}{H_i} \quad , \quad N = \frac{Q_\infty}{\rho c T_{10}}$$

$$\tau = \frac{t k_1}{\rho_1 c_1 R_i^2} \quad , \quad A_o = \frac{k_o \rho_1 c_1 R_i^2}{k_1}$$

$$A_1 = \frac{E}{R_g T_{10}} \quad , \quad \tau_o = \frac{t_o k_1}{\rho_1 c_1 R_i^2} \quad , \quad T^* = \frac{T_o}{T_{10}}$$

where T_{10} is the initial temperature of the rubber compound (ambient temperature) and R_g is the gas constant. Therefore, equations (1) to (4) generate the following dimensionless problem,

$$\frac{\partial \theta_1}{\partial \tau} = \frac{1}{R} \frac{\partial}{\partial R} R \frac{\partial \theta_1}{\partial R} + \Lambda^2 \frac{\partial^2 \theta_1}{\partial Z^2} + N \frac{\partial f}{\partial \tau} \tag{5}$$

$$\frac{\partial f}{\partial \tau} = A_o \, exp(-\frac{A_1}{\theta_o}) \tag{6}$$

$$\tau_i = \int_o^{\tau(\theta_1)} \frac{d\tau}{\tau_o \, exp(T^*/\theta_1)} \tag{7}$$

with the following constraints,

$$f = 0 \quad for \quad \tau_i < 0 \quad , \quad f \neq 0 \quad for \quad \tau_i \geq 1 \tag{8}$$

It is then easy to prove that the initial condition for equation (5) is,

$$\tau < 0 \quad , \quad 0 \leq R \leq 1 \quad , \quad 0 \leq Z \leq 1 \quad , \quad \theta = 1 \tag{9}$$

and the boundary condition for $\tau \geq 0$ are,

$$R = 0 \quad , \quad 0 \leq Z \leq 1 \quad , \quad \frac{\partial \theta_1}{\partial R} = 0 \tag{10}$$

$$0 \leq R \leq 1 \quad , \quad Z = 0 \quad , \quad \frac{\partial \theta_1}{\partial Z} = 0 \tag{11}$$

at the centers of symmetry,

$$R = 1 \quad , \quad 0 \leq Z \leq 1 \quad , \quad \frac{\partial \theta_1}{\partial R} = K_{21} \frac{\partial \theta_2}{\partial R} \quad \textit{and} \quad \theta_1 = \theta_2 \tag{12}$$

at the rubber - wall interface with $K_{21} = k_2/k_1$ and $\theta_2 = T_2/T_{10}$, and

$$0 \leq R \leq 1 \quad , \quad Z = 1 \quad , \quad \frac{\partial \theta_1}{\partial Z} = K_{31} \frac{\partial \theta_3}{\partial Z} \quad \textit{and} \quad \theta_1 = \theta_3 \tag{13}$$

at the disk - rubber interface, with $K_{31} = k_3/k_1$ and $\theta_3 = T_3/T_{10}$. It is also clear that equations (12) and (13) imply equal heat fluxes at interfaces.

* *Heat Balance in the Wall*

We define $c_{21} = \frac{\rho_2 c_2}{\rho_1 c_1}$, to find that,

$$c_{12} \frac{\partial \theta_2}{\partial \tau} = \frac{1}{R} \frac{\partial}{\partial R} R \frac{\partial \theta_2}{\partial R} + \Lambda^2 \frac{\partial^2 \theta_2}{\partial Z^2} \tag{14}$$

Equation (14) has the following initial condition,

$$\tau < 0 \quad , \quad 0 \leq R \leq \frac{R_o}{R_i} \quad , \quad 0 \leq Z \leq 1 \quad , \quad \theta_2 = \frac{T_2}{T_{10}} \tag{15}$$

Boundary conditions are,

$$R = 1 \quad , \quad 0 \leq Z \leq 1 \quad , \quad \frac{\partial \theta_1}{\partial R} = K_{21} \frac{\partial \theta_2}{\partial R} \quad \textit{and} \quad \theta_1 = \theta_2 \tag{16}$$

at the rubber - wall interface, with $K_{21} = k_2/k_1$, and

$$R = \frac{R_o}{R_i} \quad , \quad 0 \leq Z \leq 1 \quad , \quad \frac{\partial \theta_2}{\partial R} = -B_i \left(\theta_2 - \frac{T_\infty}{T_{10}}\right) \tag{17}$$

at the wall - air interface. T_∞ being the air temperature far away from the wall. $B_i = \frac{h R_i}{k_2}$ is the Biot number and h is the heat transfer coefficient by natural convection. Also,

$$0 \leq R \leq \frac{R_o}{R_i} \quad , \quad Z = 1 \quad , \quad \frac{\partial \theta_2}{\partial Z} = K_{32} \frac{\partial \theta_3}{\partial Z} \quad \textit{and} \quad \theta_2 = \theta_3 \tag{18}$$

at the wall - disk interface, with $K_{32} = k_3/k_2$. Finally, the symmetry assumption requires,

$$0 \leq R \leq \frac{R_o}{R_i} \quad , \quad Z = 0 \quad , \quad \frac{\partial \theta_2}{\partial Z} = 0 \tag{19}$$

