

HEAT TRANSFER MODELLING IN A POLYMER SAMPLE LOCATED IN A MICROWAVE FIELD

II. Transient state

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Abstract

This work presents the modelling of heat transfer in a polymer sample submitted to a microwave field in the quartz column of a dilatometer surrounded by vacuum to avoid convection. The temperature rise is studied in transient state by the finite element method. It is assumed that a uniform and constant heat production is maintained in the entire volume of the sample. It is shown that it is possible to design the set composed of the sample and of the column to achieve a nearly uniform temperature in the whole volume of the sample while its temperature is raised from 20 to 250°C at a heating rate of 5 deg·min⁻¹.

Keywords: dilatometer, heat transport phenomenon, modelling

Introduction

This work presents research on the construction of a dilatometer for studying polymer samples, the low thermal conductivity of which may be the cause of significant temperature gradients in the polymer, that have to be avoided in practical applications. In a previous work [1] mathematical modelling showed that a nominal temperature up to 250°C, nearly uniform throughout the sample, can be achieved at steady state with a convenient geometric configuration of the dilatometer column. The corresponding model supposed the absence of convective heat transfer; in practice, the column was surrounded by vacuum. Such steady state situations should be in principle suitable for step by step dilatometric measurements but the time necessary to achieve these steady states may be

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excessively long. On the other hand, continuous dilatometric measurements during heating of the sample are more convenient and consequently their feasibility should be considered.

The purpose of this work was first to study the change in temperature of the sample as a function of time before steady state is attained, and secondly, to investigate various geometric configurations of the column, which are feasible, to find out if it is possible to heat the sample from 20 to 250°C at a heating rate of 5 deg·min⁻¹, without observing a difference greater than 10°C between the highest and the lowest temperature inside the sample.

Mathematical model and resolution method

The modelling concerns the practical situation of a polymer sample located between a fixed quartz piece called the 'buffer' and a mobile quartz piece called the 'pusher'. These parts correspond to mathematical domains termed Ω_1 , Ω_2 and Ω_3 , respectively. It is assumed that the materials are isotropic and that their thermal properties are independent of temperature. As the column is surrounded by vacuum, in practice no convective heat transfer is considered. The temperature in domain Ω_i ($i = 1, 2, 3$) is the solution of the equation:

$$\rho_i \frac{\delta T}{\delta t} - \lambda_i \Delta T = q_i \quad \text{in} \quad \Omega_i \quad (i = 1, 2, 3) \quad (1)$$

In our case, $q_1 \neq 0$ and $q_2 = q_3 = 0$.

The boundary conditions are:

$$\begin{aligned} T &= T_e & \text{on} & \Gamma_{i0} \\ \frac{\delta T}{\delta n} &= 0 & \text{on} & \Gamma_{i1} \end{aligned} \quad (2)$$

and the initial conditions is

$$T = T_e \quad \text{in} \quad \Omega_i \quad (i = 1, 2, 3) \quad (3)$$

The following symbols have been employed:

- T temperature
- T_e external fixed temperature
- t time
- ρ_i product of density by heat capacity in Ω_i
- q_i power supplied in Ω_i by unit volume
- λ_i thermal conductivity in Ω_i
- Γ_{i0} part of the boundary of Ω_i maintained at T_e
- Γ_{i1} part of the boundary of Ω_i with no heat transfer.

The system of Eqs (1–3) was solved by the finite element method [2, 3]. The software Modulef [4] was employed. All the geometries studied in this work have a symmetry of revolution (y axis in Fig. 1). Consequently, calculations were carried out in a domain of dimension 2 consisting of the cut of the system by a half plane supported by the axis of revolution. Quadrangular axisymmetric finite elements with an interpolation by Lagrange polynomials of degree 2 have been employed according to the previous study [1]. The transient problem was solved by a non-constant time step and local error control procedure through the program 'EVOLGE' of the software Modulef [5].

The values chosen for the thermal parameters appearing in Eqs (1–3) are given in Table 1. The external temperature was 20°C in all cases.