* *Heat Balance in the Disks*

We define $c_{31} = c_{21} = \frac{\rho_2 c_2}{\rho_1 c_1}$, to obtain in this case the following heat balance equation,

$$c_{31} \frac{\partial \theta_3}{\partial \tau} = \frac{1}{R} \frac{\partial}{\partial R} R \frac{\partial \theta_3}{\partial R} + A^2 \frac{\partial^2 \theta_3}{\partial Z^2} \tag{20}$$

Equation (20) requires the initial condition,

$$\tau < 0 \quad , \quad 0 \leq R \leq \frac{R_t}{R_i} \quad , \quad 1 \leq Z \leq \frac{H_o}{H_i} \quad , \quad \theta_3 = 1 \tag{21}$$

Boundary conditions are,

$$0 \leq R \leq \frac{R_t}{R_i} \quad , \quad Z = \frac{H_o}{H_i} \quad , \quad \theta_3 = \frac{T_c}{T_{10}} \tag{22}$$

where T_c is the temperature of the heat source in contact with the disk,

$$0 \leq R \leq 1 \quad , \quad Z = 1 \quad , \quad \frac{\partial \theta_1}{\partial Z} = K_{31} \frac{\partial \theta_3}{\partial Z} \quad and \quad \theta_1 = \theta_3 \tag{23}$$

at the rubber - disk interface,

$$1 \leq R \leq \frac{R_o}{R_i} \quad , \quad Z = 1 \quad , \quad \frac{\partial \theta_2}{\partial Z} = K_{32} \frac{\partial \theta_3}{\partial Z} \quad and \quad \theta_2 = \theta_3 \tag{24}$$

at the disk - wall interface, and

$$\frac{R_o}{R_i} \leq R \leq \frac{R_t}{R_i} \quad , \quad Z = 1 \quad , \quad \frac{\partial \theta_3}{\partial Z} = \widehat{B}_i (\theta_3 - \frac{T_\infty}{T_{10}}) \tag{25}$$

at the disk - air horizontal interface; $\widehat{B}_i = \frac{hH_i}{k_2}$ being the Biot number at this interface. In addition,

$$R = \frac{R_t}{R_i} \quad , \quad 1 \leq Z \leq \frac{H_o}{H_i} \quad , \quad \frac{\partial \theta_3}{\partial Z} = -B_i (\theta_3 - \frac{T_\infty}{T_{10}}) \tag{26}$$

at the disk - air vertical interface; $B_i = \frac{hR_i}{k_2}$ being the Biot number at this interface. Finally, symmetry implies,

$$R = 0 \quad , \quad 0 \leq Z \leq \frac{H_o}{H_i} \quad , \quad \frac{\partial \theta_3}{\partial R} = 0 \tag{27}$$

COORDINATE TRANSFORMATIONS

It is clear that the range of variations of coordinates, described by equations (15), (21), (25) and (27) and summarized as follows,

$$\begin{gathered} 1 \leq R \leq \frac{R_o}{R_i} \\ \frac{R_o}{R_i} \leq R \leq \frac{R_t}{R_i} \\ 1 \leq Z \leq \frac{H_o}{H_i} \end{gathered} \tag{28}$$

are not suitable for the purposes of writting the coupled heat transfer problem in finite differences, with an appropriate degree of freedon in the choice of grid sizes in each computational sub-domain. This problem can be solved with the following coordinate transformations in each domain:

* *Rubber Domain*

Coordinates are kept the same.

* *Wall Domain*

We propose to transform radial coordinate according to,

$$\hat{R} = \frac{r - R_i}{R_o - R_i} \quad , \quad 0 \leq \hat{R} \leq 1 \tag{29}$$

and define the corresponding differential operator,

$$\frac{\partial}{\partial R} = \frac{1}{(\kappa - 1)} \frac{\partial}{\partial \hat{R}} \tag{30}$$

where $\kappa = R_o/R_i$.

* *Disk Domain*

The transformation is,

$$\hat{\hat{R}} = \frac{r}{R_t} = \frac{R}{\kappa'} \quad , \quad 0 \leq \hat{\hat{R}} \leq 1 \tag{31}$$

and we define the corresponding differential operator,

$$\frac{\partial}{\partial R} = \frac{1}{\kappa'} \frac{\partial}{\partial \hat{\hat{R}}} \tag{32}$$

where $\kappa' = R_t/R_i$.

In addition, it is necessary a new axial variable,

$$\hat{\hat{Z}} = \frac{z - H_i}{H_o - H_i} = \frac{Z - 1}{\kappa'' - 1} \quad , \quad 0 \leq \hat{\hat{Z}} \leq 1 \tag{33}$$

where $\kappa'' = H_o/H_i$. The corresponding differential operator is,

$$\frac{\partial}{\partial Z} = \frac{1}{(\kappa'' - 1)} \frac{\partial}{\partial \hat{\hat{Z}}} \tag{34}$$

It is then clear that new coordinates in the disks and the wall and old coordinates in the rubber vary in the range (0,1) as wished for the numerical algorithm. Nevertheless, we have to match derivatives at interfaces with different coordinates and this must be solved by an appropiate consideration of the metrics in each domain.

MATCHING OF DOMAINS

Since we have to equate temperatures and their derivatives at interfaces from each side, and the physical distances are measured with different dimensionless radial and axial coordinates, it is necessary to localize a point at any interface by requiring that the metrics measured from any side of the interface be both equal. Thus, if ds is the arc length, we have,

$$ds = ds_i = ds_j \, \varphi_{ij} \tag{35}$$

where ds_i and ds_j are arc lengths defined in domains i and j respectively, and φ_{ij} is a scaling function as follows,

$$ds_i = \varphi_{ij} \, ds_j = \begin{cases} dR = \kappa' \, d\hat{\hat{R}} \\ d\hat{R} = \dfrac{\kappa}{(\kappa - 1)} d\hat{\hat{R}} \\ d\hat{\hat{Z}} = \dfrac{1}{(\kappa'' - 1)} dZ \end{cases}$$

Consider the interface of two domains designated now a and b. Let Δa be the grid size for domain a and Δb for domain b. If i_a and i_b are integers so that,

$$i_a = 1 \ldots N_a \quad , \quad i_b = 1 \ldots N_b \tag{36}$$

and

$$\Delta a = \frac{1}{N_a} \quad , \quad \Delta b = \frac{1}{N_b} \tag{37}$$

it is clear that for a node i_a of domain a we can find a real number i_b' of domain b that satisfies,

$$i_b' \, \Delta b = i_a \, \Delta a \, \varphi_{ab} \tag{38}$$

hence,

$$i_b' = i_a \frac{\Delta a}{\Delta b} \varphi_{ab} \tag{39}$$

Therefore, we define,

$$w = | i_b' - i_b | \tag{40}$$

where i_b is the integer part of i_b'. Then, any function F evaluated at i_a in domain a can also be evaluated at the same node on the other side of interface (domain b) with the following weighted approximation,

$$F_{i_a}^b = F_{i_b} (1 - w) + F_{i_b+1} \, w \tag{41}$$

where the upper index b indicates that the function F is evaluated at the interface from the side of domain b at a place that is coincident with node i_a on the side of domain a.

Thus, since nodes of grids in different domains are not necessarilly coincident at interfaces and grid sizes are chosen according to the needs for computing sharp temperature profiles, it is clear that the above equations allow us to match temperature and their derivative from different domains. We can choose freely the grid sizes in each domain according to different physical situations and manage any desired grid refinement for the accuracy of results. Finally, we have to mention that transient partial differential equations are solved through the Alternating Direction Implicit (ADI). Figure 3 shows isotherms in the rubber and lines of constant degree of vulcanization for a typical run (see Table I). It is observed a thermal boundary layer on the rubber - disk interface.

Table I: Data used in the run of Figure 3.

k_1	$6.807\ 10^{-4}$	$\frac{cal}{°K\ gr\ cm\ seg}$
ρ_1	1.195	$\frac{gr}{cm^3}$
$\rho_2 = \rho_3$	7.85	$\frac{gr}{cm^3}$
$k_2 = k_3$	0.09	$\frac{cal}{°K\ gr\ cm\ seg}$
c_1	0.344	$\frac{cal}{gr\ °K}$
$c_2 = c_3$	0.128	$\frac{cal}{gr\ °C}$
E	$22.651\ 10^3$	$\frac{cal}{grmol}$
n	1	
k_o	$3.6\ 10^8$	$\frac{1}{seg}$
T_e	180	°C
T_∞	25	°C

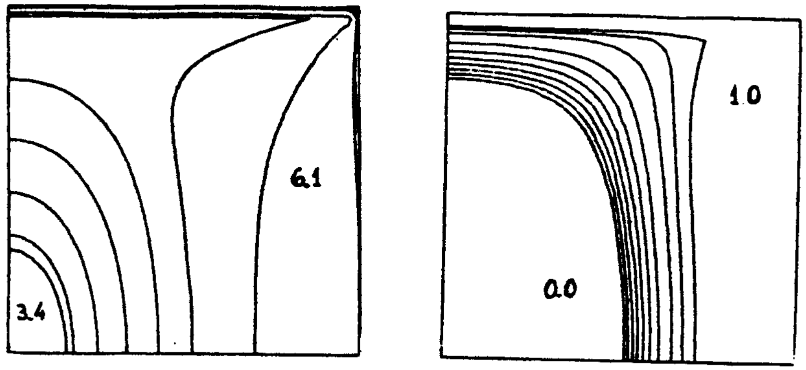

Figure 3: Isotherms and degree of vulcanization in the rubber.

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REFERENCES

1. Isayev, A. I. and Deng, J. S., " Non Isothermal Vulcanization of Rubber Compounds", Rubber Chemistry and Technology, Vol. 61, 1989, p. 340-361.

2. Schlanger, H. P., " A One - Dimensional Numerical Model of Heat Transfer in the Process of Tire Vulcanization", Rubber Chemistry and Technology, Vol. 56, 1989, p. 304-321.