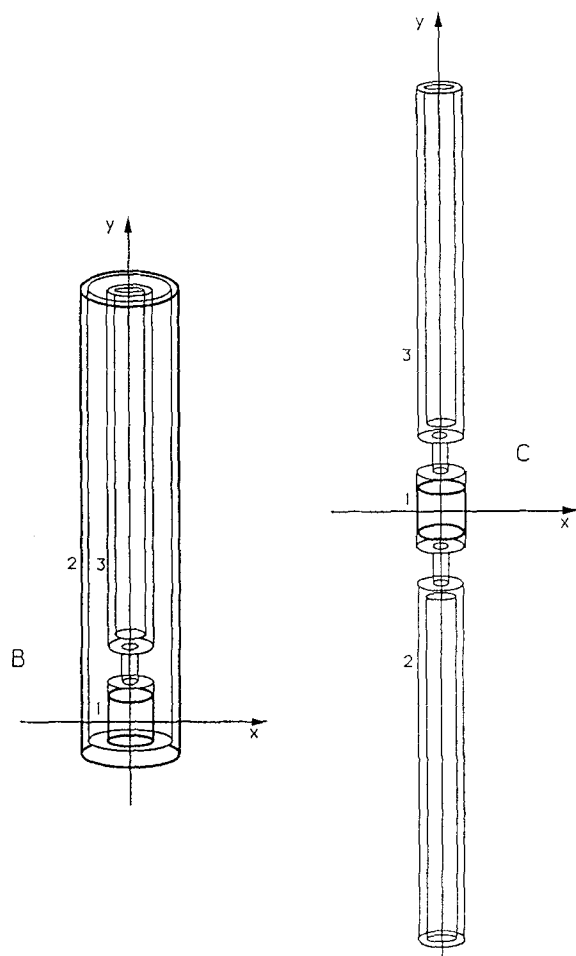


Fig. 1 Schemes of columns *B* and *C*. 1: sample; 2: buffer; 3: pusher

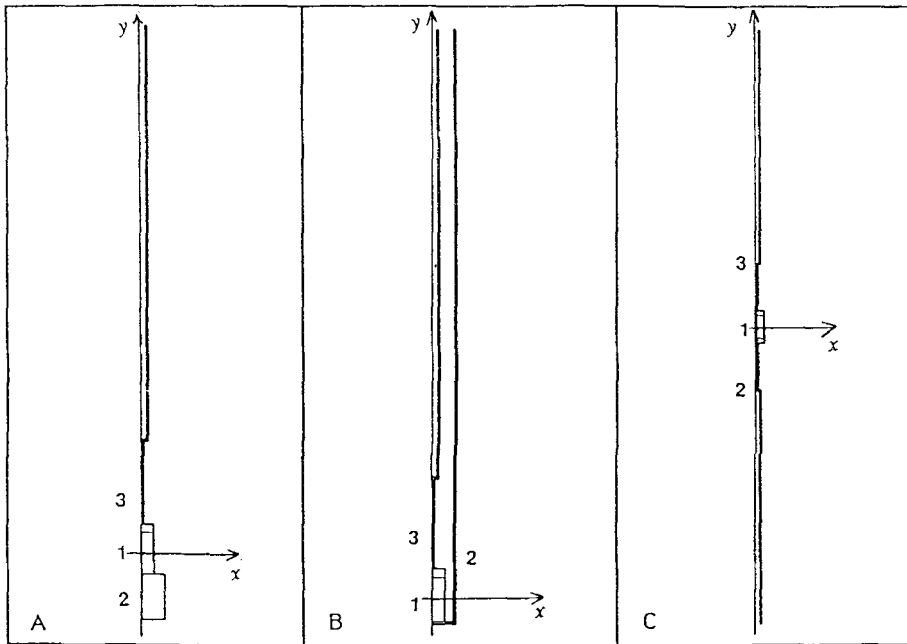


Fig. 2 Domain of study for geometries *A*, *B* and *C*. 1: sample; 2: buffer; 3: pusher

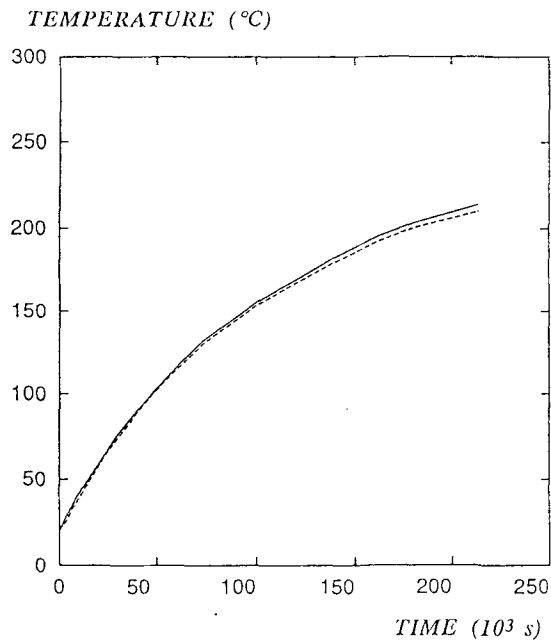


Fig. 3 Temperature rise in the sample for geometry *A* with $q_1 = 0.02 \text{ W}\cdot\text{cm}^{-3}$. (—) T_h , the highest temperature. (---) T_l , the lowest temperature

Table 1 Physical parameters

	Sample	Buffer	Pusher
Domain Ω_i	Ω_1	Ω_2	Ω_3
$\lambda_i / \text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	0.2	1.3	1.3
$\rho_i / \text{J}\cdot\text{m}^{-3}\cdot\text{K}^{-1}$	$2\cdot 10^6$	$1.65\cdot 10^6$	$1.65\cdot 10^6$

Three different geometries, termed *A*, *B* and *C*, of a dilatometer column were considered. They include an identical sample, a cylinder of height $L=1$ cm and of radius $R=3$ mm, and an identical hollow cylindrical pusher. In geometry *A*, which has been described previously [1], the buffer is a rod. In geometry *B*, the buffer consists of a hollow cylinder surrounding the sample and the pusher. The pusher and the buffer have the same design and they are symmetrically placed on both sides of the sample in geometry *C*. The schemes of the geometries *B* and *C* are presented in Fig. 1. The domains of calculus for the three geometries with their corresponding scales are depicted in Fig. 2. The total number of elements in the triangulation of these domains was 1796, 1168 and 1340, and the number of nodes was 5871, 4199 and 4825 for the geometries *A*, *B* and *C*, respectively.

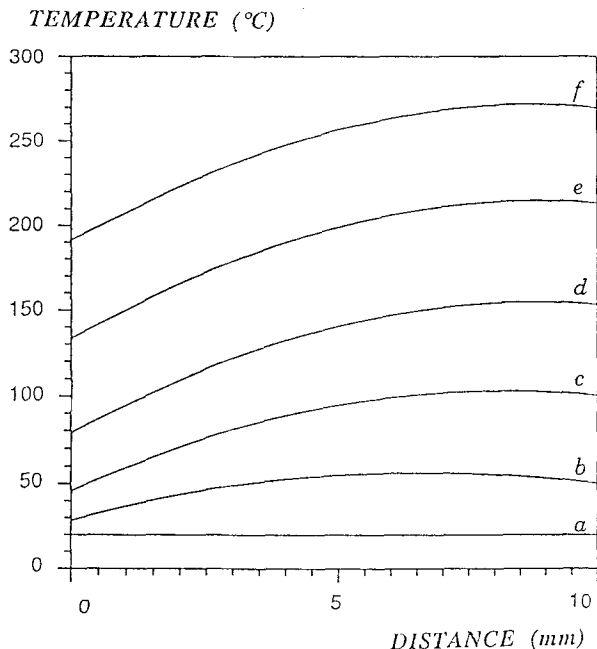


Fig. 4 Change in temperature along the axis of the sample for geometry *A* with $q_1=0.6 \text{ W}\cdot\text{cm}^{-3}$, in the course of time: a: 0 s; b: 207 s; c: 546 s; d: 1095 s; e: 2010 s; f: 2952 s

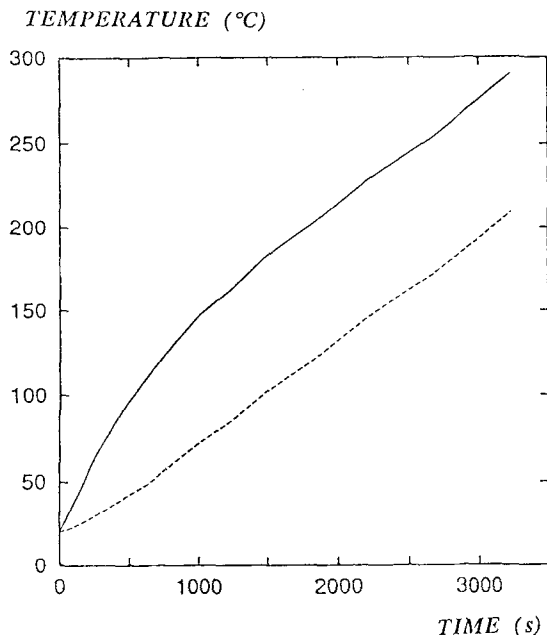


Fig. 5 Temperature rise in the sample for geometry *A* with $q_1 = 0.6 \text{ W}\cdot\text{cm}^{-3}$. (—) T_h , the highest temperature. (---) T_l , the lowest temperature

For all the geometries, the end of the pusher that is not in contact with the sample is maintained at the external temperature T_e . The buffer is submitted to the same conditions in the geometries *B* and *C* while no temperature condition is imposed to the buffer in geometry *A*.

Results

We have seen previously that a nearly uniform temperature close to 240°C was obtained at steady state with geometry *A* when the power q_1 created by unit volume of the sample was 0.02 Wcm^{-3} [1]. Figure 3 shows how this steady state is reached in time. T_h and T_l , respectively denote the highest and the lowest temperature calculated in the sample during heating. It is seen that $\delta T = T_h - T_l$ does not exceed 4°C while the temperature is raised up to 212°C . Nevertheless, this temperature is attained in a time longer than $2 \cdot 10^5 \text{ s}$, which is not acceptable for our practical purposes.

Figure 4 presents results obtained with the same geometry for a value of q_1 equal to 0.6 Wcm^{-3} that allows the temperature at the centre of the sample to reach 252°C in 2952 s. The temperature profiles along the axis of the sample at different times clearly show the preponderance of the buffer rod in creating un-

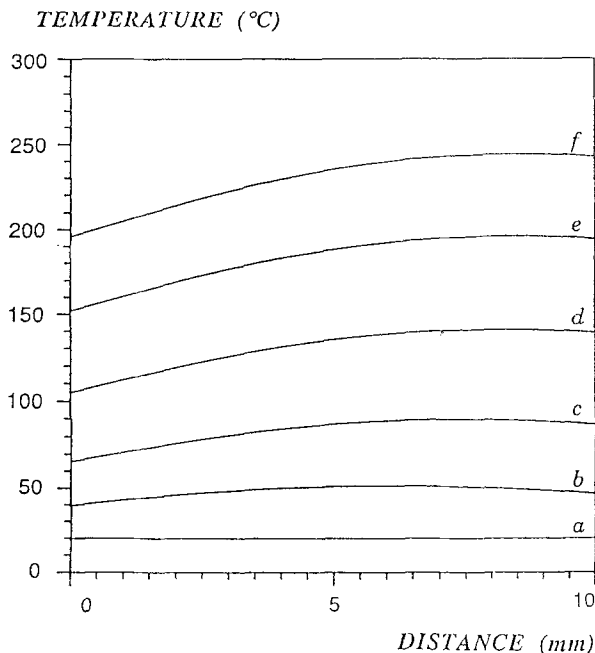


Fig. 6 Change in temperature along the axis of the sample for geometry *B* with $q_1 = 0.4 \text{ W}\cdot\text{cm}^{-3}$, in the course of time: a: 0 s; b: 250 s; c: 638 s; d: 1269 s; e: 2184 s; f: 3232 s

desirable temperature gradients in the sample. The highest and the lowest temperatures found in the sample are shown in Fig. 5.

Geometry *B* represents an attempt to reduce the thermal conductance and heat capacity of the buffer. The corresponding curves obtained for $q_1 = 0.4 \text{ W}\cdot\text{cm}^{-3}$, chosen to achieve a heating rate similar to that of the preceding case, are reported in Fig. 6. It is seen that almost no improvement in temperature homogeneity is obtained.

Table 2 Extremum temperature (T_h , T_l) in the sample in simulations at transient state up to a time t_m for various heating powers q_1

$q_1 / \text{W}\cdot\text{cm}^{-3}$	$T_h / ^\circ\text{C}$	$T_l / ^\circ\text{C}$	t_m / s
0.04	229	227	53285
0.25	244	238	2953
0.40	253	244	1865
4	260	200	158
40	244	103	13
400	263	86	1.4

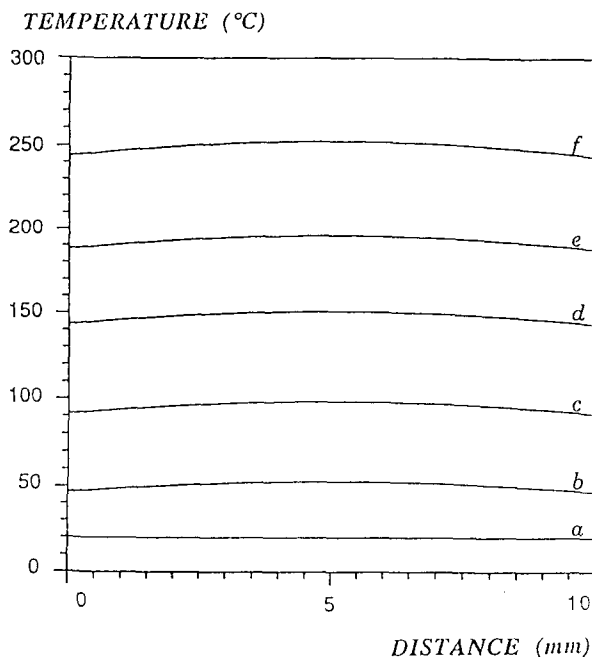


Fig. 7 Change in temperature along the axis of the sample for geometry *C* with $q_1 = 0.4 \text{ W}\cdot\text{cm}^{-3}$, in the course of time: a: 0 s; b: 259 s; c: 604 s; d: 1025 s; e: 1368 s; f: 1865 s

The symmetrical geometry *C* is much more satisfactory. Calculations were carried out for various values of q_1 ranging from 0.04 to $400 \text{ W}\cdot\text{cm}^{-3}$. Table 2 lists the results at time t_m for which the temperature T_h at the centre of the sample approximately reaches 250°C that is the maximum value attained in the dilatometric measurements.

Results for the smallest power are close to those of the stationary state calculated independently ($T_h = 247^\circ\text{C}$ and $T_l = 245^\circ\text{C}$). During the temperature rise from 20 to 227°C , the difference δT between the highest and the lowest temperature in the sample does not exceed 2.3°C but the heating rate is again too low for practical purposes. However, acceptably low values of δt were observed for powers up to $0.4 \text{ W}\cdot\text{cm}^{-3}$ that correspond to a nearly constant heating rate of $7.5 \text{ deg}\cdot\text{min}^{-1}$. Figure 7 shows the change in temperature along the sample axis in this case. The corresponding isotherms are shown in Fig. 8. It can be seen that, in the sample, the temperature is nearly uniform in planes perpendicular to the axis of revolution.

For heating powers greater than $0.4 \text{ W}\cdot\text{cm}^{-3}$, significant temperature gradients were observed in the vicinity of the ends of the sample but a plateau was observed in its centre. Nevertheless, even when $q_1 = 400 \text{ W}\cdot\text{cm}^{-3}$ (or $t_m = 1.4 \text{ s}$), this plateau is not sufficiently wide to allow thermodilatometric measurements to be correctly performed (Fig. 9).

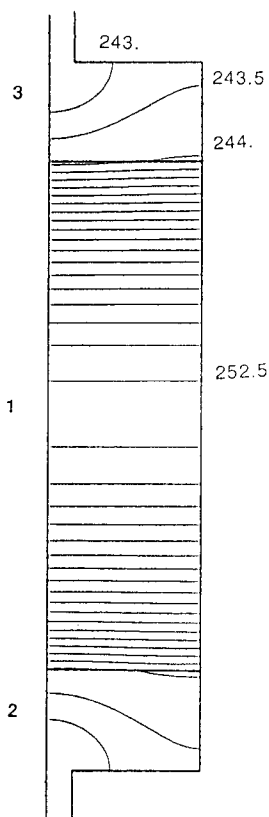


Fig. 8 Isotherms (temperature gaps = 0.5°C) with $q_1 = 0.4 \text{ W}\cdot\text{cm}^{-3}$, at time $t = 1865 \text{ s}$. 1: sample; 2: buffer; 3: pusher

Conclusion

We have seen in a previous study that stationary states with a nearly uniform temperature in the sample were possible with a convenient geometry of the dilatometer column. The requirement of temperature homogeneity in the sample during the temperature rise is, in principle, met in two extreme cases. First, when the heating rate is sufficiently low so that a quasi-stationary state with a uniform temperature is achieved. Secondly, when the heat production rate is very high and heat transfer may be considered sufficiently slow to be neglected. Modelling of the behaviour of dilatometer columns composed of a polymer sample located between a buffer and a pusher made of quartz, have shown that the first case may be satisfactorily approached in practical cases. Thus, geometry *C* allows values of δT smaller than 10°C for heating rates lower than $7 \text{ deg}\cdot\text{min}^{-1}$. These results show the feasibility of the project.

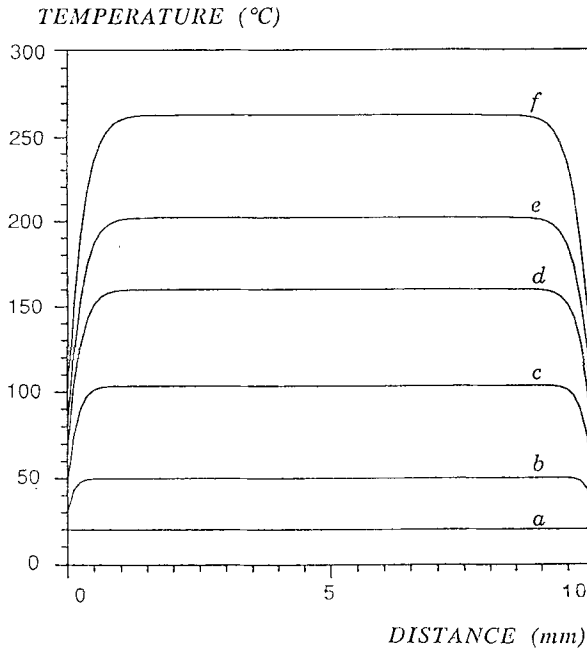


Fig. 9 Change in temperature along the axis of the sample for geometry *C* with $q_1 = 400 \text{ W}\cdot\text{cm}^{-3}$, in the course of time: a: 0 s; b: 0.2 s; c: 0.5 s; d: 0.8 s; e: 1 s; f: 1.4 s

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Zusammenfassung — Vorliegend wird das Modell eines Wärmetransportes in einer Polymerprobe dargelegt, die in der Quarzsäule eines zur Vermeidung von Konvektion durch Vakuum umgebenen Dilatometers einem Mikrowellenfeld ausgesetzt wurde. Der Temperaturanstieg im Übergangszustand wurde mittels der Elementenmethode untersucht. Es wird angenommen, daß im gesamten Probenvolumen eine gleichmäßige und konstante Wärmeproduktion beibehalten wird. Es wird die Möglichkeit gezeigt, das Doppel aus Probe und Säule so zu konstruieren, daß im gesamten Probenvolumen eine annähernd gleichmäßige Temperatur erzielt wird, während die Temperatur mit einer Aufheizgeschwindigkeit von 5 deg/min von 20 auf 250°C angehoben wird.